

Nikita V. Chukanov  
Marina F. Vigasina

# Vibrational (Infrared and Raman) Spectra of Minerals and Related Compounds

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# Vibrational (Infrared and Raman) Spectra of Minerals and Related Compounds



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*Alexandr Dmitrievich Chervonnyi  
1948–2017*

*This book is dedicated to the memory of the outstanding scientist, a specialist in the field of inorganic materials and chemistry of rare-earth elements Dr. Alexandre Dmitrievich Chervonnyi. Him belongs the idea to publish this book.*

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## Preface

This volume is the third and final part of the series of reference books on vibrational spectra of minerals. Unlike the two previous parts (Chukanov 2014; Chukanov and Chervonnyi 2016), this book contains not only infrared (IR) spectra of minerals but also data on their Raman spectra.

In Chap. 1, numerous examples of the application of IR spectroscopy to the analysis of crystal-chemical features of minerals are considered. In particular, spectral bands that characterize different local situations around OH<sup>-</sup> and BO<sub>3</sub><sup>3-</sup> groups in vesuvianite-group minerals are revealed. The effect of symmetry on the parameters of IR spectra of vesuvianite-group minerals is discussed. By means of IR and Raman spectroscopic methods, it is shown that the clathrate mineral melanophlogite is not a single species but a mineral group including minerals with different combinations of small molecules (CO<sub>2</sub>, CH<sub>4</sub>, H<sub>2</sub>S, N<sub>2</sub>, H<sub>2</sub>O, C<sub>2</sub>H<sub>6</sub>) entrapped in structural cages. Based on numerous IR spectra of nakauriite samples from different localities, it is demonstrated that this mineral does not contain sulfate groups, and its tentative simplified formula (Mg<sub>3</sub>Cu<sup>2+</sup>)(OH)<sub>6</sub>(CO<sub>3</sub>)·4H<sub>2</sub>O is suggested. A close crystal chemical relationship between nepskoeite and shabynite is demonstrated based on their IR spectra, compositional, and X-ray diffraction data. Contrary to the formula Mg<sub>4</sub>Cl(OH)<sub>7</sub>·6H<sub>2</sub>O accepted for nepskoeite, this mineral is a borate with the tentative simplified formula Mg<sub>5</sub>(BO<sub>3</sub>)(Cl, OH)<sub>2</sub>(OH)<sub>5</sub>·nH<sub>2</sub>O ( $n > 4$ ). Consequently, shabynite may be a product of nepskoeite dehydration. Based on IR spectroscopic data, it is also shown that some nominally boron-free lead carbonate minerals (molybdophyllite, hydrocerussite, plumbonacrite, somersetite) often contain minor BO<sub>3</sub><sup>3-</sup> admixture which is overlooked in structural and chemical analyses.

Chapter 2 contains IR spectra of 1024 minerals and related compounds which were not included in the preceding reference books of this series (Chukanov 2014; Chukanov and Chervonnyi 2016). Most spectra are accompanied by the information about the origin of reference samples, methods of their identification, and analytical data.

In Chap. 3, possibilities, advantages, and shortcomings of Raman spectroscopy as a method of investigation and identification of minerals are discussed. Numerous examples illustrate capabilities of Raman spectroscopy in identification of minerals and analysis of their crystal chemical features, orientation, and polarization effects, selection rules, as well as difficulties encountered in

the study of microscopic inclusions in minerals and minerals that are unstable under laser beam.

Chapter 4 contains data on 2104 Raman spectra of more than 2000 mineral species taken from various periodicals. The data are accompanied by some experimental details and information on the reference samples used.

A supplementary chapter provides comments on published IR spectra which are erroneous, dubious, or of poor quality. This chapter is provided by a separate list of references.

This work was carried out with assistance of numerous colleagues. The working partnership with Prof. I.V. Pekov, Dr. A.D. Chervonnyi, and Dr. S.A. Vozchikova was the most important.

Reference samples and valuable analytical data were kindly granted by A.V. Kasatkin, S. Jančev, E. Jonssen, R. Hochleitner, E.V. Galuskin, S. Weiss, N.V. Sorokhtina, Ł. Kruszewski, and many other mineralogists, as well as mineral collectors, of which the contribution of R. Kristiansen, G. Möhn, W. Schüller, B. Ternes, G. Blass, B. Dünkel, S. Möckel, and C. Schäfer was the most important. Collaboration with the crystallographers N.V. Zubkova, R.K. Rastsvetaeva, S.M. Aksenov, D.I. Pushcharovsky, T.L. Panikorovskii, O.I. Siidra, S.N. Britvin, M.G. Krzhizhanovskaya, D.A. Ksenofontov, S.V. Krivovichev, and I. Grey, as well as with specialists in different areas of geosciences and analytical methods (J. Göttlicher, K.V. Van, D.A. Varlamov, V.N. Ermolaeva, D.I. Belakovskiy, Yu.S. Polekhovsky, P. Voudouris, A. Magganas, A. Katerinopoulos, N.V. Shchipalkina, V.O. Yapaskurt, L.A. Pautov, V.S. Rusakov, R. Scholz, A.R. Kampf, S. Encheva, P. Petrov, Ya.V. Bychkova, N.N. Koshlyakova, P. Yu. Plechov, C.L.A. de Oliveira, I.S. Lykova, and T.S. Larikova) was especially fruitful. All of them are kindly appreciated.

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## Reference

Chukanov NV, Chervonnyi AD (2016) Infrared spectroscopy of minerals and related compounds. Springer, Cham. (1109 pp)

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# Contents

|  |           |
|--|-----------|
| <b>1 Some Examples of the Use of IR Spectroscopy in Mineralogical Studies . . . . .</b>                          | <b>1</b>  |
| 1.1 Characteristic Bands in IR Spectra of Vesuvianite-Group Minerals . . . . .                                   | 1         |
| 1.1.1 O–H-Stretching Vibrations . . . . .  | 1         |
| 1.1.2 B–O-Stretching Vibrations . . . . .  | 3         |
| 1.1.3 Stretching and Bending Vibrations of $\text{SiO}_4^{4-}$ and $\text{Si}_2\text{O}_7^{6-}$ Groups . . . . . | 5         |
| 1.2 Problem of Melanophlogite . . . . .  | 5         |
| 1.3 Problem of Nakaurite . . . . .   | 9         |
| 1.4 Relationship Between Nepskoeite and Shabynite . . . . .  | 13        |
| 1.5 Orthoborate Groups in Lead Carbonate Minerals . . . . .  | 14        |
| <b>2 IR Spectra of Minerals and Related Compounds, and Reference Samples Data . . . . .</b>                      | <b>19</b> |
| 2.1 Borates, Including Arsenatoborates and Carbonatoborates . . . . .  | 21        |
| 2.2 Carbonates . . . . .   | 78        |
| 2.3 Organic Compounds and Salts of Organic Acids . . . . .   | 98        |
| 2.4 Nitrides and Nitrates . . . . .  | 111       |
| 2.5 Oxides and Hydroxides . . . . .  | 117       |
| 2.6 Fluorides and Fluorochlorides . . . . .  | 226       |
| 2.7 Silicates . . . . .  | 236       |
| 2.8 Phosphides and Phosphates . . . . .  | 350       |
| 2.9 Sulfides, Sulfites, Sulfates, Carbonato-Sulfates, Phosphato-Sulfates, and Tellurato-Sulfates . . . . .       | 470       |
| 2.10 Chlorides and Hydroxychlorides . . . . .  | 537       |
| 2.11 Vanadates and Vanadium Oxides . . . . .   | 555       |
| 2.12 Chromates . . . . .   | 590       |
| 2.13 Germanates . . . . .  | 597       |
| 2.14 Arsenides, Arsenites, Arsenates, and Sulfato-Arsenates . . . . .  | 597       |
| 2.15 Selenides, Selenites, and Selenates . . . . .   | 639       |
| 2.16 Bromides . . . . .  | 664       |
| 2.17 Molybdates . . . . .  | 665       |
| 2.18 Tellurides, Tellurites, and Tellurates . . . . .  | 680       |

|                   |   |             |
|-------------------|---|-------------|
| 2.19              | Iodides, Iodites, and Iodates . . . . .   | 699         |
| 2.20              | Xenates . . . . .   | 704         |
| 2.21              | Tungstates and W-Bearing Oxides . . . . .   | 706         |
| <b>3</b>          | <b>Some Aspects of the Use of Raman Spectroscopy<br/>in Mineralogical Studies . . . . .</b>       | <b>721</b>  |
| 3.1               | General Principles of Raman Spectroscopy . . . . .  | 721         |
| 3.2               | Specific Features and Possibilities of Raman Spectroscopy:<br>Practical Recommendations . . . . . | 722         |
| 3.2.1             | Advantages and Disadvantages of the Method . . . . .  | 722         |
| 3.2.2             | Spectral Band Assignment . . . . .  | 727         |
| 3.2.3             | Effect of Structural Disorder on Raman Spectra<br>of Minerals . . . . .                           | 728         |
| 3.2.4             | Selection Rules . . . . .   | 730         |
| 3.2.5             | The Longitudinal-Transverse Splitting . . . . .   | 732         |
| 3.2.6             | Orientation and Polarization Effects; Analysis<br>of Water and OH Groups . . . . .                | 733         |
| 3.2.7             | Effect of Luminescence . . . . .  | 736         |
| 3.2.8             | Destructive Effect of Laser Radiation . . . . .   | 736         |
| <b>4</b>          | <b>Raman Spectra of Minerals . . . . .</b>  | <b>741</b>  |
| <b>References</b> |   | <b>1257</b> |
| <b>Index</b>      |   | <b>1351</b> |



# Some Examples of the Use of IR Spectroscopy in Mineralogical Studies

1

## 1.1 Characteristic Bands in IR Spectra of Vesuvianite-Group Minerals

Vesuvianite-group minerals (VGM) are widespread and occur in different geological formations including regional metamorphic rocks, skarns, rodingites, etc. Specific crystal-chemical features of these minerals reflect conditions of their crystallization. As a rule, high-temperature VGM have high-symmetry structures (space group  $P4/nnc$ ), whereas low-temperature samples are characterized by the symmetry  $P4/n$  or  $P4nc$  (Allen and Burnham 1992). The simplified crystal-chemical formula of VGM is  $X_{18}(X'Y_1Y_2)_4Y_3T_{0-5}(SiO_4)_{10}(Si_2O_7)_4O_{1-2}W_9$  where  $X$ ,  $X'$  = Ca, Na, K,  $Fe^{2+}$ , and REE (cations with coordination numbers from 7 to 9);  $Y_1$  = Al, Mg,  $Fe^{2+}$ ,  $Fe^{3+}$ ,  $Mn^{2+}$ ,  $Mn^{3+}$ , Ti, Cr, Cu, Zn;  $T$  = B, Al,  $\square$ ;  $W$  = OH, F, O. The  $Y_1$  cations have tetragonal-pyramidal coordination, whereas the  $Y_2$  and  $Y_3$  cations occur in octahedra.

IR spectra of VGM are discussed in numerous publications (Palusziewicz and Żabiński 1992; Groat et al. 1995; Kurazhkovskaya and Borovikova 2003; Kurazhkovskaya et al. 2005; Borovikova and Kurazhkovskaya 2006); however, in most cases their interpretation is ambiguous. We have obtained IR spectra of 33 VGM

samples from different kinds of localities which have been preliminarily investigated in detail using electron microprobe (including determination of boron), single-crystal X-ray structural analysis, DSC,  $^{27}Al$  NMR, ICP-MS, and Mössbauer spectroscopy. As a result, characteristic IR bands corresponding to different local situations in the structures of VGM have been revealed. Data on crystal structures, crystal chemistry, and IR spectra of these samples are published by Britvin et al. (2003), Panikorovskii et al. (2016a-d, 2017a-d), and Aksenov et al. (2016). The most important results of this investigation are listed below in comparison with data published elsewhere.

### 1.1.1 O-H-Stretching Vibrations

The following empirical correlations between O–H stretching frequencies in IR spectra of minerals and O···O and H···O distances (from structural data) were established by E. Libowitzky (1999):

$$\nu \left( cm^{-1} \right) = 3592 - 304 \cdot 10^9 \cdot \exp[-d(O \cdots O)/0.1321] \quad (1.1)$$

$$\nu \left( cm^{-1} \right) = 3632 - 1.79 \cdot 10^6 \cdot \exp[-d(H \cdots O)/0.2146] \quad (1.2)$$

Two decades ago this publication was of a great importance because it emphasized the existence of such correlations as a general trend. However, over time it became obvious that the Eqs. (1.1) and (1.2) are a very rough approximation and have a restricted applicability. First, it is to be noted that at high frequencies (above  $3500\text{ cm}^{-1}$ ) substantial deviations from the correlations (1.1) and (1.2) are common because O–H stretching frequencies depend not only on O···O and H···O distances, but also on the nature of cations coordinating O–H groups and  $\text{H}_2\text{O}$  molecules, as well as on the angle O–H···O, and the influence of these factors becomes most evident in case of weak hydrogen bonds. The Eqs. (1.1) and (1.2) predict that maximum possible values of O–H stretching frequencies for minerals are 3592 and  $3632\text{ cm}^{-1}$  respectively. However, in many minerals including magnesium serpentines, brucite, kaolinite, amphiboles, etc. observed frequencies are much higher and even can exceed  $3700\text{ cm}^{-1}$ .

In the IR spectra of VGM some absorption bands of O–H stretching vibrations are poorly resolved. In such cases, band component analysis is the most important source of errors and artifacts during data processing because of low correctness of inverse mathematical problems: small errors in experimental data lead to strong uncertainty of the final result. Additional uncertainty is connected with arbitrary choice of the band shape (Gauss, Lorentz, Voigt, or Lorentz-Gauss cross-product function), the number of components, and the acceptable values of the correlation coefficient  $R$  (e.g., 0.99, 0.995, or 0.999). This matter is discussed in detail by Chukanov and Chervonnyi (2016) (the section 1.1 “Sources of Errors and Artifacts in IR Spectroscopy of Minerals”) where it is shown that different variants of band shape analysis may give a good and almost identical approximation accuracy (say,  $R^2 \approx 0.9995$ ), but lead to totally different results.

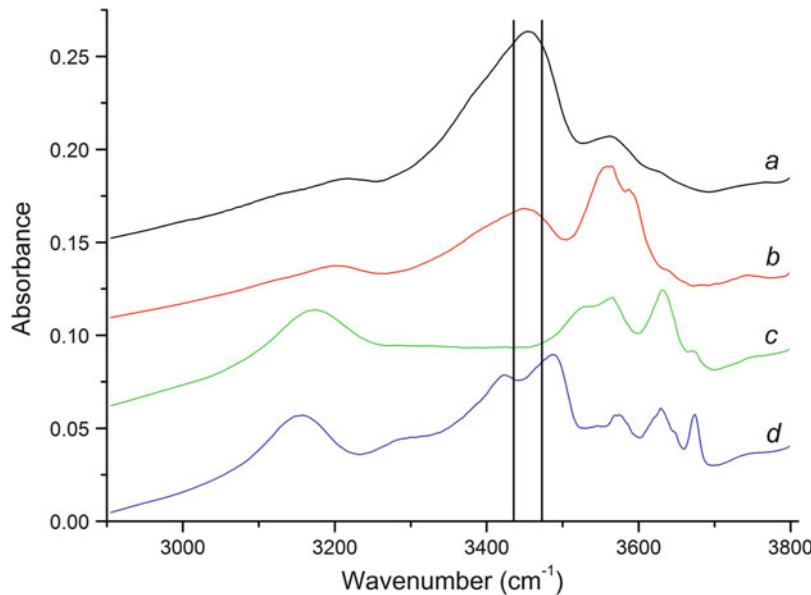
For most VGM investigated by Chukanov et al. (2018) there are significant discrepancies between wavenumbers of observed O–H stretching bands and  $\nu$  values calculated using correlations suggested by Libowitzky (1999). The above considerations explain why the attempts to apply Eqs. (1.1) and (1.2) to VGM failed.

Groat et al. (1995) distinguished 13 bands of O–H stretching vibrations in IR spectra of VGM, which have absorption maxima at the following wavenumbers ( $\text{cm}^{-1}$ ): 3670 (A), 3635 (B), 3596 (C), 3567 (D), 3524 (E), 3487 (F), 3430 (G), 3383 (H), 3240 (I), 3210 (J), 3156 (K), 3120 (L), and 3054 (M). The polarization of these bands with respect to the fourfold  $c$  axis is as follows:  $E \wedge c < 35^\circ$  for the A–H bands,  $E \perp c$  for the I band, and  $E \parallel c$  for the J–M bands (Groat et al. 1995; Bellatreccia et al. 2005). Consequently, the bands A–H and J–M can be assigned to the vibrations of differently coordinated O11–H1 and O10–H2 groups, respectively. The I band was tentatively assigned to O–H stretching vibrations of silanol group (Chukanov et al. 2018).

Our data show that actually significant deviations of the A–M band positions from the “ideal” values indicated by Groat et al. (1995) take place. In particular, IR spectra of many VGM samples contain a band in the range  $3440$ – $3470\text{ cm}^{-1}$ , i.e., between F and G bands. Taking into account that in the group of 33 chemically and structurally investigated samples the intensity of this band shows distinct positive correlation with Ti content, it was assigned to vibrations of the O11–H1 group coordinated by Ti (Chukanov et al. 2018). Most Ti-rich samples are characterized by the space group  $P4/nnc$ . The only exception is a sample from the Ahkmatovskaya open pit, South Urals with  $1.54\text{ apfu}$  Ti, space group  $P4/n$  showing bands at  $3488\text{ cm}^{-1}$  (with a shoulder at  $3460\text{ cm}^{-1}$ ) and  $3424\text{ cm}^{-1}$  instead of a single band in the range  $3440$ – $3470\text{ cm}^{-1}$  (Fig. 1.1).

Vesuvianite from the Ahkmatovskaya open pit is the only Ti-bearing VGM having space group  $P4/n$  among 33 samples investigated by Chukanov et al. (2018). The observed splitting of the band of  $\text{TiO}-\text{H}$  stretching vibrations is the result of distribution of Ti between the sites Y3A and Y3B, whereas in high-temperature VGM having the space group  $P4/nnc$  Ti is accumulated in the single Y3 site.

IR band in the range  $3375$ – $3380\text{ cm}^{-1}$  which is close to the H band by Groat et al. (1995) was observed by us only for two samples with the symmetry  $P4/n$  and high contents of Cu and



**Fig. 1.1** IR spectra of vesuvianite-group minerals with different contents of Ti in the region of O–H-stretching vibrations: a sample from Alchuri, Shigar Valley, Pakistan (Aksenov et al. 2016) with  $\text{Ti}_{2.21}$  (a); a sample from Hazlov, Karlovy Vary Region, Czech Republic with  $\text{Ti}_{0.48}$  (b); a sample from Myrster area, Drammen,

Buskerud, Norway with  $\text{Ti}_{0.00}$  (c); VGM from the Akhmatovskaya open pit, South Urals, Russia with  $\text{Ti}_{1.54}$  (anomalous Ti-rich sample, space group  $P4/n$ ) (d). Two vertical lines outline the region of the band corresponding to the  $\text{Ti}\cdots\text{O}11\text{--H}1$  group in  $P4/nnc$  VGM

$\text{Mn}^{3+}$ . This band is more intense in the IR spectrum of the sample from the N'Chwaning III mine, Kuruman, South Africa with a relatively higher content of  $\text{Mn}^{3+}$  ( $1.83 \text{ apfu}$ ). Based on these data, the band in the range  $3375\text{--}3380 \text{ cm}^{-1}$  can be assigned to the  ${}^y\text{Mn}^{3+}\cdots\text{O}11\text{--H}1$  group.

The nominal position of the D band is  $3567 \text{ cm}^{-1}$  (Groat et al. 1995), but in IR spectra of some samples this band is shifted towards lower wavenumbers (up to  $3560 \text{ cm}^{-1}$ ). The D band is not observed in IR spectra of F-poor VGM and has the highest intensities in IR spectra of samples with most high contents of F (Britvin et al. 2003; Galuskin et al. 2003; Chukanov et al. 2018; see Fig. 1.2). Taking into account polarization  $E\wedge c < 35^\circ$  (Groat et al. 1995), the D band is to be assigned to the group  $\text{O}11\text{--H}1$  in the situation when F occupies neighboring  $\text{O}11$  site.

Galuskin et al. (2003) supposed that the J band corresponds to OH groups in the  $\text{O}10$  site coordinating Fe in  $\text{Y}1$  and forming hydrogen bond with F in the neighboring  $\text{O}10$  site. However, this assumption was not confirmed by our investigations: IR spectra of most VGM,

including F- and Fe-poor ones, contain distinct J band whose wavenumber varies from  $3190$  to  $3225 \text{ cm}^{-1}$ . These values correspond to strong hydrogen bonds, which is hardly possible in cases when F is the H-bond acceptor.

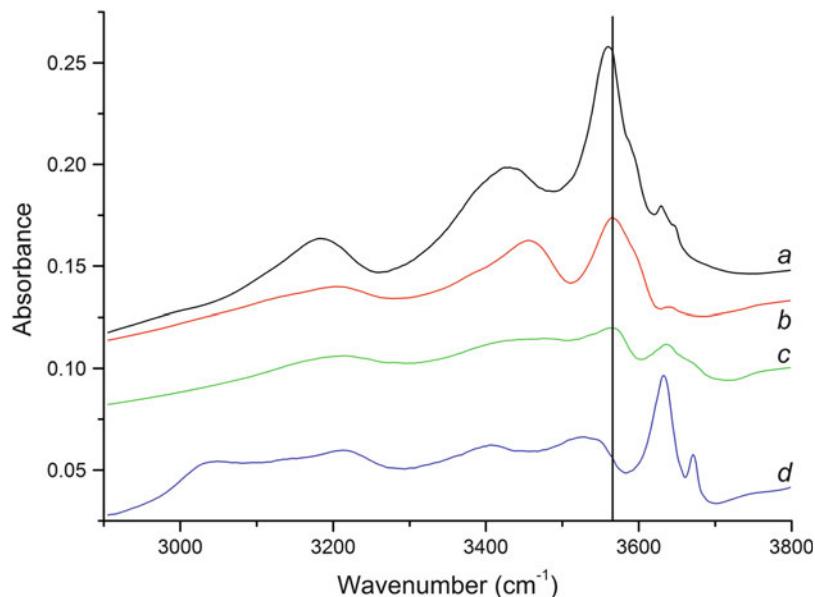
The weak B band (in the range from  $3628$  to  $3632 \text{ cm}^{-1}$ ) is often observed in IR spectra of low-symmetry VGM. This band corresponds to very weak H-bonds formed by the groups  $\text{O}11\text{--H}1$  with low values of the angle between  $\text{O}11\text{--H}1$  and  $\text{H}1\cdots\text{O}7$  (see Lager et al. 1999).

### 1.1.2 B-O-Stretching Vibrations

In VGM boron can occupy sites with coordination numbers 3 or 4. IR spectra of most VGM samples contain shoulders in the range  $1070\text{--}1170 \text{ cm}^{-1}$  corresponding to stretching vibrations of  $[\text{BO}_4]$  tetrahedra.

$\text{BO}_3$  groups are connected with  $\text{Y}1\text{O}_6\text{O}10$  polyhedra via  $\text{O}10$  oxygen atom to form the cluster  $T2\text{Y}1\text{O}_7$  (Fig. 1.3) where  $T2 = \text{B}$  and  $\text{Y}1 = \text{Fe}^{3+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Mn}^{3+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Al}$ , or  $\text{Mg}$ . As a result, four

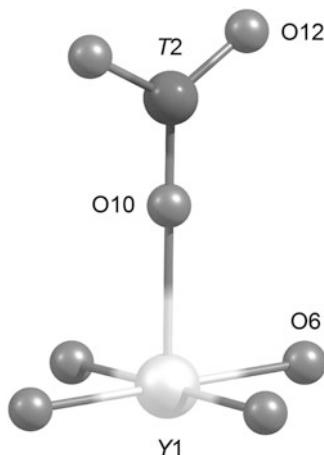
**Fig. 1.2** IR spectra of vesuvianite-group minerals with different contents of F in the region of O–H-stretching vibrations: fluorvesuvianite holotype with 7.16 *apfu* F (*a*); VGM from Sakharyok massif, Keyvy Mts., Kola Peninsula with 3.06 *apfu* F (*b*); VGM from Gulshad, Kazakhstan with 0.24 *apfu* F (*c*); F-free alumovesuvianite holotype (*d*). Vertical line corresponds to the nominal position of the D band



degrees of freedom corresponding to the bond lengths  $T_2$ –O12 ( $\times 2$ ),  $T_2$ –O10, and Y1–O10 are involved in stretching vibrations of  $BO_3^{3-}$ . This results in four nondegenerate modes and, consequently, the expected number of absorption bands in the region of stretching vibrations of  $BO_3$  groups (i.e., 1200–1570  $cm^{-1}$ ) is equal to 4. However, in the IR spectrum of wiluite only three bands are observed in this region: the peaks at 1267 and 1373  $cm^{-1}$  and the shoulder at

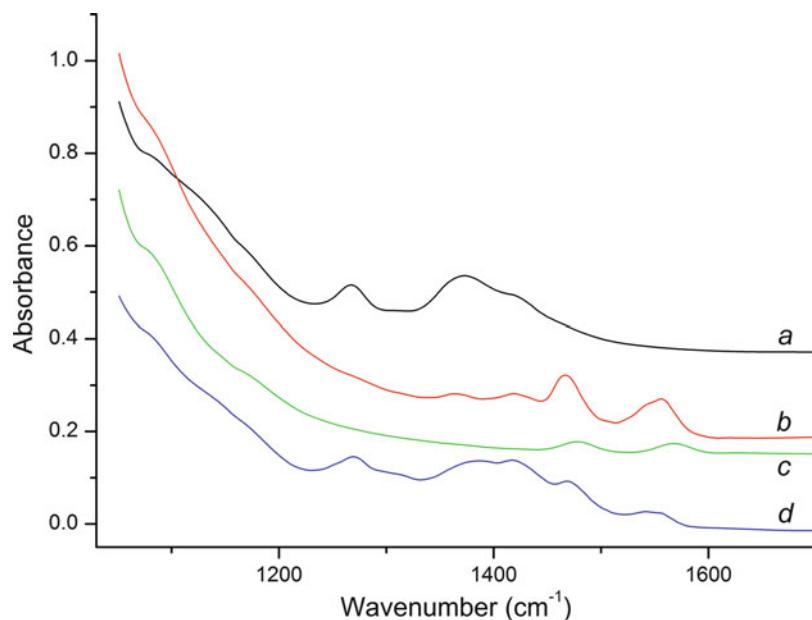
1415  $cm^{-1}$  (Panikorovskii et al. 2017b; see Fig. 1.4). The fourth band corresponding to symmetric vibrations of  $BO_3^{3-}$  is forbidden for a regular  $BO_3$  triangle and is weak in case of weakly distorted  $BO_3$  triangle. The latter case takes place in wiluite: the bond lengths  $T_2$ –O10 and  $T_2$ –O12 are 1.39–1.40 and 1.32 Å, respectively (Panikorovskii et al. 2017b). Weak absorption between 1267 and 1373  $cm^{-1}$  may correspond to the symmetric stretching mode of  $BO_3^{3-}$  groups (Fig. 1.4).

Unlike wiluite, most boron-rich VGM contain significantly distorted  $BO_3$  triangle. For example, in a sample from Gulshad, Kazakhstan the bond lengths  $T_2$ –O10 and  $T_2$ –O12 are equal to 1.384 and 1.20 Å, respectively. As a result, four distinct IR bands (at 1557, 1467, 1419, and 1365  $cm^{-1}$ ) are observed in the range 1200–1570  $cm^{-1}$  (curve *b* in Fig. 1.4). As compared to wiluite, these bands are substantially shifted towards high frequencies because of shorter B–O bonds and shortened Y1–O bond (2.044 Å for the mineral from Gulshad and 2.15 Å for wiluite: Chukanov et al. 2018; Panikorovskii et al. 2017b). These differences may be due to different predominant cations in the Y1 site: Mg in wiluite and  $Fe^{3+}$  in the sample from Gulshad.



**Fig. 1.3** Local environment of the  $T_2$  and Y1 sites in vesuvianite-group minerals

**Fig. 1.4** IR spectra of vesuvianite-group minerals in the region of B–O-stretching vibrations: wiluite from its type locality (*a*), B-rich VGM from Gulshad (*b*), a typical B-bearing vesuvianite from Somma-Vesuvius complex, Italy (*c*), and anomalous B-rich VGM from Titivskoe (*d*)



An anomalous IR spectrum with six absorption bands in the range 1200–1570 cm<sup>−1</sup> shows boron-rich VGM from Titivskoe boron deposit, Yakutia, Russia (curve *d* in Fig. 1.4). Structural investigation of this sample (Panikorovskii et al. 2016a) showed the presence of domains with different symmetry (*P*4/*nnc* and *P*4/*n*).

### 1.1.3 Stretching and Bending Vibrations of SiO<sub>4</sub><sup>4−</sup> and Si<sub>2</sub>O<sub>7</sub><sup>6−</sup> Groups

Based on the available data on IR spectra of a restricted set of VGM Kurazhkowskaya and Borovikova (2003) concluded that for low-symmetry samples the band of Si–O-stretching vibrations in the range from 960 to 990 cm<sup>−1</sup> is shifted on 10–15 cm<sup>−1</sup> towards lower frequencies as compared to high-symmetry VGM. Our data confirm this conclusion only partly. Indeed, among nine samples with the space group *P*4/*n*, eight samples show strong IR bands in the range 962–968 cm<sup>−1</sup>, and in the IR spectrum of one more sample a band at 973 cm<sup>−1</sup> is observed. Among 21 boron-poor samples with the space group *P*4/*nnc*, for 16 samples bands in the range

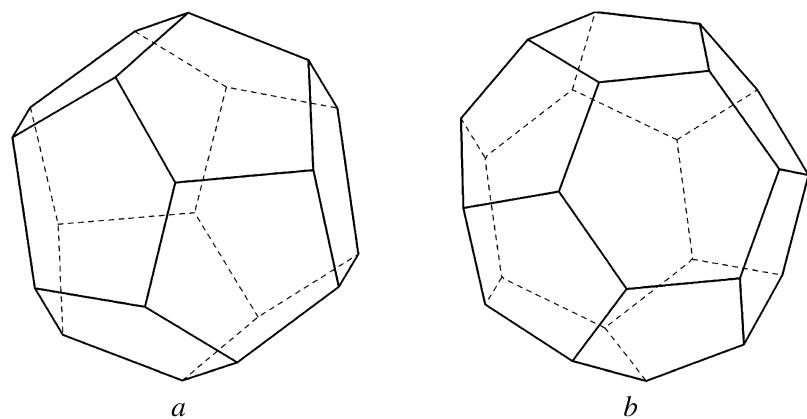
976–986 cm<sup>−1</sup> are observed, but 5 samples show bands between 962 and 968 cm<sup>−1</sup>.

Another specific feature of low-symmetry VGM indicated by Kurazhkowskaya and Borovikova (2003), as well as by Borovikova and Kurazhkowskaya (2006) is the doublet ~575 +615 cm<sup>−1</sup> corresponding to O–Si–O bending vibrations. This regularity was confirmed by us as a general trend; however, among 21 boron-poor samples with the space group *P*4/*nnc*, 3 samples show doublets in the range ~575–615 cm<sup>−1</sup> with components of approximately equal intensity.

## 1.2 Problem of Melanophlogite

Melanophlogite is a clathrate compound which contains guest molecules N<sub>2</sub>, CO<sub>2</sub>, and CH<sub>4</sub> entrapped within the cages of the 3D framework built by SiO<sub>4</sub> tetrahedra (Gies 1983; Nakagawa et al. 2001; Kolesov and Geiger 2003). The cubic unit cell of the structure of melanophlogite includes two [5<sup>12</sup>] cages and six [5<sup>12</sup>6<sup>2</sup>] cages (Fig. 1.5). The former are considered to be occupied mainly by CH<sub>4</sub> molecules and the latter by N<sub>2</sub> and CO<sub>2</sub> (Gies et al. 1982; Gies 1983). In

**Fig. 1.5**  $[5^{12}]$  cages (a) and  $[5^{12}6^2]$  cages (b) in the structure of melanophlogite

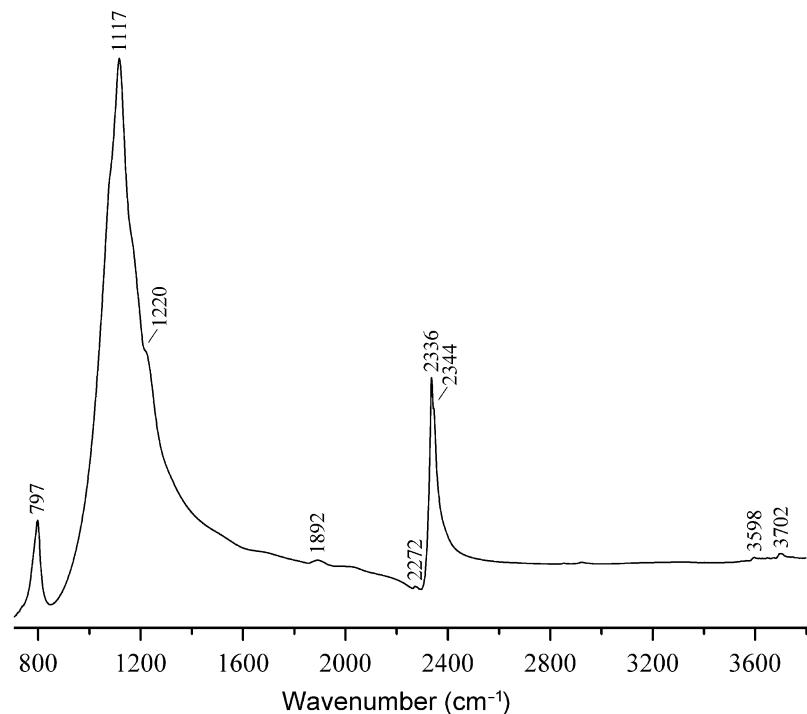


melanophlogite from Mt. Hamilton, California, USA, the occupancy factor of the  $\text{CH}_4$  site in the  $[5^{12}]$  cage is about 90% (Gies 1983). The molecules of carbon dioxide located in the  $[5^{12}6^2]$  cages can rotate and are statistically distributed between 12 possible equivalent orientations. Most part of  $\text{N}_2$  and  $\text{CO}_2$  occurs in the  $[5^{12}6^2]$  cage, but minor part of these molecules can be present in the  $[5^{12}]$  cage (Gies 1983; Kolesov and Geiger 2003). Based on the

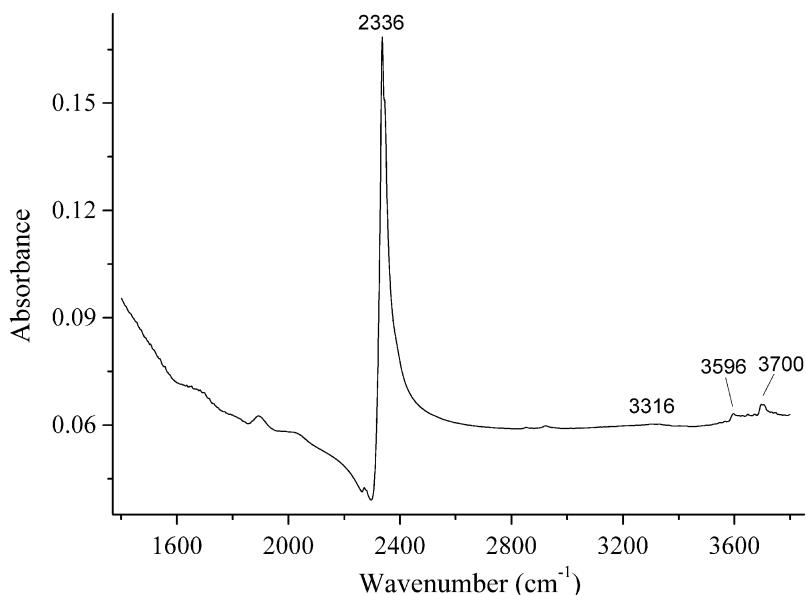
available structural data, the general formula of melanophlogite can be written as follows:  $(\text{CH}_4, \text{N}_2, \text{CO}_2)_{2-x}(\text{N}_2, \text{CO}_2)_{6-y}(\text{Si}_{46}\text{O}_{92})$ .

The IR spectrum of melanophlogite from Fortullino, Livorno province, Tuscany, Italy (cubic, with  $a = 13.4051(13)$  Å, according to single-crystal X-ray diffraction data) contains a strong band at  $2330\text{--}2336\text{ cm}^{-1}$  corresponding to antisymmetric vibrations of  $\text{CO}_2$  molecules (Chukanov and Chervonnyi 2016; see Fig. 1.6).

**Fig. 1.6** Powder IR spectrum of melanophlogite from Fortullino, Italy



**Fig. 1.7** IR spectrum of melanophlogite from Fortullino in the  $1400\text{--}3800\text{ cm}^{-1}$  range. Very weak bands in the range from  $2800$  to  $3000\text{ cm}^{-1}$  correspond to grease impurity



A weaker peak at  $\sim 2375\text{ cm}^{-1}$  present in IR spectra of some melanophlogite samples from this locality (Chukanov 2014) may be due to rotational splitting or correspond to a minor amount of  $\text{CO}_2$  molecules in the  $[5^{12}]$  cages, which are predominantly occupied by  $\text{CH}_4$ . Weak bands at  $3700$  and  $3596\text{ cm}^{-1}$  (Fig. 1.7) are, respectively, due to asymmetric and symmetric stretching vibrations of  $\text{H}_2\text{O}$  molecules that do not form hydrogen bonds. The band at  $3316\text{ cm}^{-1}$  can be tentatively assigned to silanol groups or H-bonded  $\text{H}_2\text{O}$  molecules.

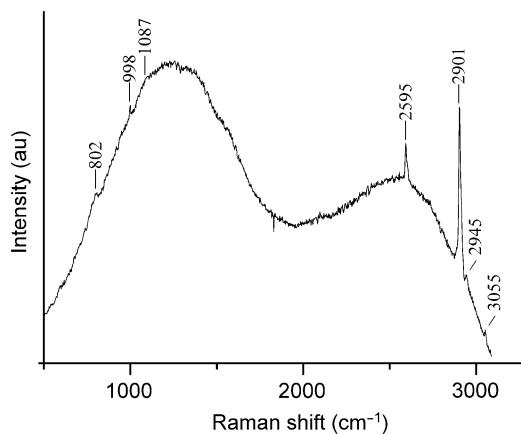
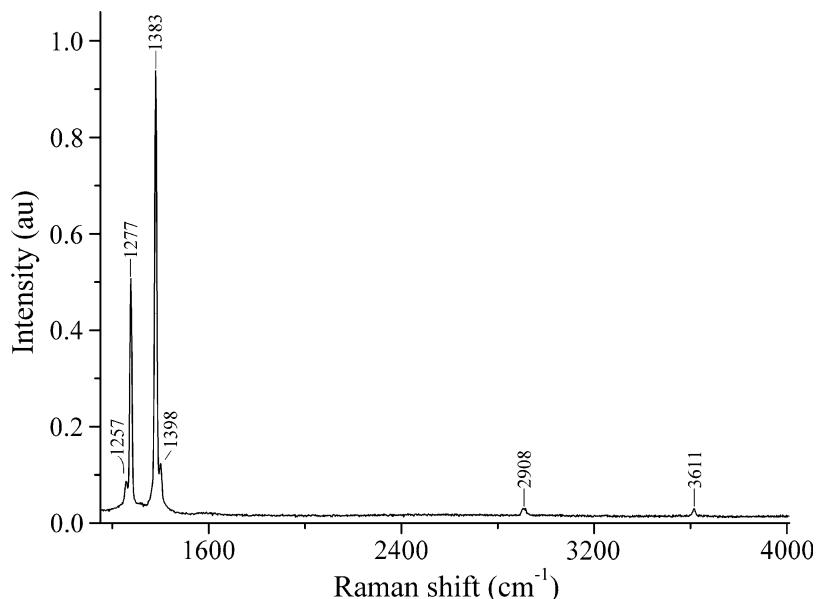
Two  $\text{CO}_2$  modes at  $1277$  and  $1378\text{ cm}^{-1}$  observed in the Raman spectrum of melanophlogite from Mt. Hamilton, California, USA correspond to the first overtone of the  $\nu_2$ -bending mode and the symmetric  $\nu_1$ -stretching mode, respectively, both bands being components of a vibrational system coupled via Fermi resonance (Kolesov and Geiger 2003).

Raman spectrum of melanophlogite from Mt. Hamilton has been investigated previously at  $4\text{ K}$  (Kolesov and Geiger 2003). The bands at  $2900$  and  $2909\text{ cm}^{-1}$  in the single-crystal Raman spectrum of melanophlogite from this locality have been assigned to asymmetric stretching modes of  $\text{CH}_4$  located in the  $[5^{12}]$  and  $[5^{12}6^2]$  cages, respectively. Along with the main band at

$1378.5\text{ cm}^{-1}$  assigned to  $\text{CO}_2$  molecules in the  $[5^{12}6^2]$  cages, the shoulder at  $1376\text{ cm}^{-1}$  was registered and was attributed to  $\text{CO}_2$  in the  $[5^{12}]$  cages. Kolesov and Geiger (2003) also reported the presence of the band of symmetric  $\text{N}\equiv\text{N}$ -stretching vibrations located at  $2321\text{ cm}^{-1}$  which corresponds to  $\text{N}_2$  molecules. The IR forbidden band of  $\text{N}_2$  in binary mixtures with other molecules has been observed at about  $2328\text{ cm}^{-1}$  (Bernstein and Sandford 1999). It is to be noted that this value is close to the wavenumber of antisymmetric vibrations of  $\text{CO}_2$  molecules, which is forbidden in Raman spectra. However, this band is not observed by us in Raman spectra of melanophlogite from different Italian localities (Figs. 1.8, 1.9 and 1.10).

Raman spectrum of the sample from Fortullino (Fig. 1.8) exhibits strong bands of  $\text{CO}_2$  at  $1277$  and  $1383\text{ cm}^{-1}$ . Two weak bands at  $1257$  and  $1398\text{ cm}^{-1}$  accompanying the components of the Fermi-doublet are the so-called hot bands arising from the transitions from an excited vibrational level to the ground vibrational level (Wang et al. 2011). In accordance with Frezzotti et al. (2012) and Wang et al. (2011), carbon dioxide in this mineral is in the high density fluid state with  $D \approx 1\text{ g/cm}^3$ . This is confirmed by the down shift of the Fermi doublet frequencies from  $1388$

**Fig. 1.8** Raman spectrum of melanophlogite from Fortullino



**Fig. 1.9** Raman spectrum of melanophlogite from Racalmuto

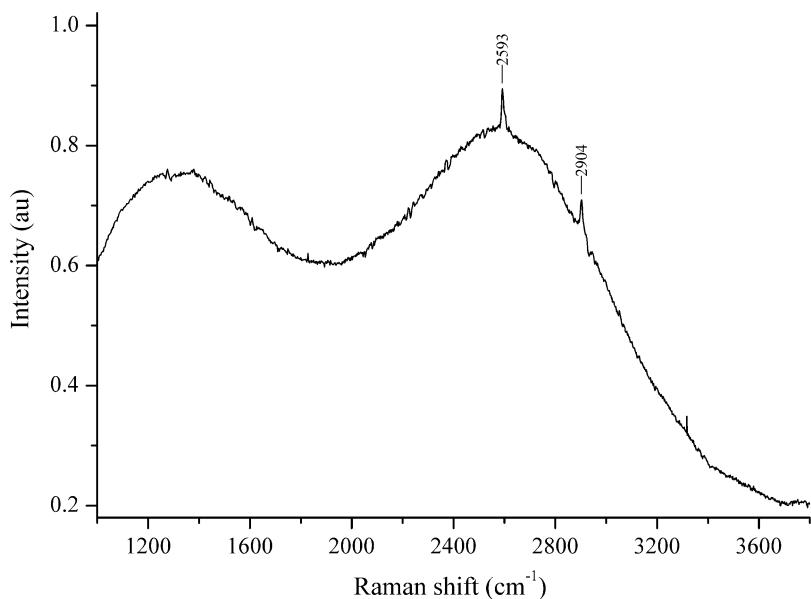
and  $1285\text{ cm}^{-1}$  ( $\Delta = 103\text{ cm}^{-1}$ ) for  $\text{CO}_2$  at normal conditions to the values  $1383$  and  $1277\text{ cm}^{-1}$  ( $\Delta = 106\text{ cm}^{-1}$ ); the increased value of  $\Delta$  in the spectrum of melanoflogite from Fortullino (Fig. 1.8) also corresponds to a high-density  $\text{CO}_2$  fluid. The very weak band at  $2908\text{ cm}^{-1}$  which is attributed to  $\text{CH}_4$  and the band at  $3611\text{ cm}^{-1}$  attributed to OH-groups are in a good agreement with the IR spectrum of this sample (Chukanov and Chervonnyi 2016). Thus, nitrogen, which is a substantial component in

melanophlogite from Mt. Hamilton, is absent in the sample from Rio Fortullino.

Melanophlogite from Racalmuto, Sicily (Fig. 1.9) is characterized by a higher content of  $\text{CH}_4$  detected by the bands at  $2901$  and  $3055\text{ cm}^{-1}$  and by a trace amount of  $\text{C}_2\text{H}_6$  detected by the very weak bands at  $998$  and  $2945\text{ cm}^{-1}$  (Kohlrausch 1943; Momma et al. 2011). The presence of  $\text{H}_2\text{S}$  molecules is detected by the presence in the Raman spectrum of the band at  $2595\text{ cm}^{-1}$ . This sample does not contain  $\text{N}_2$  and  $\text{CO}_2$  molecules in detectable amounts. The sample of melanophlogite from Racalmuto contains a small amount of mineral impurities of calcite or aragonite (the band at  $1087\text{ cm}^{-1}$ : Edwards et al. 2005) and celestine ( $998\text{ cm}^{-1}$ : Frezzotti et al. 2012). The weak band at  $802\text{ cm}^{-1}$  and the bands at  $363$  and  $276\text{ cm}^{-1}$  relate to the spectrum of the melanophlogite-type silicon-oxygen framework.

Melanophlogite from Miniera Giona, Sicily (Fig. 1.10) contains  $\text{H}_2\text{S}$  molecules (the band of H–S-stretching vibrations at  $2593\text{ cm}^{-1}$ ) and a low amount of  $\text{CH}_4$  molecules ( $2904\text{ cm}^{-1}$ ) whereas bands of  $\text{N}_2$  and  $\text{CO}_2$  are not observed in its Raman spectrum. This sample contains anhydrite admixture detected by the Raman bands at  $1132$  and  $1004\text{ cm}^{-1}$  (Frezzotti et al.

**Fig. 1.10** Raman spectrum of melanophlogite from Miniera Giona



2012). Broad peaks in Figs. 1.9 and 1.10 are due to fluorescence.

Powder IR spectra of melanophlogite from some other localities do not show any presence of methane molecules. In the frequency range from 2800 to 3000 cm<sup>-1</sup>, a sample from Chvaletice, Bohemia shows the presence of three overlapping, relatively broad bands indicative of the contamination by a polyatomic aliphatic hydrocarbon, most probably grease. Similar but much weaker bands are present in the IR spectrum of melanophlogite from Fortullino, Italy (Fig. 1.7), but no characteristic bands of methane are observed in this spectrum too.

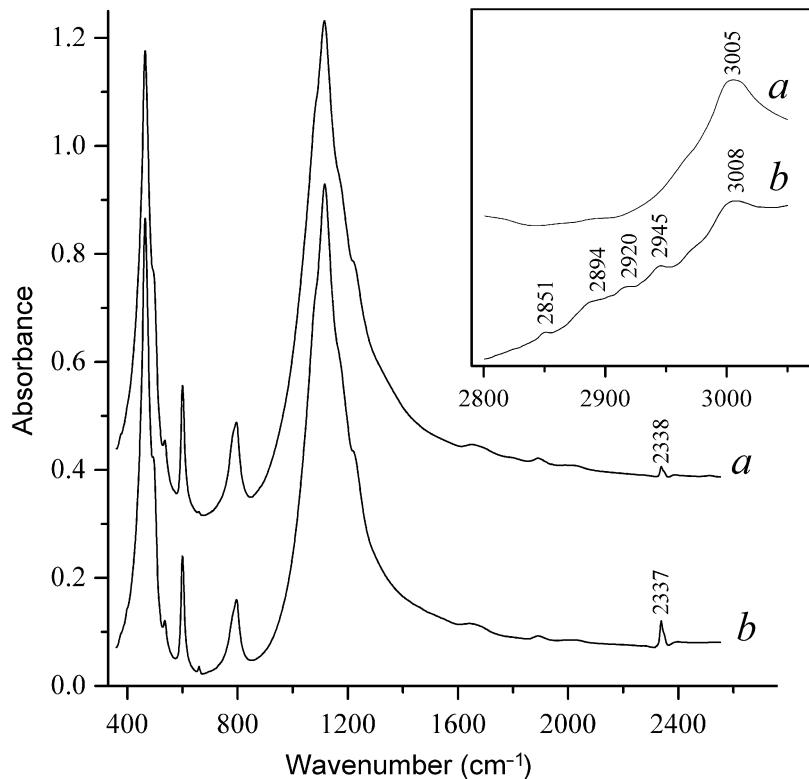
The IR spectra of melanophlogite samples from Racalmuto and Miniera Giona (Fig. 1.11) show much lower contents of CO<sub>2</sub> (the bands at 2337–2338 cm<sup>-1</sup>) and substantially higher contents of CH<sub>4</sub> (the bands at 3005–3008 cm<sup>-1</sup>) as compared with the sample from Fortullino. Moreover, the bands in the range from 2850 to 2950 cm<sup>-1</sup> in the IR spectrum of melanophlogite samples from Miniera Giona indicate the presence of hydrocarbons heavier than methane. IR spectrum of the sample from Racalmuto confirms the presence of H<sub>2</sub>S (Fig. 1.12).

The band assignment and the distribution of different components between [5<sup>12</sup>] and [5<sup>12</sup>6<sup>2</sup>] cages in melanophlogite samples from different localities are given in Table 1.1. These examples show that, in all probability, melanophlogite is not a single mineral species, but a mineral group including minerals with different combinations of small molecules (CO<sub>2</sub>, CH<sub>4</sub>, H<sub>2</sub>S, N<sub>2</sub>, H<sub>2</sub>O, C<sub>2</sub>H<sub>6</sub>) entrapped in the [5<sup>12</sup>] and [5<sup>12</sup>6<sup>2</sup>] cages. In particular, the mineral from Fortullino may be the CO<sub>2</sub>-dominant analogue of melanophlogite, and in the samples from Racalmuto and Miniera Giona H<sub>2</sub>S may be a species-defining component.

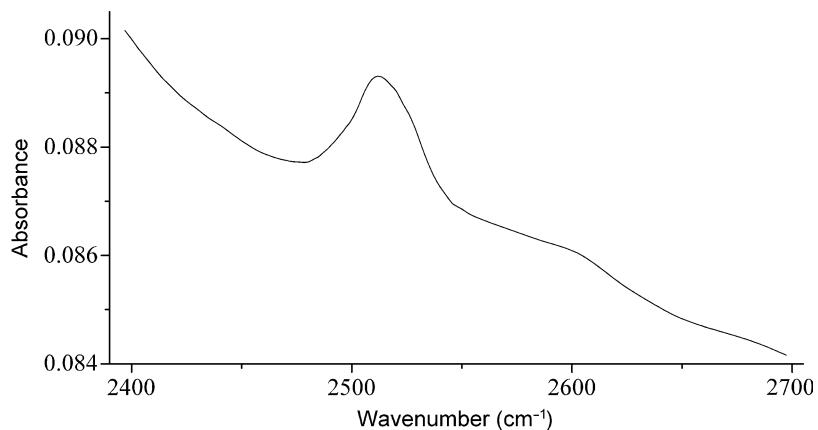
### 1.3 Problem of Nakauriite

Nakauriite was initially described as a new mineral with the general formula (Mn,Ni,Cu)<sub>8</sub>(SO<sub>4</sub>)<sub>4</sub>(CO<sub>3</sub>)(OH)<sub>6</sub>·48H<sub>2</sub>O (Suzuki et al. 1976). The mineral occurs in fissure-fillings in brucite-bearing serpentine at Nakauri, Aichi Prefecture, Japan, and is intimately intergrown with chrysotile. Most analytical data for nakauriite, including powder X-ray diffraction pattern, chemical composition and IR spectrum, have been obtained for a polymineral mixture, in

**Fig. 1.11** Powder IR spectra of melanophlogite from Racalmuto (*a*) and Miniera Giona (*b*)



**Fig. 1.12** IR spectrum of melanophlogite from Racalmuto in the region of S–H-stretching vibrations



which chrysotile is the main phase. The above formula does not conform to analytical data of Suzuki et al. (1976). Taking into account strong predominance of Cu over Mn and Ni, the simplified formula  $\text{Cu}_8(\text{SO}_4)_4(\text{CO}_3)(\text{OH})_6 \cdot 48\text{H}_2\text{O}$  is given for nakauriite in the IMA list of minerals. Published IR spectrum of nakauriite from its type

locality contains strong bands of admixed chrysotile at 1075, 950 and 613  $\text{cm}^{-1}$  (Suzuki et al. 1976; see curve *a* in Fig. 1.13), but characteristic bands of sulfate anions are not observed.

Later nakauriite was reported from several localities in Great Britain, USA, Austria, Italy, and Russia (Braithwaite and Pritchard 1983;

**Table 1.1** The assignment of IR and Raman bands and the distribution of different enclathrated components between  $[5^{12}]$  and  $[5^{12}6^2]$  cages for melanophlogite samples from different localities

| Locality                  | Wavenumber ( $\text{cm}^{-1}$ ) | Assignment   |
|---------------------------|---------------------------------|--|
| Mt. Hamilton <sup>a</sup> | 3050w (R)                       | $\text{CH}_4$ (first overtone of the doubly degenerate $\nu_2$ -bending mode?)                           |
|                           | 2909w (R)                       | $\text{CH}_4$ in $[5^{12}6^2]$ (symmetric stretching mode)   |
|                           | 2900 (R)                        | $\text{CH}_4$ in $[5^{12}]$ (symmetric stretching mode)  |
|                           | 2321 (R)                        | $\text{N}_2$ in $[5^{12}6^2]$  |
|                           | 1378.5 (R)                      | $\text{CO}_2$ in $[5^{12}6^2]$ (symmetric stretching mode)   |
|                           | 1376 (R)                        | $\text{CO}_2$ in $[5^{12}]$ (symmetric stretching mode)  |
|                           | 1277 (R)                        | $\text{CO}_2$ : Fermi resonance between symmetric stretching mode and first overtone of the bending mode |
| Fortullino                | 3700 (IR)                       | $\text{H}_2\text{O}$ (antisymmetric stretching mode)   |
|                           | 3611 (R)                        | $\text{H}_2\text{O}$ (?) O-H-stretching mode   |
|                           | 3596 (IR)                       | $\text{H}_2\text{O}$ (symmetric stretching mode)   |
|                           | 3316 (IR)                       | $\text{H}_2\text{O}$ (?) O-H-stretching mode (H-bonded OH)   |
|                           | 2908w (R)                       | $\text{CH}_4$ in $[5^{12}6^2]$   |
|                           | 2344 (IR)                       | $^{12}\text{CO}_2$ in $[5^{12}]$ (antisymmetric stretching mode)   |
|                           | 2336 (IR)                       | $^{12}\text{CO}_2$ in $[5^{12}6^2]$ (antisymmetric stretching mode)                                      |
|                           | 2273w (IR)                      | $^{13}\text{CO}_2$ (antisymmetric stretching mode)   |
|                           | 1398w (R)                       | $\text{CO}_2$ ("hot band")   |
|                           | 1383 (R)                        | $\text{CO}_2$ in $[5^{12}6^2]$ (symmetric stretching mode)   |
|                           | 1377 (R)                        | $\text{CO}_2$ in $[5^{12}]$ (symmetric stretching mode)  |
|                           | 1277 (R)                        | $\text{CO}_2$ : Fermi resonance between symmetric stretching mode and first overtone of the bending mode |
|                           | 1257w (R)                       | $\text{CO}_2$ ("hot band")   |
| Racalmuto                 | 3055w (R)                       | Hydrocarbon other than methane   |
|                           | 3005w (IR)                      | $\text{CH}_4$ in $[5^{12}]$ (asymmetric stretching mode)   |
|                           | 2945w (R)                       | $\text{C}_2\text{H}_6$ ?   |
|                           | 2901 (R)                        | $\text{CH}_4$ in $[5^{12}]$ (symmetric stretching mode)  |
|                           | 2595 (R)                        | $\text{H}_2\text{S}$ (symmetric stretching mode)   |
|                           | 2512 (IR)                       | $\text{H}_2\text{S}$ (antisymmetric stretching mode)   |
|                           | 2338w (IR)                      | $^{12}\text{CO}_2$ in $[5^{12}6^2]$ (antisymmetric stretching mode)                                      |
| Miniera Giona             | 3008w (IR)                      | $\text{CH}_4$ in $[5^{12}]$ (asymmetric stretching mode)   |
|                           | 2945w (IR)                      | Hydrocarbon other than methane   |
|                           | 2920w (IR)                      | Hydrocarbon other than methane   |
|                           | 2904w (R)                       | $\text{CH}_4$ in $[5^{12}]$ (symmetric stretching mode)  |
|                           | 2894w (IR)                      | Hydrocarbon other than methane   |
|                           | 2851w (IR)                      | Hydrocarbon other than methane   |
|                           | 2593 (R)                        | $\text{H}_2\text{S}$ (symmetric stretching mode)   |
|                           | 2337 (IR)                       | $^{12}\text{CO}_2$ in $[5^{12}6^2]$ (antisymmetric stretching mode)                                      |

R Raman spectrum, IR infrared spectrum, w weak band

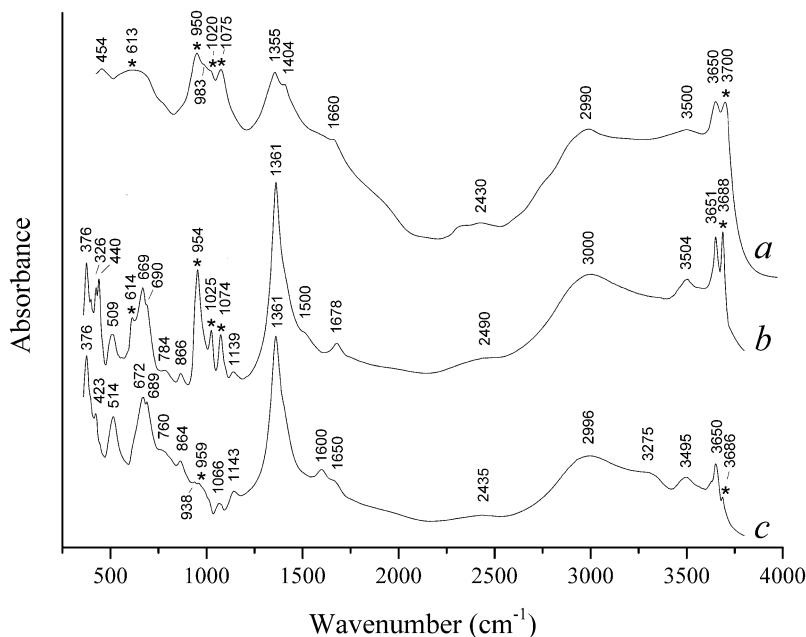
<sup>a</sup>Data from Kolesov and Geiger (2003)

Barnes 1986; Postl and Moser 1988; Palenzona and Martinelli 2007; Popov et al. 2016), as well as a secondary product in metallurgic slags. All available data indicate that nakauriite (1) does not contain sulfate anion and (2) usually forms fine intergrowths with magnesium serpentine-group minerals (see curve *b* in Fig. 1.13). In

particular, electron microprobe analyses of nakauriite from Japan and from Nevada (Peacor et al. 1982) do not show substantial amounts of sulfur. Microchemical tests show only traces of  $\text{SO}_4^{2-}$  (Braithwaite and Pritchard 1983).

We managed to obtain an almost pure fraction of nakauriite from its type locality. Its IR

**Fig. 1.13** IR spectra of nakaurite-bearing samples from Nakauri drawn using data from Suzuki et al. (1976) (a), and from Karkodin, South Urals, Russia (b) and IR spectrum of an almost pure nakaurite from Nakauri (c). Bands of admixed serpentine are marked by asterisk



spectrum is given in Fig. 1.13 (curve c). Specific features of the mineral are unusually low frequency of the non-split band of C–O-stretching vibrations ( $1361\text{ cm}^{-1}$ ), as well as relatively low intensity and high width of the band of out-of-plane bending vibrations of  $\text{CO}_3^{2-}$  groups at  $864\text{ cm}^{-1}$ . The bands at  $1600$  and  $1650\text{ cm}^{-1}$  indicate the presence of  $\text{H}_2\text{O}$  molecules. The same features are inherent in carbonate members of the hydrotalcite group (Chukanov 2014) whose structures contain brucite-like layers and interlayer  $\text{CO}_3^{2-}$  anions and water molecules. Weak bands at  $1066$  and  $1143\text{ cm}^{-1}$  may be due to the presence of trace amounts of  $\text{SO}_4^{2-}$  anions.

Our electron microprobe analyses of nakaurite samples from Nakauri (Japan), Karkodin, (Russia) and Monte Ramazzo mine (Italy) show that this mineral is Mg-dominant. Only three metal cations have been found, namely Mg,  $\text{Cu}^{2+}$ , and  $\text{Ni}^{2+}$ . The atomic ratio Mg:Cu:Ni in a sample from Nakauri is  $0.75:0.23:0.02$ . In another sample from Nakauri Mg:Cu:Ni =  $0.80:0.19:0.01$ . In the sample from Karkodin Mg:Cu:Ni =  $0.75:0.23:0.02$ . Nakaurite from Monte Ramazzo does not contain Ni in detectable amounts; Mg:Cu =  $0.80:0.20$ . In all

analyzed samples the content of sulfur is below its detection limit. The predominance of Mg over Cu in nakaurite from Karkodin was noted also by Popov et al. (2016).

Thermal data for nakaurite from Suzuki et al. (1976) are nearly consistent with the general simplified formula  $(\text{Mg}_3\text{Cu}^{2+})(\text{OH})_6(\text{CO}_3)_4\text{H}_2\text{O}$ . Hypothetically, nakaurite can be an interstratification of brucite and copper carbonate modules. Powder X-ray diffraction data of nakaurite from South Urals kindly provided by I.V. Pekov are given in Table 1.2.

Suzuki et al. (1976) reported the absence of the reflection near  $7.8\text{ \AA}$  in some samples from Nakauri. It was supposed that this reflection may be due to an impurity (Peacor et al. 1982; Braithwaite and Pritchard 1983). However, nakaurite from Karkodin shows a relatively strong reflection at  $7.88\text{ \AA}$  (Table 1.2). In our opinion, the reflections at  $7.32$  and  $7.88\text{ \AA}$  may correspond to nakaurite-type phases with different contents of interlayer water.

A further detailed investigation of nakaurite and revision of its chemical formula are required.

**Table 1.2** Powder X-ray diffraction data of nakauriite from Karkodin, South Urals, Russia (MoK $\alpha$  radiation)

| $d, \text{\AA}$ | $I, \%$ | $d, \text{\AA}$ | $I, \%$ | $d, \text{\AA}$ | $I, \%$ |
|-----------------|---------|-----------------|---------|-----------------|---------|
| 7.88            | 19      | 2.845           | 4       | 1.5947          | 1       |
| 7.32            | 100     | 2.677           | 4       | 1.5762          | 1       |
| 5.11            | 12      | 2.612           | 8       | 1.5447          | 12      |
| 4.835           | 17      | 2.536           | 4       | 1.5185          | 5       |
| 4.629           | 12      | 2.365           | 43      | 1.5107          | 4       |
| 4.485           | 14      | 2.258           | 7       | 1.4569          | 5       |
| 4.217           | 4       | 2.221           | 4       | 1.4210          | 3       |
| 3.928           | 12      | 2.096           | 1       | 1.4035          | 3       |
| 3.642           | 13      | 2.037           | 2       | 1.3523          | 1       |
| 3.539           | 15      | 1.956           | 3       | 1.2985          | 4       |
| 3.335           | 6       | 1.910           | 24      | 1.2910          | 4       |
| 3.305           | 8       | 1.820           | 2       | 1.2404          | 1       |
| 3.105           | 4       | 1.782           | 3       | 1.2281          | 2       |
| 3.065           | 4       | 1.7206          | 4       | 1.2170          | 2       |
| 2.976           | 3       | 1.6951          | 2       | 1.2021          | 2       |
| 2.939           | 3       | 1.6657          | 2       | 1.1973          | 2       |
| 2.874           | 4       | 1.6439          | 5       | 1.1082          | 1       |

## 1.4 Relationship Between Nepskoeite and Shabynite

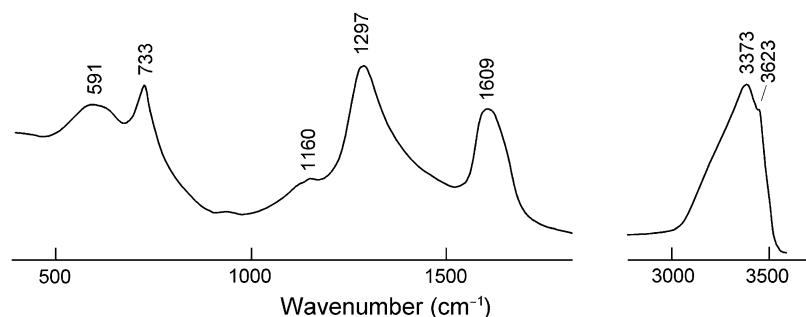
Nepskoeite was initially described as a new chloride-hydroxide mineral with the formula  $\text{Mg}_4\text{Cl}(\text{OH})_7 \cdot 6\text{H}_2\text{O}$  (Apollonov 1998). However, IR spectrum of nepskoeite published by Apollonov (1998) contains very strong band at  $1297 \text{ cm}^{-1}$  corresponding to stretching vibrations of orthoborate groups, as well as distinct band at  $591 \text{ cm}^{-1}$  that may correspond to bending vibrations of orthoborate groups (Fig. 1.14).

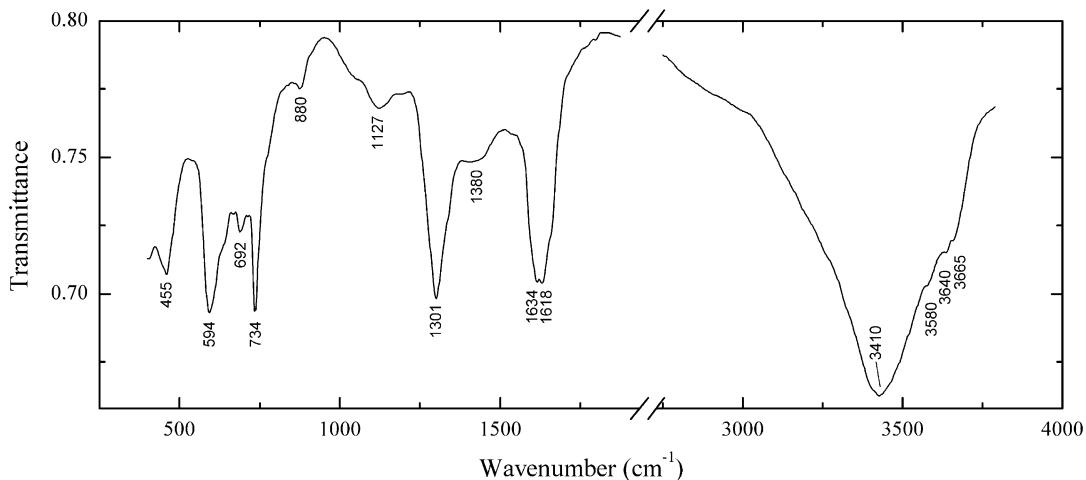
Our reinvestigation of nepskoeite from the type material confirmed the presence of boron in this mineral. In particular, IR spectrum contains strong bands at  $1301$  and  $734 \text{ cm}^{-1}$  corresponding to stretching and bending vibrations of  $\text{BO}_3^{3-}$  anions, respectively (Chukanov 2014; see Fig. 1.15). Moreover, color reaction with quinalizarin shows a high content of boron in nepskoeite.

IR spectrum of nepskoeite shows similarity with that of shabynite  $\text{Mg}_5(\text{BO}_3)(\text{Cl},\text{OH})_2(\text{OH})_5 \cdot 4\text{H}_2\text{O}$  (Fig. 1.16). In particular, the IR spectrum of shabynite contains strong bands at  $1302$  and  $732 \text{ cm}^{-1}$ . However, substantial differences between these spectra are observed in the region of vibrations of  $\text{H}_2\text{O}$  molecules above  $1500 \text{ cm}^{-1}$ .

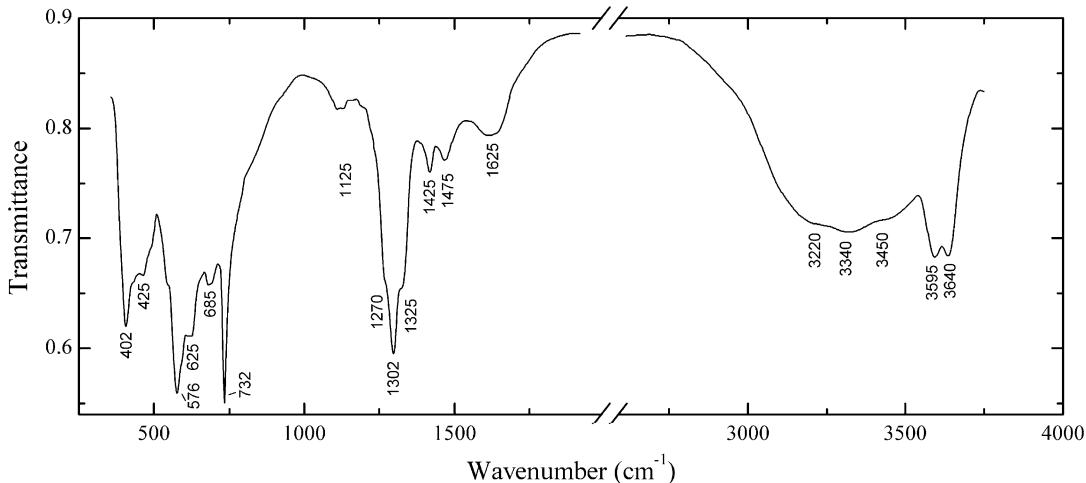
There is also close similarity between powder X-ray diffraction (PXRD) patterns of nepskoeite and shabynite (Table 1.3). However, nepskoeite shows strong reflections at  $10.64$  and  $3.498 \text{ cm}^{-1}$  that are absent in the PXRD pattern of shabynite. On the other hand, strongest reflections of different shabynite samples are observed at  $9.62$  and  $3.191 \text{ cm}^{-1}$ . Refraction indices of nepskoeite ( $\alpha = 1.532$ ,  $\beta \approx \gamma = 1.562$ ) are somewhat lower than those of shabynite ( $\alpha = 1.543$ ,  $\beta = 1.571$ ,  $\gamma = 1.577$ ).

Based on these data, nepskoeite can be tentatively considered as a hydrous orthoborate chloride, a high-hydrated analogue of shabynite. Both minerals need further investigations, first of all, determination of unit-cell dimensions and  $\text{H}_2\text{O}$  content by means of direct methods.

**Fig. 1.14** IR spectrum of nepskoeite drawn using data from Apollonov (1998)



**Fig. 1.15** IR spectrum of nepskoeite drawn using data from Chukanov (2014)



**Fig. 1.16** IR spectrum of shabynite drawn using data from Chukanov (2014)

## 1.5 Orthoborate Groups in Lead Carbonate Minerals

The  $\text{CO}_3^{2-}$  and  $\text{BO}_3^{3-}$  anions have the same trigonal planar configuration, but in most orthoborate and carbonate minerals these groups do not show appreciable isomorphous substitutions. The main causes of the absence of isomorphous substitutions between these groups are differences in their charges and sizes. In addition,  $\text{BO}_3^{3-}$  groups are often significantly distorted (see, e.g., Kolitsch et al. 2012, as well as Sect. 1.1). However, some

lead carbonate minerals are exceptions from this regularity. For example, IR spectra of some samples of molybdophyllite  $\text{Pb}_8\text{Mg}_9(\text{Si}_{10}\text{O}_{28})(\text{CO}_3)_3(\text{OH})_8\text{O}_2\text{H}_2\text{O}$ , which is nominally a boron-free mineral, show weak IR bands of B–O-stretching vibrations at 1170 and 1240  $\text{cm}^{-1}$  (Fig. 1.17), whereas Raman spectrum of the structurally investigated molybdophyllite sample does not show bands of borate groups (Kolitsch et al. 2012).

The crystal structure of molybdophyllite (Kolitsch et al. 2012) does not contain boron-

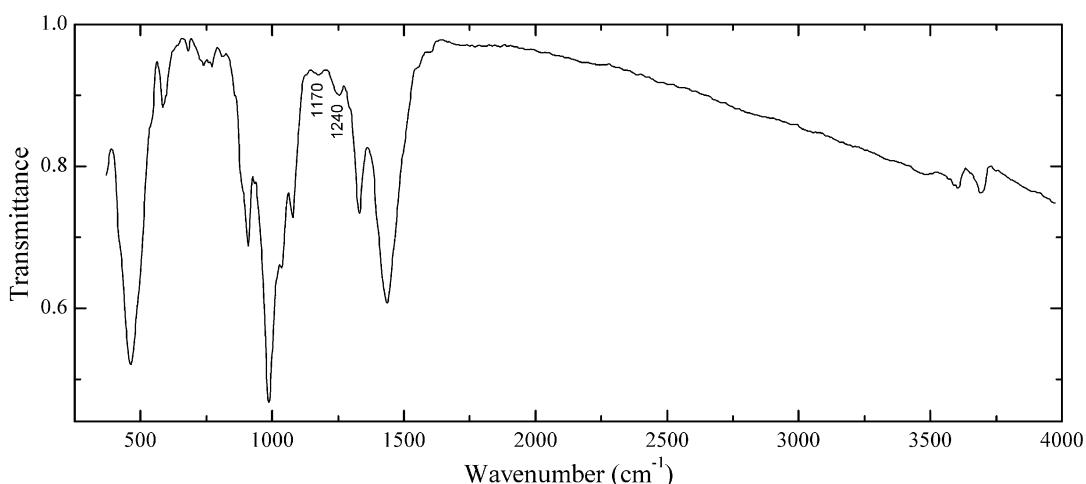
**Table 1.3** Strongest lines (with  $I \geq 10\%$ ) of the PXRD patterns of nepskoeite and shabynite

| Nepskoeite<br>(Apollonov 1998) | Shabynite, sample No. 3<br>(Pertsev et al. 1980) |                 |                |
|--------------------------------|--|-----------------|----------------|
| $d, \text{\AA}$                | $I, \%$  | $d, \text{\AA}$ | $I, \%$        |
| 11.41                          | 29   | 11.33           | 10             |
| 10.64                          | 18   | — <sup>a</sup>  | — <sup>a</sup> |
| 9.78                           | 46   | 9.72            | 17             |
| 9.60                           | 38   | —               | —              |
| 5.57                           | 17   | —               | —              |
| 5.48                           | 16   | 5.48            | 16             |
|                                |  | 5.41            | 16             |
| —                              | —  | 4.86            | 19             |
| 4.78                           | 15   | 4.77            | 19             |
| 4.25                           | 20   | 4.266           | 16             |
|                                |  | 4.230           | 17             |
| —                              | —  | 4.133           | 29             |
| 3.726                          | 15   | 3.726           | 17             |
| 3.624                          | 14   | 3.648           | 10             |
| 3.498                          | 100  | —               | —              |
| —                              | —  | 3.191           | 100            |
| 3.184                          | 10   | —               | —              |
| 2.977                          | 10   | —               | —              |
| 2.739                          | 16   | —               | —              |
| 2.448                          | 18   | 2.447           | 19             |
| 2.395                          | 17   | 2.390           | 11             |
| 2.284                          | 11   | —               | —              |
| 1.749                          | 10   | —               | —              |

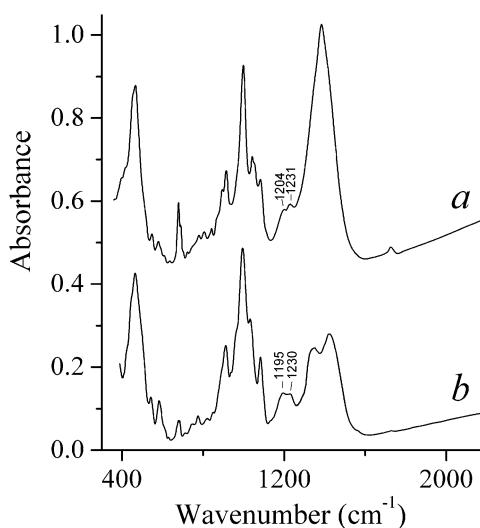
<sup>a</sup>The strongest reflection of the powder X-ray diffraction pattern of shabynite sample No. 2 (Pertsev et al. 1980) is observed at 9.62 Å

dominant sites and, consequently,  $\text{BO}_3^{3-}$  anions occur in  $\text{CO}_3^{2-}$ -dominant positions, unlike roymillerite  $\text{Pb}_{24}\text{Mg}_9(\text{Si}_9\text{AlO}_{28})(\text{SiO}_4)(\text{BO}_3)(\text{CO}_3)_{10}(\text{OH})_{14}\text{O}_4$  and britvinitite  $\text{Pb}_{15}\text{Mg}_9(\text{Si}_{10}\text{O}_{28})(\text{CO}_3)_2(\text{BO}_3)_4(\text{OH})_{12}\text{O}_2$ , in which orthoborate and carbonate groups are ordered in different sites (Yakubovich et al. 2008; Chukanov et al. 2017b; see Fig. 1.18).

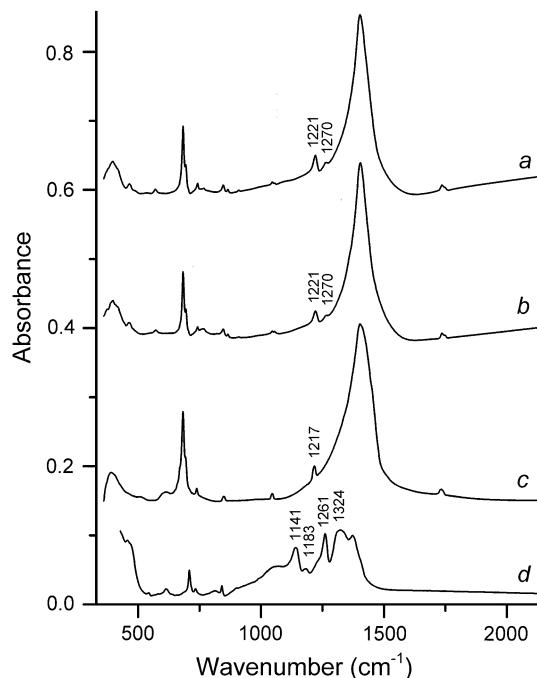
The IR spectrum of hydrocerussite  $\text{Pb}_3(\text{OH})_2(\text{CO}_3)_2$  from Långban (curve *b* in Fig. 1.19) contains weak bands at 1230 (shoulder), 742, and 470  $\text{cm}^{-1}$ . These bands may be assigned to stretching and bending vibrations of orthoborate anions partly substituting regular  $\text{CO}_3$  triangles in the hydrocerussite structure. Indeed, in the IR spectrum of fluoborite containing regular  $\text{BO}_3$  triangle strong bands of B–O-stretching and O–B–O bending vibrations are observed at 1241, 743, and 468  $\text{cm}^{-1}$  (Chukanov 2014). It is important to note that bands of orthoborate groups are absent in the IR spectra of hydrocerussite from Merehead quarry, England (curve *a* in Fig. 1.19), some related minerals (curves *c* and *d* in Fig. 1.19), as well as synthetic analogues of hydrocerussite and plumbonacrite (Brooker et al. 1983). In all probability, the presence of borate groups in hydrocerussite from Långban is the result of high activity of boron that accompanied formation of this deposit where different borate minerals are common.



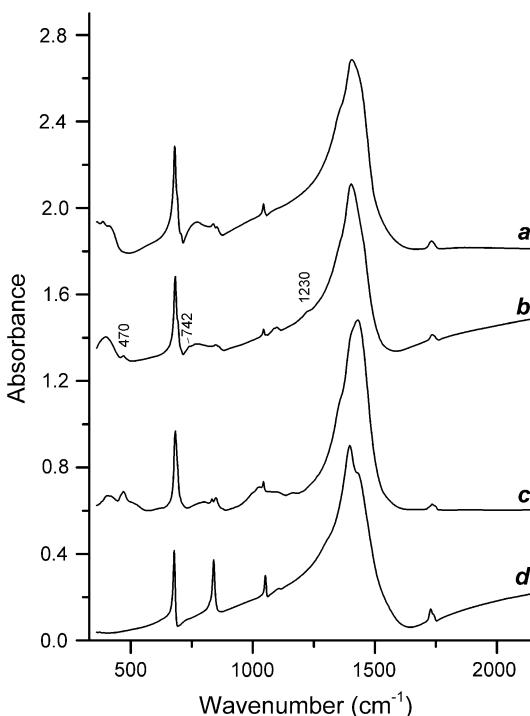
**Fig. 1.17** IR spectrum of molybdophyllite from the Långban deposit, Bergslagen ore region, Filipstad district, Värmland, Sweden (Chukanov 2014, sample Sil247). The wavenumbers of  $\text{BO}_3^{3-}$  groups are indicated



**Fig. 1.18** IR spectra of (a) roymillerite and (b) britvinitie from Långban, Värmland, Sweden. Bands of stretching vibrations of  $\text{BO}_3^{3-}$  groups are indicated



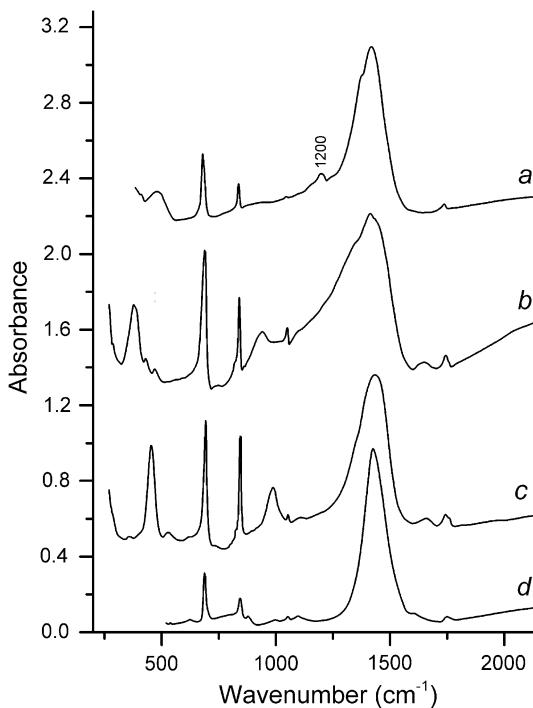
**Fig. 1.20** IR spectra of (a) plumbonacrite from Merehead quarry, (b) plumbonacrite from Långban, (c) somersetite, and (d) mereheadite. Bands of stretching vibrations of  $\text{BO}_3^{3-}$  groups are indicated



**Fig. 1.19** IR spectra of (a) hydrocerussite from Merehead quarry, (b) hydrocerussite from Långban, (c) hydrocerussite-related phase  $\text{NaPb}_5(\text{CO}_3)_4(\text{OH})_3$  from Lavrion, and (d) cerussite from Merehead quarry. Bands of  $\text{BO}_3^{3-}$  groups are indicated

The IR spectra of plumbonacrite  $\text{Pb}_5\text{O}(\text{OH})_2(\text{CO}_3)_3$  from Merehead and Långban (Fig. 1.20) are similar and differ from the IR spectra of synthetic plumbonacrite analogue (Brooker et al. 1983) by additional bands of  $\text{BO}_3^{3-}$  groups at 1270, 1221, 742, and 464–465 cm<sup>-1</sup>. Unlike hydrocerussite, a mineral with the only site of  $\text{CO}_3^{2-}$  groups, in the crystal structure, plumbonacrite is characterized by five positions of carbonate groups (Krivovichev and Burns 2000). The IR spectrum of plumbonacrite contains two bands of asymmetric B–O-stretching vibrations (at 1270 and 1221 cm<sup>-1</sup>), which indicates the presence of  $\text{BO}_3^{3-}$  groups in different sites.

The IR spectrum of somersetite (curve c in Fig. 1.20) is similar to those of plumbonacrite and hydrocerussite and contains bands of  $\text{BO}_3^{3-}$  groups at 1217 and 738 cm<sup>-1</sup>. The crystal structure of somersetite consists of electroneutral  $[\text{Pb}_3(\text{OH})_2(\text{CO}_3)_2]$  hydrocerussite block and electroneutral  $[\text{Pb}_5\text{O}_2(\text{CO}_3)_3]$  block with the structure derivative from plumbonacrite. The



**Fig. 1.21** IR spectra of (a) grootfonteinite holotype, (b) synthetic compound  $\text{KPb}_2(\text{CO}_3)_2(\text{OH})$  (Brooker et al. 1983), (c) synthetic compound  $\text{NaPb}_2(\text{CO}_3)_2(\text{OH})$  (Brooker et al. 1983), and (d) abellaite holotype (Ibáñez-Insa et al. 2017). Band of stretching vibrations of  $\text{BO}_3^{3-}$  groups is indicated

only band of B–O-stretching vibrations observed in the IR spectrum of somersetite indicates that all admixed  $\text{BO}_3^{3-}$  groups belong to the hydrocerussite block.

The relatively weak bands at 480 and  $1200\text{ cm}^{-1}$  in the IR spectrum of grootfonteinite  $\text{Pb}_3\text{O}(\text{CO}_3)_2$  indicate the presence of minor amounts of undistorted orthoborate groups, but these groups are absent in most samples of structurally related minerals and compounds (see Fig. 1.21).

In hydrocerussite, plumbonacrite, somersetite, and grootfonteinite  $\text{CO}_3/\text{BO}_3$  are undistorted. As a result, bands of admixed B–O-stretching vibrations of  $\text{BO}_3^{3-}$  anions are observed in the narrow wavenumber range from  $1200$  to  $1270\text{ cm}^{-1}$ . In contrast to these minerals, in mereheadite  $\text{Pb}_{47}\text{O}_{24}(\text{OH})_{13}\text{Cl}_{25}(\text{BO}_3)_2(\text{CO}_3)$   $\text{BO}_3$  triangles are significantly distorted with B–O distances varying from  $1.23$  to  $1.32\text{ \AA}$  (Krivovichev et al. 2009). This results in splitting of the band of B–O-stretching vibrations into several components (at  $1141$ ,  $1183$ , and  $1261\text{ cm}^{-1}$ ); in addition, broad band at  $1324\text{ cm}^{-1}$  corresponding to a mixed mode involving B–O- and C–O-stretching vibrations appears (curve d in Fig. 1.20).



## IR Spectra of Minerals and Related Compounds, and Reference Samples Data

2

This chapter contains IR spectra of mineral species and varieties, most of which was not included in the preceding reference books (Chukanov 2014; Chukanov and Chervonnyi 2016). Along with spectra obtained by us, we provide most reliable new data on infrared spectra of 791 minerals and related synthetic compounds published elsewhere. Each spectrum is accompanied with analytical data on the reference sample, its occurrence and general appearance, associated minerals, as well as kind of sample preparation and/or method of registration of the spectrum.

The Sects. 2.1, 2.2, 2.3, etc. are arranged in ascending order of the atomic number  $Z_a$  of the main species-defining element for a given class of minerals: first for borate minerals (with  $Z_a = 5$  for boron), then for carbon, carbides, carbonates, and organic substances (with  $Z_a = 6$  for carbon), for nitrates (with  $Z_a = 7$  for nitrogen), for oxides and hydroxides (with  $Z_a = 8$  for oxygen), and so on.

A total of 174 spectra presented in this chapter have been obtained by one of the authors (NVC). In order to obtain absorption infrared spectra, powdered mineral samples have been mixed with anhydrous KBr, pelletized, and analyzed using an ALPHA FT IR spectrometer (Bruker Optics, Ettlingen, Germany) with a resolution of  $4 \text{ cm}^{-1}$  and 16 scans. IR spectrum of an analogous disc of pure KBr was used as a reference. It is important to note that reflectance mode IR spectra, IR spectra obtained without immersion medium (e.g., KBr), as well as IR spectra of

single crystals, coarse-grained, or textured aggregates cannot be considered as stable and reliable diagnostic characteristics of mineral species due to specific effects induced by orientation, polarization, scattering, and reflection conditions. For example, in case of a single crystal, bands corresponding to normal vibrations with polarization vector parallel to the direction of propagation of IR radiation are absent in the spectrum. However these bands can be observed at another orientation of the crystal. In more detail these aspects were considered above (see Chukanov and Chervonnyi 2016, the section “Sources of Errors and Artifacts in IR Spectroscopy of Minerals”). For the above reasons, *only transmittance or absorbance IR spectrum of a pulverized sample dispersed in an immersion medium is a stable characteristic of a mineral and can be used as a diagnostic tool*.

Additional information includes general appearance, associated minerals, methods of the mineral species identification, and the list of wavenumbers of absorption bands with the indication of strong bands, weak bands, and shoulders. IR spectroscopy itself can be considered as an adequate identification method if IR spectrum is unique for a given mineral and coincides with IR spectrum of a well-investigated sample. For most synthetic samples the method of synthesis is shortly characterized.

For more than 100 samples (mainly holotypes of mineral species), a more detailed information is given including unit-cell dimensions, symmetry,

strongest reflections of the powder X-ray diffraction pattern, empirical formula, optical data, density, etc.

The following *abbreviations* are used in this chapter:

|                       |  |
|-----------------------|--|
| Mt.                   | mountain   |
| Co.                   | county   |
| IR                    | infrared   |
| D                     | density  |
| $D_{\text{meas}}$     | measured density   |
| $D_{\text{calc}}$     | calculated density   |
| apfu                  | atoms per formula unit   |
| Z                     | the number of formula units per unit cell                            |
| $\alpha, \beta$ ,     | refractive indices for biaxial minerals                              |
| $\gamma$              |  |
| $\omega, \varepsilon$ | refractive indices for uniaxial minerals                             |
| n                     | refractive index for isotropic minerals                              |
| 2V                    | angle between optic axes   |
| d                     | interplanar spacing  |
| I                     | relative intensity of a line in the powder X-ray diffraction pattern |
| REE                   | rare-earth elements  |
| Ln                    | lanthanides  |
| s                     | strong band  |

|    |           |
|----|-----------|
| w  | weak band |
| sh | shoulder  |
| □  | vacancy   |

In most cases, the terms “strong band” and “weak band” mean band having transmittance minimum below and above any conventional values, respectively. As a rule, “shoulder” means inflection point of the spectral curve. For the convenience of visual perception, the positions of all peaks and shoulders in most figures are indicated by arrows.

For the numeration of samples, double letter-figure symbols are used. This numbering is a continuation of the numbering used in the previous books of this series (Chukanov 2014; Chukanov and Chervonnyi 2016). The meaning of letter parts of the symbols is explained in Table 2.1. It is to be noted that these designations are conventional and not unambiguous. For example, zirsilite-(Ce),  $\text{Na}_{12-x}(\text{Ce}, \text{Na})_3\text{Ca}_6\text{Mn}_3\text{Zr}_3\text{NbSi}_{25}\text{O}_{73}(\text{OH})_3(\text{CO}_3)\cdot\text{H}_2\text{O}$ , can be classified as cyclosilicate, as zirconosilicate or as carbonatosilicate.

**Table 2.1** The meaning of letter symbols used in the numbering of reference samples

| Symbol | Meaning of the symbol   | Symbol | Meaning of the symbol  |
|--------|---|--------|--|
| Bo     | Borates with isolated orthogroups $\text{BO}_3$   | PSi    | Phosphato-silicates  |
| B      | Other borates   | SSi    | Sulfato-silicates  |
| BC     | Carbonatoborates  | TiSi   | Titanosilicates and related zircono-, niobo-, and stannosilicates      |
| BAs    | Arsenatoborates   | AsSi   | Arsenato-silicates   |
| C      | Carbon and carbonates   | USi    | Silicates with uranyl groups $\text{UO}_2^{2+}$ (except nesosilicates) |
| Org    | Organic compounds and salts of organic acids  | P      | Phosphides and phosphates  |
| N      | Nitrides and nitrates   | S      | Sulfates   |
| O      | Oxides and hydroxides   | SC     | Carbonato-sulfates   |
| F      | Fluorides   | SP     | Phosphato-sulfates   |
| Sio    | Nesosilicates (i.e., silicates with orthogroups $\text{SiO}_4$ )                                | SMo    | Sulfatomolybdates  |
| Sid    | Sorosilicates (i.e., silicates with diorthogroups $\text{Si}_2\text{O}_7$ or $\text{SiAlO}_7$ ) | Cl     | Chlorides and hydroxychlorides   |
| Siod   | Silicates containing both orthogroups $\text{SiO}_4$ and diorthogroups $\text{Si}_2\text{O}_7$  | V      | Vanadates, V oxides, and hydroxides                                    |
| Sit    | Triorthosilicates with groups $\text{Si}_3\text{O}_{10}$  | Cr     | Chromates  |
| Siot   | Ortho-triorthosilicates   | Ge     | Germanates   |
| Sir    | Cyclosilicates (“r” means “ring”)   | As     | Arsenic, arsenides, arsenites, arsenates, and sulfato-arsenates        |
| Sic    | Inosilicates with chains formed by $\text{SiO}_4$ and $\text{AlO}_4$ tetrahedra                 | UAs    | Uranyl arsenates   |

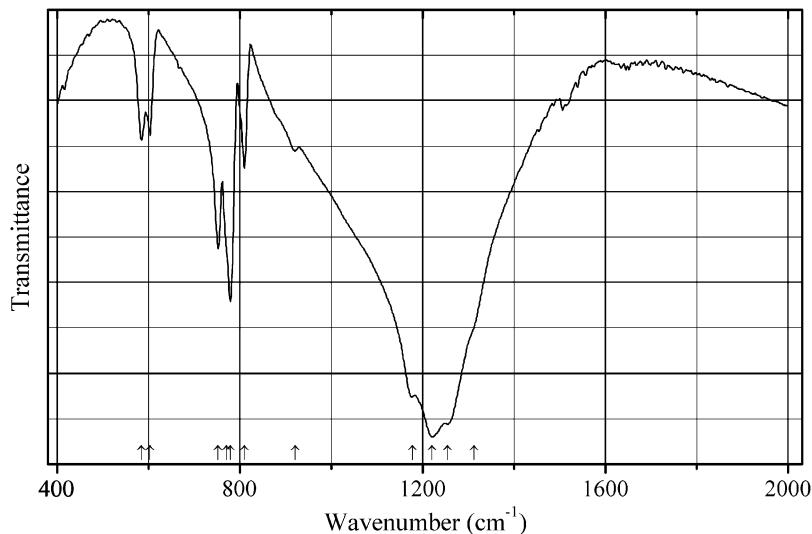
(continued)

**Table 2.1** (continued)

| Symbol | Meaning of the symbol  | Symbol | Meaning of the symbol                  |
|--------|--|--------|--|
| Sib    | Inosilicates with bands formed by $\text{SiO}_4$ and $\text{AlO}_4$ tetrahedra   | AsS    | Sulfato-arsenates                      |
| Sil    | Phyllosilicates with layers formed by $\text{SiO}_4$ and $\text{AlO}_4$ tetrahedra   | Se     | Selenium, selenides, and selenites     |
| Sif    | Tectosilicates (aluminosilicates with 3d frameworks formed by $\text{SiO}_4$ and $\text{AlO}_4$ tetrahedra), except zeolites | Br     | Bromides and bromates                  |
| Sif_Z  | Zeolites   | Mo     | Molybdates and Mo-bearing oxides       |
| Si     | Silicon, silicides, and silicates with unknown or complex structures   | Te     | Tellurides, tellurites, and tellurates |
| Sia    | Amorphous silicates  | I      | Iodides, iodites, and iodates          |
| BeSi   | Beryllosilicates   | Xe     | Xenates                                |
| BSi    | Borosilicates and borato-silicates   | W      | Tungstates and W-bearing oxides        |
| CSi    | Carbonato-silicates  |        |  |

## 2.1 Borates, Including Arsenatoborates and Carbonatoborates

**Bo36 Barium strontium orthoborate fluoride**  $\text{Ba}_3\text{Sr}_4(\text{BO}_3)_3\text{F}_5$



**Origin:** Synthetic.

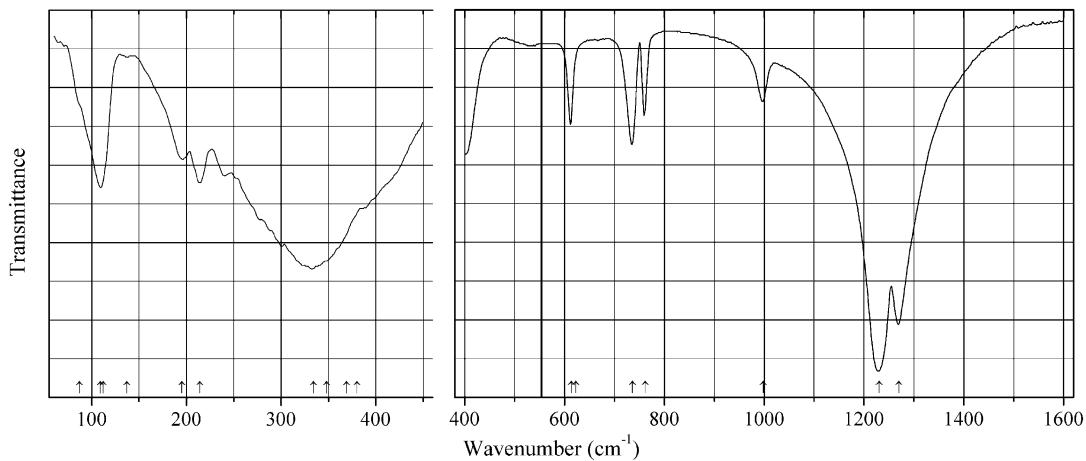
**Description:** Prepared from  $\text{BaF}_2$ ,  $\text{BaCO}_3$ ,  $\text{SrCO}_3$ , and  $\text{H}_3\text{BO}_3$  by using a high-temperature solid-state technique. The crystal structure is solved. Hexagonal, space group  $P6_3mc$ ,  $a = 10.8953(16)$ ,  $c = 6.9381(15)$  Å,  $V = 713.3(2)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{calc}} = 4.814$  g/cm $^3$ . Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Zhang et al. (2009a).

**Wavenumbers (cm $^{-1}$ ):** 1312sh, 1255s, 1221s, 1177s, 921w, 810, 779, 771sh, 753, 604, 585.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**Bo37 Barium zirconium orthoborate**  $\text{BaZr}(\text{BO}_3)_2$ 

**Origin:** Synthetic.

**Description:** Powder obtained by means of standard solid-state reaction from the stoichiometric mixture of  $\text{BaCO}_3$ ,  $\text{ZrO}_2$ , and  $\text{B}_2\text{O}_3$  pressed into a pellet and heated first at  $550^\circ\text{C}$  for 48 h and thereafter heated twice at  $910^\circ\text{C}$  for 20 h. Trigonal,  $a = 5.167$ ,  $c = 33.913 \text{ \AA}$ .

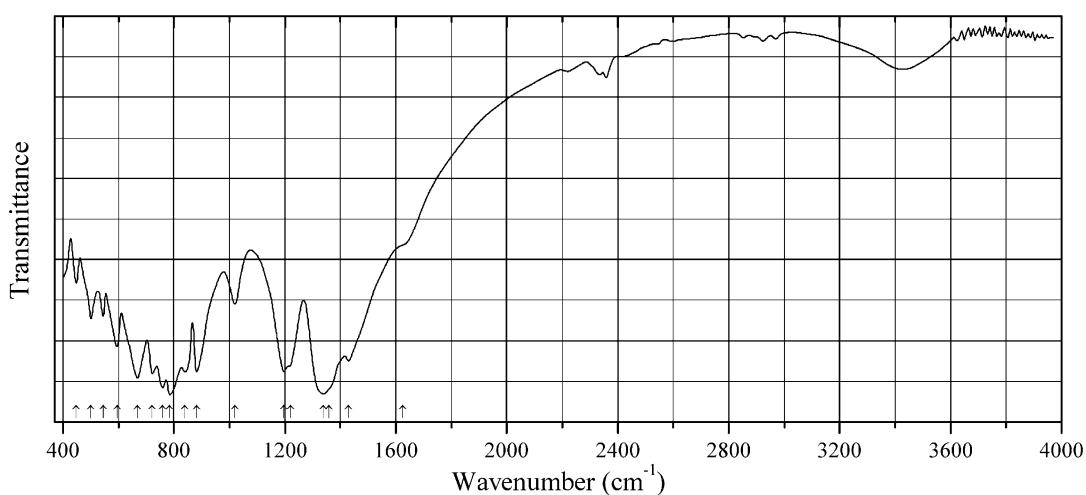
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc (in the  $1500$ – $400 \text{ cm}^{-1}$  region) and Nujol suspension (in the  $500$ – $50 \text{ cm}^{-1}$  region). Transmission.

**Source:** Mączka et al. (2015).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1270s, 1230s, 998w, 761, 736, 613, 380sh, 369sh, 334s, 214, 195w, 137w, 109, 87sh.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1272w, 1258w, 1250w, 1228s, 739w, 622w, 380s, 369s, 348w, 137, 112w, 59.

**Bo38 Cesium beryllium orthoborate**  $\text{CsBe}_4(\text{BO}_3)_3$ 

**Origin:** Synthetic.

**Description:** Prepared from  $\text{Cs}_2\text{CO}_3$ ,  $\text{BeO}$ , and  $\text{B}_2\text{O}_3$  by solid-state reaction at  $800\text{ }^\circ\text{C}$  for 48 h in air. The crystal structure is solved. Orthorhombic, space group  $Pnma$ ,  $a = 8.3914(5)$ ,  $b = 13.3674(7)$ ,  $c = 6.4391(3)$  Å,  $V = 722.28(7)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 3.176$  g/cm $^3$ . Characterized by powder X-ray diffraction data.

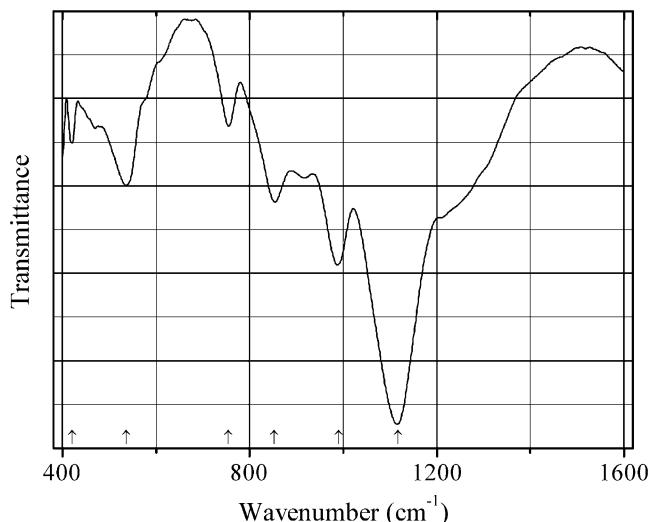
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Huang et al. (2013a).

**Wavenumbers (cm $^{-1}$ ):** (3430), (1625sh), 1430, 1360sh, 1339s, 1220sh, 1197s, 1020, 881, 840, 785s, 760, 722, 669, 595, 545, 501, 448.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The bands at  $3430$  and  $1625\text{ cm}^{-1}$  may correspond to adsorbed water. Weak bands in the range from  $2300$  to  $2400\text{ cm}^{-1}$  correspond to atmospheric  $\text{CO}_2$ .

### Bo39 Calcium orthoborate fluoride $\text{Ca}_5(\text{BO}_3)_3\text{F}$



**Origin:** Synthetic.

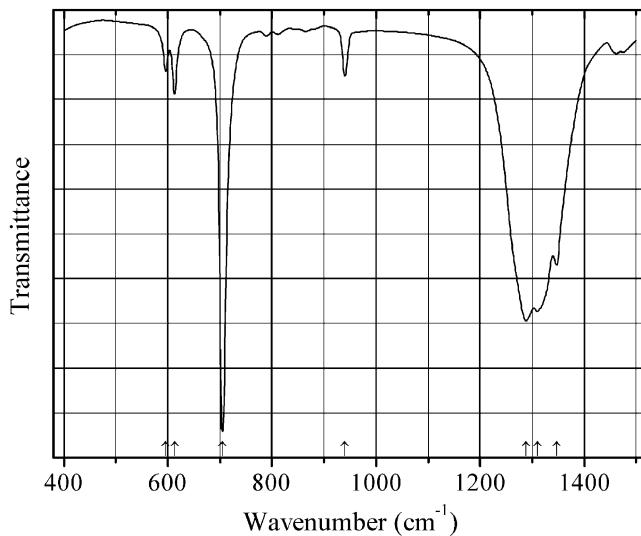
**Description:** Synthesized by high-temperature solid-state reaction from the mixture of  $\text{CaCO}_3$ ,  $\text{H}_3\text{BO}_3$ , and  $\text{CaF}_2$  with the molar ratio 9:6:1. After heating at  $500\text{ }^\circ\text{C}$  for 1 day, the mixture was cooled down to room temperature, ground again, then pressed and sintered at  $1000\text{ }^\circ\text{C}$  for 2 days. Monoclinic, space group  $a = 8.125(3)$ ,  $b = 16.051(5)$ ,  $c = 3.538(2)$  Å,  $\beta = 100.90(4)^\circ$ ,  $Z = 2$ . Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Chen et al. (2006a).

**Wavenumbers (cm $^{-1}$ ):** 1117s, 990, 852, 755w, 536, 420w.

**Note:** The IR spectrum contains additional bands in the range from  $1500$  to  $4000\text{ cm}^{-1}$  that correspond to adsorbed (?) water molecules.

**Bo40 Lanthanum orthoborate La(BO<sub>3</sub>)**

**Origin:** Synthetic.

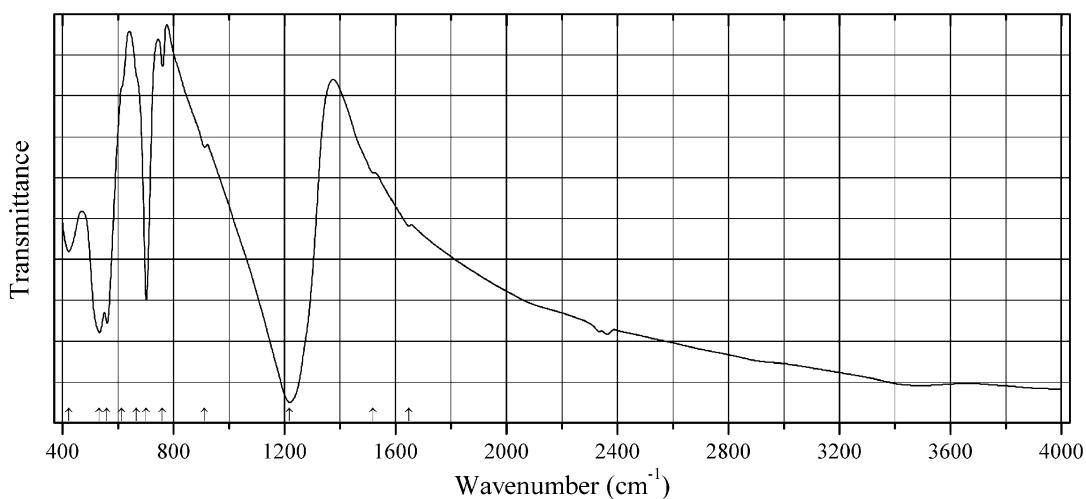
**Description:** Prepared hydrothermally from La<sub>2</sub>O<sub>3</sub> and B<sub>2</sub>O<sub>3</sub> at 200 °C for 24 h. Characterized by powder X-ray diffraction data. Orthorhombic,  $a = 5.0960(8)$ ,  $b = 8.2514(4)$ ,  $c = 5.8726(6)$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** Absorption. Kind of sample preparation is not indicated.

**Source:** Ma et al. (2007).

**Wavenumbers (cm<sup>-1</sup>):** 1347, 1310s, 1288s, 940, 705s, 613, 596w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Bo41 Lead aluminium orthoborate fluoride Pb<sub>6</sub>Al(BO<sub>3</sub>)<sub>2</sub>OF<sub>7</sub> Pb<sub>6</sub>Al(BO<sub>3</sub>)<sub>2</sub>OF<sub>7</sub>**

**Origin:** Synthetic.

**Description:** Prepared from a stoichiometric mixture of  $\text{PbF}_2$ ,  $\text{Al}_2\text{O}_3$ , and  $\text{H}_3\text{BO}_3$  at  $430^\circ\text{C}$  with several intermediate grindings. Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group  $Cmca$ ,  $a = 11.649(7)$ ,  $b = 18.300(11)$ ,  $c = 6.394(4)$  Å,  $V = 1363.1(15)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 7.488$  g/cm $^3$ . In the structure, Al atoms coordinated by F (to form slightly distorted  $\text{AlF}_6$  octahedra) are situated between the  $[\text{Pb}_6\text{BO}_{11}\text{F}_{10}]$  layers.

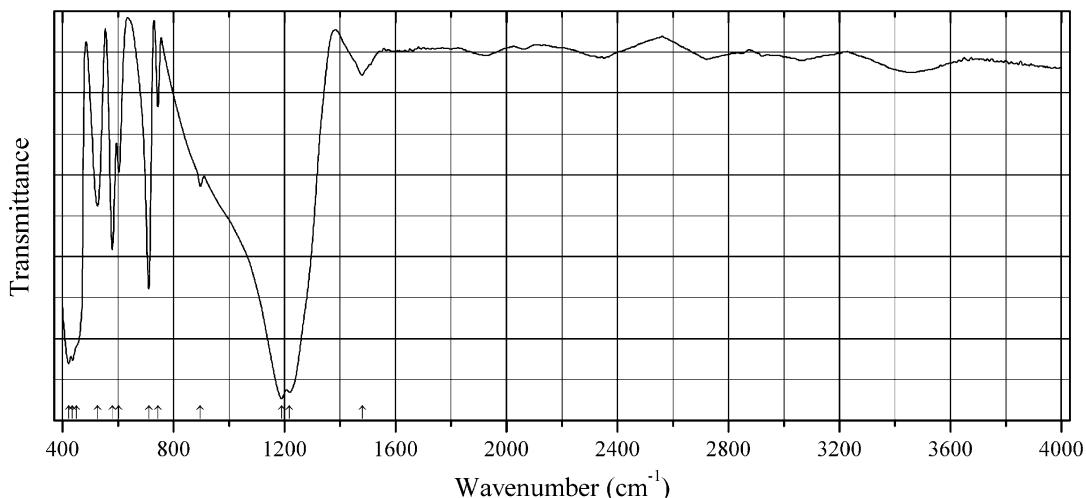
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Dong et al. (2012).

**Wavenumbers (cm $^{-1}$ ):** 1648w, 1520w, 1219s, 912w, 761w, 702s, 665sh, 612sh, 561s, 533s, 423.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### Bo42 Lead bismuth orthoborate $\text{PbBi}(\text{BO}_3)\text{O}$



**Origin:** Synthetic.

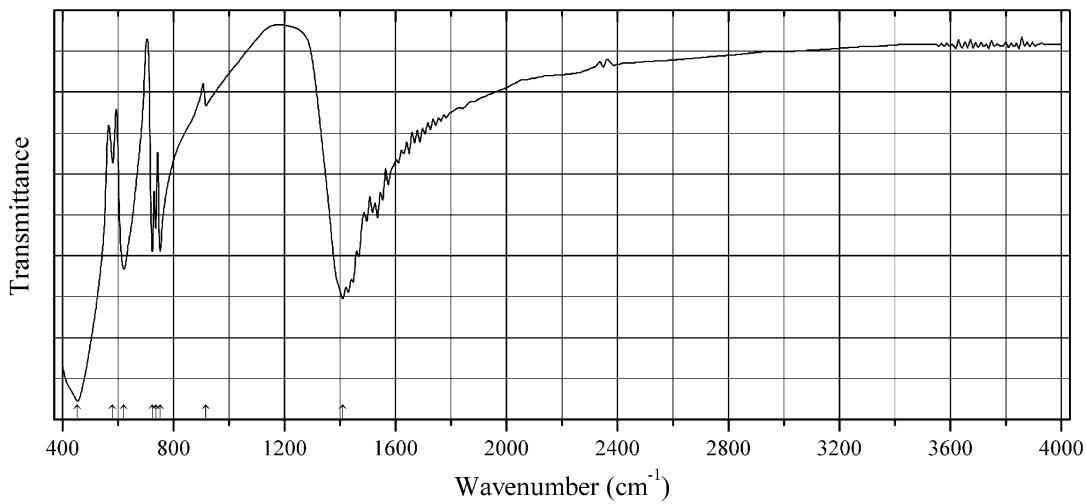
**Description:** Synthesized by solid-state reaction of a stoichiometric mixture of  $\text{PbO}$ ,  $\text{Bi}_2\text{O}_3$ , and  $\text{H}_3\text{BO}_3$  powders. The crystal structure is solved. Orthorhombic, space group  $Cmca$ ,  $a = 10.782(3)$ ,  $b = 10.502(3)$ ,  $c = 7.477(2)$  Å,  $V = 846.7(4)$  Å $^3$ ,  $Z = 8$ .  $D_{\text{calc}} = 7.704$  g/cm $^3$ . Each Bi atom is coordinated to six O atoms. The  $\text{BiO}_6$  octahedra are connected via common vertices and edges to form infinite  $[\text{BiO}_4]$  layer.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Zhao et al. (2011).

**Wavenumbers (cm $^{-1}$ ):** 1480w, 1219s, 1189s, 897, 744, 711s, 603, 579, 526, 452sh, 437s, 422s.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**Bo43 Lead cadmium orthoborate  $\text{Pb}_8\text{Cd}(\text{BO}_3)_6$** 

**Origin:** Synthetic.

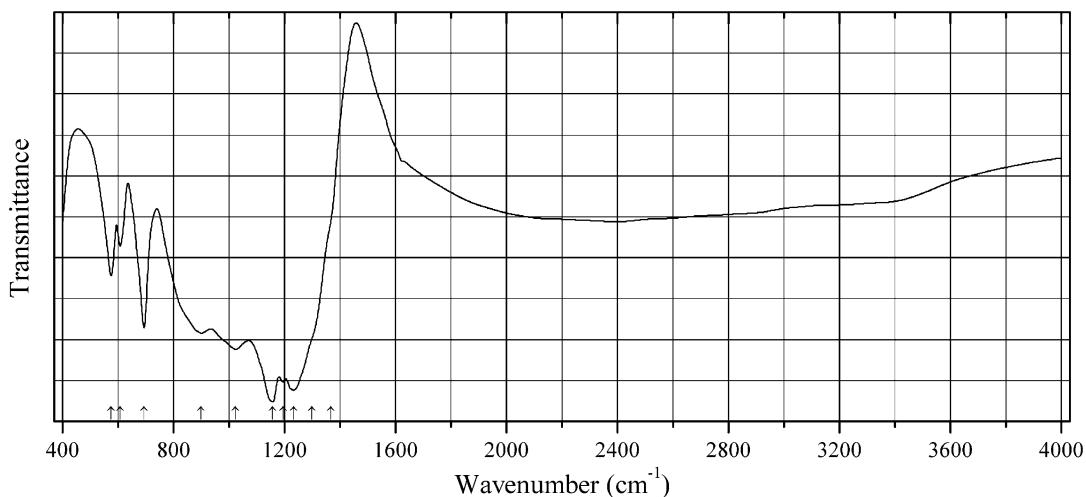
**Description:** Synthesized via solid-state reaction. Characterized by powder X-ray diffraction data. The crystal structure is solved. Trigonal, space group  $R\bar{3}$ ,  $a = 9.5584(16)$ ,  $c = 18.670(3)$  Å,  $V = 1477.2$  (4) Å<sup>3</sup>,  $Z = 3$ .  $D_{\text{calc}} = 7.159$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Huang et al. (2013c).

**Wavenumbers (cm<sup>-1</sup>):** 1411, 917, 752, 736, 724, 621, 581, 454.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**Bo44 Lead copper orthoborate  $\text{Pb}_2\text{Cu}(\text{BO}_3)_2$** 

**Origin:** Synthetic.

**Description:** Prepared by a solid-state reaction method using PbO, CuO, and B<sub>2</sub>O<sub>3</sub> as the starting components in the molar ratio 2:1:1. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group *P2<sub>1</sub>/c*, *a* = 5.6311(6), *b* = 8.7628(9), *c* = 6.2025(6) Å,  $\beta$  = 115.7060(10) $^\circ$ , *V* = 275.77(5) Å<sup>3</sup>, *Z* = 2. *D*<sub>calc</sub> = 7.172 g/cm<sup>3</sup>. Cu atoms have rectangular planar coordination.

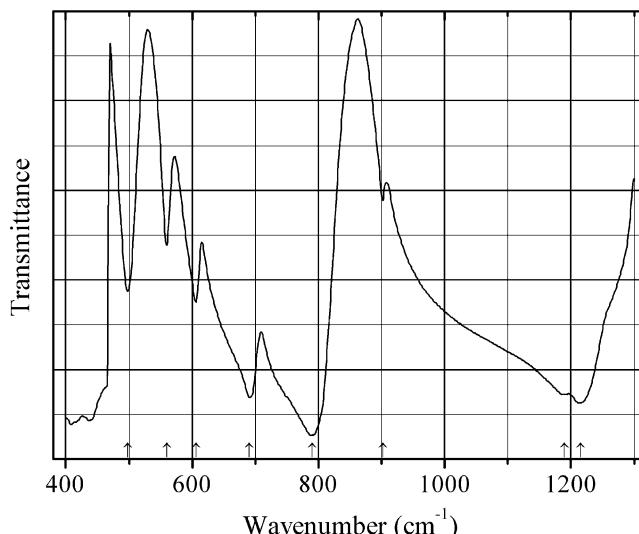
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Pan et al. (2006).

**Wavenumbers (cm<sup>-1</sup>):** 1368sh, 1300sh, 1232s, 1195s, 1156s, 1024, 900, 694, 608, 575.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

#### Bo45 Lead orthoborate tungstate Pb<sub>6</sub>(BO<sub>3</sub>)<sub>2</sub>(WO<sub>4</sub>)O<sub>2</sub>



**Origin:** Synthetic.

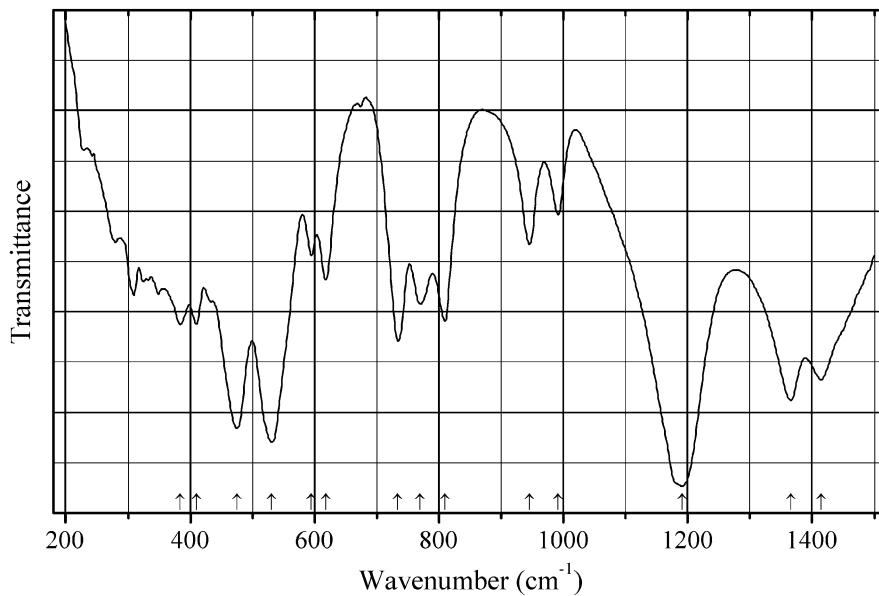
**Description:** Crystals obtained from the melt of Bi<sub>2</sub>O<sub>3</sub>, PbO, WO<sub>3</sub>, and H<sub>3</sub>BO<sub>3</sub> with the molar ratio of 3:12:2:2. Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group *Cmcm*, *a* = 18.4904(5), *b* = 6.35980(10), *c* = 11.6789(2) Å, *V* = 1373.38 (5) Å<sup>3</sup>, *Z* = 4. *D*<sub>calc</sub> = 7.935 g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Li et al. (2011b).

**Wavenumbers (cm<sup>-1</sup>):** 1215s, 1190, 902w, 790s, 690s, 606, 560, 498.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Bo46 Lithium aluminium orthoborate**  $\text{Li}_3\text{Al}(\text{BO}_3)_2$ 


**Origin:** Synthetic.

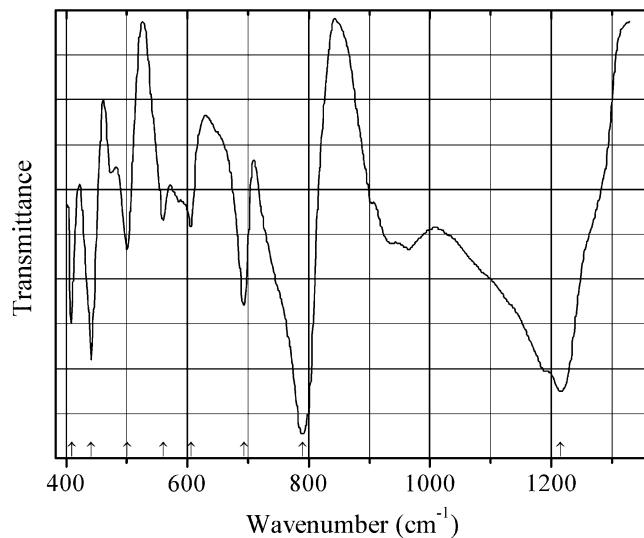
**Description:** Prepared from the mixture of  $\text{Li}_2\text{CO}_3$ ,  $\text{Al}_2\text{O}_3$ , and  $\text{H}_3\text{BO}_3$  in stoichiometric proportion, at 690 °C for 1–2 days, with one intermediate grinding. Characterized by powder X-ray diffraction data. The crystal structure is solved. Triclinic, space group  $P-1$ ,  $a = 4.876(8)$ ,  $b = 6.191(16)$ ,  $c = 7.910(20)$  Å,  $\alpha = 74.46(18)^\circ$ ,  $\beta = 89.44(17)^\circ$ ,  $\gamma = 89.52(18)^\circ$ ,  $V = 230.0(9)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 2.388$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** He et al. (2002).

**Wavenumbers (cm<sup>-1</sup>):** 1415, 1366, 1191s, 992, 946, 810, 770, 734, 618, 595, 531s, 475s, 410, 384.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Bo47 Lead orthoborate tungstate**  $\text{Pb}_6(\text{BO}_3)_2(\text{WO}_4)\text{O}_2$ 

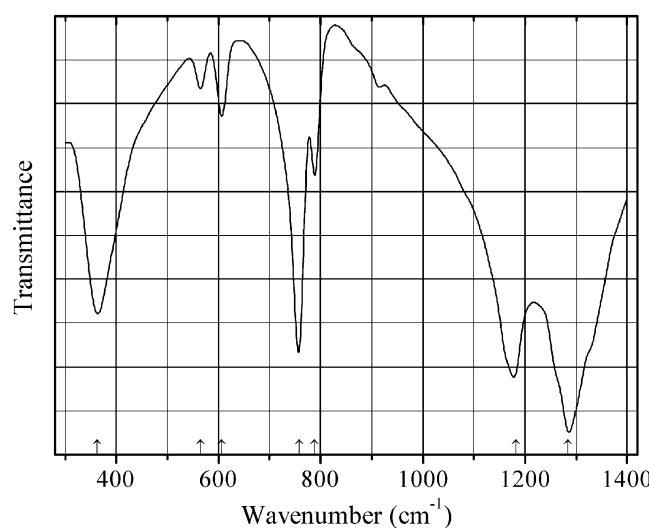
**Origin:** Synthetic.

**Description:** Obtained by a solid-state reaction method. The crystal structure is solved. Orthorhombic, space group  $Cmcm$ ,  $a = 18.480(4)$ ,  $b = 6.3567(13)$ ,  $c = 11.672(2)$  Å,  $V = 1371.1(5)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 7.948$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Reshak et al. (2012b).

**Wavenumbers (cm<sup>-1</sup>):** 1216s, 790s, 694, 606.5, 561, 500.5, 441, 409.

**Bo48 Lithium strontium orthoborate**  $\text{LiSr}_4(\text{BO}_3)_3$ 

**Origin:** Synthetic.

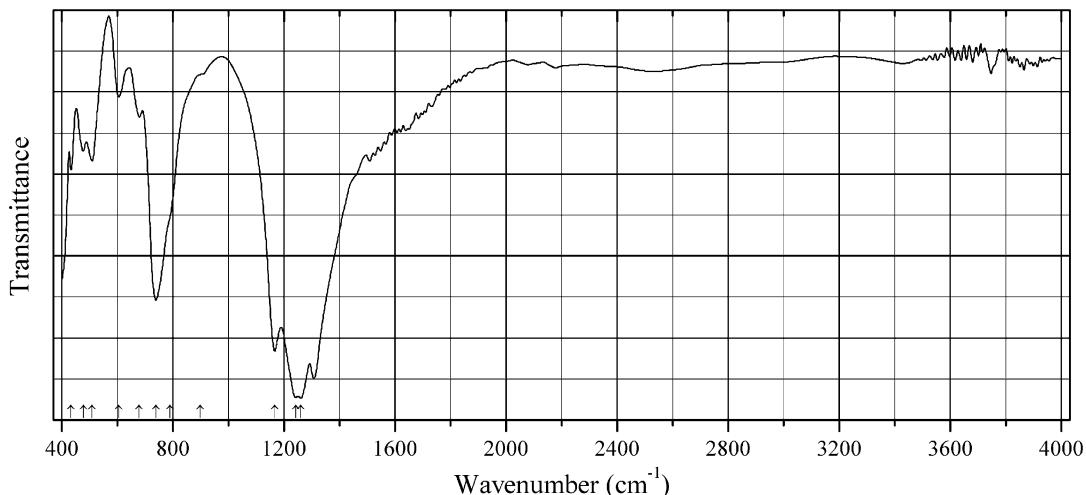
**Description:** Obtained in the solid-state reaction from the stoichiometric mixture of  $\text{Li}_2\text{CO}_3$ ,  $\text{SrCO}_3$ , and  $\text{H}_3\text{BO}_3$  at 750 °C, with several grindings. Characterized by powder X-ray diffraction data. The crystal structure is solved. Cubic, space group  $Ia-3d$ ,  $a = 14.95066(5)$  Å,  $V = 3341.80(3)$  Å<sup>3</sup>,  $Z = 16$ .  $D_{\text{calc}} = 4.243$  g/cm<sup>3</sup>. In the structure, isolated  $\text{BO}_3$  groups are perpendicular to each other.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Wu et al. (2005).

**Wavenumbers (cm<sup>-1</sup>):** 1284s, 1182s, 788, 758s, 607, 565w, 362.

#### Bo49 Magnesium orthoborate fluoride $\text{Mg}_5(\text{BO}_3)_3\text{F}$



**Origin:** Synthetic.

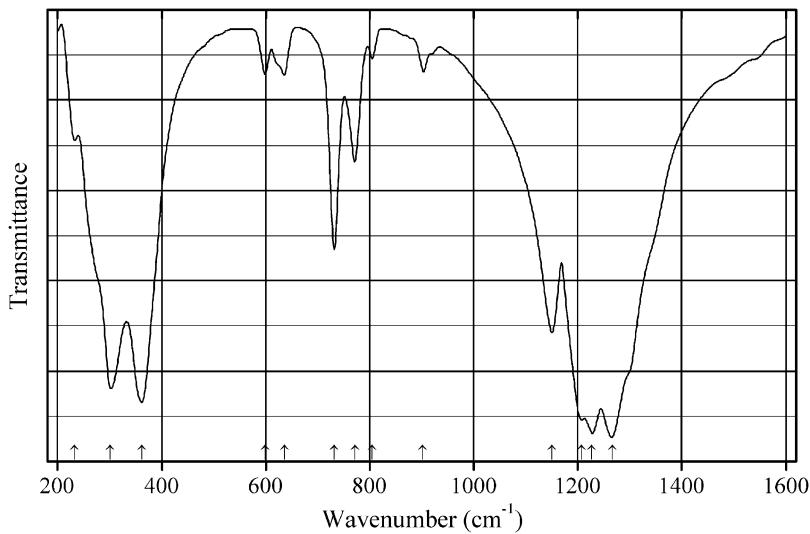
**Description:** Crystals grown from the flux prepared from  $\text{MgF}_2$ ,  $\text{LiF}$ ,  $\text{Na}_2\text{CO}_3$ , and  $\text{H}_3\text{BO}_3$ . Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group  $Pnma$ ,  $a = 10.068(5)$ ,  $b = 14.858(7)$ ,  $c = 4.540(2)$  Å,  $V = 679.2(6)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 3.100$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Bai et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 1308s, 1262s, 1243s, 1168s, 900sh, 790sh, 739s, 680, 606, 510, 478, 433.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The band designed by the authors as 1275 cm<sup>-1</sup> is a doublet 1262+1243 cm<sup>-1</sup>.

**Bo50 Potassium calcium orthoborate**  $\text{KCa}_4(\text{BO}_3)_3$ 

**Origin:** Synthetic.

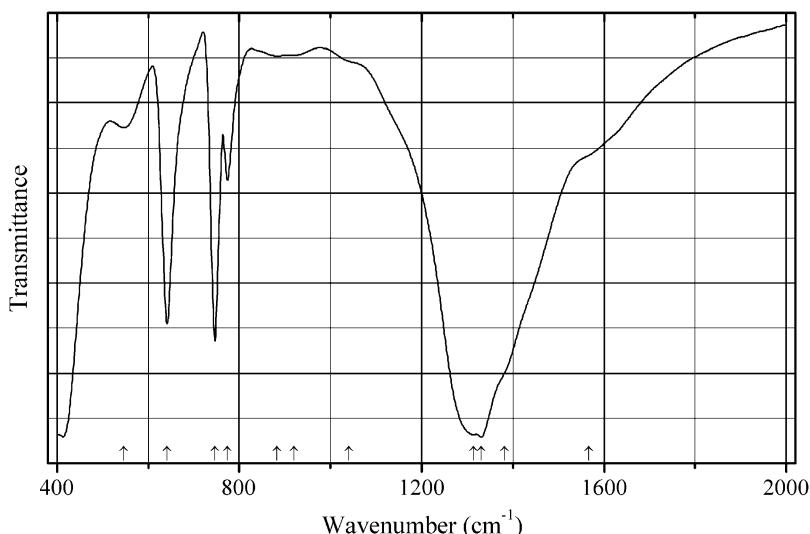
**Description:** Obtained by heating stoichiometric mixture of  $\text{K}_2\text{CO}_3$ ,  $\text{CaCO}_3$ , and  $\text{H}_3\text{BO}_3$  first at  $600^\circ\text{C}$  to decompose carbonates, and thereafter at  $900^\circ\text{C}$  for 72 h. The crystal structure is solved. Orthorhombic, space group  $\text{Ama}2$ ,  $a = 10.63455(10)$ ,  $b = 11.51705(11)$ ,  $c = 6.51942(6)$  Å,  $V = 798.49(2)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 3.161$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Wu et al. (2006a).

**Wavenumbers (cm<sup>-1</sup>):** 1266s, 1226s, 1207s, 1150, 902, 804w, 772, 731, 636, 599, 362s, 301s, 232.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Bo51 Potassium magnesium orthoborate**  $\text{KMg}(\text{BO}_3)_3$ 

**Origin:** Synthetic.

**Description:** Prepared through solid-state reaction from the stoichiometric mixture of metal carbonates and  $\text{H}_3\text{BO}_3$ . Characterized by powder X-ray diffraction data. The crystal structure is solved. Cubic, space group  $P2_13$ ,  $a = 6.83443(4)$  Å,  $V = 319.23(1)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 2.543$  g/cm $^3$ .

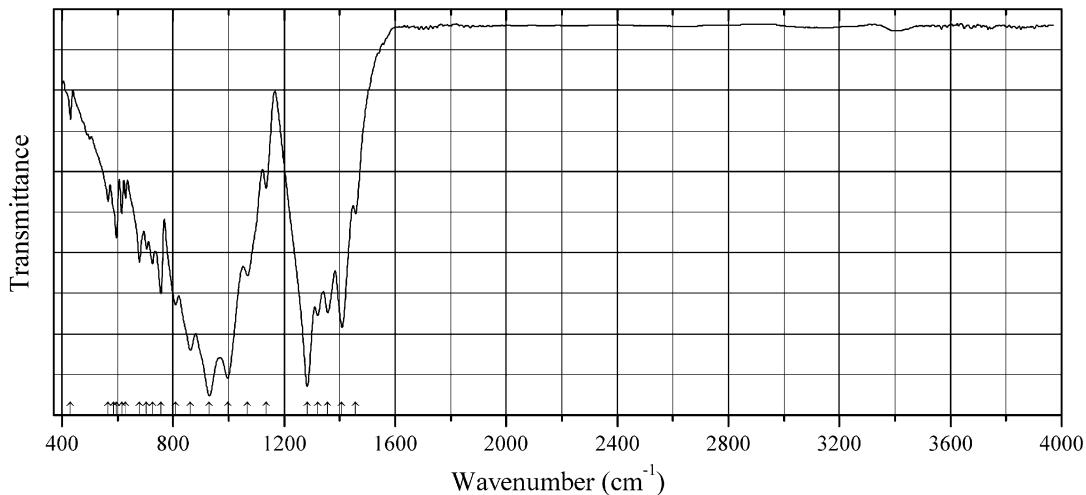
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Wu et al. (2010a).

**Wavenumbers (cm $^{-1}$ ):** 1567sh, 1381sh, 1331s, 1314s, 1040sh, 920w, 882w, 774, 747s, 641s, 547.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The band designed by the authors as 1318 cm $^{-1}$  is a doublet 1331+1314 cm $^{-1}$ .

### Bo52 Potassium strontium orthoborate $\text{KSr}_4(\text{BO}_3)_3$



**Origin:** Synthetic.

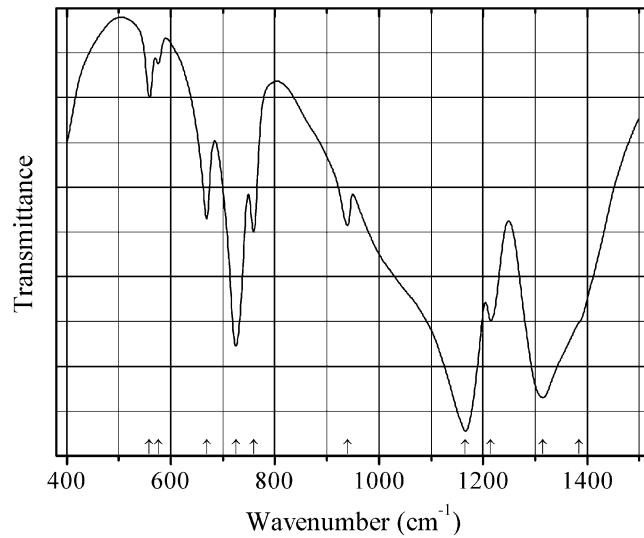
**Description:** Synthesized by solid-state reaction of a stoichiometric mixture of  $\text{K}_2\text{CO}_3$ ,  $\text{SrCO}_3$ , and  $\text{H}_3\text{BO}_3$ , heated first at 400 °C for 5 h and thereafter at 900 °C for 48 h with several intermediate grindings. Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group  $Ama2$ ,  $a = 11.025(10)$ ,  $b = 11.977(10)$ ,  $c = 6.872(6)$  Å,  $V = 907.4(14)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 4.143$  g/cm $^3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** No data.

**Source:** Zhao et al. (2012).

**Wavenumbers (cm $^{-1}$ ):** 1458, 1408s, 1357, 1321, 1284s, 1135w, 1067, 997s, 931s, 862s, 930, 862, 809, 756, 726, 705, 679, 629, 615, 596, 586sh, 566w, 431w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Bo53 Samarium orthoborate Sm(BO<sub>3</sub>)**

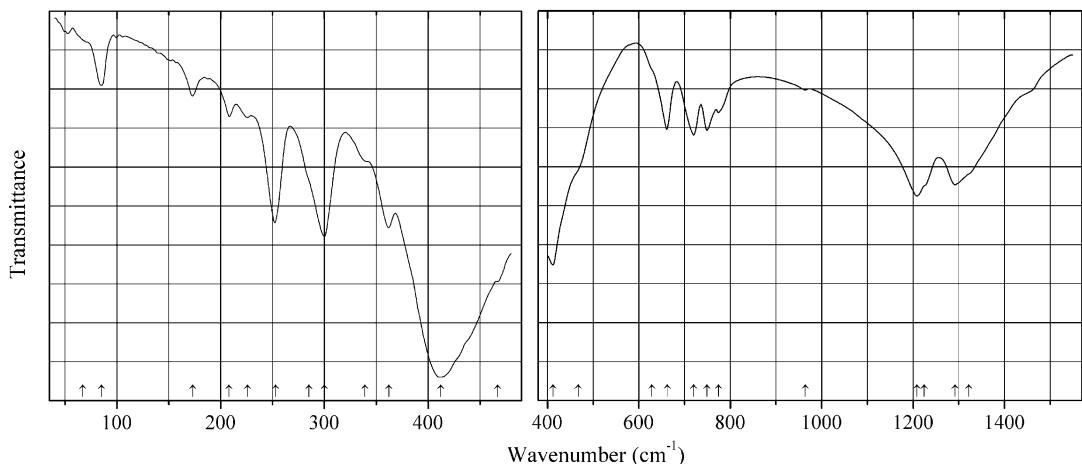
**Origin:** Synthetic.

**Description:** Synthesized by a solid-state method from stoichiometric amounts of H<sub>3</sub>BO<sub>3</sub> and Sm<sub>2</sub>O<sub>3</sub> first at 500 °C for 5 h, thereafter at 700 °C for 5 h, and finally at 900 °C for 5 h with intermediate grindings. Characterized by powder X-ray diffraction data. Triclinic (see JCPDS card No. 13-0489). Contains minor admixture of the vaterite-type polymorph.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Velchuri et al. (2011a).

**Wavenumbers (cm<sup>-1</sup>):** 1384sh, 1315s, 1215, 1166s, 939, 759, 725, 669, 576w, 559w.

**Bo54 Scandium lanthanum orthoborate LaSc<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>**

**Origin:** Synthetic.

**Description:** Bi-doped single crystals obtained by means of spontaneous crystallization from flux at starting molar composition of the melt  $\text{La}_2\text{O}_3:\text{Sc}_2\text{O}_3:\text{Bi}_2\text{O}_3:\text{B}_2\text{O}_3 = 1:1.5:13:13$ . The crystal structure is solved. Trigonal, space group  $R\bar{3}2$ ,  $a = 9.8370(14)$  Å,  $c = 7.9860(14)$  Å,  $Z = 3$ . The empirical formula is (electron microprobe):  $\text{Bi}_{0.21}\text{La}_{0.91}\text{Sc}_{2.88}(\text{BO}_3)_4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc and Nujol mull. Absorption.

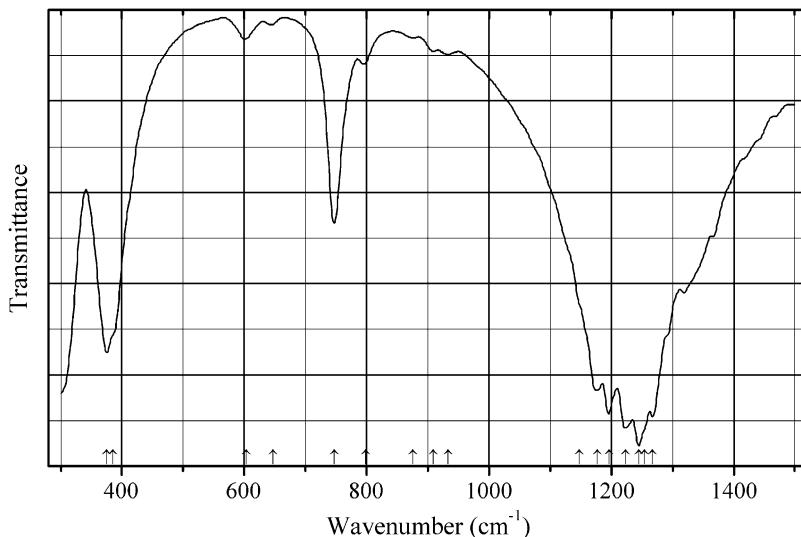
**Source:** Mączka et al. (2010).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1322sh, 1292s, 1224sh, 1208s, 964w, 774w, 749, 720, 662, 628w, 467sh, 412s, 362w, 339w, 300, 285sh, 253, 226w, 208w, 173w, 85, 67w.

**Note:** In the cited paper, polarized Raman spectra of an oriented single crystal are given.

**Wavenumbers (Raman, for the  $x(yy)x$  polarization,  $\text{cm}^{-1}$ ):** 1406, 1278, 1248sh, 1232, 1223, 983, 968w, 738, 712w, 663, 626, 607, 590, 457, 430s, 393sh, 384, 339s, 307sh, 298, 293, 248, 230, 227, 222sh, 207w, 176, 155, 90.

### Bo55 Sodium calcium orthoborate $\text{NaCa}(\text{BO}_3)$



**Origin:** Synthetic.

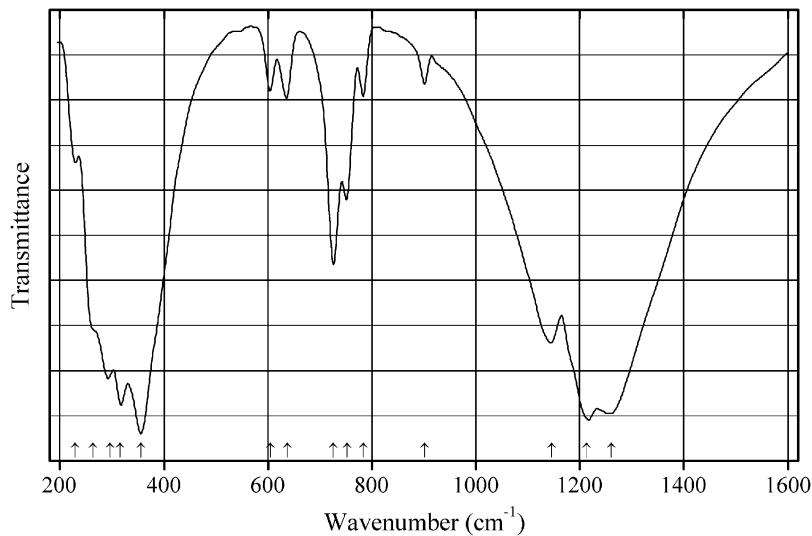
**Description:** Orthorhombic. In the crystal structure, Na and Ca atoms are disordered.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Wu et al. (2006b).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1267s, 1254sh, 1245s, 1223s, 1196s, 1177s, 1148sh, 933w, 909w, 876w, 798, 747w, 647w, 603, 385sh, 375.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Bo56 Sodium calcium orthoborate**  $\text{NaCa}_4(\text{BO}_3)_3$ 

**Origin:** Synthetic.

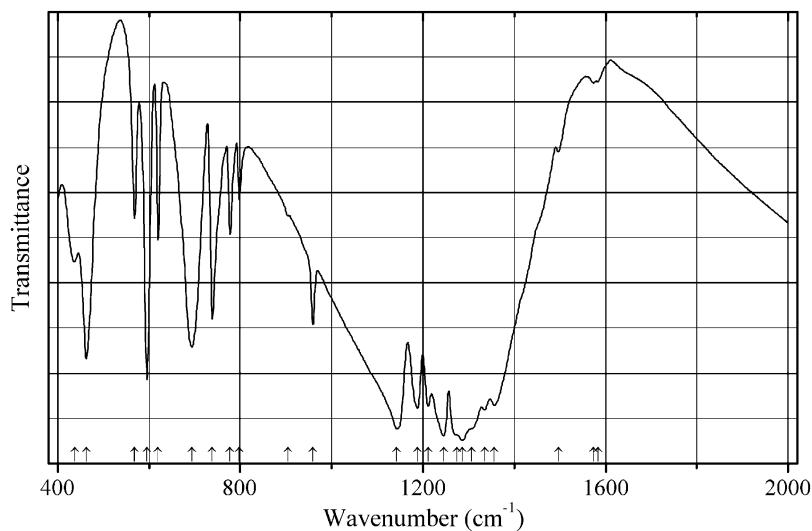
**Description:** Polycrystalline sample prepared by sintering a stoichiometric mixture of  $\text{Na}_2\text{CO}_3$ ,  $\text{CaCO}_3$ , and  $\text{H}_3\text{BO}_3$ , first at 600 °C and thereafter at 880 °C for 72 h with intermediate grinding. Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group  $\text{Ama}2$ ,  $a = 10.68004(11)$ ,  $b = 11.28574(11)$ ,  $c = 6.48521(6)$  Å,  $V = 781.68(2)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 3.056$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Wu et al. (2006a).

**Wavenumbers (cm<sup>-1</sup>):** 1261s, 1213s, 1146, 901w, 784w, 752, 726, 638w, 605w, 356s, 316s, 296s, 263sh, 229w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Bo57 Sodium lanthanum orthoborate**  $\text{Na}_3\text{La}_9(\text{BO}_3)_8\text{O}_3$ 

**Origin:** Synthetic.

**Description:** Synthesized from  $\text{La}_2\text{O}_3$ ,  $\text{Na}_2\text{CO}_3$ , and  $\text{H}_3\text{BO}_3$  by using high-temperature solid-state techniques, first at  $600^\circ\text{C}$  for 10 h and thereafter at  $1100^\circ\text{C}$  for 36 h with intermediate grinding. Characterized by powder X-ray diffraction data and elemental analysis. Hexagonal,  $a = 78.9214$ ,  $c = 8.7267 \text{ \AA}$ . The strongest lines of the powder X-ray diffraction pattern [ $d, \text{ \AA}$  ( $I, \%$ ) ( $hkl$ )] are: 4.3378 (46) (002), 3.1032 (100) (112), 2.9038 (60) (210), 2.2140 (56) (302), 2.1724 (34) (004), 2.1682 (38) (221), 2.0724 (32) (311), 1.5661 (53) (412).

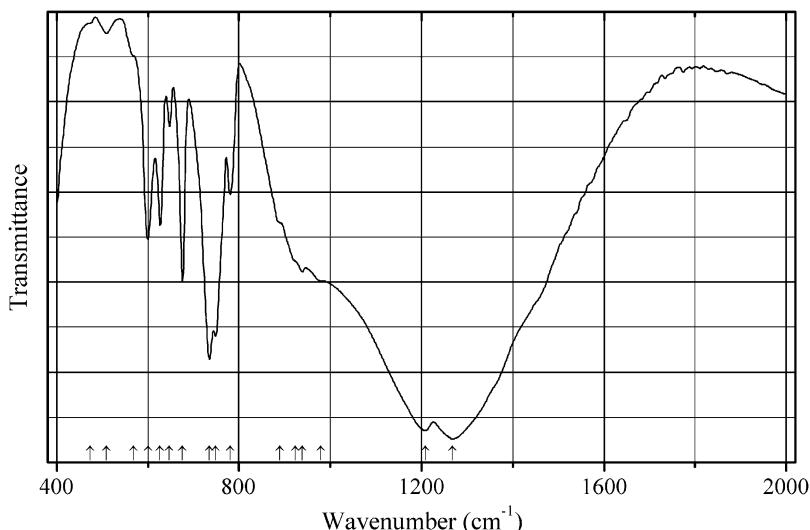
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Zhang et al. (2005).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1583w, 1574w, 1497w, 1356s, 1335s, 1307sh, 1287s, 1274sh, 1245s, 1212s, 1188s, 1143s, 959, 904, 798, 778, 739, 694, 620, 596, 568, 463, 437.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

### Bo58 Sodium samarium orthoborate $\text{Na}_3\text{Sm}_2(\text{BO}_3)_3$



**Origin:** Synthetic.

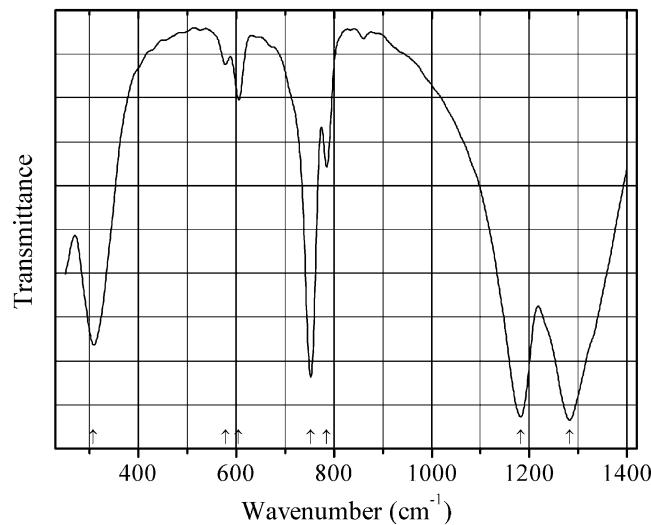
**Description:** Synthesized by heating a mixture of  $\text{Sm}_2\text{O}_3$ ,  $\text{Na}_2\text{CO}_3$ , and  $\text{H}_3\text{BO}_3$  first at  $500^\circ\text{C}$  for 10 h, and thereafter (after intermediate grinding) at  $800^\circ\text{C}$  for 24 h. Orthorhombic,  $a = 5.0585$ ,  $b = 11.0421$ ,  $c = 7.0316 \text{ \AA}$ . The strongest lines of the powder X-ray diffraction pattern [ $d, \text{ \AA}$  ( $I, \%$ ) ( $hkl$ )] are: 5.5210 (58) (020), 5.0521 (80) (100), 3.7232 (69) (120), 2.9685 (65) (022), 2.8851 (81) (102), 2.5602 (100) (122).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Zhang et al. (2002b).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1268s, 1208s, 980, 939, 923sh, 890sh, 781, 749, 735s, 676, 647w, 627, 600, 568sh, 509w, 473sh.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**Bo59 Sodium strontium orthoborate**  $\text{NaSr}_4(\text{BO}_3)_3$ 

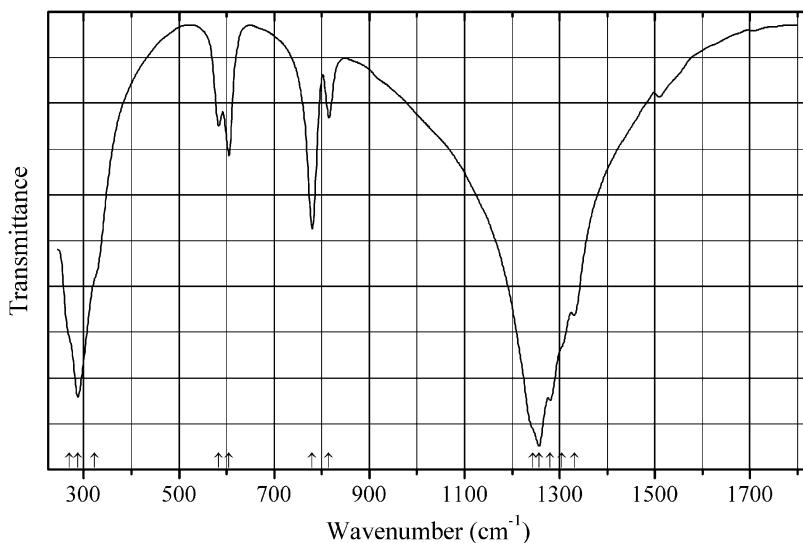
**Origin:** Synthetic.

**Description:** Obtained in the solid-state reaction from the stoichiometric mixture of  $\text{Na}_2\text{CO}_3$ ,  $\text{SrCO}_3$ , and  $\text{H}_3\text{BO}_3$  at  $800^\circ\text{C}$ , with several grindings. Characterized by powder X-ray diffraction data. The crystal structure is solved. Cubic, space group  $Ia-3d$ ,  $a = 15.14629(6)$ ,  $V = 3474.71(4)$   $\text{\AA}^3$ ,  $Z = 16$ .  $D_{\text{calc}} = 4.203$   $\text{g/cm}^3$ . In the structure, isolated  $\text{BO}_3$  groups are perpendicular to each other.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Wu et al. (2005).

**Wavenumbers (cm<sup>-1</sup>):** 1283s, 1182s, 785, 753s, 605, 578w, 307s.

**Bo60 Sodium strontium orthoborate**  $\text{NaSr}(\text{BO}_3)_3$ 

**Origin:** Synthetic.

**Description:** Prepared by heating a mixture of  $\text{Na}_2\text{CO}_3$ ,  $\text{SrCO}_3$ , and  $\text{H}_3\text{BO}_3$  first at  $650\text{ }^\circ\text{C}$  and thereafter at  $850\text{ }^\circ\text{C}$  for 72 h with intermediate grinding. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 5.32446(7)$ ,  $b = 9.2684(1)$ ,  $c = 6.06683(8)\text{ \AA}$ ,  $\beta = 100.589(1)^\circ$ ,  $V = 294.30(8)\text{ \AA}^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 3.824\text{ g/cm}^3$ .

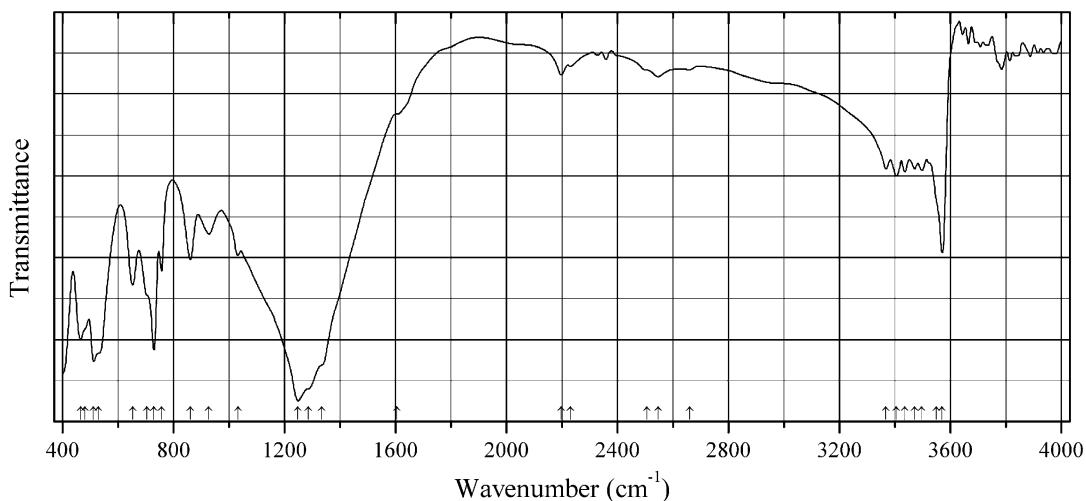
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Wu et al. (2006b).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1331, 1305sh, 1280s, 1257s, 1243sh, 815, 780, 605, 583, 323sh, 287s, 270sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### Bo61 Zinc orthoborate hydroxide $\text{Zn}_8(\text{BO}_3)_3\text{O}_2(\text{OH})_3$



**Origin:** Synthetic.

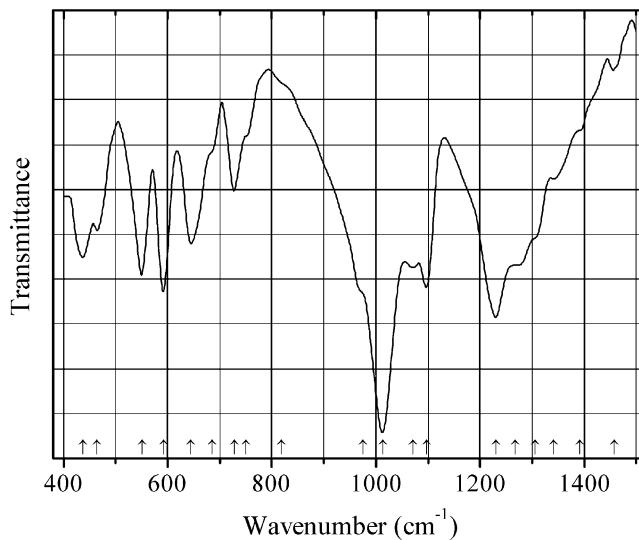
**Description:** Prepared hydrothermally from a mixture of 0.637 mmol of  $\text{Zn}_3\text{B}_2\text{O}_6$ , 0.2 ml of  $\text{CH}_3\text{COOH}$ , 0.2 ml of  $\text{NH}_2\text{CH}_2\text{CH}_2\text{NH}_2$ , and 1 ml of  $\text{H}_2\text{O}$ , at  $170\text{ }^\circ\text{C}$  for 1 week. Characterized by powder X-ray diffraction data. The crystal structure is solved. Trigonal, space group  $R\bar{3}2$ ,  $a = 8.006(2)$ ,  $c = 17.751(2)\text{ \AA}$ ,  $V = 985.3(4)\text{ \AA}^3$ ,  $Z = 3$ .  $D_{\text{calc}} = 3.956\text{ g/cm}^3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Chen et al. (2006b).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3570, 3550sh, (3497), (3471), (3435), (3405), (3368), 2660w, 2546w, 2505sh, 2230w, 2197w, 1605sh, 1334sh, 1285sh, 1249s, 1032w, 927w, 861, 758, 730s, 705sh, 653, 530sh, 513s, 481sh, 465.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Bo62 Zinc orthoborate orthophosphate**  $\text{Zn}_3(\text{BO}_3)(\text{PO}_4)$ 

**Origin:** Synthetic.

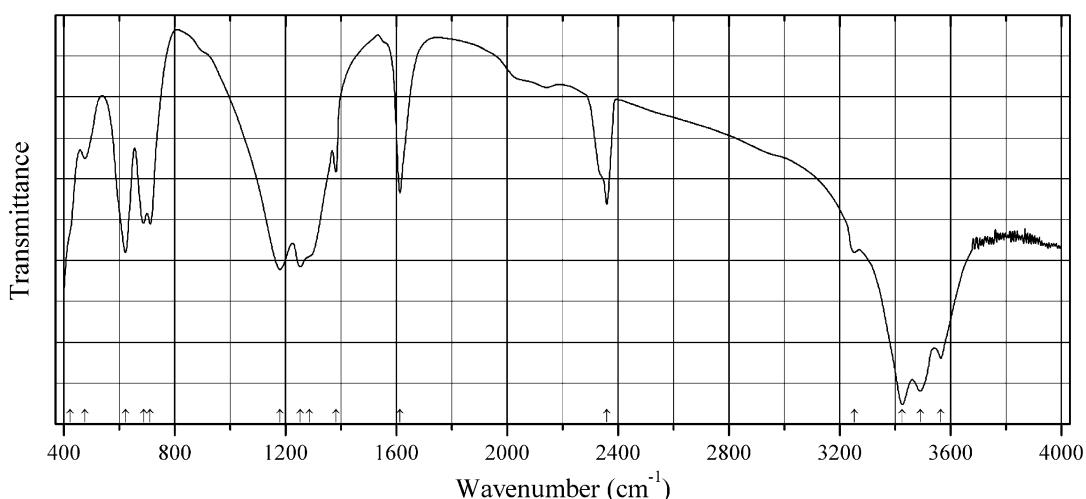
**Description:** Prepared by heating a mixture of  $\text{ZnCO}_3$ ,  $\text{H}_3\text{BO}_3$ , and  $(\text{NH}_4)_2(\text{HPO}_4)$ , taken in stoichiometric amounts, at  $870^\circ\text{C}$ . Characterized by powder X-ray diffraction data. Hexagonal,  $a = 8.435$  (4),  $c = 13.032(6)$  Å. The strongest reflections are observed at 4.2113 and 2.5761 Å.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Wang et al. (2002).

**Wavenumbers (cm<sup>-1</sup>):** 1458w, 1392w, 1342w, 1306sh, 1268, 1230s, 1098, 1071, 1013s, 975sh, 819sh, 751sh, 728, 685sh, 645, 592, 552, 464, 438.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Bo63 Cobalt dinickel orthoborate**  $\text{CoNi}_2(\text{BO}_3)_2$ 

**Origin:** Synthetic.

**Description:** Synthesized by heating a stoichiometric mixture of cobalt nitrate, nickel nitrate, and boric acid, first at 450 °C for 4 h, thereafter (after cooling to room temperature and grinding) at 600 °C for 3 h, and finally at 900 °C for 48 h. Characterized by powder X-ray diffraction data. Isostructural with kotoite. Orthorhombic, space group  $Pnmn$ ,  $a = 5.419(9)$ ,  $b = 8.352(0)$ ,  $c = 4.478(8)$  Å,  $Z = 2$ .  $D_{\text{meas}} = 4.48$  g/cm<sup>3</sup>. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 3.9420 (38) (011), 2.6591 (100) (121), 2.4755 (36) (130), 2.2339 (55) (211), 1.7258 (30) (202), 1.6610 (33) (132).

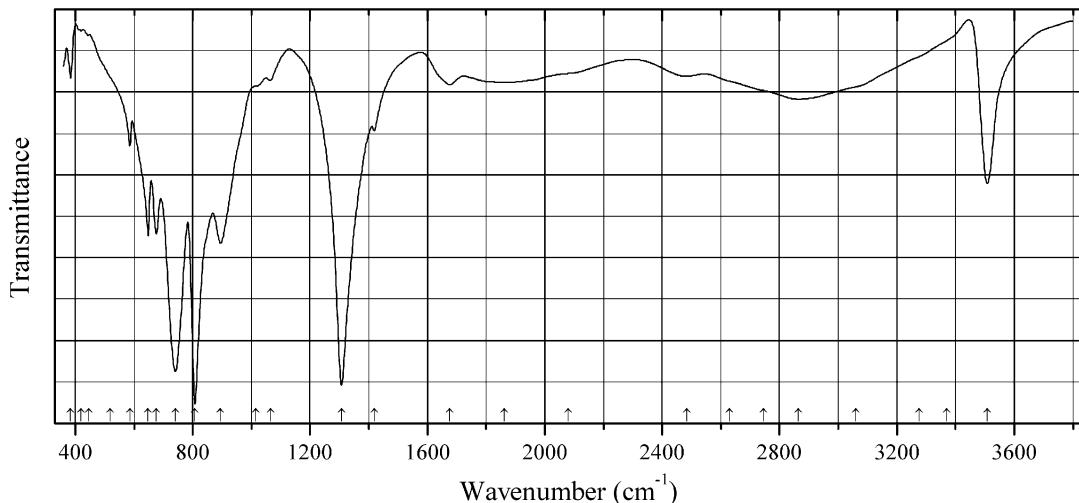
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Güler and Tekin (2009).

**Wavenumbers (cm<sup>-1</sup>):** 3564, 3490, 3426, 2360, 2340sh, 1613, 1382, 1285sh, 1253, 1180, 712, 688, 622, 476, 422sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The sample is strongly contaminated with a hydrous phase (the bands at 3564, 3490, 3426, and 1613 cm<sup>-1</sup>). The bands at 2360 and 2340 cm<sup>-1</sup> may correspond to atmospheric CO<sub>2</sub>.

#### Bo64 Berborite $\text{Be}_2(\text{BO}_3)(\text{OH},\text{F}) \cdot \text{H}_2\text{O}$



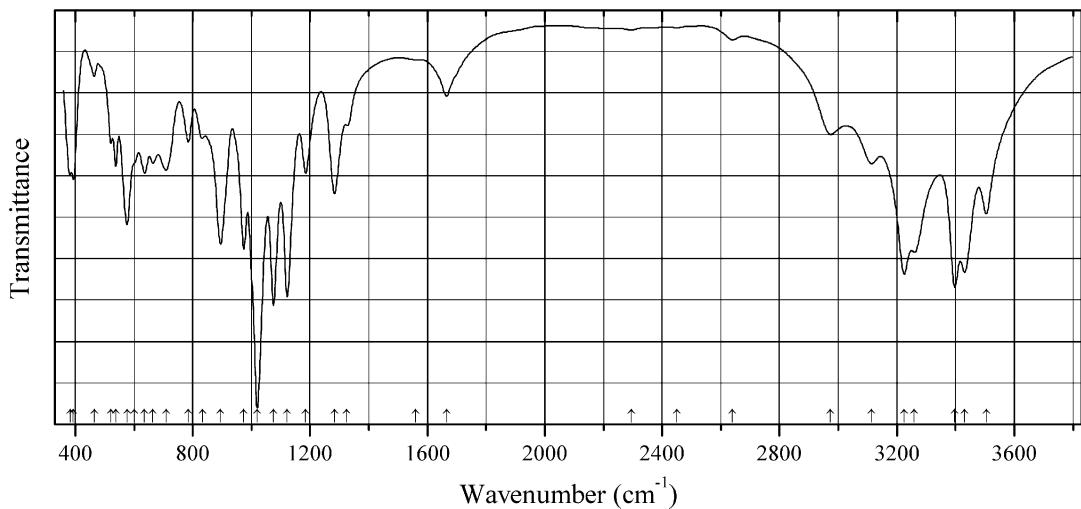
**Origin:** Vevja quarry, Tvedalen, Larvik, Vestfold, Norway.

**Description:** Colorless crystals from the association with natrolite. Holotype sample. Characterized by single-crystal X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3508, 3370sh, 3275sh, 3060sh, 2865, 2745sh, 2630sh, 2483, 2080sh, 1862, 1676, 1420, 1307s, 1065w, 1015sh, 895, 807s, 741s, 676, 648, 586, 520sh, (445w), (419w), 384w.

**Note:** The spectrum was obtained by N.V. Chukanov.

**B160 Lüneburgite**  $Mg_3[B_2(OH)_6(PO_4)_2] \cdot 6H_2O$ 

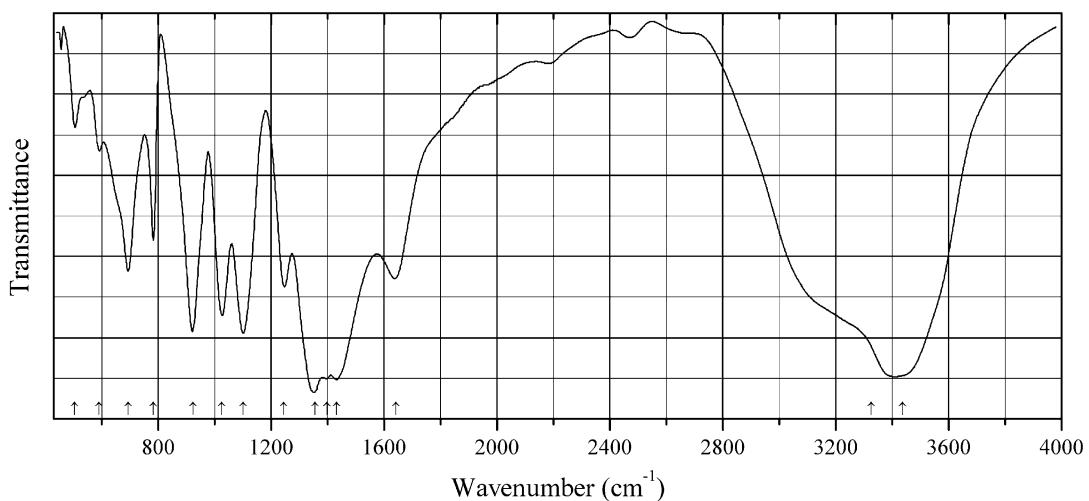
**Origin:** Morro Mejillones, Mejillones Peninsula, Mejillones, Antofagasta, II Region, Chile.

**Description:** Yellow nodule from clay. Investigated by I.V. Pekov. Identified by IR spectrum and qualitative electron microprobe analyses.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3505, 3431s, 3397s, 3258, 3225s, 3113, 2974, 2639w, 2450w, 2295w, 1665, (1560w), 1326, 1283, 1185, 1122s, 1075s, 1020s, 974, 895, 834, 785, 709, 665, 636, 600sh, 576, 538, 522, 465w, 393, 383.

**Note:** The spectrum was obtained by N.V. Chukanov.

**B161 Ammonium pentaborate**  $(\text{NH}_4)\text{B}_5\text{O}_8$ 

**Origin:** Synthetic.

**Description:** Crystals of commercially available ammonium pentaborate grown from aqueous solution. Characterized by powder X-ray diffraction data. Monoclinic,  $a = 7.189(5)$ ,  $b = 11.308(5)$ ,  $c = 7.217(6)$  Å,  $\beta = 100.12(7)^\circ$ ,  $V = 578(2)$  Å<sup>3</sup>.

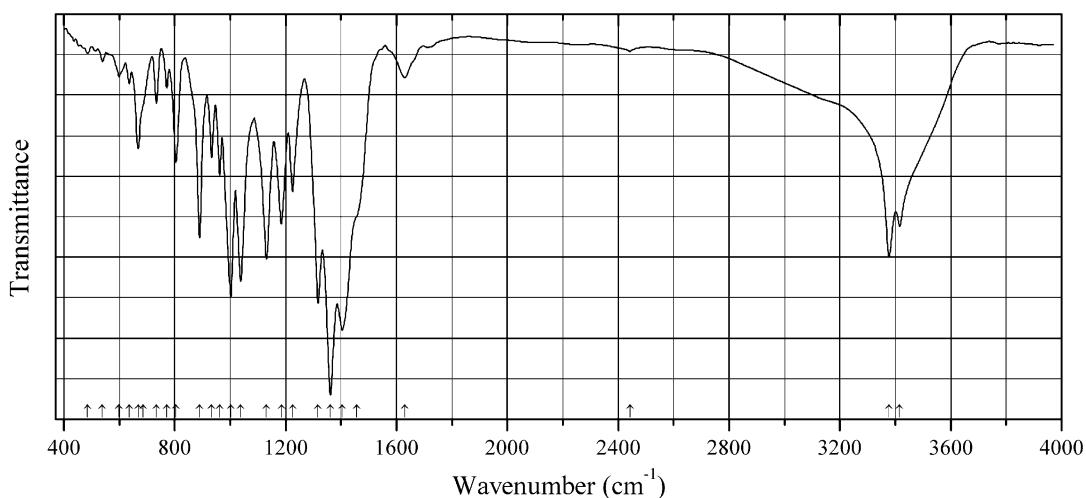
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Balakrishnan et al. (2008).

**Wavenumbers (cm<sup>-1</sup>):** 3436s, 3327sh, 1642, 1433s, 1397s, 1355s, 1245, 1102, 1024, 924, 782, 695, 591w, 504w.

**Note:** In the cited paper, the wavenumber 1245 cm<sup>-1</sup> is erroneously indicated as 1345 cm<sup>-1</sup>.

### B162 Barium borate BaB<sub>8</sub>O<sub>11</sub>(OH)<sub>4</sub>



**Origin:** Synthetic.

**Description:** Synthesized from Ba(NO<sub>3</sub>)<sub>2</sub> and H<sub>3</sub>BO<sub>3</sub> by using a low-temperature molten salt technique at 458 K. The crystal structure is solved at 173 K. It is built from borate layers consisting of [B<sub>6</sub>O<sub>9</sub>(OH)] clusters. Monoclinic, pseudo-orthorhombic, space group P2<sub>1</sub>/n,  $a = 7.9080(16)$ ,  $b = 13.939(3)$ ,  $c = 10.047(2)$  Å,  $\beta = 90.00(3)^\circ$ ,  $V = 1107.6(4)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 2.806$  g/cm<sup>3</sup>.

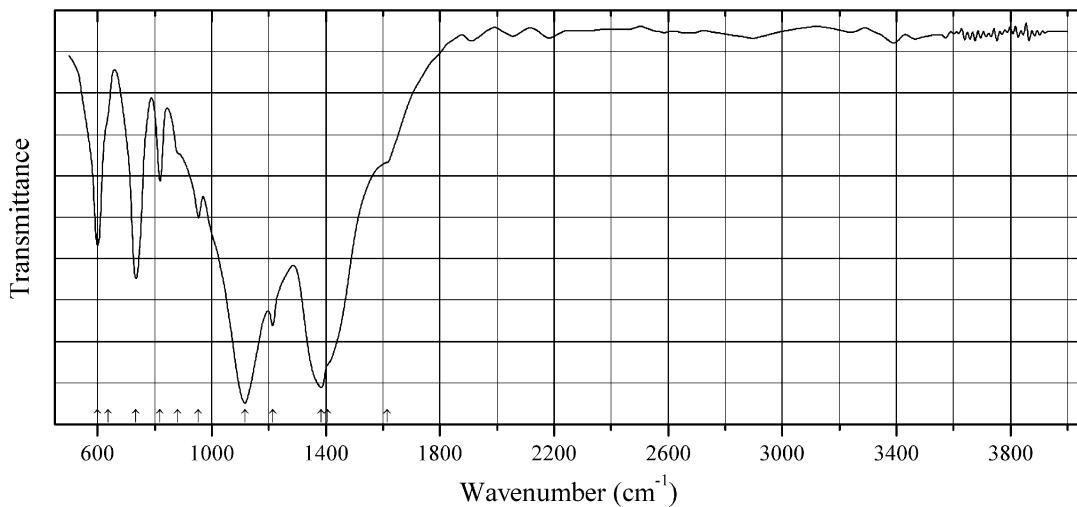
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Sun et al. (2010a).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3416, 3377s, 2443w, 1630, 1456sh, 1404s, 1361s, 1317s, 1225, 1185, 1131, 1038s, 1003s, 962, 933, 890, 804, 771w, 734, 686sh, 668, 635, 599w, 539w, 486w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1305, 1170w, 1112w, 1011s, 1050w, 987s, 886w, 858, 822, 761s, 736s, 658, 638, 540, 472s, 453s, 434, 424, 410, 367s, 243, 202w, 166w, 135w, 116s.

**B163 Barium calcium diborate** BaCa(B<sub>2</sub>O<sub>5</sub>)

**Origin:** Synthetic.

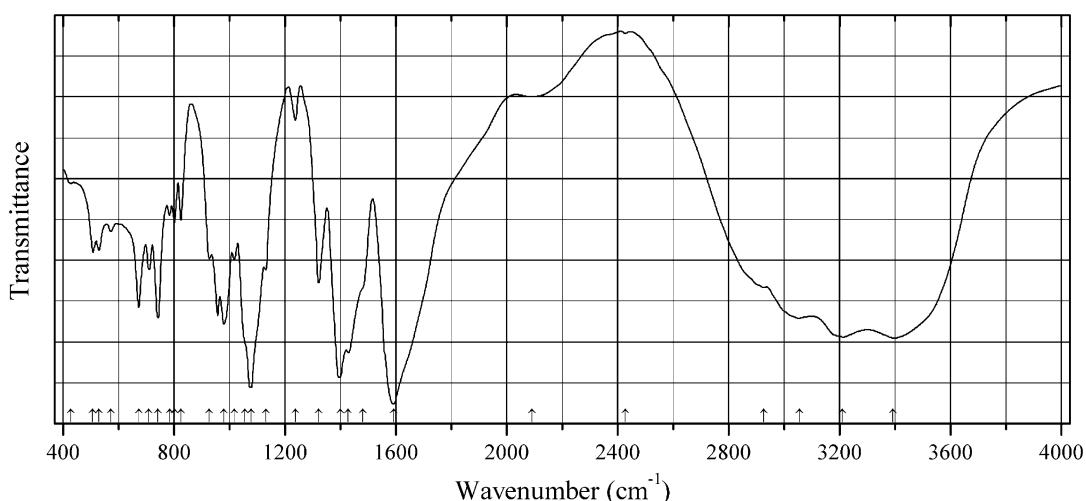
**Description:** Crystals grown from the mixture of barium nitrate, calcium oxide, and boric acid first preheated at 500 °C for 7 h, then gradually heated to 900 °C, and kept at this temperature for 72 h with several intermediate grindings and mixing. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 6.568(2)$ ,  $b = 20.545(7)$ ,  $c = 8.201(2)$  Å,  $\beta = 117.00(2)^\circ$ ,  $Z = 4$ .  $D_{\text{calc}} = 3.759$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Liu et al. (2015b).

**Wavenumbers (cm<sup>-1</sup>):** 1615sh, 1405sh, 1383s, 1214, 1117s, 954, 881sh, 819, 735, 637sh, 600.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**B164 Ammonium calcium borate** (NH<sub>4</sub>)<sub>2</sub>Ca[B<sub>4</sub>O<sub>5</sub>(OH)<sub>4</sub>]<sub>2</sub>·8H<sub>2</sub>O

**Origin:** Synthetic.

**Description:** Synthesized through slow evaporation of a solution containing  $\text{CaCl}_2$ ,  $\text{H}_3\text{BO}_3$  and  $\text{NH}_3$ . Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group  $P2_12_12_1$ ,  $a = 11.556(7)$ ,  $b = 12.583(8)$ ,  $c = 16.679(8)$  Å,  $V = 2425.2(2)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 1.651$  g/cm<sup>3</sup>.

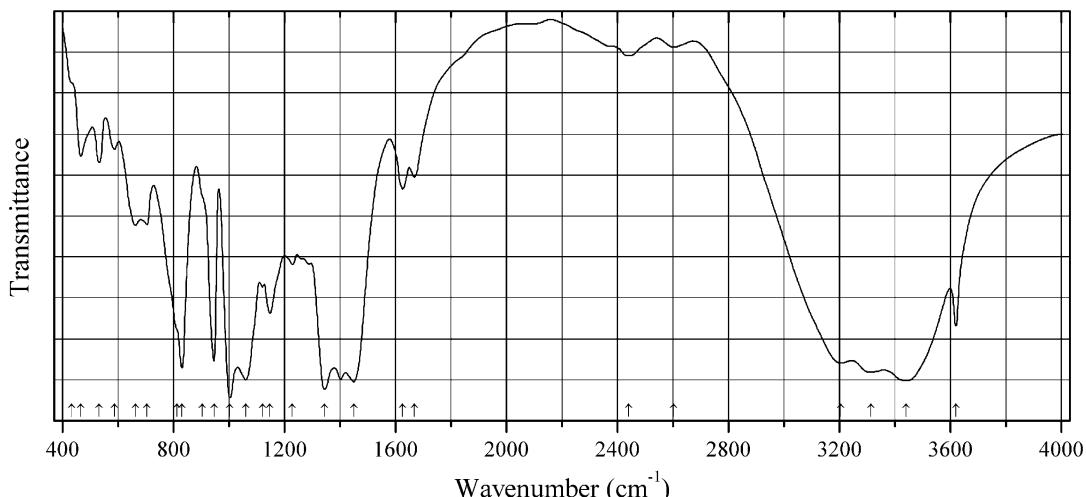
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Li et al. (2011a).

**Wavenumbers (cm<sup>-1</sup>):** 3392s, 3210s, 3055, 2927, 2427, 2090, 1592s, 1482sh, 1429s, 1399s, 1322, 1238w, 1131, 1078s, 1057sh, 1018, 980, 957, 928, 825, 802, 784, 743, 710, 673, 572, 529, 507, 428.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### B165 Cesium calcium borate $\text{Cs}_2\text{Ca}[\text{B}_4\text{O}_5(\text{OH})_4]_2 \cdot 8\text{H}_2\text{O}$



**Origin:** Synthetic.

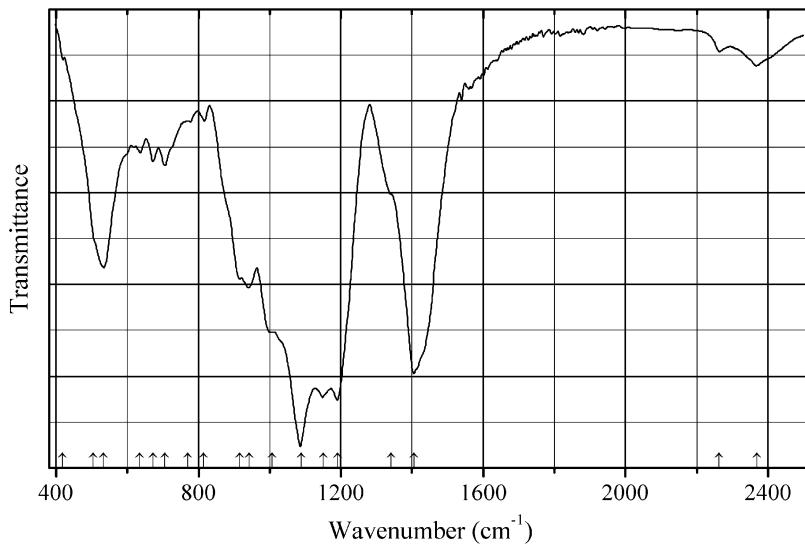
**Description:** Crystals grown by slow evaporation from the 2:1 (vol.) aqueous acetone solution of  $\text{Cs}_2\text{CO}_3$ ,  $\text{CaCl}_2$ , and  $\text{H}_3\text{BO}_3$  with a molar ratio of 2:1:8. The crystal structure is solved. Orthorhombic, space group  $P2_12_12_1$ ,  $a = 11.5158(7)$ ,  $b = 12.8558(7)$ ,  $c = 16.7976(10)$  Å,  $V = 2486.8(3)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 2.224$  g/cm<sup>3</sup>. Characterized by DSC and TG data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Huang et al. (2013b).

**Wavenumbers (cm<sup>-1</sup>):** 3620, 3440s, 3313s, 3205s, 2602w, 2440w, 1668, 1626, 1450s, 1345s, 1229w, 1147, 1121, 1060s, 1003s, 946s, 904sh, 831s, 814sh, 705, 663, 588, 532, 466, 434sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**B166 Calcium borate**  $\text{CaB}_6\text{O}_{10}$ 

**Origin:** Synthetic.

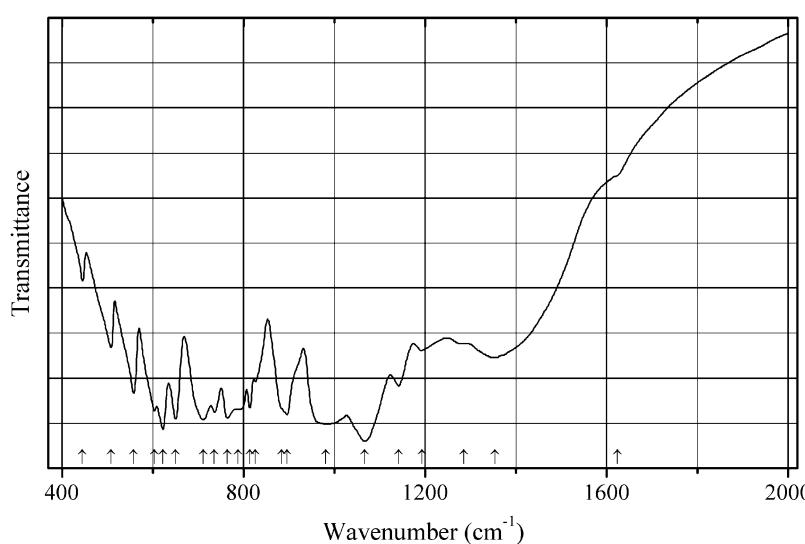
**Description:** Colorless crystals prepared from corresponding oxides by solid-state reaction at 735 °C for 2 weeks. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 9.799(1)$ ,  $b = 8.705(1)$ ,  $c = 9.067(1)$  Å,  $\beta = 116.65(1)$ °,  $V = 691.23(13)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 2.546$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Chen et al. (2008b).

**Wavenumbers (cm<sup>-1</sup>):** 2369w, 2264w, 1406s, 1342sh, 1150s, 1191s, 1088s, 1008sh, 942, 916, 815w, 769sh, 705w, 672w, 635w, 533, 504sh, 418w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**B167 Calcium tetraborate**  $\beta\text{-CaB}_4\text{O}_7$ 

**Origin:** Synthetic.

**Description:** High-pressure  $\beta$ -modification isotopic with orthorhombic  $\text{SnB}_4\text{O}_7$ .

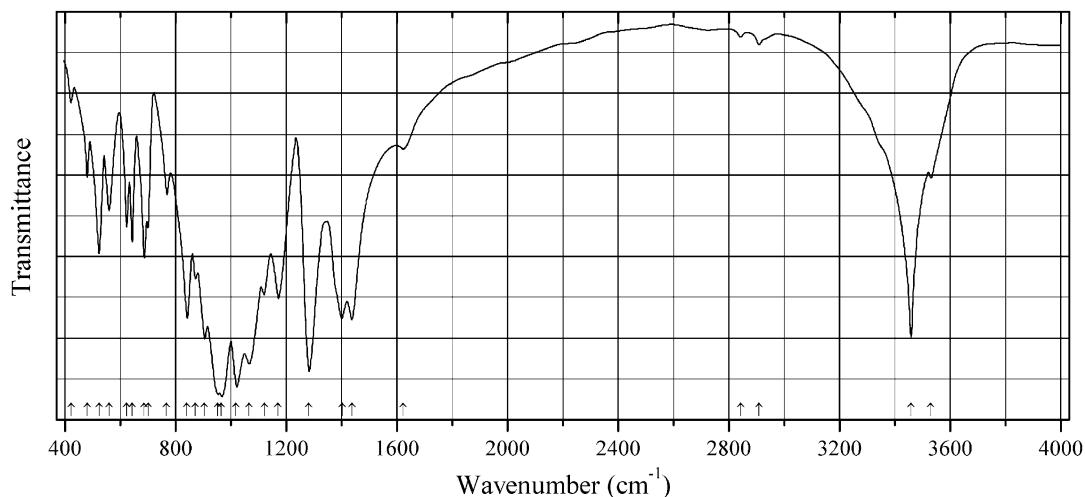
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Knyrim et al. (2007).

**Wavenumbers (cm<sup>-1</sup>):** 1623sh, 1353, 1285sh, 1193, 1142, 1067s, 982s, 896, 884sh, 826, 814, 788sh, 765, 736, 712, 650, 623s, 604, 558, 509, 446w.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

### B168 Dicalcium hexaborate monohydrate $\text{Ca}_2\text{B}_6\text{O}_{11}\cdot\text{H}_2\text{O}$



**Origin:** Synthetic.

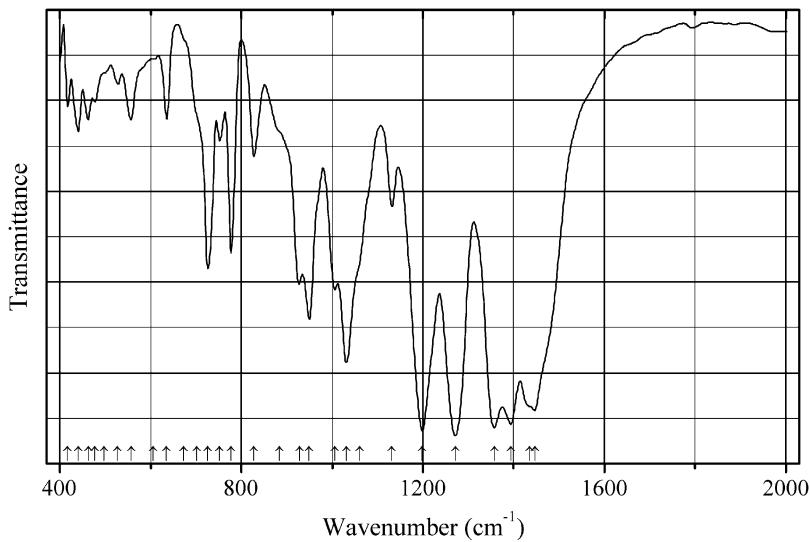
**Description:** Synthesized hydrothermally from  $\text{H}_3\text{BO}_3$  and  $\text{CaO}$  mixed with the mole ratio ranging from 1.5:1 to 2:1, at 234–300 °C for 48–96 h. Characterized by powder X-ray diffraction data. Orthorhombic, space group  $Pbn2_1$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Guo et al. (2000).

**Wavenumbers (cm<sup>-1</sup>):** 3530, 3458s, 2908w, 2842w, 1623w, 1438, 1403, 1282s, 1171, 1121, 1066s, 1019s, 966s, 953s, 905, 871, 842, 767, 701, 686, 643, 623, 559, 524, 482, 422w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**B169 Dipotassium sodium zinc pentaborate**  $K_2NaZnB_5O_{10}$ 

**Origin:** Synthetic.

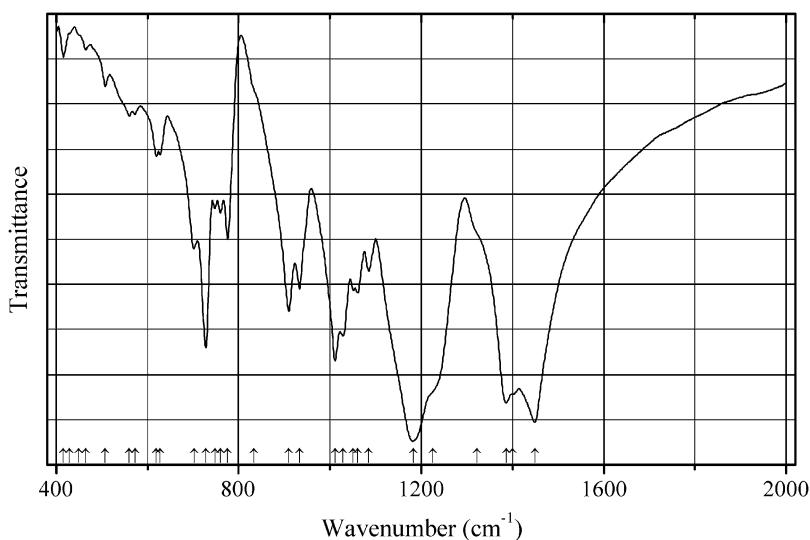
**Description:** Synthesized by employing a high-temperature solution reaction method. The crystal structure is solved. Monoclinic, space group  $C2/c$ ,  $a = 7.9244(16)$ ,  $b = 12.805(3)$ ,  $c = 18.962(4)$  Å,  $\beta = 99.39(3)$ °,  $V = 1898.4(7)$  Å<sup>3</sup>,  $Z = 8$ .  $D_{\text{calc}} = 2.663$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Chen et al. (2010).

**Wavenumbers (cm<sup>-1</sup>):** 1447s, 1436sh, 1394s, 1358s, 1272s, 1199s, 1132, 1060sh, 1032, 1006, 949, 928, 883sh, 827, 777, 752, 726, 702sh, 673sh, 635w, 606sh, 557w, 527w, 498sh, 477w, 462w, 440w, 417w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**B170 Double-ring borate ( $Na,K)_3Sr(B_5O_{10}$ ) ( $Na,K)_3Sr(B_5O_{10}$ )**

**Origin:** Synthetic.

**Description:** Synthesized from the melt prepared from  $\text{Na}_2\text{CO}_3$ ,  $\text{SrCO}_3$ ,  $\text{H}_3\text{BO}_3$ , and  $\text{K}_2\text{B}_4\text{O}_7$  in the molar ratio 3:2:10:2 at 800 °C for 10 days. Triclinic, space group  $P-1$ ,  $a = 7.3900(15)$ ,  $b = 7.6490(15)$ ,  $c = 9.773(2)$  Å,  $\alpha = 79.31(2)^\circ$ ,  $\beta = 70.85(2)^\circ$ ,  $\gamma = 62.09(1)^\circ$ ,  $V = 460.82(17)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 2.766$  g/cm<sup>3</sup>.

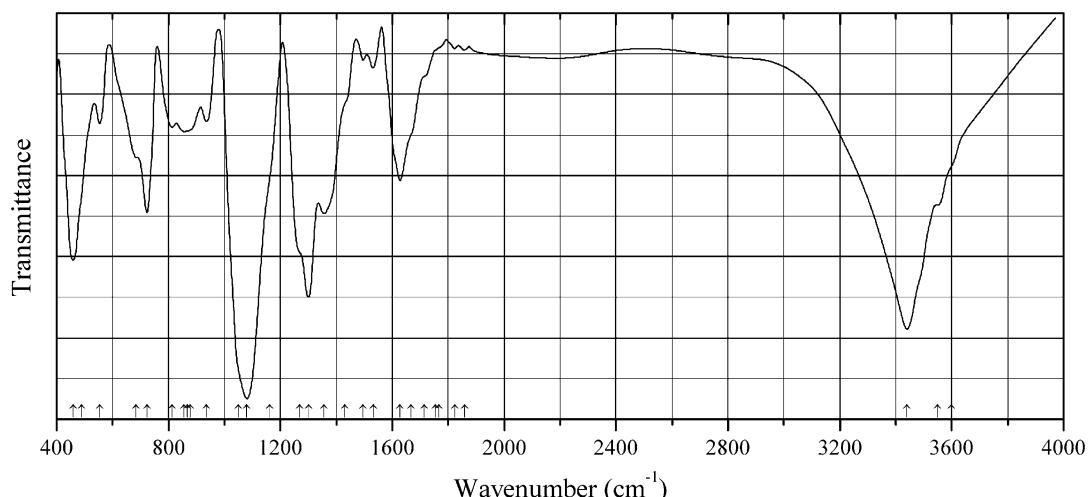
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Chen et al. (2011).

**Wavenumbers (cm<sup>-1</sup>):** 1449s, 1400sh, 1386s, 1322sh, 1225sh, 1183s, 1085, 1061, 1051, 1029, 1011, 934, 910, 834sh, 776, 760, 748, 728, 702, 628w, 620w, 573w, 560w, 508w, 465w, 450sh, 430w, 416w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

## B171 Lead borate $Pb_6B_{11}O_{18}(OH)_9$ $Pb_6B_{11}O_{18}(OH)_9$



**Origin:** Synthetic.

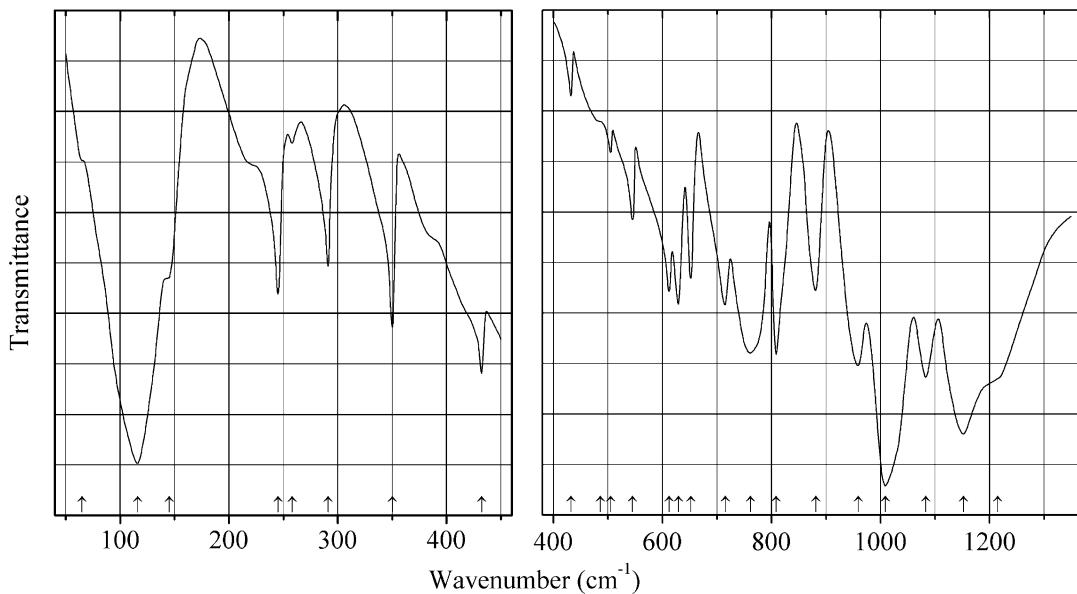
**Description:** Synthesized hydrothermally from  $\text{Pb}(\text{CH}_3\text{COO})_2$  and  $\text{H}_3\text{BO}_3$  in the presence of  $\text{H}_2\text{NCH}_2\text{CH}_2\text{NH}_2$  and  $\text{CH}_3\text{COOH}$ , at  $180^\circ$  for 2 days. The crystal structure is solved. Trigonal, space group  $P3_2$ ,  $a = 11.7691(7)$ ,  $c = 13.3361(12)$  Å,  $V = 1599.7(2)$  Å $^3$ ,  $Z = 3$ .  $D_{\text{calc}} = 5.615$  g/cm $^3$ . The structure is based on infinite and finite chains built up from  $\text{BO}_4$  and  $\text{BO}_3$  units.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

Source: Yu et al. (2002)

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3600sh, 3550sh, 3440s, 1858w, 1823w, 1768sh, 1755sh, 1715sh, 1668sh, 1628, 1532w, 1495w, 1430sh, 1357, 1300s, 1270sh, 1162sh, 1080s, 1051sh, 936, 877sh, 867sh, 856, 814, 723, 685sh, 554, 490sh, 459.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**B172 Lead borate  $\text{PbB}_4\text{O}_7$   $\text{PbB}_4\text{O}_7$** 

**Origin:** Synthetic.

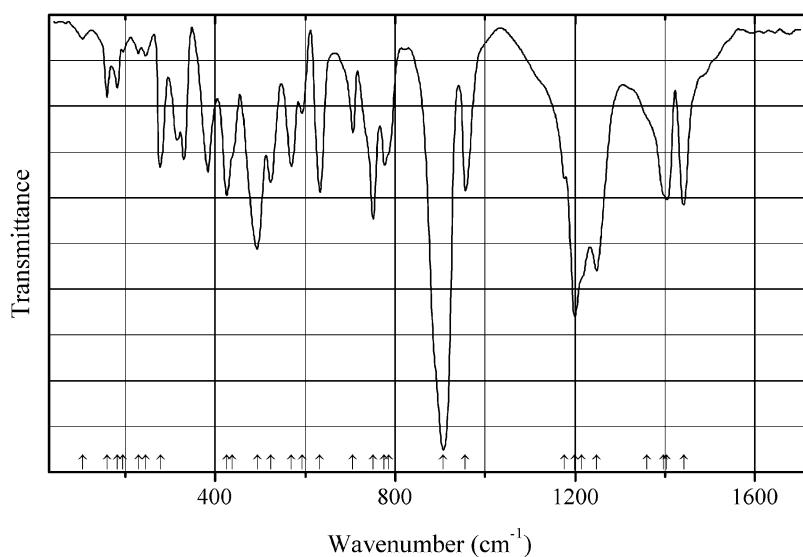
**Description:** Obtained from stoichiometric melt of  $\text{PbO}$  and  $\text{B}_2\text{O}_3$  heated to 1060 K. Orthorhombic  $P21nm$ , space group,  $a = 4.251$ ,  $b = 4.463$ ,  $c = 10.86 \text{ \AA}$ ,  $Z = 2$ . Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc (for the 1500–400  $\text{cm}^{-1}$  region) and Nujol mull (for the 500–50  $\text{cm}^{-1}$  region). Transmission.

**Source:** Hanuza et al. (2008b).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1215sh, 1152s, 1083s, 1009s, 959s, 881, 808, 761, 715, 652, 629, 612, 545, 505w, 486sh, 432w, 350w, 291w, 258w, 245w, 145sh, 116, 65sh.

**Note:** In the cited paper, Raman spectra are given for different polarization and crystal orientation.

**B173 Lithium aluminoborate  $\text{Li}_2\text{AlBO}_4$** 

**Origin:** Synthetic.

**Description:** Prepared from a stoichiometric mixture of  $\text{Li}_2\text{CO}_3$ ,  $\text{B}_2\text{O}_3$ , and  $\text{Al}_2\text{O}_3$  (corundum) by solid-state reaction at 600 °C for ca. 2 months. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 6.2720(3)$ ,  $b = 5.0701(3)$ ,  $c = 10.2989(6)$  Å,  $\beta = 95.882(2)$ °,  $V = 325.78$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 2.63$  g/cm<sup>3</sup>. The structure is based on the sheets consisting of metaboroaluminate rings,  $\text{B}_2\text{Al}_2\text{O}_8$ , which are formed of alternating corner-sharing  $\text{AlO}_4$  tetrahedra and  $\text{BO}_3$  triangles.

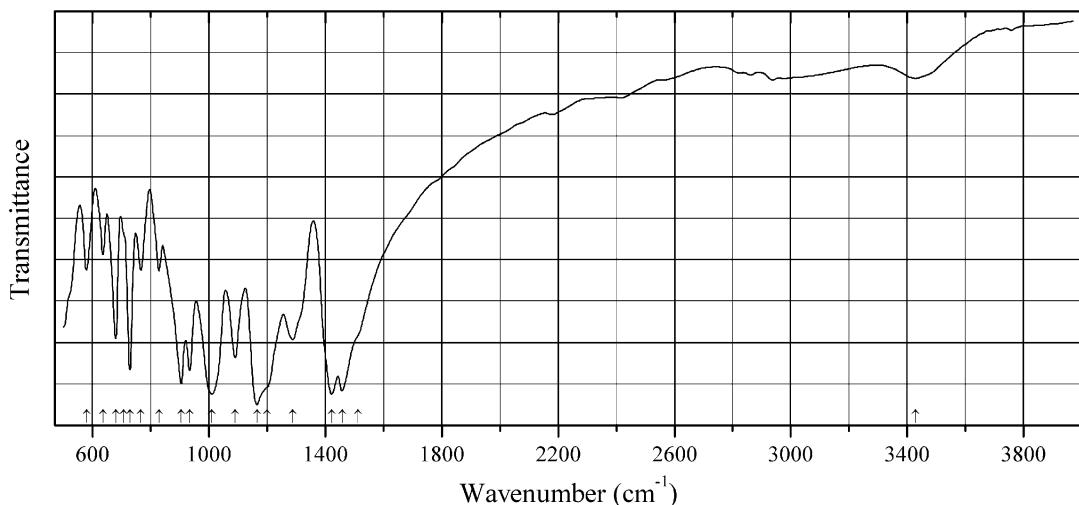
**Kind of sample preparation and/or method of registration of the spectrum:** Reflectance data for a pelletized sample have been transformed by Kramers-Kronig analysis and presented in the absorption coefficient formalism.

**Source:** Pscharis et al. (1999).

**Wavenumbers (cm<sup>-1</sup>):** 1441, 1404, 1396sh, 1360sh, 1248, 1215sh, 1176, 1199s, 956, 907s, 786sh, 776, 751, 705, 632, 593, 569, 523, 493s, 438sh, 426, 384, 330, 315, 278, 245w, 229w, 195w, 182w, 159w, 105w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

#### B174 Lithium cesium borate $\text{Li}_4\text{Cs}_3\text{B}_7\text{O}_{14}$ $\text{Li}_4\text{Cs}_3\text{B}_7\text{O}_{14}$



**Origin:** Synthetic.

**Description:** Synthesized via solid-state reaction from the mixture of  $\text{Li}_2\text{CO}_3$ ,  $\text{Cs}_2\text{CO}_3$ , and  $\text{H}_3\text{BO}_3$  in a molar ratio of 4:3:14, at 560 °C, for 48 h, with several intermediate grindings and mixings. Characterized by powder X-ray diffraction data. The crystal structure is solved. Trigonal, space group  $P3_121$ ,  $a = 6.9313(6)$ ,  $c = 26.799(3)$  Å,  $V = 1115.01(19)$  Å<sup>3</sup>,  $Z = 3$ .  $D_{\text{calc}} = 3.244$  g/cm<sup>3</sup>. The crystal structure contains isolated tricyclic  $\text{B}_7\text{O}_{14}$  units in which five trigonal  $\text{BO}_3$  units and two tetrahedral  $\text{BO}_4$  units are linked by vertical oxygen atoms.

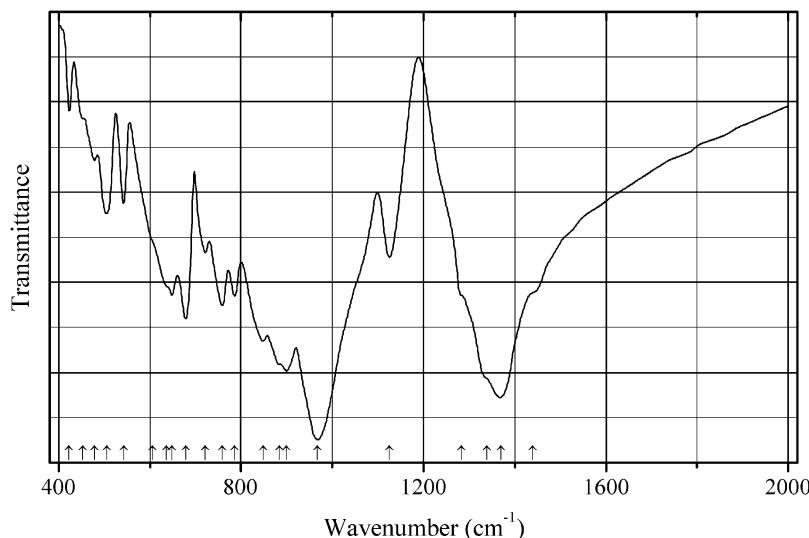
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Yang et al. (2011e).

**Wavenumbers (cm<sup>-1</sup>):** (3428w), 1512sh, 1458s, 1421s, 1288, 1201sh, 1165s, 1090, 934, 905, 828, 766, 728, 707sh, 679, 635, 579.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The wavenumber at 1129 cm<sup>-1</sup> given by the authors is erroneous.

### B175 Lithium sodium borate LiNaB<sub>4</sub>O<sub>7</sub> LiNaB<sub>4</sub>O<sub>7</sub>



**Origin:** Synthetic.

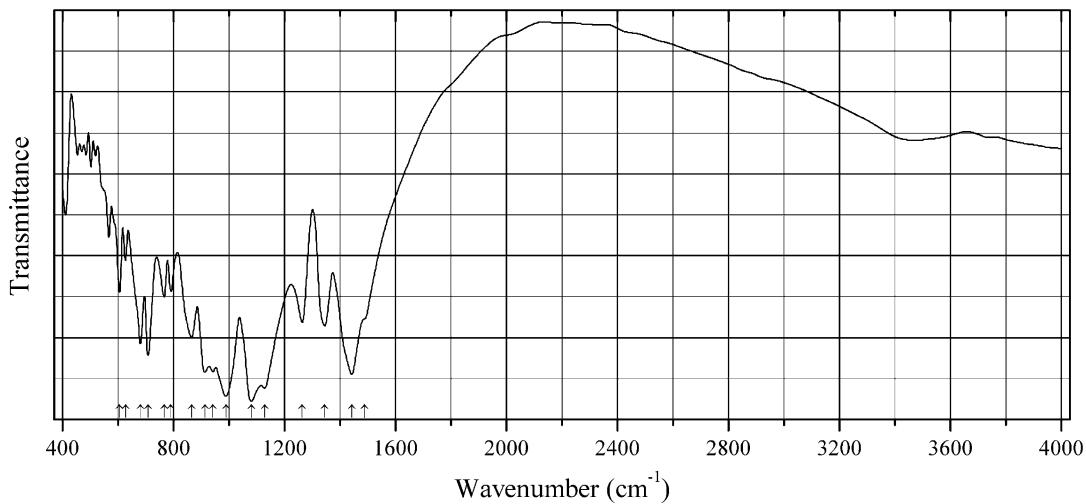
**Description:** Synthesized from the mixture of Na<sub>2</sub>CO<sub>3</sub>, Ga<sub>2</sub>O<sub>3</sub>, H<sub>3</sub>BO<sub>3</sub>, and Li<sub>2</sub>B<sub>4</sub>O<sub>7</sub> in the molar ratio 2:1:8:1 by employing high temperature solution reaction method. Ga<sub>2</sub>O<sub>3</sub> acted as a flux for the crystal growth. Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group *Fdd2*, *a* = 13.326(3), *b* = 14.072(3), *c* = 10.238(2) Å, *V* = 1919.9 (7) Å<sup>3</sup>, *Z* = 16. *D*<sub>calc</sub> = 2.563 g/cm<sup>3</sup>. The basic structural unit is a bicyclic B<sub>4</sub>O<sub>9</sub> group that consists of two vertex-sharing BO<sub>4</sub> tetrahedra and two bridging BO<sub>3</sub> triangles.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Reshak et al. (2012a).

**Wavenumbers (cm<sup>-1</sup>):** 1440sh, 1369s, 1339sh, 1283sh, 1126, 968s, 900, 885sh, 848, 786, 759, 722, 678, 648, 637sh, 605sh, 543, 505, 479w, 453w, 423w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**B176 Lithium strontium borate  $\text{Li}_2\text{Sr}_4\text{B}_{12}\text{O}_{23}$   $\text{Li}_2\text{Sr}_4\text{B}_{12}\text{O}_{23}$** 

**Origin:** Synthetic.

**Description:** Synthesized from stoichiometric mixture of  $\text{Li}_2\text{CO}_3$ ,  $\text{SrCO}_3$ , and  $\text{H}_3\text{BO}_3$  by solid-state reaction method at  $710^\circ\text{C}$  for 60 h, with several intermediate grindings and mixings. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 6.4664(4)$ ,  $b = 8.4878(4)$ ,  $c = 15.3337(8)$  Å,  $\beta = 102.024(3)^\circ$ ,  $V = 823.13(8)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{calc}} = 3.478$  g/cm $^3$ . The structure is based on the  $\text{B}_{10}\text{O}_{18}$  network, consisting of  $\text{BO}_4$  tetrahedra and  $\text{BO}_3$  triangles, and isolated  $\text{B}_2\text{O}_5$  unit.

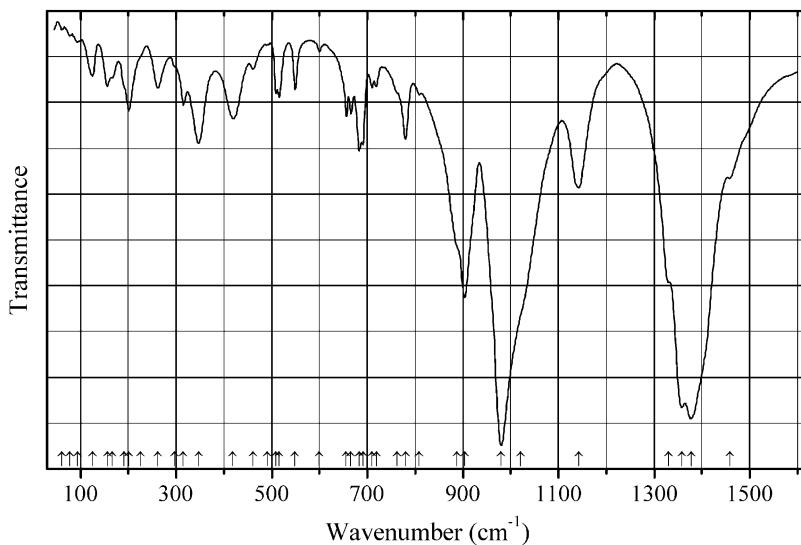
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Zhang et al. (2012a).

**Wavenumbers (cm $^{-1}$ ):** 1488sh, 1442, 1345, 1264, 1129s, 1081s, 989s, 942s, 913s, 865, 791, 767, 708, 681, 627, 606, and a series of weak bands below 600 cm $^{-1}$ .

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

## B177 Lithium tetraborate $\text{Li}_2\text{B}_4\text{O}_7$



**Origin:** Synthetic.

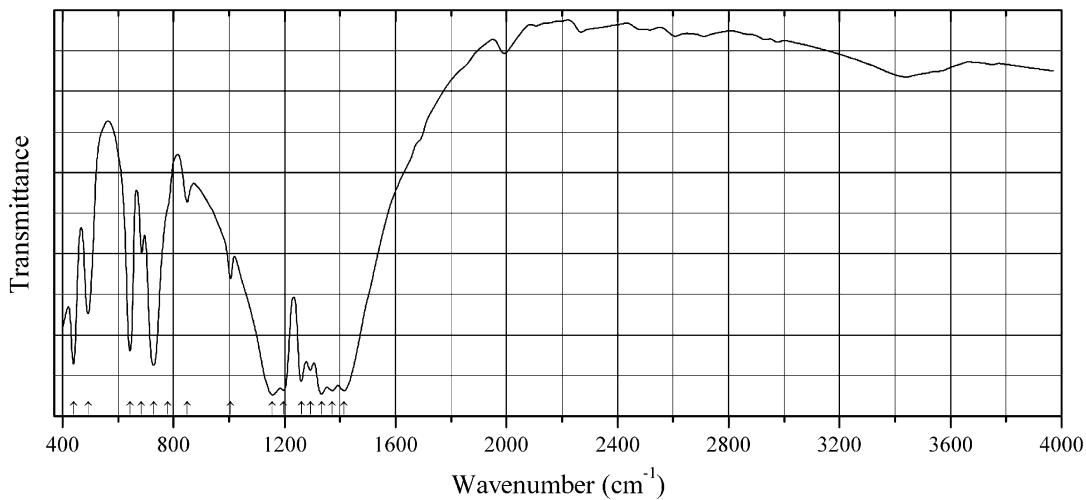
**Description:** Single crystals grown by the Czochralski method from a stoichiometric melt. Characterized by powder X-ray diffraction data. The crystal structure is solved. Tetragonal, space group  $I4_1cd$ ,  $a = 9.477$ ,  $c = 10.286$  Å,  $Z = 8$ . The structure contains pairs of  $\text{BO}_4$  tetrahedra linked by a common O atom to form a  $\text{B}_2\text{O}_7$  group.  $\text{BO}_3$  triangles join these groups to yield a  $\text{B}_4\text{O}_7$  network.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc (for the region 500–1600  $\text{cm}^{-1}$ ), CsI disc (200–700  $\text{cm}^{-1}$ ), and polyethylene disc (50–300  $\text{cm}^{-1}$ ). Absorption.

**Source:** Zhigadlo et al. (2001).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1458, 1378s, 1358s, 1330, 1142, 1021sh, 980s, 904s, 888sh, 809w, 780, 763sh, 719, 710, 691, 683, 666, 656, 600w, 549, 516, 509, 491w, 461w, 419, 348, 315, 297sh, 262, 226sh, 201, 191sh, 167, 156, 125, 94w, 77w, 61w.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**B178 Magnesium strontium diorthoborate  $MgSr(B_2O_5)$** 

**Origin:** Synthetic.

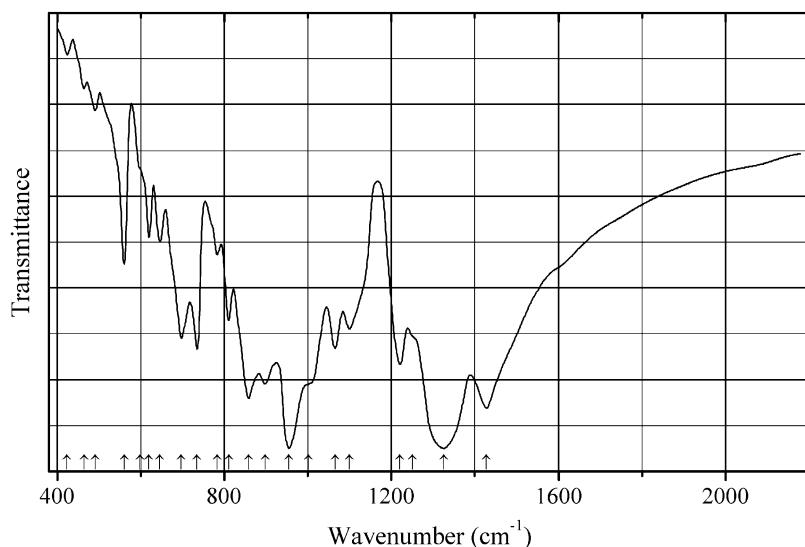
**Description:** Synthesized by solid-state reaction from the stoichiometric mixture of  $MgO$ ,  $Sr(NO_3)_2$ , and  $H_3BO_3$  heated first at 500 °C for 24 h and then at 900 °C for 72 h with several intermediate grindings and mixings. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 6.478(4)$ ,  $b = 5.327(4)$ ,  $c = 12.048(8)$  Å,  $\beta = 102.805(8)^\circ$ ,  $V = 405.4(5)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 3.499$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Guo et al. (2014b).

**Wavenumbers (cm<sup>-1</sup>):** 1415s, 1372s, 1333s, 1293s, 1260s, 1197s, 1157s, 1006, 849w, 780sh, 729, 685, 643, 492, 440.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**B179 Potassium barium borate  $KBaB_5O_9$ ,  $KBaB_5O_9$** 

**Origin:** Synthetic.

**Description:** Prepared by the solid-state reaction of a stoichiometric mixture containing  $\text{KNO}_3$ ,  $\text{Ba}(\text{NO}_3)_2$ , and  $\text{H}_3\text{BO}_3$ , first at  $500^\circ\text{C}$  for 4 h, and thereafter (after regrinding) at  $650^\circ\text{C}$  and for 48 h. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 6.7168(11)$ ,  $b = 8.2724(13)$ ,  $c = 14.262(2)$  Å,  $\beta = 92.724(2)^\circ$ ,  $V = 791.5(2)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 5.572$  g/cm $^3$ .

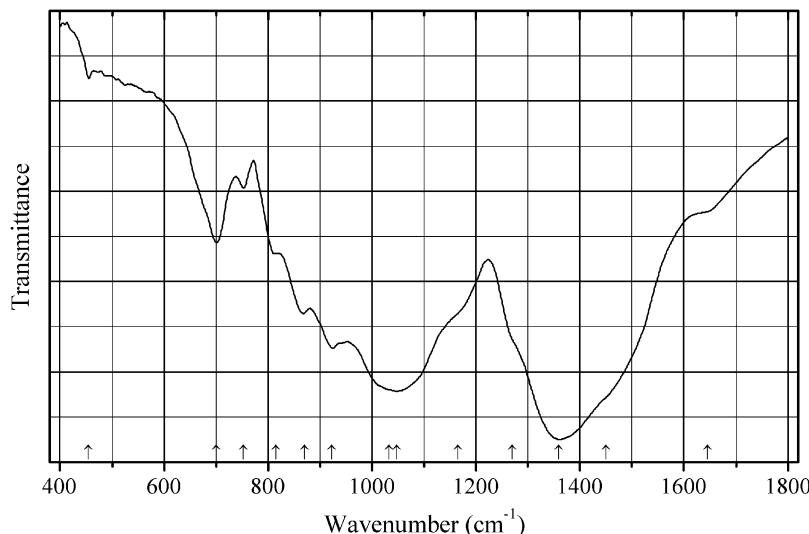
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Yu et al. (2014).

**Wavenumbers (cm $^{-1}$ ):** 1428s, 1325s, 1251sh, 1221, 1100, 1065, 1002sh, 955s, 898s, 858s, 811, 784, 735, 697, 646, 620, 598sh, 560, 491w, 464w, 424w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### B180 Potassium borate $\text{KB}_3\text{O}_5 \cdot \text{H}_2\text{O}$ $\text{KB}_3\text{O}_5 \cdot \text{H}_2\text{O}$



**Origin:** Synthetic.

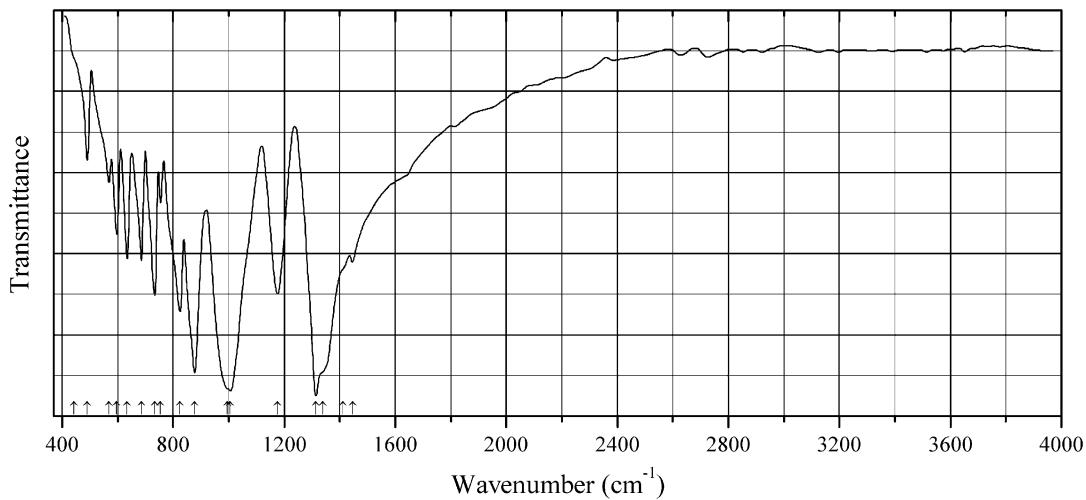
**Description:** Prepared in the reaction between fine powders of  $\text{K}_2\text{B}_4\text{O}_7 \cdot 4\text{H}_2\text{O}$  and  $\text{KB}_5\text{O}_8 \cdot 4\text{H}_2\text{O}$  under exposure of water vapor, with subsequent heating to  $110^\circ\text{C}$ . X-ray amorphous. Characterized by DTA.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Salentine (1987).

**Wavenumbers (cm $^{-1}$ ):** 1645sh, 1450sh, 1360s, 1270sh, 1165sh, 1048s, 1033sh, 923, 870, 816sh, 753, 701, 455w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**B181 Potassium chloride borate perovskite-related  $K_3B_6O_{10}Cl$** 

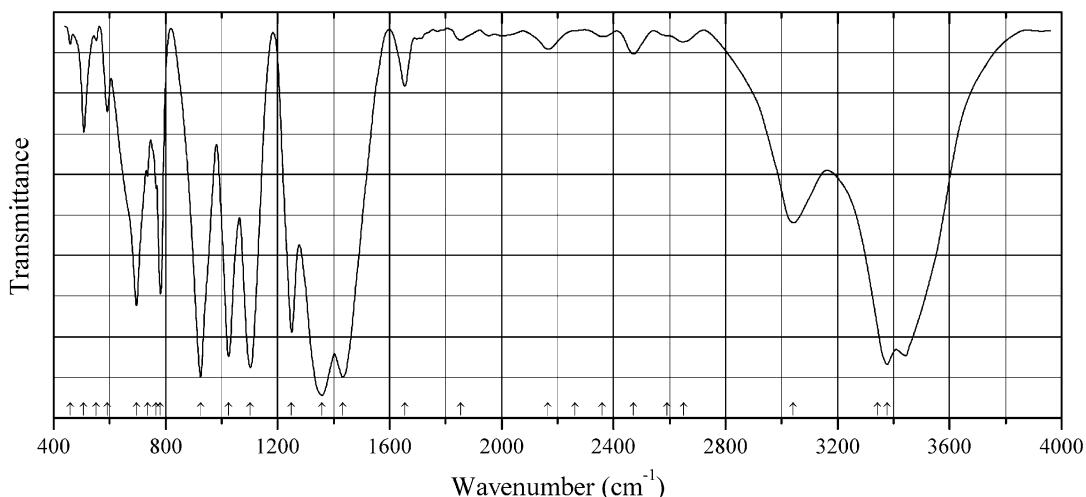
**Origin:** Synthetic.

**Description:** Prepared by heating stoichiometric mixture of  $K_2CO_3$ , KCl, and  $H_3BO_3$ , first at 500 °C for 10 h and thereafter (after intermediate grinding) at 720 °C for 2 days. Characterized by powder X-ray diffraction data. The crystal structure is solved. Trigonal, space group  $R\bar{3}m$ ,  $a = 10.0624(14)$ ,  $c = 8.8361(18)$  Å,  $V = 774.8(2)$  Å $^3$ ,  $Z = 3$ .  $D_{\text{calc}} = 2.428$  g/cm $^3$ . The structure is based on a 3D framework containing  $[B_6O_{10}]$  units in which three  $BO_4$  tetrahedra are shared by the oxygen vertex and are connected with three  $BO_3$  triangles.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Wu et al. (2011).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1446, 1411sh, 1340sh, 1315s, 1176, 1006s, 996sh, 877s, 825, 755, 734, 686, 634, 597, 568, 491, 444sh.

**B182 Potassium pentaborate  $KB_5O_8$** 

**Origin:** Synthetic.

**Description:** Crystals obtained by slow evaporation of aqueous solution containing potassium carbonate and boric acid in the stoichiometric ratio. Characterized by powder X-ray diffraction data. Orthorhombic, space group  $Aba2$ ,  $a = 11.065$ ,  $b = 11.171$ ,  $c = 9.054$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission. The procedure of baseline correction has been applied.

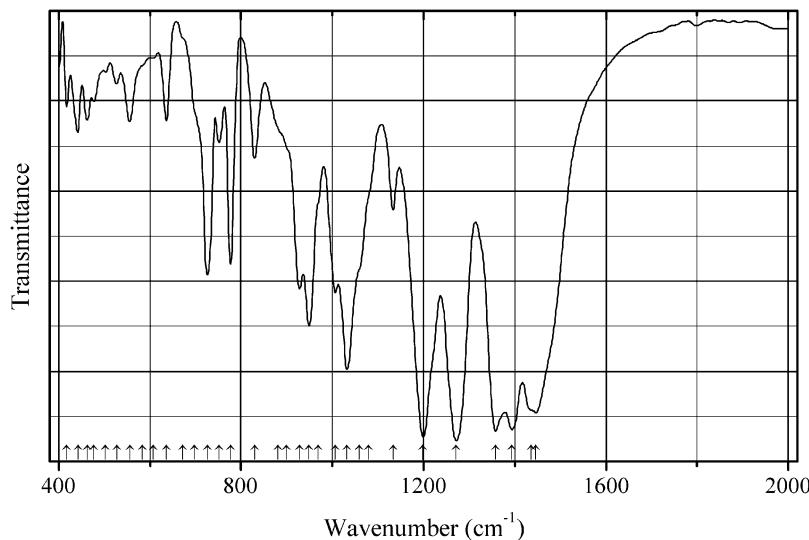
**Source:** Mary et al. (2008).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3443s, 3377s, 3042, 2650w, 2590sh, 2472w, 2360w, 2263sh, 2166w, 1854w, 1654, 1433s, 1358s, 1250, 1103s, 1025s, 925s, 782, 766, 735, 696, 591, 552w, 508, 459w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 917s, 786, 730, 559s, 456s, 373 (weak bands are not indicated).

### B183 Potassium sodium zinc borate $\text{K}_2\text{NaZnB}_5\text{O}_{10}$ $\text{K}_2\text{NaZnB}_5\text{O}_{10}$



**Origin:** Synthetic.

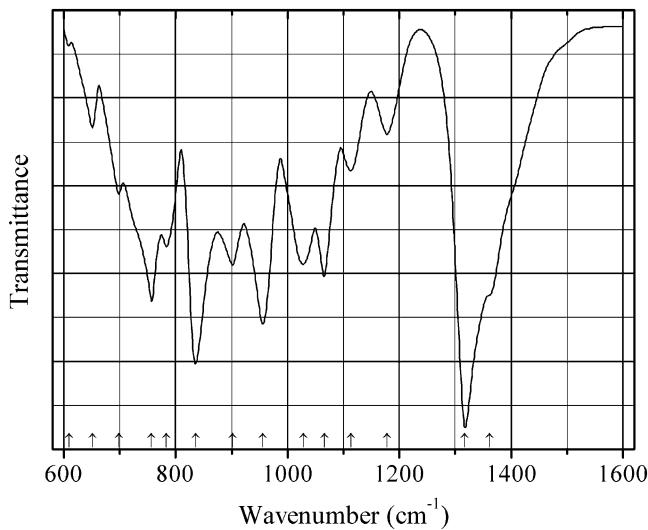
**Description:** Colorless prismatic crystals obtained from  $\text{K}_2\text{CO}_3$ ,  $\text{ZnO}$ ,  $\text{H}_3\text{BO}_3$ , and  $\text{Na}_2\text{B}_4\text{O}_7 \cdot 10\text{H}_2\text{O}$  in the molar ratio of 3:2:10:2 by employing a high-temperature solution reaction method. The crystal structure is solved. Monoclinic, space group  $C2/c$ ,  $a = 7.9244(16)$ ,  $b = 12.805(3)$ ,  $c = 18.962(4)$  Å,  $\beta = 99.39$  (3)°,  $V = 1898.4(7)$  Å³,  $Z = 8$ .  $D_{\text{calc}} = 2.663$  g/cm³. The structure is based on the  $[\text{B}_5\text{O}_{10}]^{5-}$  group that consists of one  $\text{BO}_4$  tetrahedron and four  $\text{BO}_3$  triangles condensed to a double ring via the common tetrahedron.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Chen et al. (2010).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1447s, 1436sh, 1394s, 1358s, 1272s, 1199s, 1133, 1080sh, 1059sh, 1032s, 1006, 969sh, 949, 928, 900sh, 880sh, 830, 777, 752, 726, 698sh, 672sh, 636w, 607w, 583sh, 556w, 527w, 503w, 477w, 463w, 442w, 417w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**B184 Potassium triborate  $\text{KB}_3\text{O}_5$** 

**Origin:** Synthetic.

**Description:** A high-pressure monoclinic polymorph. Characterized by powder X-ray diffraction data.

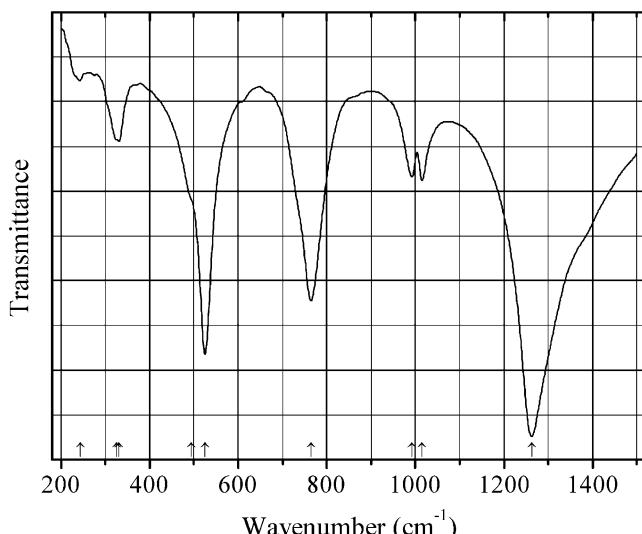
The crystal structure is solved. Monoclinic, space group  $C2/c$ ,  $a = 9.608(2)$ ,  $b = 8.770(2)$ ,  $c = 9.099(2) \text{ \AA}$ ,  $\beta = 104.4(1)^\circ$ ,  $V = 742.8(3) \text{ \AA}^3$ ,  $Z = 8$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection (?).

**Source:** Sohr et al. (2014).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1362sh, 1317s, 1178, 1113, 1066, 1028, 956s, 902, 836s, 783, 757s, 698, 651, 609w.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**B185 Sodium aluminum borate  $\text{Na}_2\text{Al}_2\text{B}_2\text{O}_7$   $\text{Na}_2\text{Al}_2\text{B}_2\text{O}_7$** 

**Origin:** Synthetic.

**Description:** Prepared by heating stoichiometric mixture of  $\text{NaHCO}_3$ ,  $\text{Al}_2\text{O}_3$ , and  $\text{H}_3\text{BO}_3$ , first at  $400^\circ\text{C}$  for 10 h and thereafter at  $950^\circ\text{C}$  for 2 days. The crystal structure is solved by the Rietveld technique. Trigonal, space group  $P-31c$ ,  $a = 4.8113(1)$ ,  $c = 15.2781(3)$  Å,  $V = 306.29(2)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{calc}} = 2.532$  g/cm $^3$ . The structure contains infinite  $[\text{Al}_2\text{B}_2\text{O}_7]$  sheets. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 4.02 (59) (101), 3.820 (55) (004), 2.815 (100) (104), 2.406 (33) (110), 2.295 (36) (112).

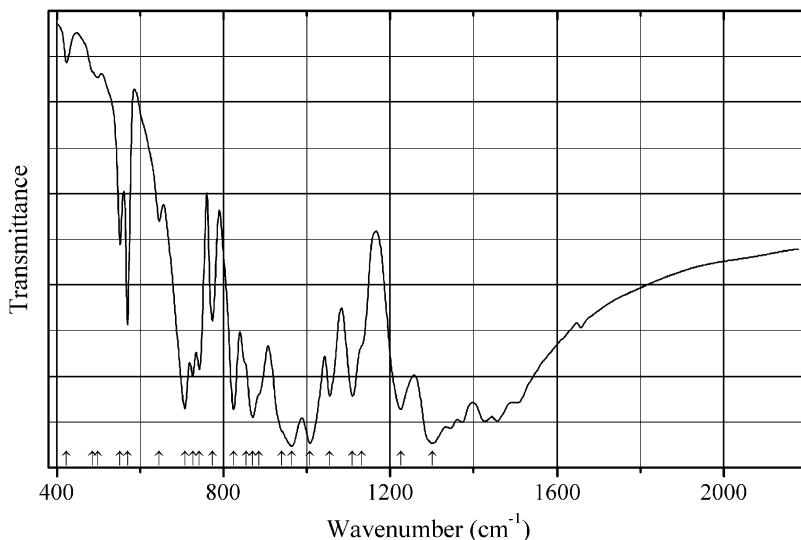
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** He et al. (2001).

**Wavenumbers (cm $^{-1}$ ):** 1263s, 1015, 992, 765s, 525s, 495sh, 331, 325sh, 244w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### B186 Sodium barium borate $\text{NaBaB}_5\text{O}_9$ $\text{NaBaB}_5\text{O}_9$



**Origin:** Synthetic.

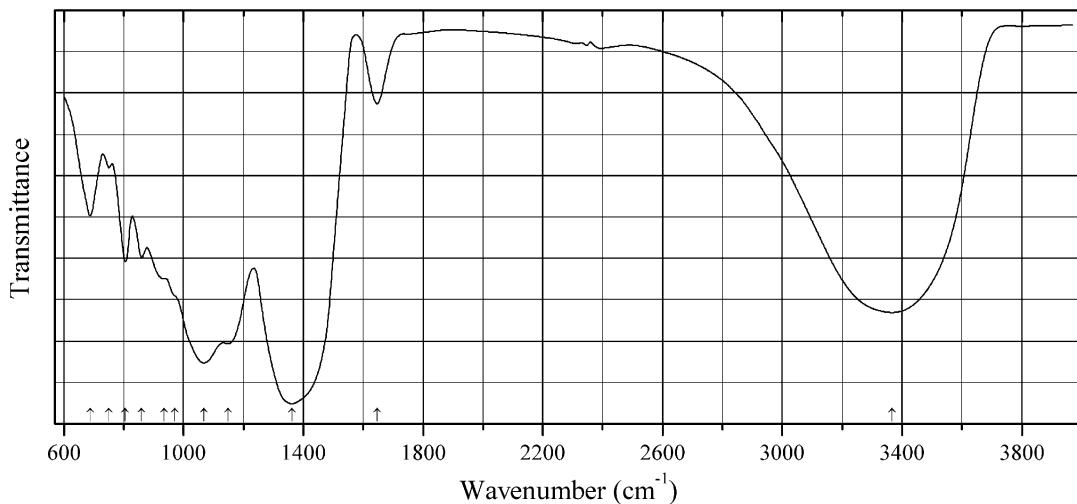
**Description:** Prepared by solid-state reaction techniques from a stoichiometric ratio of  $\text{NaNO}_3$ ,  $\text{Ba}(\text{NO}_3)_2$ , and  $\text{H}_3\text{BO}_3$  preheated at  $500^\circ\text{C}$  for 4 h and thereafter (after intermediate grinding) heated at  $650^\circ\text{C}$  for 48 h. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 6.5773(19)$ ,  $b = 13.872(4)$ ,  $c = 8.371(2)$  Å,  $\beta = 105.393(3)^\circ$ ,  $V = 736.4(4)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 3.232$  g/cm $^3$ . The structure is based on infinite corrugated layers containing  $\text{B}_5\text{O}_9^{3-}$  double rings.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Yu et al. (2014).

**Wavenumbers (cm $^{-1}$ ):** 1301s, 1225s, 1132sh, 1110, 1055, 1008s, 964s, 940sh, 885sh, 870s, 854sh, 824s, 773, 742, 726, 707s, 646, 570, 552, 498w, 486sh, 424w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**B187 Sodium borate  $\text{Na}_2\text{B}_5\text{O}_8(\text{OH})\cdot 2\text{H}_2\text{O}$   $\text{Na}_2\text{B}_5\text{O}_8(\text{OH})\cdot 2\text{H}_2\text{O}$** 

**Origin:** Synthetic.

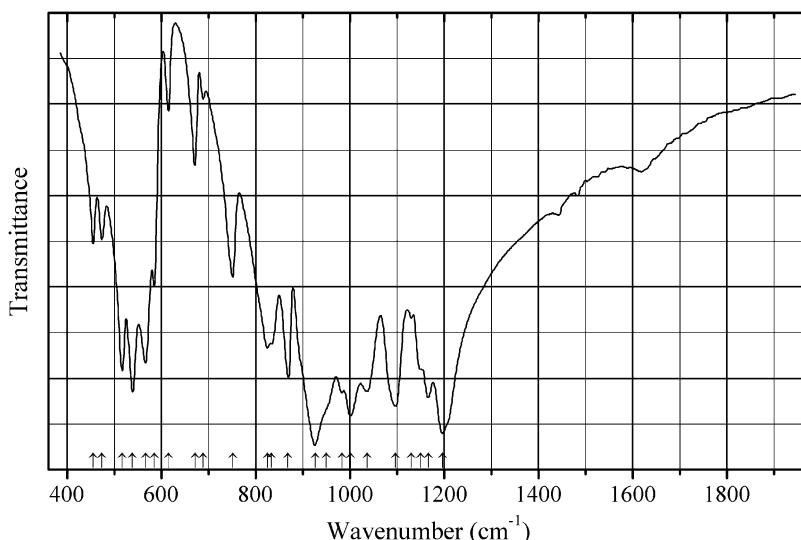
**Description:** Synthesized hydrothermally from  $\text{Na}_2\text{B}_4\text{O}_7\cdot 10\text{H}_2\text{O}$  and  $\text{H}_3\text{BO}_3$  at  $180^\circ\text{C}$  for 3 days, with subsequent cooling to room temperature for 9 days. Characterized by powder X-ray diffraction data and elemental analysis. The crystal structure is solved. Orthorhombic, space group  $Pna2_1$ ,  $a = 11.967(2)$ ,  $b = 6.5320(13)$ ,  $c = 11.126(2)$  Å,  $V = 869.7(3)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 2.146$  g/cm $^3$ . The structure is based on the double hexagonal ring  $\text{B}_5\text{O}_8(\text{OH})^{2-}$  containing three  $\text{BO}_3$  triangles and two  $\text{BO}_4$  tetrahedra.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Wang et al. (2009b).

**Wavenumbers (cm $^{-1}$ ):** 3367s, 1646, 1362s, 1149s, 1067s, 970sh, 936sh, 860, 806, 750, 688.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**B188 Sodium borophosphate  $\text{Na}_5(\text{B}_2\text{P}_3\text{O}_{13})$   $\text{Na}_5(\text{B}_2\text{P}_3\text{O}_{13})$** 

**Origin:** Synthetic.

**Description:** Prepared by solid-state reaction techniques, by heating the mixture of  $\text{Na}_2\text{CO}_3$ ,  $\text{H}_3\text{BO}_3$ , and  $(\text{NH}_4)(\text{H}_2\text{PO}_4)$  in the molar ratio 2.5:2:(3.01–3.05) first at 500 °C for 10 h and thereafter at 700 °C for 24 h with intermediate grinding. Monoclinic, space group  $C2$ . Characterized by powder X-ray diffraction data.  $D_{\text{meas}} = 2.68 \text{ g/cm}^3$ .

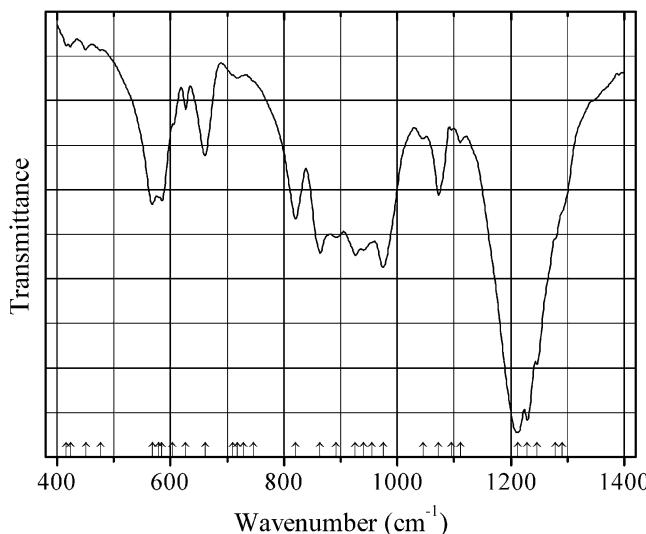
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission.

**Source:** Li et al. (2003).

**Wavenumbers (cm<sup>-1</sup>):** 1197s, 1166, 1150sh, 1130, 1097s, 1036, 1002s, 983, 950sh, 926s, 869, 834, 825, 751, 688w, 671, 615w, 585, 566, 539, 517, 473, 455.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

### B189 Sodium borosulfate $\text{Na}_5[\text{B}(\text{SO}_4)_4]$ $\text{Na}_5[\text{B}(\text{SO}_4)_4]$



**Origin:** Synthetic.

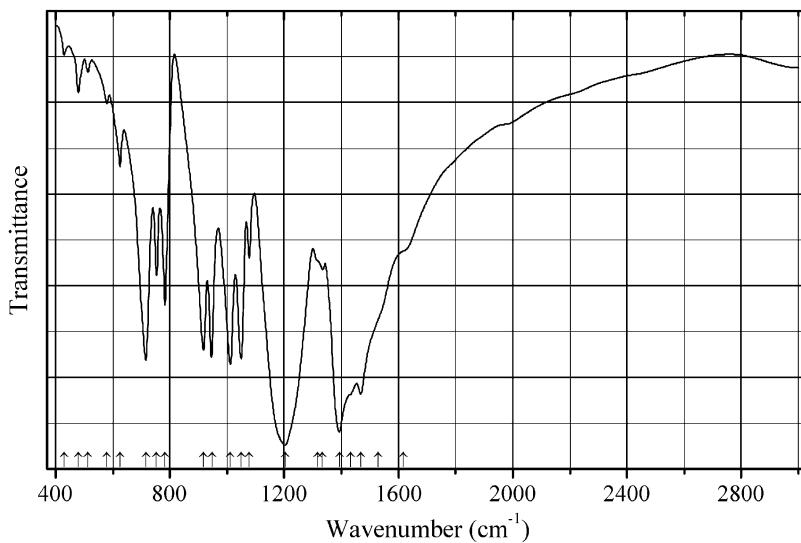
**Description:** Colorless crystals prepared by solid-state reaction techniques, by heating the mixture of  $\text{NaHSO}_4 \cdot \text{H}_2\text{O}$  and  $\text{B}(\text{OH})_3$  at 673 K for 12 h. Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group  $Pca2_1$ ,  $a = 10.730(2)$ ,  $b = 13.891(3)$ ,  $c = 18.197(4)$  Å,  $Z = 8$ .  $D_{\text{calc}} = 2.498 \text{ g/cm}^3$ . The structure contains open-branched pentameric anion  $[\text{B}(\text{SO}_4)_4]^{5-}$  with the borate tetrahedron in the center.

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection.

**Source:** Daub et al. (2013).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1290sh, 1278sh, 1246s, 1229s, 1212s, 1111w, 1095, 1073, 1045, 975, 955sh, 941, 926, 892, 864, 821, 746sh, 729sh, 718w, 710sh, 661, 627, 604sh, 585, 580sh, 568, 477sh, 451w, 424w, 416w.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. In the cited paper, a figure of the Raman spectrum is given.

**B190 Sodium calcium pentaborate  $\text{Na}_3\text{Ca}(\text{B}_5\text{O}_{10})$   $\text{Na}_3\text{Ca}(\text{B}_5\text{O}_{10})$** 

**Origin:** Synthetic.

**Description:** Colorless prismatic crystals obtained by heating a powder mixture of  $\text{CaCO}_3$ ,  $\text{Bi}_2\text{O}_3$ ,  $\text{H}_3\text{BO}_3$ , and  $\text{Na}_2\text{B}_4\text{O}_7 \cdot 10\text{H}_2\text{O}$  with the molar ratio 1:1:2:4.63 at 750 °C for 1 day, with subsequent cooling down to 730 °C at a rate of 1 °C/h. Characterized by energy-dispersive X-ray analyses. The crystal structure is solved. Triclinic, space group  $P-1$ ,  $a = 7.4403(6)$ ,  $b = 9.7530(10)$ ,  $c = 12.9289(9)$  Å,  $\alpha = 90.972(7)^\circ$ ,  $\beta = 90.073(7)^\circ$ ,  $\gamma = 109.656(6)^\circ$ ,  $V = 883.37(13)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 2.429$  g/cm<sup>3</sup>. The basic structural unit is a  $[\text{B}_5\text{O}_{10}]^{5-}$  group that consists of one  $\text{BO}_4$  tetrahedron and four  $\text{BO}_3$  triangles condensed to a double ring via the common tetrahedron.

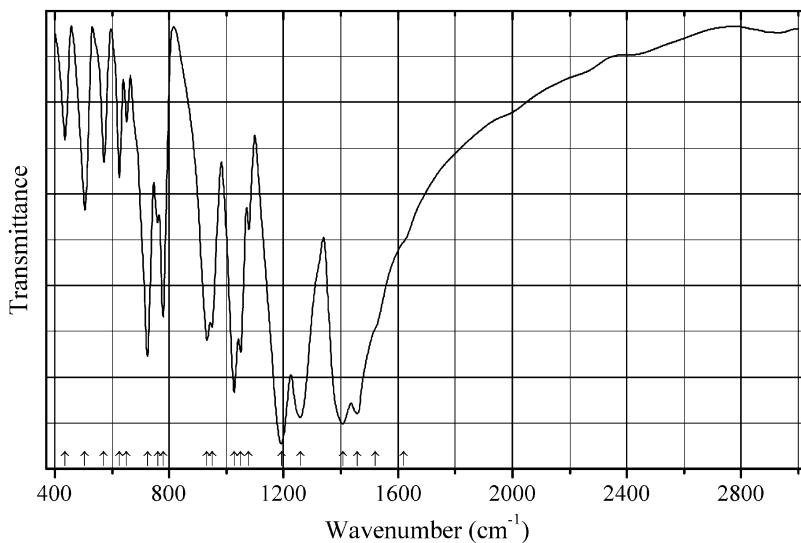
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Chen et al. (2007b).

**Wavenumbers (cm<sup>-1</sup>):** 1617sh, 1530sh, 1468s, 1434sh, 1393, 1335, 1316sh, 1204s, 1078, 1050, 1012, 947, 918, 783, 754, 716, 625, 580w, 513w, 480w, 430w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

## B191 Sodium magnesium pentaborate $\text{Na}_3\text{MgB}_5\text{O}_{10}$ $\text{Na}_3\text{MgB}_5\text{O}_{10}$



**Origin:** Synthetic.

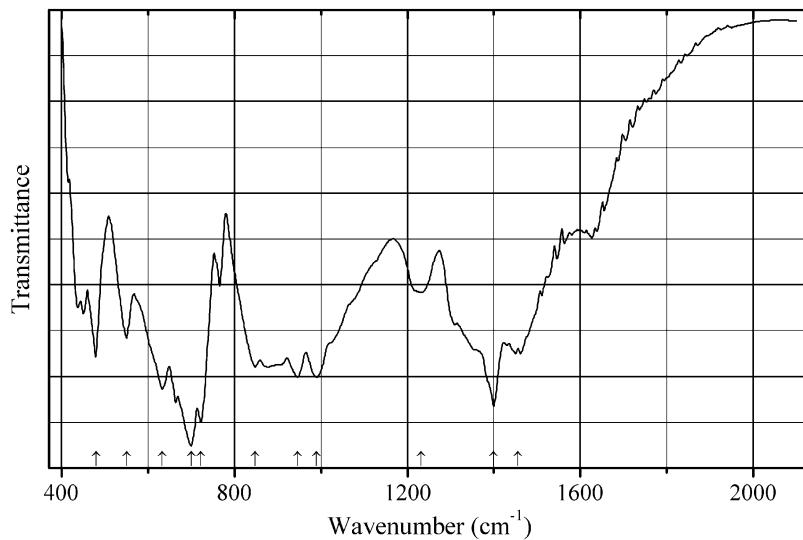
**Description:** Colorless prismatic crystals obtained by heating a powder mixture of  $\text{Na}_2\text{CO}_3$ ,  $\text{Mg}(\text{NO}_3)_2$ ,  $\text{H}_3\text{BO}_3$ , and  $\text{Na}_2\text{B}_4\text{O}_7 \cdot 10\text{H}_2\text{O}$  with the molar ratio 3.2:5.2 at 750 °C for 4 days, with subsequent cooling down to 700 °C at a rate of 1 °C/h and to 600 °C at a rate of 5 °C/h. Characterized by energy-dispersive X-ray analyses. The crystal structure is solved. Orthorhombic, space group  $Pbca$ ,  $a = 7.838(1)$ ,  $b = 12.288(1)$ ,  $c = 18.180(2)$  Å,  $V = 1751.0(3)$  Å<sup>3</sup>,  $Z = 8$ .  $D_{\text{calc}} = 2.332$  g/cm<sup>3</sup>. The basic structural unit is a  $[\text{B}_5\text{O}_{10}]^{5-}$  group that consists of one  $\text{BO}_4$  tetrahedron and four  $\text{BO}_3$  triangles condensed to a double ring via the common tetrahedron.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Chen et al. (2007b).

**Wavenumbers (cm<sup>-1</sup>):** 1620sh, 1522sh, 1458s, 1407s, 1260s, 1192s, 1079w, 1050, 1027s, 950, 932, 779, 760, 725, 651w, 626, 572, 506, 436

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**B192 Sodium strontium aluminum borate  $\text{NaSr}_7\text{AlB}_{18}\text{O}_{36}$   $\text{NaSr}_7\text{AlB}_{18}\text{O}_{36}$** 

**Origin:** Synthetic.

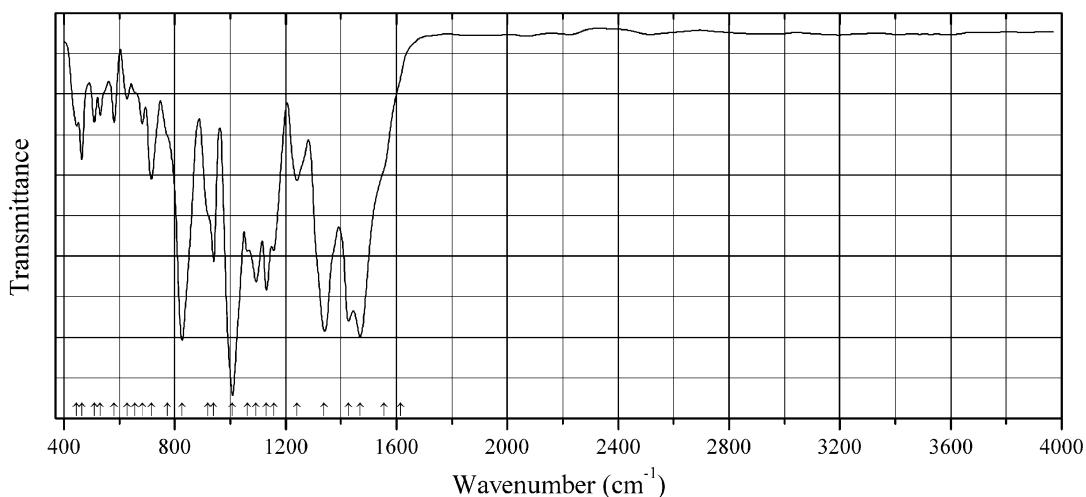
**Description:** Crystals grown from the melt prepared from  $\text{SrCO}_3$ ,  $\text{Al}(\text{OH})_3$ , and  $\text{Na}_2\text{B}_4\text{O}_7 \cdot 10\text{H}_2\text{O}$  (with the ratio 1:4:3) at  $860^\circ\text{C}$  by cooling down to  $700^\circ\text{C}$  at a rate of  $2.0^\circ\text{C}/\text{h}$ , to  $500^\circ\text{C}$  at  $5.0^\circ\text{C}/\text{h}$ , and finally to room temperature at  $20^\circ\text{C}/\text{h}$ . Characterized by powder X-ray diffraction data. The crystal structure is solved. Trigonal, space group  $R-3c$ ,  $a = 11.356(2)$ ,  $c = 36.655(7)$  Å,  $V = 4093.7(12)$  Å<sup>3</sup>,  $Z = 6$ .  $D_{\text{calc}} = 3.490$  g/cm<sup>3</sup>. The crystal structure contains a polycyclic  $\text{B}_{18}\text{O}_{36}$  building unit consisting of 12  $\text{BO}_3$  triangles and 6  $\text{BO}_4$  tetrahedra.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Chen et al. (2014a).

**Wavenumbers (cm<sup>-1</sup>):** 1456, 1400s, 1232, 990s, 946s, 847, 765w, 721s, 700s, 663, 632s, 550, 479, 450, 437.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**B193 Sodium vanadyl borate  $\text{Na}_3(\text{VO}_2)\text{B}_6\text{O}_{11}$   $\text{Na}_3(\text{VO}_2)\text{B}_6\text{O}_{11}$** 

**Origin:** Synthetic.

**Description:** Synthesized by solid-state reaction between  $\text{Na}_2\text{CO}_3$ ,  $\text{V}_2\text{O}_5$ , and  $\text{H}_3\text{BO}_3$ . A stoichiometric mixture of these reactants was heated first at 300 °C for 5 h, thereafter at 500 °C for 5 h, and finally at 600 °C for 2 days with several intermediate grindings. Orthorhombic, space group  $P2_12_12_1$ ,  $a = 7.7359(9)$ ,  $b = 10.1884(12)$ ,  $c = 12.5697(15)$  Å,  $V = 990.7(2)$  Å<sup>3</sup>,  $Z = 4$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 4.1325 (39) (121), 3.6679 (57) (103), 3.1309 (100) (004), 3.0821 (38) (220), 2.9814 (39) (032).

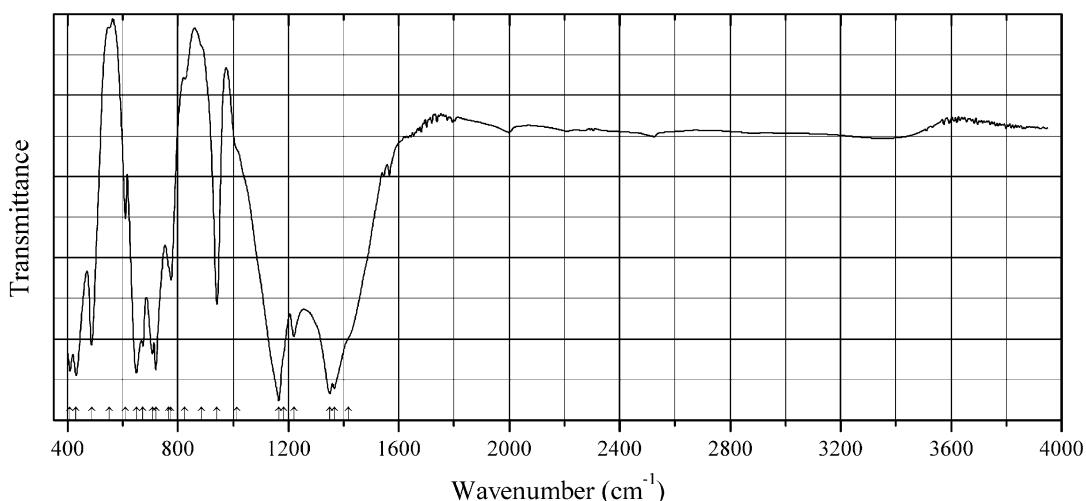
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Fan et al. (2010).

**Wavenumbers (cm<sup>-1</sup>):** 1615sh, 1555sh, 1469s, 1427s, 1340s, 1241, 1158, 1130, 1094, 1062, 1008s, 941, 921sh, 827s, 775sh, 716, 683w, 656sh, 628w, 581w, 531w, 510w, 465, 446.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### B194 Sodium yttrium tellurate borate $\text{Na}_2\text{Y}_2(\text{Te}^{6+}\text{B}_2\text{O}_{10})$ $\text{Na}_2\text{Y}_2(\text{Te}^{6+}\text{B}_2\text{O}_{10})$



**Origin:** Synthetic.

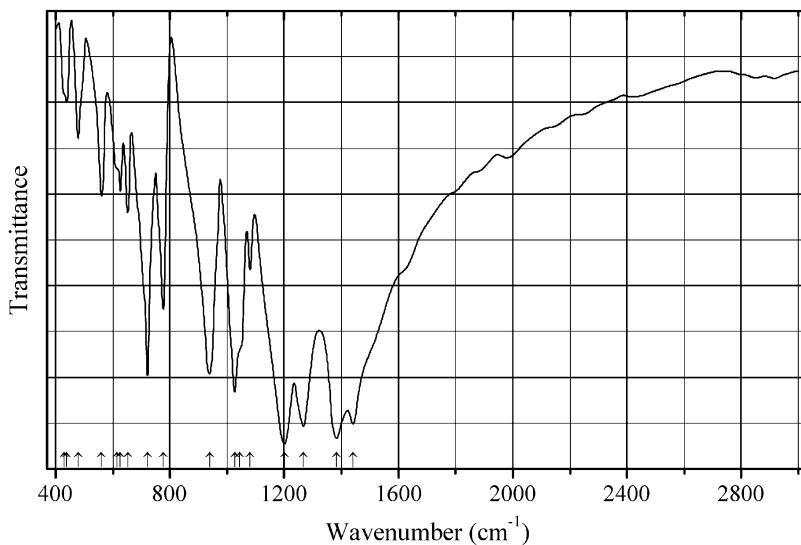
**Description:** Synthesized by heating a mixture of  $\text{NaCO}_3$ ,  $\text{TeO}_2$ ,  $\text{H}_3\text{BO}_3$ , and  $\text{Y}_2\text{O}_3$  at 830 °C for 10 h with subsequent cooling down to 600 °C at 3–5 °C/h rate. Characterized by powder X-ray diffraction data and EDS elemental analyses. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 6.3073(7)$ ,  $b = 9.9279(8)$ ,  $c = 6.7219(6)$  Å,  $\beta = 104.260(10)^\circ$ ,  $V = 407.94(7)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 4.339$  g/cm<sup>3</sup>. The structure is based on a 3D framework composed of linear  $[\text{TeO}_4(\text{BO}_3)_2]^{8-}$  anions interconnected by  $\text{Y}^{3+}$  cations.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission? Kind of sample preparation is not indicated.

**Source:** Feng et al. (2015a).

**Wavenumbers (cm<sup>-1</sup>):** 1418sh, 1366s, 1350s, 1220, 1183sh, 1165s, 1014sh, 941, 885sh, 825w, 775, 766sh, 720s, 708s, 674s, 650s, 610, 552, 488, 432s, 409s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**B195 Sodium zinc pentaborate  $\text{Na}_3\text{ZnB}_5\text{O}_{10}$   $\text{Na}_3\text{ZnB}_5\text{O}_{10}$** 

**Origin:** Synthetic.

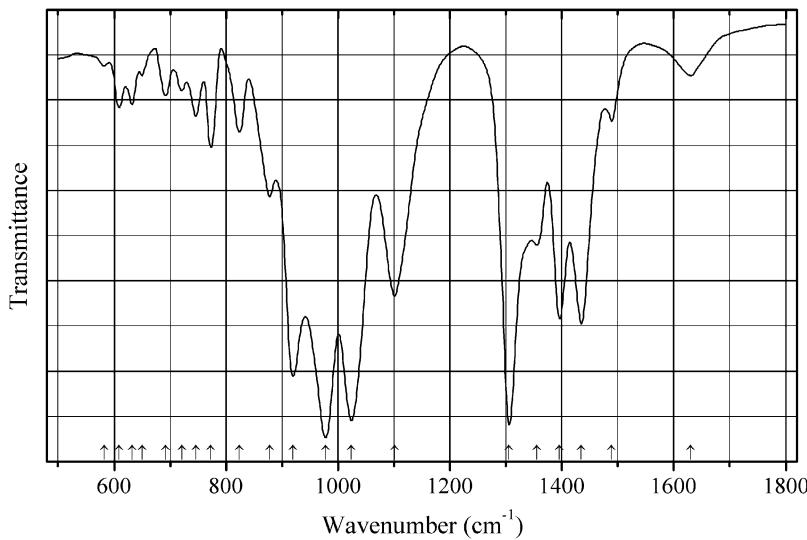
**Description:** Prepared by a solid-state reaction method, by heating the mixture of  $\text{Na}_2\text{CO}_3$ ,  $\text{ZnO}$ ,  $\text{H}_3\text{BO}_3$ , and  $\text{Na}_2\text{B}_4\text{O}_7 \cdot 10\text{H}_2\text{O}$  (with the molar ratio 1:2:2:1) at  $750^\circ\text{C}$  for 1 day with subsequent cooling down to  $730^\circ\text{C}$  at a rate of  $1^\circ\text{C}/\text{h}$ , then to  $720^\circ\text{C}$  at  $0.5^\circ\text{C}/\text{h}$ , and finally to room temperature at  $20^\circ\text{C}/\text{h}$ . Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2_1/n$ ,  $a = 6.6725(7)$ ,  $b = 18.1730(10)$ ,  $c = 7.8656(9)$  Å,  $\beta = 114.604(6)^\circ$ ,  $V = 867.18(14)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 2.668$  g/cm $^3$ . The structure contains double rings  $[\text{B}_5\text{O}_{10}]^{5-}$  bridged by  $\text{ZnO}_4$  tetrahedra through common O atoms to form a 2D layer.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Chen et al. (2007a).

**Wavenumbers (cm $^{-1}$ ):** 1441s, 1383s, 1268s, 1201s, 1081, 1045sh, 1027s, 939s, 777, 722s, 653, 627, 615sh, 561, 479, 439w, 430sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**B196 Strontium borate chloride  $\text{Sr}_2\text{B}_5\text{O}_9\text{Cl}$   $\text{Sr}_2\text{B}_5\text{O}_9\text{Cl}$** 

**Origin:** Synthetic.

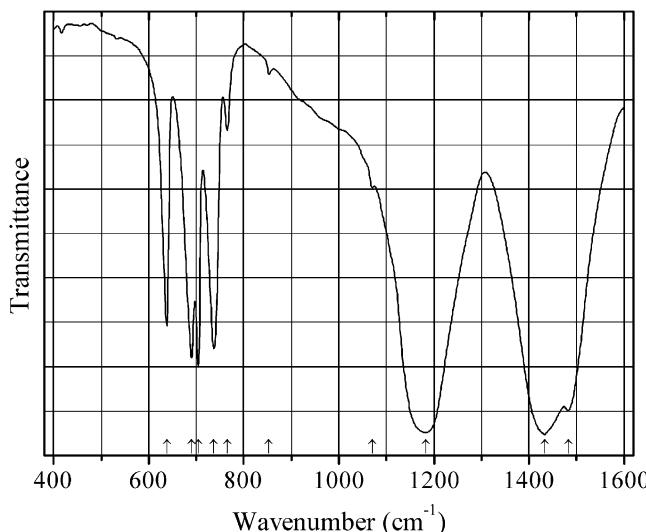
**Description:** Obtained by stepwise heating a precipitate formed by adding  $\text{SrCl}_2$  aqueous solution to  $\text{Na}_2\text{B}_4\text{O}_7$  aqueous solution at 600, 700, and 800 °C for 8 h at each temperature. Characterized by powder X-ray diffraction data. Orthorhombic,  $a = 11.381$ ,  $b = 11.319$ , and  $c = 6.498$  Å (see JCPDS Card No. 27-0835).

**Kind of sample preparation and/or method of registration of the spectrum:** No data.

**Source:** Zhu et al. (2013).

**Wavenumbers (cm⁻¹):** 1630w, 1489w, 1435, 1396, 1355, 1306s, 1101, 1024s, 978s, 920s, 878, 824, 773, 721w, 746w, 692w, 650w, 632w, 609w, 582w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**B197 Strontium borate  $\text{SrB}_2\text{O}_4$   $\text{SrB}_2\text{O}_4$** 

**Origin:** Synthetic.

**Description:** Synthesized by heating a mixture of appropriate amounts of  $\text{SrCO}_3$  and  $\text{H}_3\text{BO}_3$  at 1000 °C for 2 h in air. Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic,  $a \approx 12.01$ ,  $b \approx 4.34$ , and  $c \approx 6.59$  Å (see JCPDS card No. 84-2175).

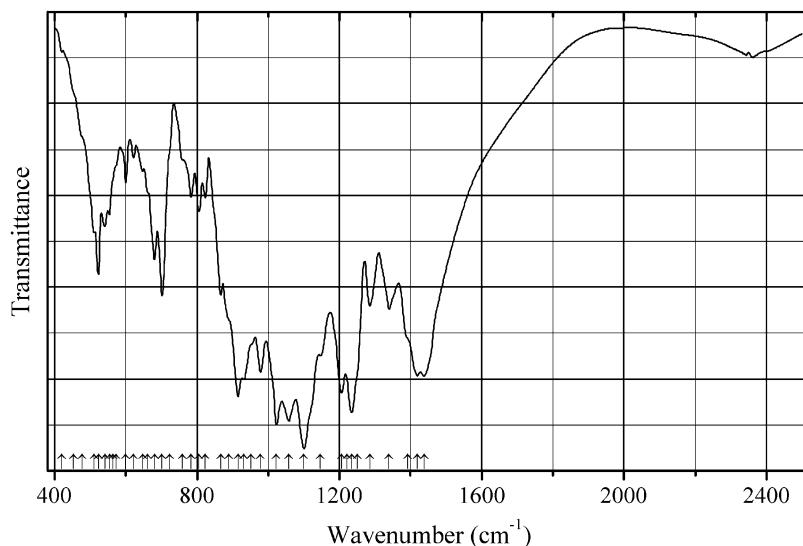
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Onodera et al. (1999).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1483s, 1433s, 1183s, 1070w, 853w, 765w, 737, 704, 690, 638.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

### B198 Strontium borate $\text{SrB}_8\text{O}_{13}$ $\text{SrB}_8\text{O}_{13}$



**Origin:** Synthetic.

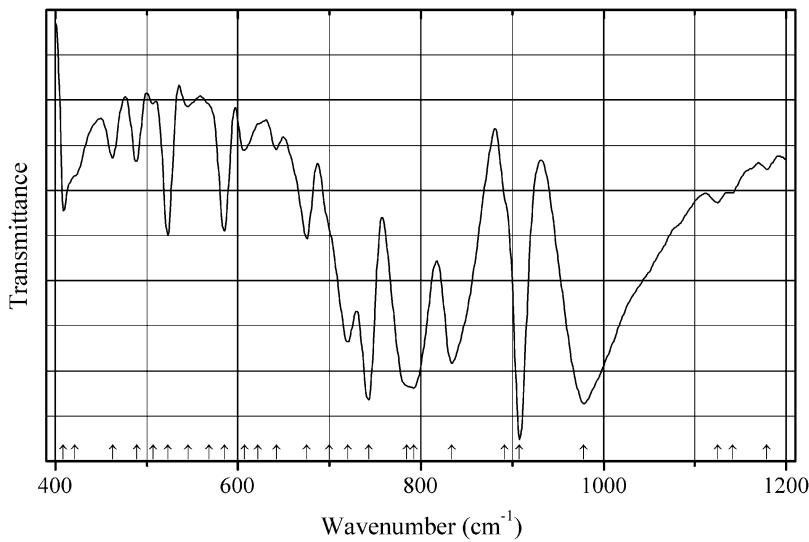
**Description:** Synthesized by heating a powder mixture of  $\text{Bi}_2\text{O}_3$ ,  $\text{SrCO}_3$ , and  $\text{H}_3\text{BO}_3$  (with a molar ratio 3:3:26) at 735 °C for 2 weeks. The product was then cooled down to 500 °C at a rate of 5 °C/h and thereafter cooled to room temperature at a rate of 20 °C/h. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 8.408(1)$ ,  $b = 16.672(2)$ ,  $c = 13.901(2)$  Å,  $\beta = 106.33(1)^\circ$ ,  $V = 1870.0(4)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 2.714$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Tang et al. (2008).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1438s, 1419s, 1392sh, 1340, 1286, 1250sh, 1235s, 1221sh, 1206s, 1147, 1101s, 1058s, 1023s, 979, 951sh, 932, 915s, 889sh, 867, 823w, 806w, 783w, 759sh, 724sh, 702, 681, 662sh, 647w, 622w, 600w, 572sh, 564sh, 554, 541, 523, 511, 477sh, 452sh, 420w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**B199 Strontium boroarsenate Sr(BAsO<sub>5</sub>) Sr(BAsO<sub>5</sub>)**

**Origin:** Synthetic.

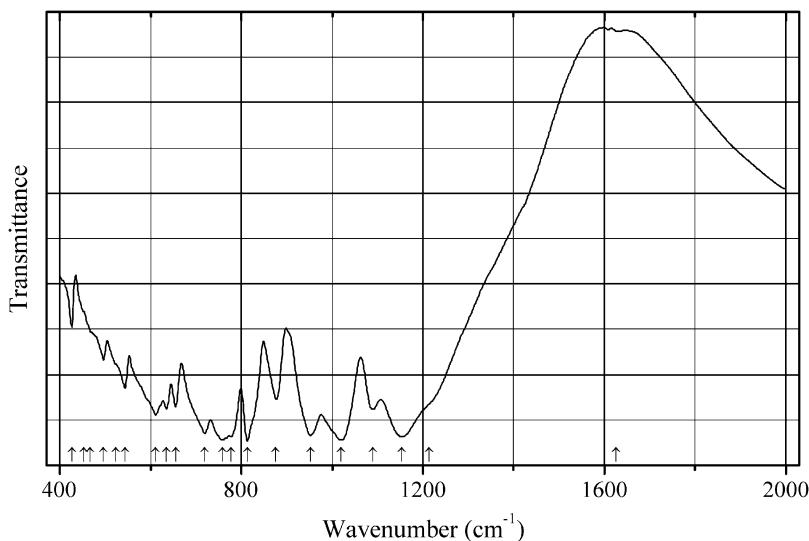
**Description:** Synthesized by heating a mixture of SrCO<sub>3</sub>, As<sub>2</sub>O<sub>5</sub>, and H<sub>3</sub>BO<sub>3</sub> in a 2:1:2 molar ratio at 900 °C for 15 h. Characterized by powder X-ray diffraction data. The crystal structure is solved. Hexagonal, space group P2<sub>1</sub>21,  $a = 7.056(3)$ ,  $c = 6.898(1)$  Å,  $V = 571.6(3)$  Å<sup>3</sup>,  $Z = 3$ . In the infinite loop-branched [BAsO<sub>5</sub>] chain, both B and As have fourfold coordination.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Birsöz and Baykal (2008).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1179w, 1141w, 1125w, 978s, 908s, 892sh, 834s, 792s, 785sh, 743s, 720s, 700sh, 675, 642w, 622sh, 607w, 585, 568sh, 545w, 523, 507w, 489, 463, 421sh, 409.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. In the cited paper, a figure of the Raman spectrum is given.

**B200 Tin tetraborate  $\beta$ -SnB<sub>4</sub>O<sub>7</sub>**

**Origin:** Synthetic.

**Description:** Prepared by compressing a mixture of  $\text{SnO}_2$  and  $\text{B}_2\text{O}_3$ , taken in stoichiometric amounts, to 7.5 GPa for 3 h with subsequent heating first at 1100 °C for 5 min and thereafter at 750 °C for 15 min. The crystal structure is solved. Orthorhombic, space group  $Pmn2_1$ ,  $a = 10.864(2)$ ,  $b = 4.4480(9)$ ,  $c = 4.2396(8)$  Å,  $V = 204.9(1)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 4.44$  g/cm<sup>3</sup>. The structure is based on a network of corner-sharing  $\text{BO}_4$  tetrahedra with channels built from four- and six-membered rings.

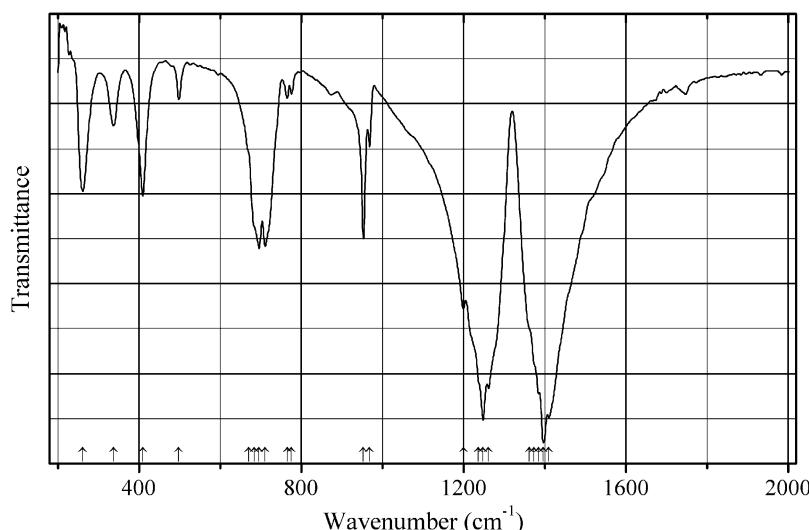
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Knyrim et al. (2007).

**Wavenumbers (cm<sup>-1</sup>):** 1213sh, 1154s, 1090, 1020s, 952s, 876, 813s, 777s, 758s, 719s, 655, 635, 611, 543, 523sh, 496, 467sh, 453sh, 426.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

### B201 Yttrium barium borate $\text{YBa}_3\text{B}_9\text{O}_{18}$ $\text{YBa}_3\text{B}_9\text{O}_{18}$



**Origin:** Synthetic.

**Description:** Crystals prepared by stepwise heating a mixture of  $\text{BaCO}_3$ ,  $\text{Y}_2\text{O}_3$ , and  $\text{H}_3\text{BO}_3$  (with the molar ratios Y:Ba:B = 1:1:9) to 1050 °C for 12 h followed by cooling down to 800 °C at a rate of 1 °C/h and from 800 to 600 °C at a rate of 2 °C/h. Characterized by powder X-ray diffraction data. The crystal structure is solved. Hexagonal, space group  $P6_3/m$ ,  $a = 7.1761(6)$ ,  $c = 16.9657(6)$  Å,  $V = 756.1(1)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 3.89$  g/cm<sup>3</sup>. The fundamental building unit of the crystal structure is the planar  $\text{B}_3\text{O}_6$  group.

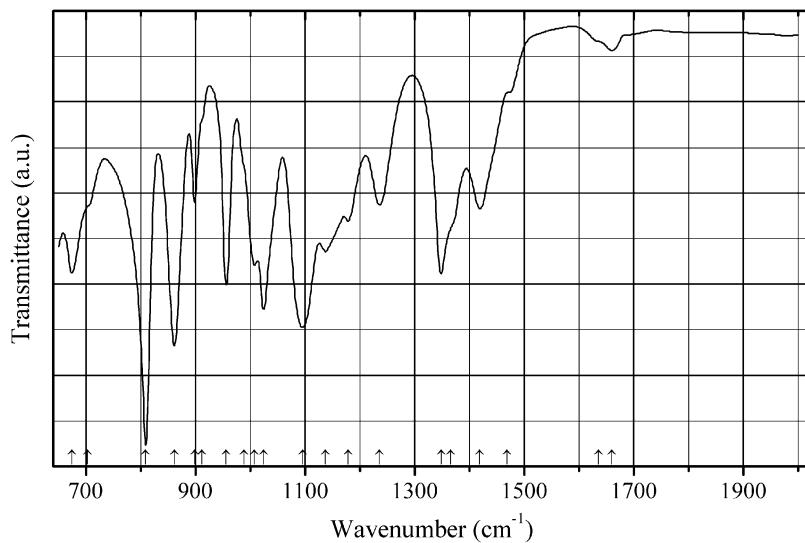
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Li et al. (2004a).

**Wavenumbers (cm<sup>-1</sup>):** 1411s, 1398s, 1385s, 1375sh, 1363sh, 1262s, 1249s, 1238sh, 1200, 969, 954, 777w, 766w, 712, 697, 684sh, 671sh, 499w, 410, 338, 262.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

## **B202 Admontite $MgB_6O_{10} \cdot 7H_2O$**



**Origin:** Synthetic.

**Description:** Prepared hydrothermally from MgO and H<sub>3</sub>BO<sub>3</sub>, taken in the molar ratio 1:6, at 100 °C for 120 min. Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of a powdered sample.

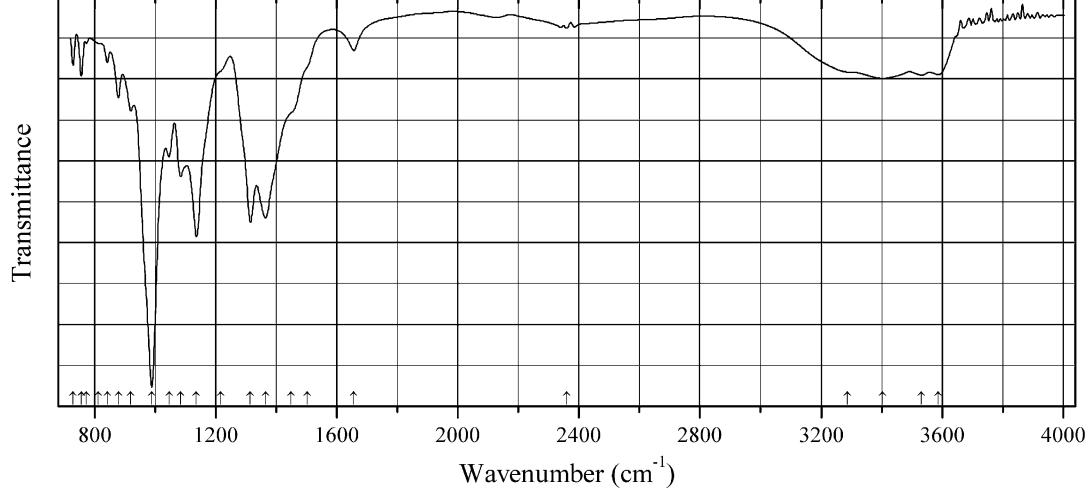
Source: Derun et al. (2015).

Wavenumbers ( $\text{cm}^{-1}$ ): 1660w 16

Note: The wavenumbers were partly determined by us based on spectral curve analysis of the

**Note.** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

## B203 Fontarnauite $(\text{Na},\text{K})_2(\text{Sr},\text{Ca})(\text{SO}_4)[\text{B}_5\text{O}_8(\text{OH})] \cdot 2\text{H}_2\text{O}$



**Origin:** Village of Doğanlar, Kütahya Province, Western Anatolia, Turkey (type locality).

**Description:** Colorless to light-brown prismatic crystals from the association with probertite, glauberite, and celestine. Holotype sample. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 6.458(2)$ ,  $b = 22.299(7)$ ,  $c = 8.571(2)$  Å,  $\beta = 103.047(13)^\circ$ ,  $V = 1202.5(10)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 2.533$  g/cm $^3$ . Optically biaxial (−),  $\alpha = 1.517(2)$ ,  $\beta = 1.517(2)$ ,  $\gamma = 1.543(2)$ ,  $2V = 46(1)^\circ$ . The empirical formula is  $(\text{Na}_{1.84}\text{K}_{0.16})(\text{Sr}_{0.82}\text{Ca}_{0.18})\text{S}_{1.00}\text{B}_5\text{H}_5\text{O}_{15}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 11.1498 (100) (020), 3.3948 (8) (061), 3.3389 (20) (042), 3.1993+3.1990 (10) (160, −142), 3.0458 (10) (052), 3.0250 (7) (220), 2.7500 (10) (−222, 142), 2.3999 (8) (260), 2.2284 (7) (0.10.0, 222), 1.9237 +1.9237 (7) (311, −224).

**Kind of sample preparation and/or method of registration of the spectrum:** The spectrum was obtained from a small cleavage sheet crushed in a diamond-cell holder.

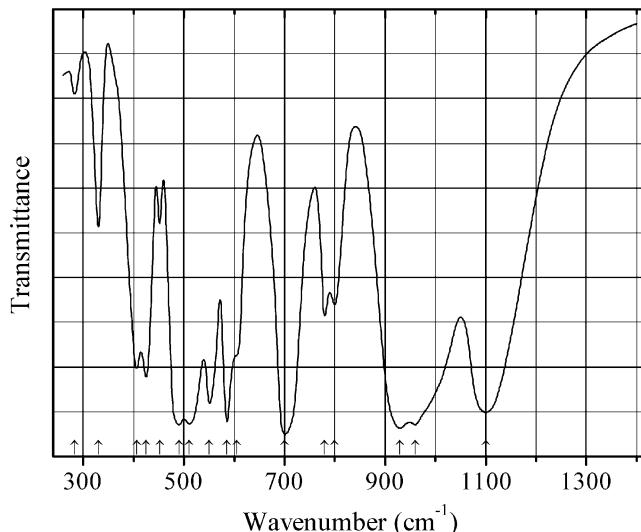
**Source:** Cooper et al. (2016b).

**Wavenumbers (IR, cm $^{-1}$ ):** 3587, 3531, 3404, 3288, 2359w, 1657, 1502sh, 1449sh, 1365s, 1315s, 1217sh, 1136s, 1085, 1046, 989s, 920, 879, 842w, 812sh, 773w, 756w, 729w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The band position denoted by Cooper et al. (2016b) as 862 cm $^{-1}$  was determined by us at 842 cm $^{-1}$ . In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 975s, 470, 430, 160, 129.

#### B204 Sinhalite $\text{MgAl}(\text{BO}_4)$



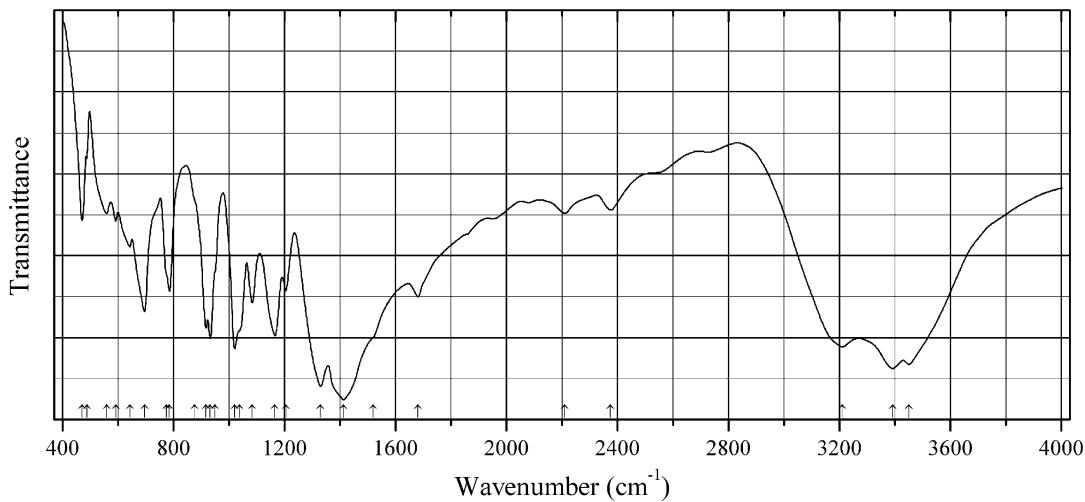
**Origin:** Synthetic.

**Description:** Synthesized hydrothermally from a gel of suitable composition at 700 °C for 500 h. Characterized by powder X-ray diffraction data. Orthorhombic, space group  $Pnma$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Tarte et al. (1985).

**Wavenumbers (cm $^{-1}$ ):** 1100s, 960s, 930s, 800, 780, 700s, 605sh, 586s, 551, 510s, 490s, 452w, 425, 406, 330, 283w.

**B205 Sborgite**  $\text{NaB}_5\text{O}_6(\text{OH})_4 \cdot 3\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Synthesized from aqueous solutions of boric acid and borax. Characterized by powder X-ray diffraction data.

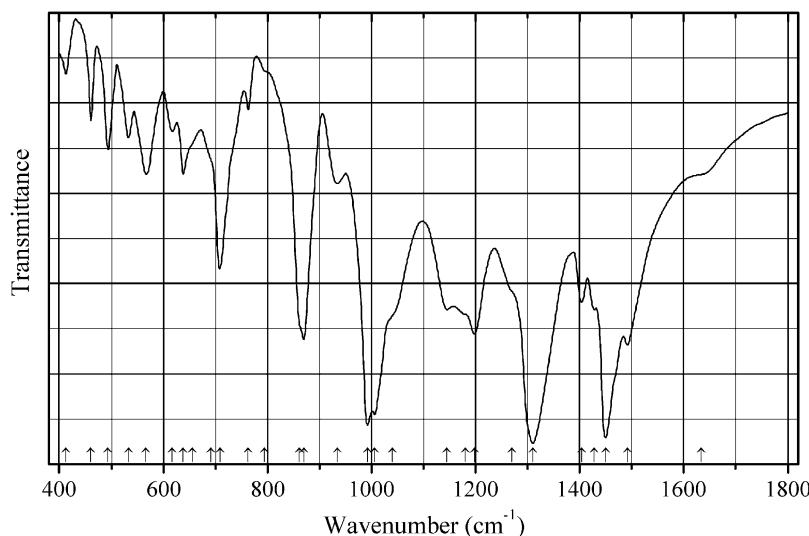
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Chen and Pei (2016).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3450s, 3392s, 3210, 2375w, 2211w, 1681, 1518sh, 1413s, 1330s, 1205, 1166, 1084, 1038sh, 1021, 950sh, 933, 917, 875sh, 786, 775sh, 696, 643, 592, 559, 488, 471.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 922, 856s, 774, 529s, 494, 468w, 386w.

**B206 Potassium borate**  $\text{KB}_3\text{O}_3(\text{OH})_4 \cdot \text{H}_2\text{O}$   $\text{KB}_3\text{O}_3(\text{OH})_4 \cdot \text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Prepared in the reaction between fine powders of  $K_2B_4O_7 \cdot 4H_2O$  and  $KB_5O_8 \cdot 4H_2O$  under exposure of water vapor. The crystal structure is solved. Monoclinic, space group  $C2/c$ ,  $a = 15.540(5)$ ,  $b = 6.821(2)$ ,  $c = 14.273(4)$  Å,  $\beta = 104.44(2)^\circ$ ,  $V = 1465.1$  Å $^3$ ,  $Z = 8$ . The structure contains an isolated  $B_3O_3(OH)_4^-$  anion formed from a  $B_3O_3$  ring consisting of one  $BO_2(OH)_2$  tetrahedron and two  $BO_2(OH)$  triangles.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

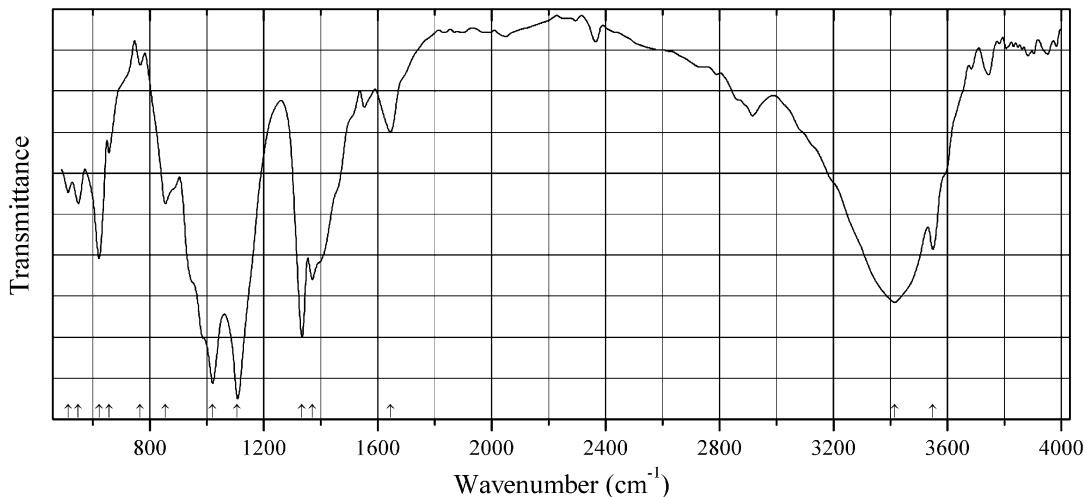
**Source:** Salentine (1987).

**Wavenumbers (IR, cm $^{-1}$ ):** 1634sh, 1492, 1450s, 1428, 1404, 1310s, 1270sh, 1198s, 1181sh, 1145, 1041sh, 1006s, 992s, 934, 870s, 862sh, 795sh, 763w, 709, 691sh, 656sh, 638, 617, 567, 533, 494, 461, 413w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given. The band position denoted by Salentine (1987) as  $1000$  cm $^{-1}$  was determined by us as doublet ( $1006+992$  cm $^{-1}$ ).

**Wavenumbers (Raman, cm $^{-1}$ ):** 1194w, 966, 753s, 624s, 488, 453, 407, 212w, 176, 137, 116.

### B207 Tyretskite (monoclinic polytype) $Ca_2B_5O_9(OH) \cdot H_2O$



**Origin:** Synthetic.

**Description:** Synthesized under solvothermal conditions. The crystal structure is solved. Monoclinic, space group  $Cc$ ,  $a = 10.790(5)$ ,  $b = 6.5174(18)$ ,  $c = 12.359(6)$  Å,  $\beta = 114.975(19)^\circ$ ,  $V = 787.8$  (6) Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 2.641$  g/cm $^3$ .

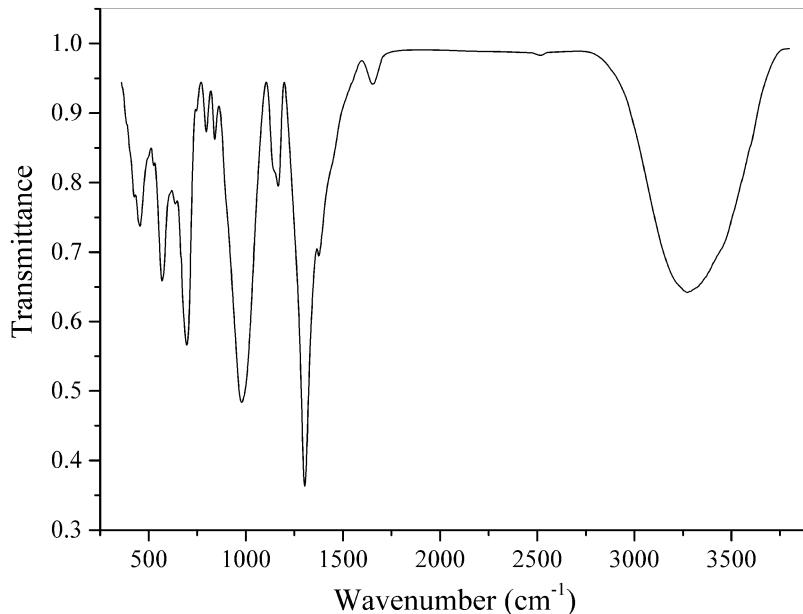
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Wei et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 3549, 3415s, 1645, ~1371s, 1335s, 1108s, 1021s, 855, 767w, 657w, 622, 550, 514.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### B208 Satimolite KNa<sub>2</sub>(Al<sub>5</sub>Mg<sub>2</sub>)[B<sub>12</sub>O<sub>18</sub>(OH)<sub>12</sub>](OH)<sub>6</sub>Cl<sub>4</sub>·4H<sub>2</sub>O



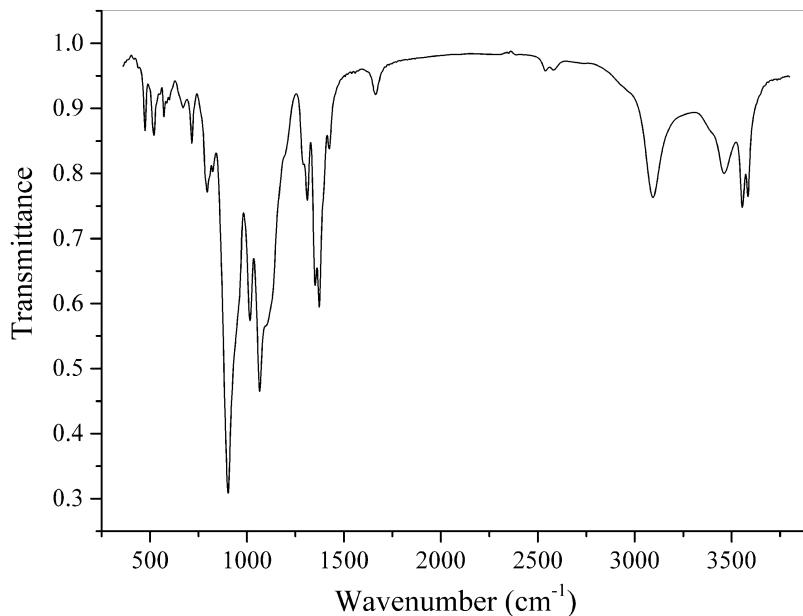
**Origin:** Chelkar salt dome, Aksai Valley, Aktobe (Aqtöbe) region, Kazakhstan.

**Description:** Isolated colorless crystals from the association with sylvite, halite, anhydrite, and boracite. Characterized by powder and single-crystal X-ray diffraction data. The crystal structure is solved. Trigonal, space group  $R\bar{3}m$ ,  $a = 15.1406(4)$ ,  $c = 14.3794(9)$  Å,  $V = 2854.7(2)$  Å<sup>3</sup>. The structural formula is  $(\square_{0.68}\text{Na}_{0.32})_6(\text{Cl}_{0.68}\text{K}_{0.22}\square\text{h}_{0.10})_6(\text{Al}_{0.66}\text{Mg}_{0.31}\text{Fe}^{3+}_{0.03})_7[\text{B}_{12}\text{O}_{18}(\text{OH})_{12}]$  (OH)<sub>6</sub>·4H<sub>2</sub>O

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3430, 3272s, 2518w, 1651, 1435sh, 1376, 1304s, 1166, 1150sh, 979s, 840, 797, 745w, 696s, 639, 568, 528, 455, 429.

**Note:** The spectrum was obtained by N.V. Chukanov.

**B209 Priceite**  $\text{Ca}_4\text{B}_{10}\text{O}_{19} \cdot 7\text{H}_2\text{O}$ 

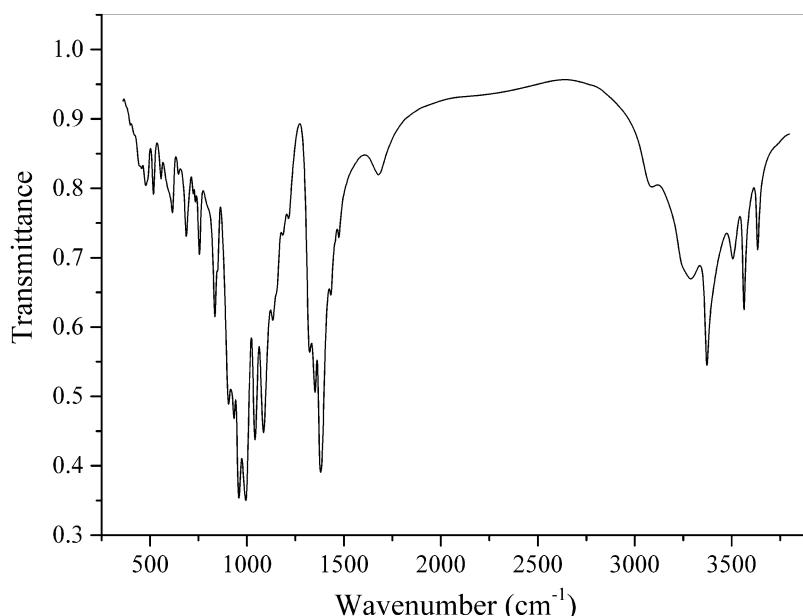
**Origin:** Inder boron deposit, Atyrau region, Kazakhstan.

**Description:** White powdery aggregate. Confirmed by the IR spectrum.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3584, 3555, 3461, 3390sh, 3094, 2960sh, 2580w, 2540w, 1663, 1424, 1373, 1352, 1311, 1293, 1195sh, 1095sh, 1065s, 1016, 903s, 825, 795, 716, 670, 599w, 587w, 572, 520, 474.

**Note:** The spectrum was obtained by N.V. Chukanov.

**B210 Probertite**  $\text{NaCaB}_5\text{O}_7(\text{OH})_4 \cdot 3\text{H}_2\text{O}$ 

**Origin:** Banderma (Pandirma), Balikesir province, Turkey.

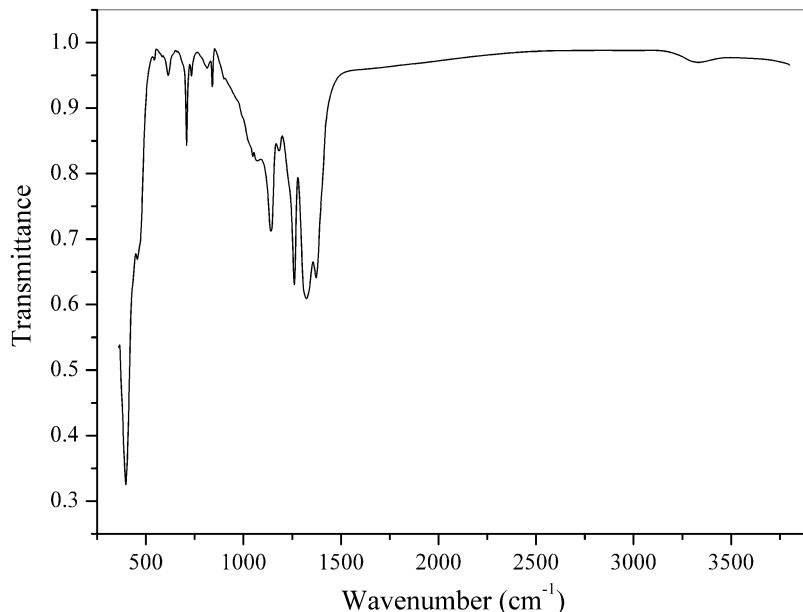
**Description:** Grey radial aggregate. Confirmed by the IR spectrum and qualitative electron microprobe analyses.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3634, 3564, 3506, 3372s, 3289, 3250sh, 3092, 1678, 1474, 1435, 1380s, 1351s, 1323, 1216, 1186, 1150sh, 1133, 1085s, 1041s, 994s, 959s, 934s, 906s, 850sh, 835, 805sh, 755, 737w, 726w, 686, 649w, 615, 600sh, 557, 517, 478, 456w, 447w, 424w, 400w.

**Note:** The spectrum was obtained by N.V. Chukanov.

#### BC10 Mereheadite Pb<sub>47</sub>Cl<sub>25</sub>(OH)<sub>13</sub>O<sub>24</sub>(CO<sub>3</sub>)(BO<sub>3</sub>)<sub>2</sub>



**Origin:** Merehead Quarry, Cranmore, Somerset, England, UK (type locality).

**Description:** Reddish-orange grains. The crystal structure is solved. Monoclinic, space group *Cm*,  $a = 17.372(1)$ ,  $b = 27.9419(19)$ ,  $c = 10.6661(6)$  Å,  $\beta = 93.152(5)^\circ$ ,  $V = 5169.6(5)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 7.236$  g/cm<sup>3</sup>.

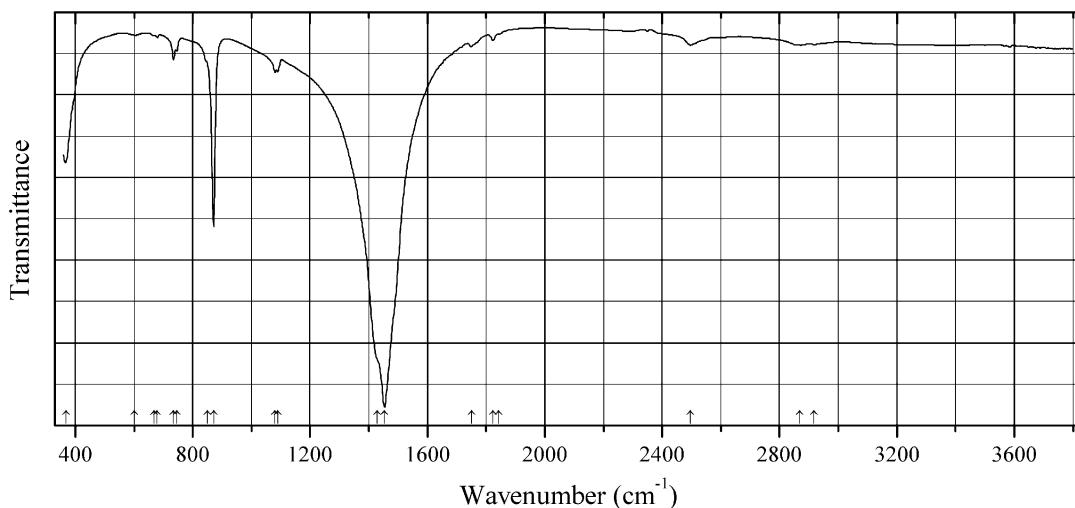
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3331, 1373s, 1324s, 1261s, 1183, 1141s, 1071, 1050, 1000sh, 902w, 841, 813w, 734, 709, 615, 542w, 457s, 398s.

**Note:** The spectrum was obtained by N.V. Chukanov.

## 2.2 Carbonates

### C342 Parisite-(La) CaLa<sub>2</sub>(CO<sub>3</sub>)<sub>3</sub>F<sub>2</sub>



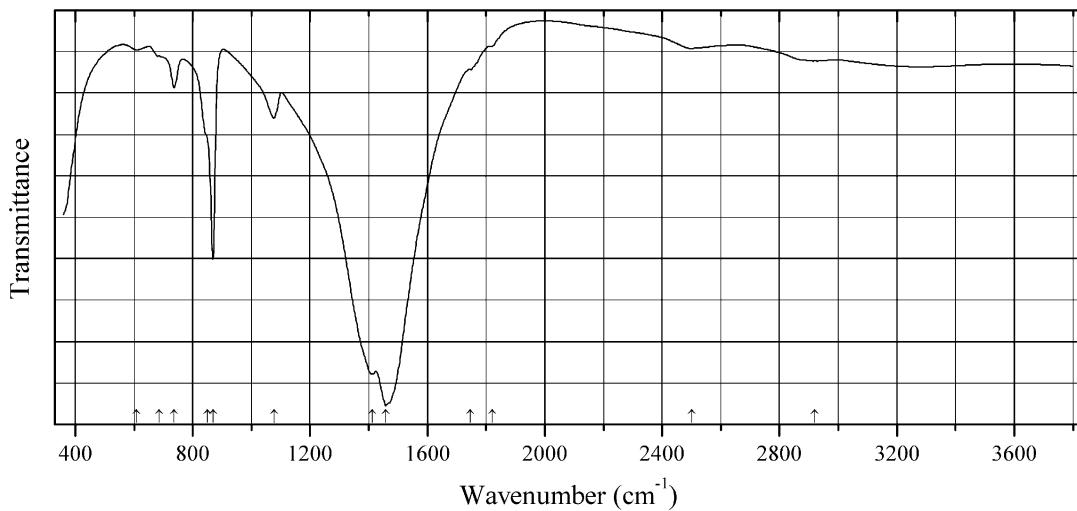
**Origin:** Rio dos Remédios Group, Mula mine, near Tapera village, Novo Horizonte Co., Bahia, Brazil (type locality).

**Description:** Greenish-yellow inner zone of a pseudohexagonal crystal from the association with hematite, rutile, almeidaite, fluocerite-(Ce), brockite, monazite-(La), rhabdophane-(La), and bastnäsite-(La). Holotype sample. Monoclinic, space group:  $C2$ ,  $Cm$ , or  $C2/m$ ,  $a = 12.356(1)$ ,  $b = 7.1368(7)$ ,  $c = 28.299(3)$  Å,  $\beta = 98.342(4)^\circ$ ,  $V = 2469.1(4)$  Å $^3$ ,  $Z = 12$ .  $D_{\text{calc}} = 4.273$  g/cm $^3$ . Optically pseudo-uniaxial (+),  $\omega = 1.670(2)$ ,  $\varepsilon = 1.782(5)$ . The empirical formula is Ca $_{0.98}$ (La $_{0.83}$ Nd $_{0.51}$ Ce $_{0.37}$ Pr $_{0.16}$ Sm $_{0.04}$ Y $_{0.03}$ )C $_{3.03}$ O $_{8.91}$ F $_{2.09}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 13.95 (55) (002), 4.655 (37) (006), 3.555 (88) (020, -311), 2.827 (100) (026, 315, -317), 2.055 (58) (-331, -602), 1.950 (38) (0.2.12, 3.1.11, -3.1.13), 1.880 (36) (335, -337, 604, -608).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 2918w, 2870w, 2497w, 1843w, 1823w, 1750w, 1454sm 1430sh, 1089, 1081, 871s, 850sh, 746w, 734, 679w, 670w, 602w, 368

**Note:** The spectrum was obtained by N.V. Chukanov.

**C343 Parisite-(Ce)  $\text{CaCe}_2(\text{CO}_3)_3\text{F}_2$** 

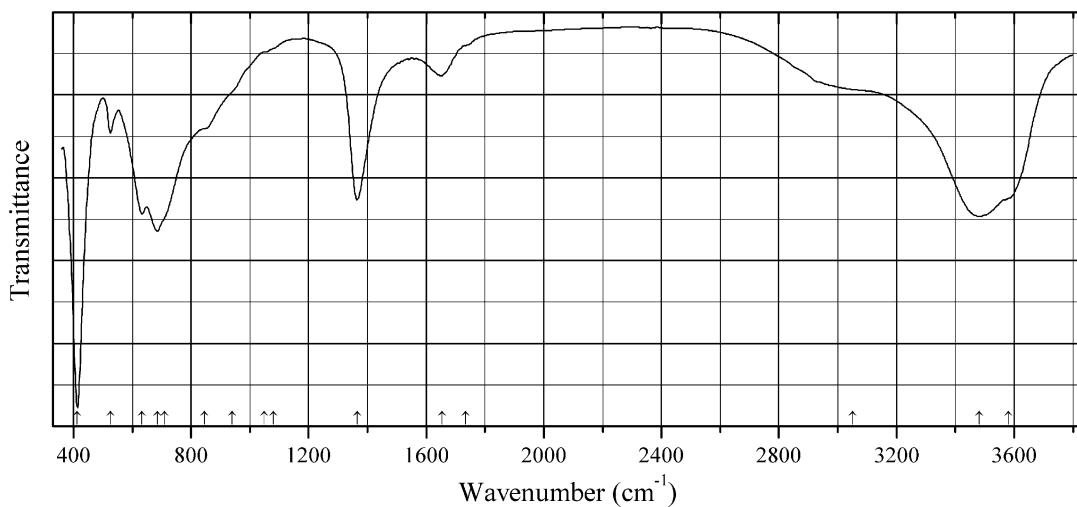
**Origin:** White Cloud Mine, Pyrites, Ravalli Co., Montana, USA.

**Description:** Beige crystal. The empirical formula is (electron microprobe):  $\text{Ca}_{1.08}(\text{Ce}_{0.93}\text{La}_{0.47}\text{Nd}_{0.32}\text{Pr}_{0.06}\text{Y}_{0.08}\text{Th}_{0.06})(\text{CO}_3)_{3.00}\text{F}_{1.88}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 2920w, 2500w, 1820w, 1746w, 1459s, 1411s, 1077, 869s, 850sh, 736, 685sh, 609w.

**Note:** The spectrum was obtained by N.V. Chukanov.

**C344 Stichtite  $\text{Mg}_6\text{Cr}_2(\text{OH})_{16}(\text{CO}_3)\cdot 4\text{H}_2\text{O}$** 

**Origin:** Kara-Uyuk stream, Terektskiy ridge, Altai Mts., Siberia, Russia.

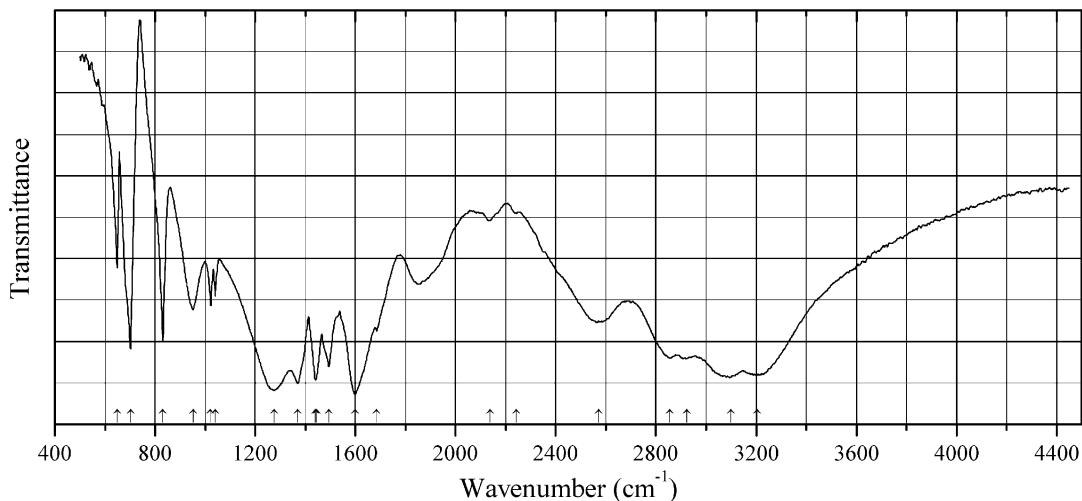
**Description:** Lilac scaly aggregate from the association with serpentine. An Al-rich variety. The empirical formula is (electron microprobe):  $Mg_{5.98}(Cr_{1.13}Al_{0.73}Fe_{0.16})(OH)_{16}(CO_3) \cdot 4H_2O$ . Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3580sh, 3482s, 3050sh, (1735sh), 1653, 1365s, 1080sh, 1050w, 940sh, 845sh, 710sh, 686s, 633s, 525, 413s.

**Note:** The spectrum was obtained by N.V. Chukanov.

### C345 Ammonium bicarbonate $\text{NH}_4\text{HCO}_3$



**Origin:** Synthetic.

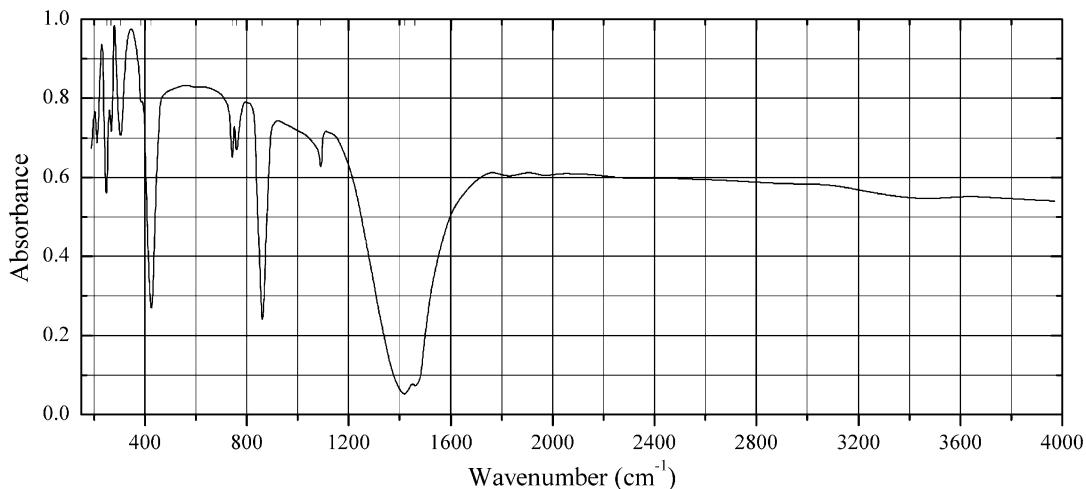
**Description:** Commercial reactant purchased from Aldrich. Characterized by elemental analysis and PXRD. The strongest lines of the powder X-ray diffraction pattern [ $d, \text{\AA}$  ( $I, \%$ )] are: 5.36 (26.5), 4.04 (19), 3.00 (100).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Meng et al. (2005).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3205s, 3098s, 2923, 2856, 2572, 2243w, 2138w, 1685w, 1600s, 1494s, 1441s, 1370s, 1275s, 1041, 1022, 952, 831, 702, 649.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**C346 Copper(II) carbonate CuCO<sub>3</sub>**

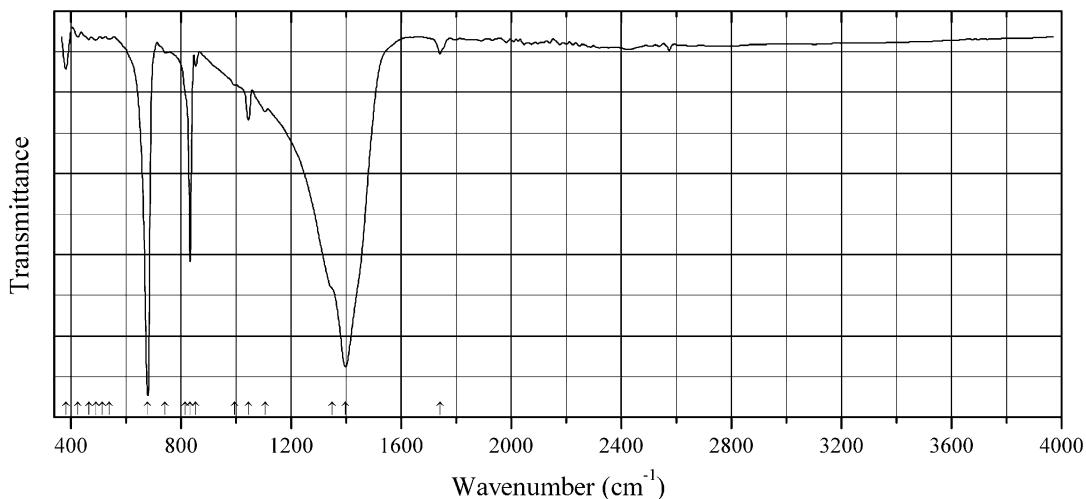
**Origin:** Synthetic.

**Description:** CuCO<sub>3</sub> can be prepared from azurite, malachite or CuO by reaction with CO<sub>2</sub> at a pressure of 20 kb and a temperature of 500 °C. Monoclinic, space group *Pa*,  $a = 6.092$ ,  $b = 4.493$ ,  $c = 7.030$  Å,  $\beta = 101.34^\circ$ ,  $V = 188.7$  Å<sup>3</sup>,  $Z = 4$ . In the structure, Cu has the fivefold (square pyramid) coordination.  $D_{\text{meas}} = 4.18$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 4.35$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc (above 190 cm<sup>-1</sup>) and polyethylene mull (below 190 cm<sup>-1</sup>). Transmission.

**Source:** Seidel et al. (1974).

**Wavenumbers (cm<sup>-1</sup>):** 1460sh, 1420s, 1090w, 860s, 760, 743, 425, 383sh, 305, 268, 250, 212, 194, 166, 158, 151, 130, 113, 103, 97, 90, 83, 61, 55, 49, 44, 38, 31.

**C347 Potassium lead carbonate fluoride KPb<sub>2</sub>(CO<sub>3</sub>)<sub>2</sub>F**

**Origin:** Synthetic.

**Description:** Synthesized by a conventional solid-state technique from the stoichiometric mixture of KF and PbCO<sub>3</sub>, at 250 °C, in flowing CO<sub>2</sub> gas, for 2 days. Characterized by powder X-ray diffraction data. The crystal structure is solved. Hexagonal, space group *P6<sub>3</sub>/mmc*,  $a = 5.3000(2)$ ,  $c = 13.9302(8)$  Å,  $V = 338.88(3)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 5.807$  g/cm<sup>3</sup>.

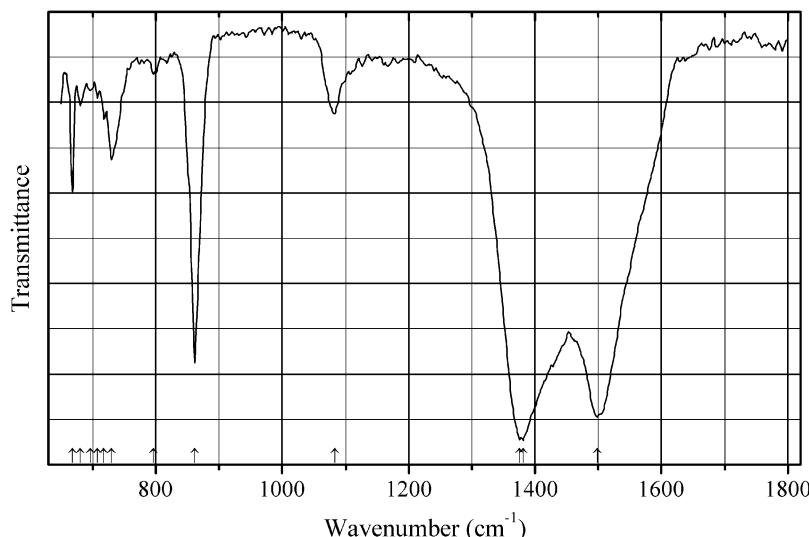
**Kind of sample preparation and/or method of registration of the spectrum:** Reflection of a powdered sample.

**Source:** Tran and Halasyamani (2013).

**Wavenumbers (cm<sup>-1</sup>):** 1741w, 1398s, 1350sh, 1107w, 1045, 995w, 855w, 833, 815sh, 743w, 680s, 541w, 515w, 491w, 466w, 425w, 382.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### C348 Sodium lithium gadolinium carbonate Na<sub>2</sub>LiGd(CO<sub>3</sub>)<sub>3</sub> Na<sub>2</sub>LiGd(CO<sub>3</sub>)<sub>3</sub>



**Origin:** Synthetic.

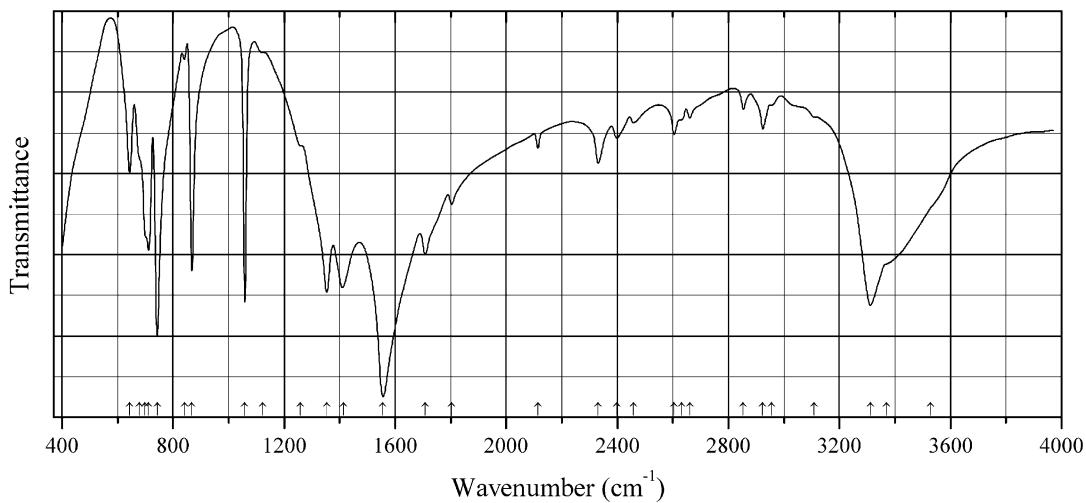
**Description:** Obtained hydrothermally from GdF<sub>3</sub>, Na<sub>2</sub>CO<sub>3</sub>, and Li<sub>2</sub>CO<sub>3</sub> with molar ratio 1:6:2 at 230 °C for 48 h. Characterized by powder X-ray diffraction data. Cubic, space group *Fd-3m*,  $a \approx 14.4$  Å,  $Z = 8$ .

**Kind of sample preparation and/or method of registration of the spectrum:** A diamond-anvil cell as a micro-sampling device was used.

**Source:** Ali et al. (2004b).

**Wavenumbers (cm<sup>-1</sup>):** 1498s, 1381+1375, 1083, 861s, 796w, 730, 718, (707), (696), 680w, 668.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. In the cited paper, a figure of the Raman spectrum is given.

**C349 Sodium scandium carbonate  $\text{Na}_5\text{Sc}(\text{CO}_3)_3 \cdot 2\text{H}_2\text{O}$   $\text{Na}_5\text{Sc}(\text{CO}_3)_3 \cdot 2\text{H}_2\text{O}$** 

**Origin:** Synthetic.

**Description:** Obtained from aqueous solutions of scandium chloride and sodium carbonate. The crystal structure is solved. Tetragonal, space group  $P-42_1c$ ,  $a = 7.4637(4)$ ,  $c = 11.570(2)$  Å,  $V = 644.55(13)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{meas}} = 2.23$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 2.246$  g/cm<sup>3</sup>.

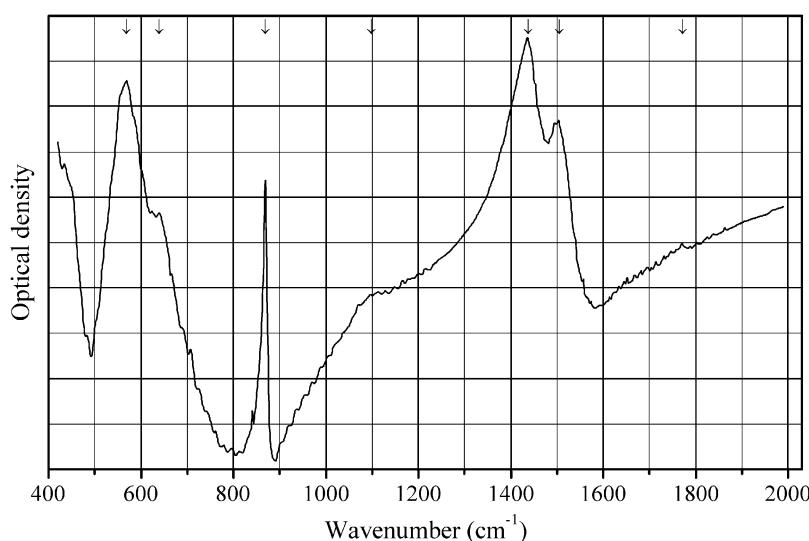
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc and Nujol mull. Transmission.

**Source:** Dahm and Adam (2001).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3528sh, 3369sh, 3311s, 3108w, 2955sh, 2924, 2854w, 2662w, 2631sh, 2604, 2458w, 2399, 2330, 2114, 1804, 1708, 1556s, 1414s, 1354s, 1259sh, 1122sh, 1059s, 868s, 841w, 743s, 712s, 699sh, 680sh, 644, 359s, 261s, 230, 215, 195sh, 180, 165, 145, 122w, 101w, 93, 63w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1739, 1702, 1601, 1575s, 1439, 1355, 1061s, 1039, 867, 764, 744s, 682, 668, 644, 354, 300, 277s, 245s, 231s, 216s, 187s, 165s, 132s.

**C350 Strontium iron(III) oxycarbonate  $\text{Sr}_4\text{Fe}_2\text{O}_6(\text{CO}_3)$** 

**Origin:** Synthetic.

**Description:** Prepared by heating an appropriate mixture of SrO, SrCO<sub>3</sub>, and Fe<sub>2</sub>O<sub>3</sub> at 1200 °C for 12 h under vacuum with subsequent cooling down to room temperature, annealing at 500 °C for 30 min in air and quenching. Characterized by EDS analysis, Mössbauer spectroscopy, powder X-ray diffraction, neutron powder diffraction, and single-crystal electron diffraction data. Orthorhombic, space group *I4/mmm*,  $a = 3.88965(3)$ ,  $c = 27.9906(1)$  Å.

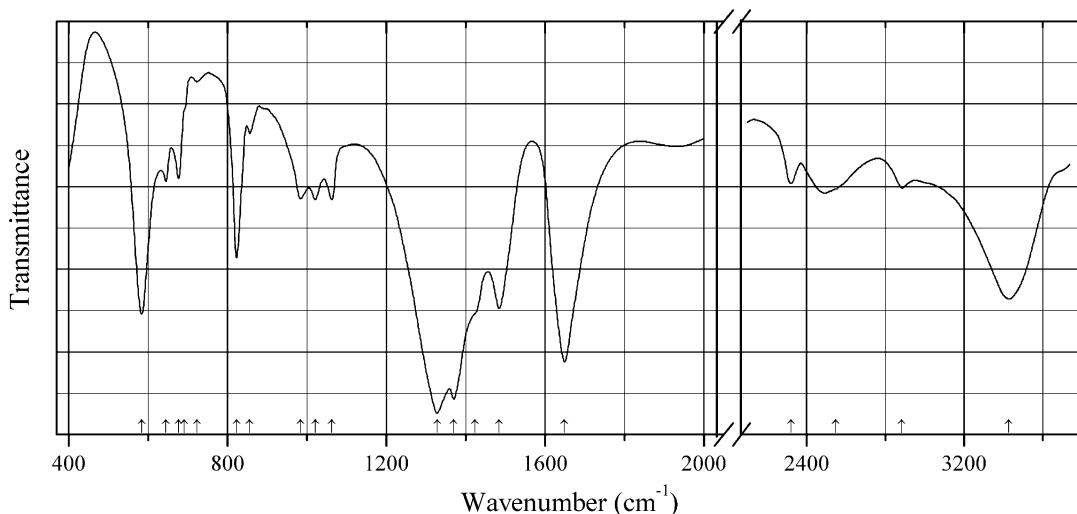
**Kind of sample preparation and/or method of registration of the spectrum:** Absorption. Kind of sample preparation is not indicated.

**Source:** Bréard et al. (2004).

**Wavenumbers (cm<sup>-1</sup>):** 1771w, 1506s, 1437s, 1098sh, 869, 640, 569s.

**Note:** The band at 569 cm<sup>-1</sup> may correspond to polymerized Fe<sup>3+</sup>O<sub>6</sub> and/or Fe<sup>3+</sup>O<sub>5</sub> polyhedra.

### C351 Barentsite Na<sub>7</sub>Al(HCO<sub>3</sub>)<sub>2</sub>(CO<sub>3</sub>)<sub>2</sub>F<sub>4</sub>



**Origin:** Restin'yun Mt., Khibiny massif, Kola Peninsula (type locality).

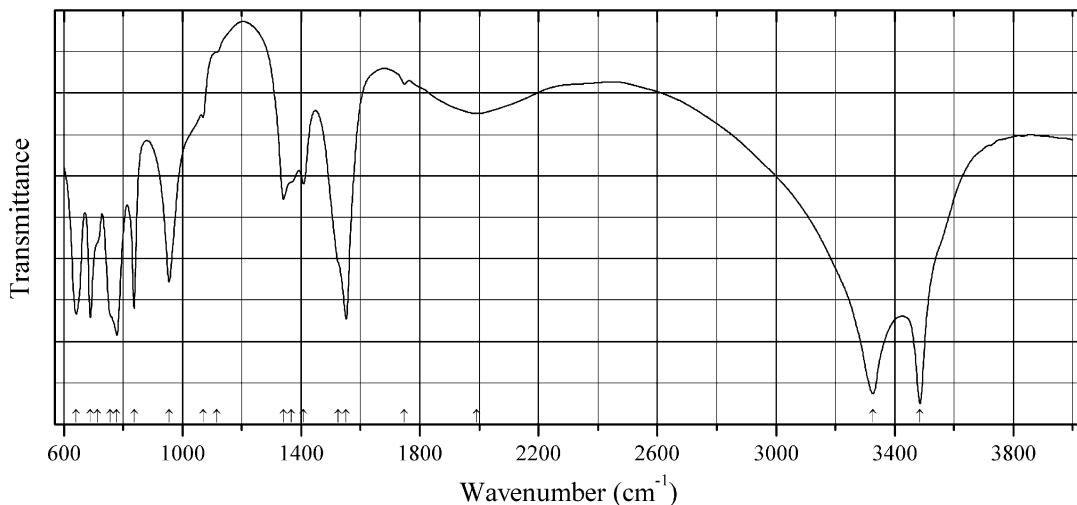
**Description:** Colorless anhedral grains from the association with shortite, albite, natrolite, trona, natrite, villiaumite, etc. Holotype sample. Triclinic,  $a = 6.472(2)$ ,  $b = 6.735(2)$ ,  $c = 8.806(2)$  Å,  $\alpha = 92.50(2)^\circ$ ,  $\beta = 97.33(2)^\circ$ ,  $\gamma = 119.32(2)^\circ$ ,  $V = 329.41$  Å<sup>3</sup>,  $Z = 1$ .  $D_{\text{meas}} = 2.56(2)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 2.55$  g/cm<sup>3</sup>. Optically biaxial (-),  $\alpha = 1.358(2)$ ,  $\beta = 1.479(2)$ ,  $\gamma = 1.530(2)$ ,  $2V = 62^\circ$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 2.887 (84) (003, 2–11), 2.778 (100) (200, -103), 2.658 (100) (2–21), 2.316 (50) (2–22), 2.169 (70) (120, 004), 1.870 (42) (-331, -204).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Khomyakov et al. (1983).

**Wavenumbers (cm<sup>-1</sup>):** 3430, 2885, 2550, 2322, 1649s, 1484, 1424sh, 1370s, 1328s, 1063, 1021, 984, 856w, 823, 723w, 692sh, 677, 645, 584s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**C352 Chukanovite**  $\text{Fe}_2(\text{CO}_3)(\text{OH})_2$ 

**Origin:** Synthetic.

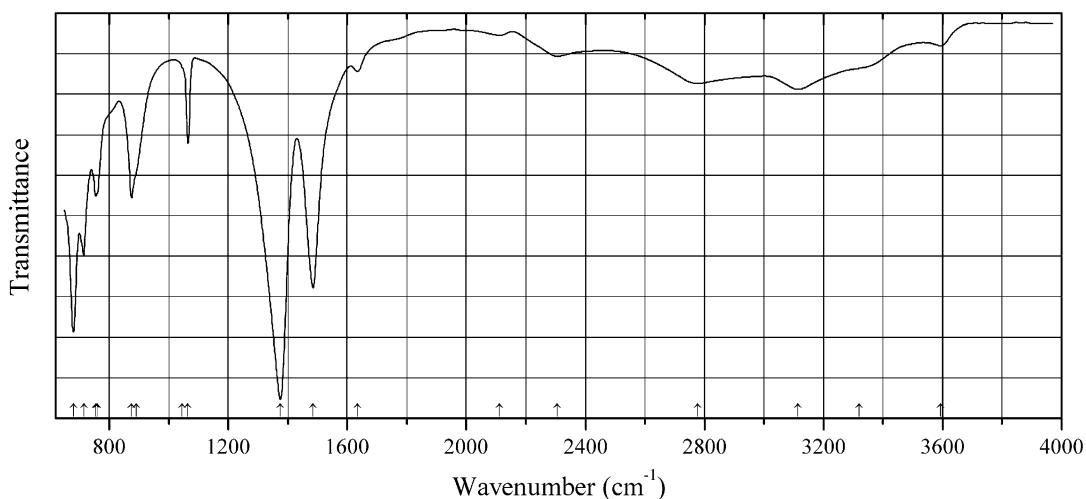
**Description:** Obtained by heating a mixture of powdered claystone (a rock containing clay minerals, Ca-Mg-Fe carbonates and quartz as the main components) and iron powder, in the presence of iron plates and an aqueous solution containing NaCl and CaCl<sub>2</sub> at 90 °C for 6 months. The synthetic analogue of chukanovite was formed as randomly oriented powder on the iron plates. Characterized by powder X-ray diffraction and electron diffraction data. Monoclinic, space group  $P2_1/a$ ,  $a = 12.5$  (3),  $b = 9.5(2)$ ,  $c = 3.2(1)$  Å,  $\beta = 97.6(5)^\circ$ ,  $V = 377(17)$  Å<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** Reflection from an iron plate covered by the synthetic analogue of chukanovite.

**Source:** Pignatelli et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 3485s, 3327s, 1992 (broad), 1748w, 1552s, 1525sh, 1408, 1368sh, 1340, 1116sh, 1069, 955, 837, 779, 757sh, 713sh, 690, 642.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**C353 Lecoqite-(Y)**  $\text{Na}_3\text{Y}(\text{CO}_3)_3 \cdot 6\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Prepared hydrothermally from  $\text{Na}_2\text{CO}_3$ ,  $\text{YF}_3$ , and  $\text{H}_2\text{O}$  in the molar ratio 25:1:55 at 220 °C for 48 h. Characterized by thermoanalytical data. The crystal structure is solved. Hexagonal, space group  $P6_3$ ,  $a = 11.347(5)$  Å,  $c = 5.935(5)$  Å,  $V = 661.8(5)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{meas}} = 2.25(5)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 2.24$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. A diamond-anvil cell as a microsampling device was used.

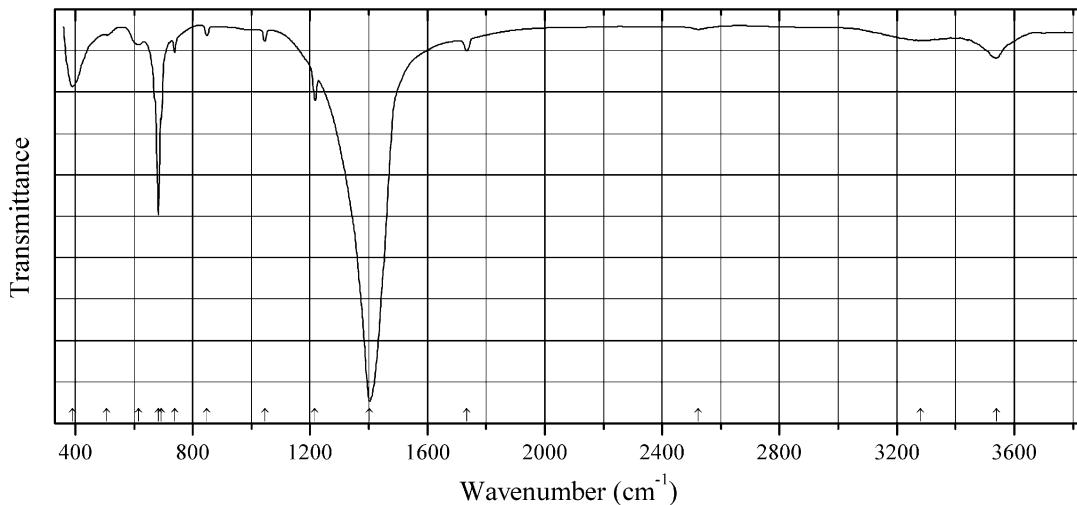
**Source:** Ali et al. (2004a).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3593w, 3320sh, 3115, 2778, 2305w, 2112w, 1634w, 1485s, 1375s, 1065, 1045sh, 890sh, 875, 760sh, 755, 715, 680s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1635, 715s, 680.

### C354 Somersetite [Pb<sub>3</sub>(OH)<sub>2</sub>(CO<sub>3</sub>)<sub>2</sub>][Pb<sub>3</sub>(Pb<sub>2</sub>O<sub>2</sub>)(CO<sub>3</sub>)<sub>3</sub>]



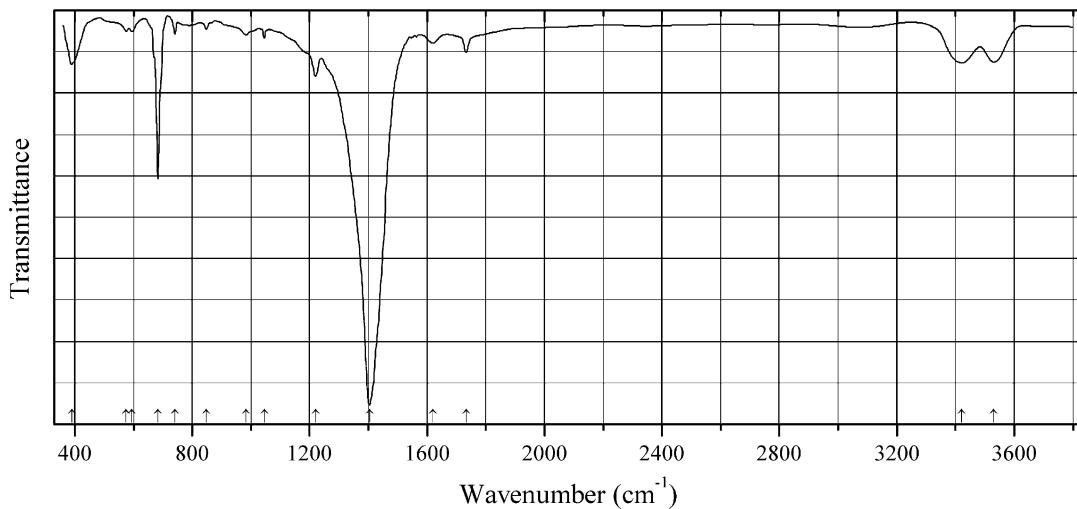
**Origin:** Torr Works ("Merehead Quarry"), Somerset, England, UK (type locality).

**Description:** Greenish grains from the association with calcite, aragonite, and quartz. Holotype sample. The crystal structure is solved. Hexagonal, space group  $P6_3/mmc$ ,  $a = 5.2427(7)$ ,  $c = 40.624(6)$  Å,  $V = 967.0(3)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 7.11$  g/cm<sup>3</sup>. The empirical formula is  $\text{Pb}_{8.004}\text{C}_{4.998}\text{H}_{1.998}\text{O}_{19}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 4.308 (33) (103), 3.581 (40) (107), 3.390 (100) (108), 3.206 (55) (109), 2.625 (78) (110), 2.544 (98) (0.016).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3539, (3280w), 2524w, 1734w, 1403s, 1217, 1046w, 849w, 738w, 690sh, 683s, 615w, 507w, 391.

**Note:** The spectrum was obtained by N.V. Chukanov. The bands at 1217 and 738 cm<sup>-1</sup> correspond to a minor admixture of  $\text{BO}_3^{3-}$  groups substituting  $\text{CO}_3^{2-}$  groups.

**C355 “Hydrucerussite-like mineral 9-40” Lead hydroxycarbonate**

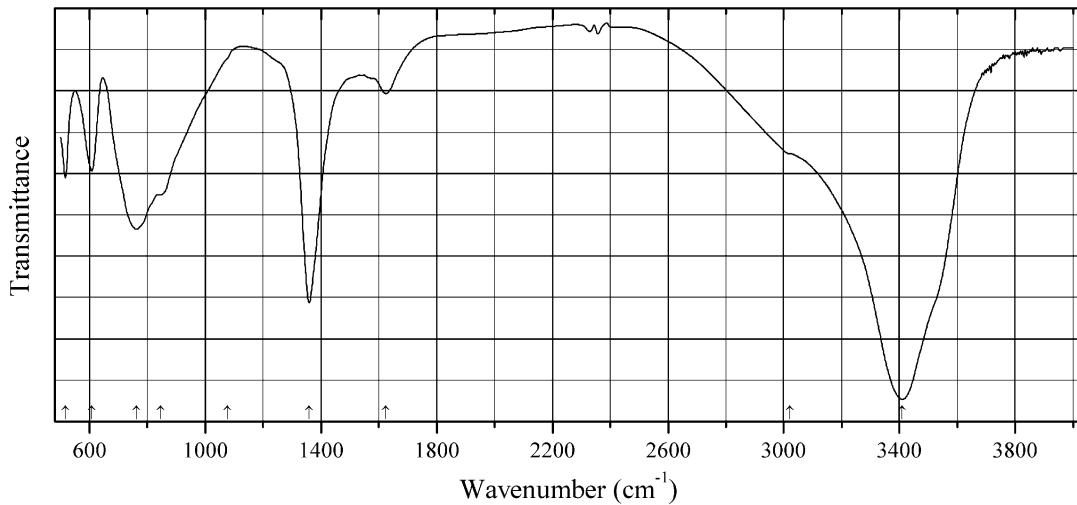
**Origin:** Torr Works (“Merehead Quarry”), Somerset, England, UK.

**Description:** Investigated by O.I. Siidra. Characterized by single-crystal X-ray diffraction data. Trigonal,  $a = 9.0929(5)$ ,  $c = 40.660(6)$  Å,  $V = 2911.42(9)$  Å<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3531, (3422), 1733, (1619w), 1404s, 1220, 1046w, 984w, 848w, 741w, 683s, 595w, 575w, 391.

**Note:** The spectrum was obtained by N.V. Chukanov. The bands at 1220 and 741 cm<sup>-1</sup> correspond to a minor admixture of BO<sub>3</sub><sup>3-</sup> groups substituting CO<sub>3</sub><sup>2-</sup> groups.

**C356 Quintinite-related hydroxyde carbonate Mg<sub>4</sub>Cr<sub>2</sub>(OH)<sub>12</sub>(CO<sub>3</sub>)·nH<sub>2</sub>O Mg<sub>4</sub>Cr<sub>2</sub>(OH)<sub>12</sub>(CO<sub>3</sub>)·nH<sub>2</sub>O**

**Origin:** Synthetic.

**Description:** Synthesized by the coprecipitation method from  $Mg(NO_3)_2$ ,  $Cr(NO_3)_3$ , and  $Na_2(CO_3)$  in the presence of NaOH. Characterized by thermoanalytical and powder X-ray diffraction data, and by atomic absorption spectrometry. The empirical formula is  $Mg_{0.68}Cr_{0.32}(OH)_2(CO_3)_{0.16}\cdot 0.86H_2O$ . The strongest line of the powder X-ray diffraction pattern is observed at 22.92 Å.

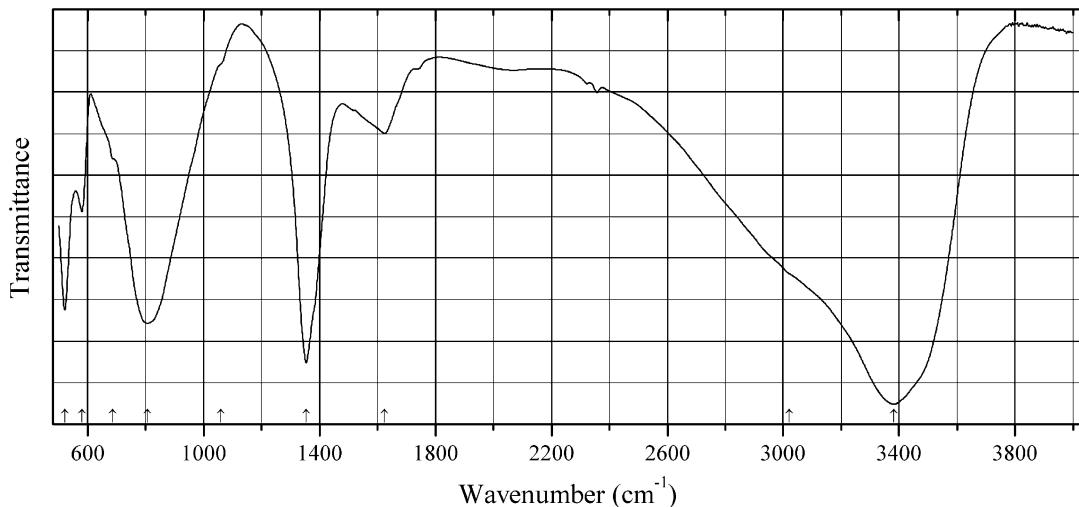
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Labajos and Rives (1996).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3410s, 3020sh, 1625w, 1360s, 1077sh, 845sh, 762, 608, 517.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**C357 Quintinite-related hydroxyde carbonate  $Ni_4Cr_2(OH)_{12}(CO_3)\cdot nH_2O$   $Ni_4Cr_2(OH)_{12}(CO_3)\cdot nH_2O$**



**Origin:** Synthetic.

**Description:** Synthesized by the coprecipitation method from  $Ni(NO_3)_2$ ,  $Cr(NO_3)_3$ , and  $Na_2(CO_3)$  in the presence of NaOH. Characterized by thermoanalytical and powder X-ray diffraction data, and by atomic absorption spectrometry. The empirical formula is  $Ni_{0.65}Cr_{0.35}(OH)_2(CO_3)_{0.15}\cdot 0.99H_2O$ . The strongest line of the powder X-ray diffraction pattern is observed at 22.50 Å.

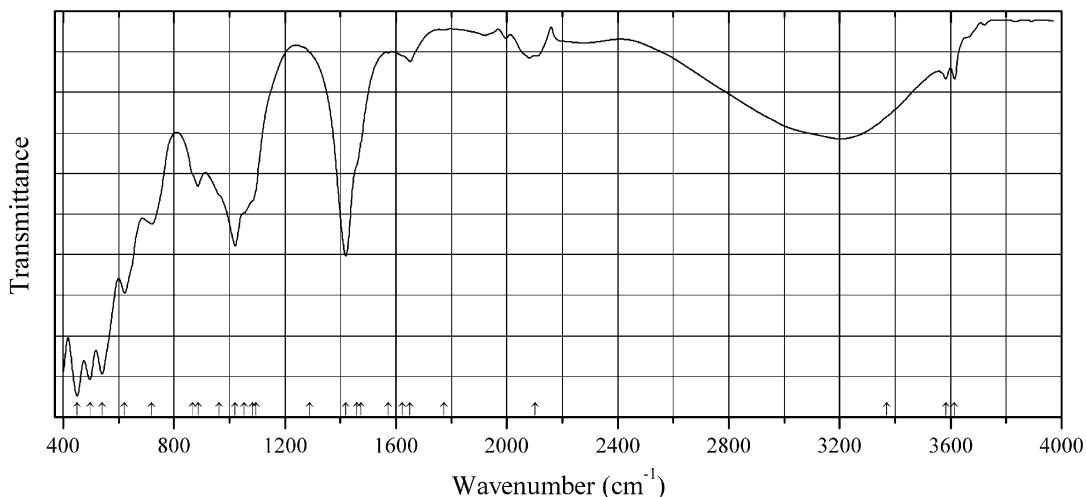
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Labajos and Rives (1996).

**Wavenumbers (cm<sup>-1</sup>):** 3382s, 3020sh, 1624w, 1354s, 1060sh, 806s, 687sh, 580, 521.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### C358 Scarbroite Al<sub>5</sub>(CO<sub>3</sub>)(OH)<sub>13</sub>·5H<sub>2</sub>O



**Origin:** The former Fonte Civillina, the town of Recoaro Terme, Vicenza, NE Italy.

**Description:** Nests of microcrystalline aggregates from the association with quartz, baryte, galena, cerussite, etc. Characterized by powder X-ray diffraction data and semiquantitative electron microprobe analyses. Triclinic,  $a = 9.892(1)$ ,  $b = 14.934(2)$ ,  $c = 26.321(4)$  Å,  $\alpha = 98.89(1)^\circ$ ,  $\beta = 97.49(1)^\circ$ ,  $\gamma = 89.04(1)^\circ$ .

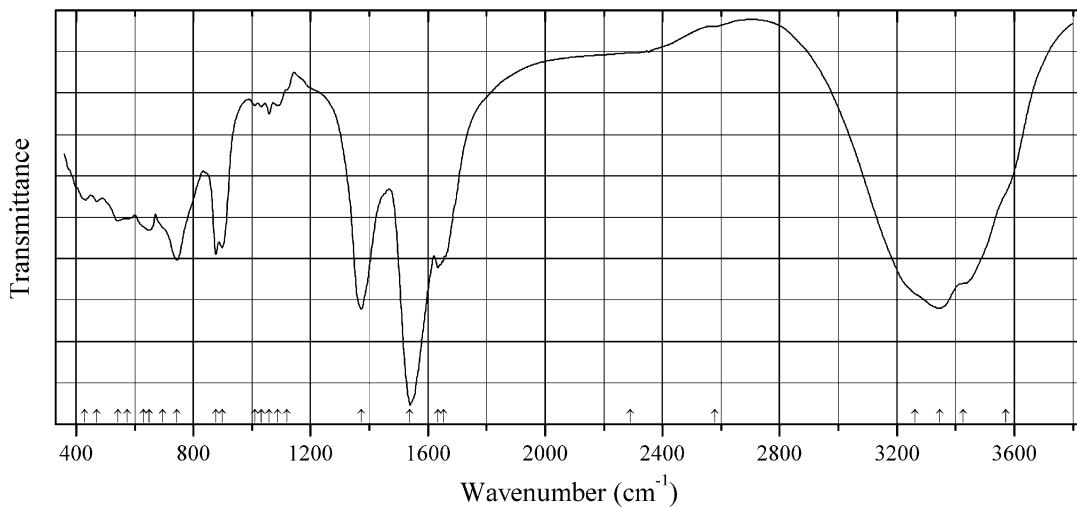
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Boscardin et al. (2009).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3614w, 3583w, 3370 (broad), 2102w, (1773w), 1651w, 1622sh, (1573w), 1474sh, 1459sh, 1419s, 1288sh, 1096sh, 1084sh, 1052sh, 1020s, 963sh, 886, 868sh, 720, 622s, 540s, 497s, 451s.

**Note:** In the cited paper, the wavenumber 720 cm<sup>-1</sup> is erroneously indicated as 750 cm<sup>-1</sup>. The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 3668, 3614s, 3593, 2994s, 1421, 1342, 1107s, 983, 889, 696, 600s, 449, 376, 267.

**C359 Bayleyite**  $Mg_2(UO_2)_2(CO_3)_3 \cdot 18H_2O$ 

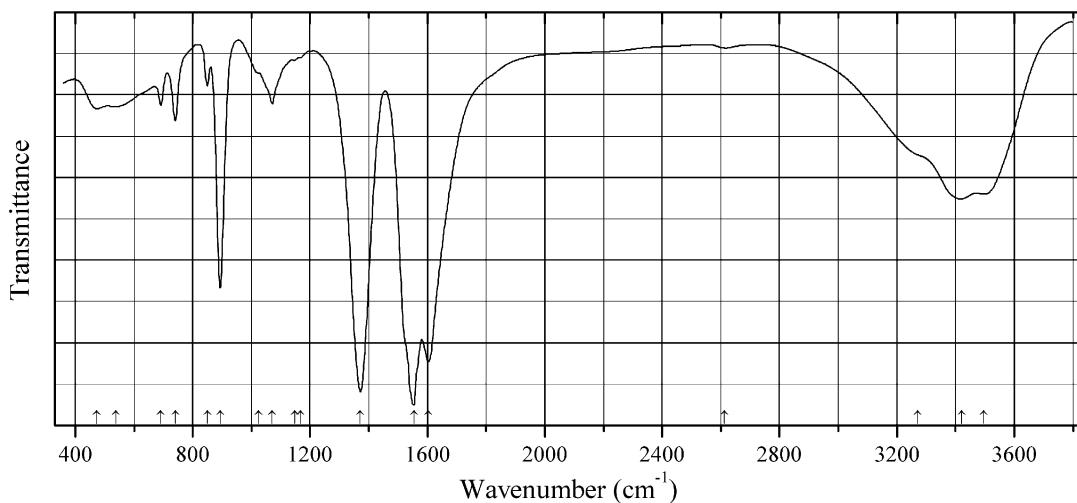
**Origin:** Hideout #1 mine, San Juan Co., Utah, USA.

**Description:** Yellow crystals from the association with gypsum. The sample was kindly provided by A.V. Kasatkin.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3570sh, 3425, 3346s, 3260sh, 2579w, 2290sh, 1655sh, 1635, 1539s, 1373s, 1120sh, 1088w, 1059w, 1031w, 1009w, 898, 876, 744, 695sh, 649, 630sh, 575sh, 542, 471, 430.

**Note:** The spectrum was obtained by N.V. Chukanov.

**C360 Línekite**  $K_2Ca_3[(UO_2)(CO_3)_3]_2 \cdot 8H_2O$ 

**Origin:** Geschieber vein, Svornost Mine, Jáchymov, Jáchymov District, Krušné Hory Mts, Karlovy Vary Region, Bohemia, Czech Republic (type locality).

**Description:** Greenish-yellow tabular crystals from the association with braunerite. Investigated by A.V. Kasatkin. The empirical formula is (electron microprobe):  $K_{1.94}Ca_{3.03}(UO_2)_{2.00}(CO_3)_6 \cdot nH_2O$ .

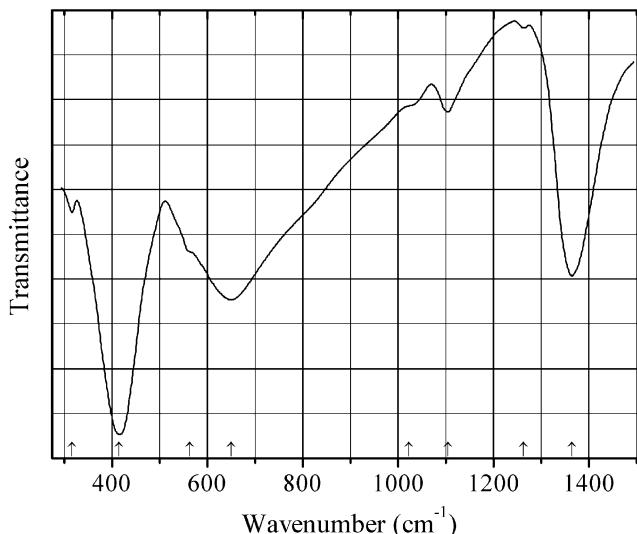
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3496s, 3420s, 3270sh, 2612w, 1604s, 1555s, 1372s, 1168w, 1148w, 1071,

1025sh, 893s, 850, 741, 691, 538, 474.

**Note:** The spectrum was obtained by N.V. Chukanov.

### C361 Wermlandite carbonate analogue $Mg_7Al_2(OH)_{18}[Ca(H_2O)_6](CO_3,SO_4)_2 \cdot 6H_2O$



**Origin:** Långban deposit, Bergslagen ore region, Filipstad district, Värmland, Sweden (type locality).

**Description:** Pale greenish-gray hexagonal platelets on calcite crystals. The crystal structure is solved.

Trigonal, space group  $P-3c1$ ,  $a = 9.303(3)$ ,  $c = 22.57(1)$  Å,  $V = 1692$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{meas}} = 1.93$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 1.96$  g/cm<sup>3</sup>.

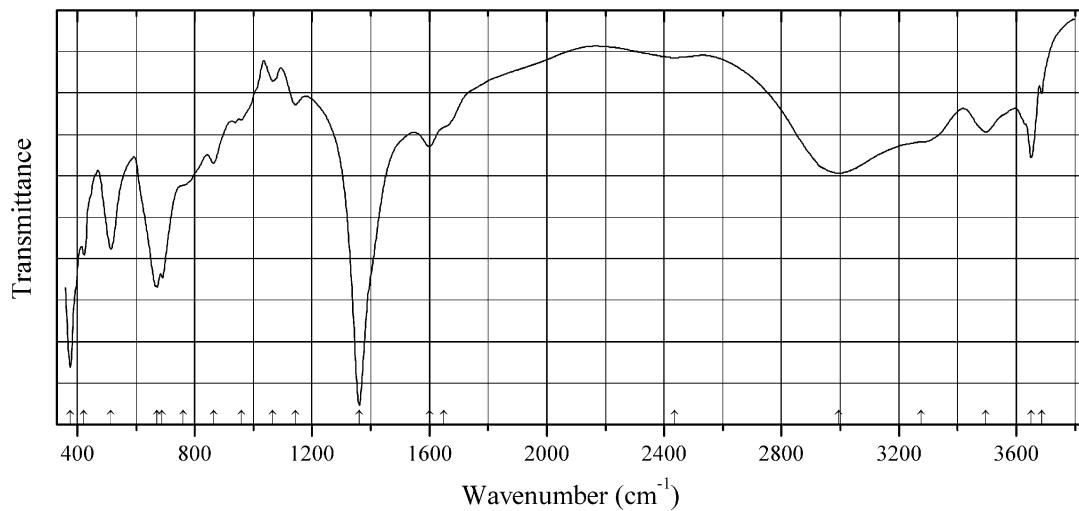
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Rius and Allmann (1984).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1365s, 1264, 1105w, 1024sh, 650s, 564sh, 416s, 317w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, the mineral is described as wermlandite s.s.,  $Mg_7Al_2(OH)_{18}[Ca(H_2O)_6](SO_4)_2 \cdot 6H_2O$ . However the intensities of the bands of asymmetric vibrations of carbonate and sulfate anions (at 1365 and 1105 cm<sup>-1</sup>, respectively) indicate that it is a CO<sub>3</sub>-dominant mineral. The value of measured density confirms this conclusion.

**C362 Nakauriite** Cu<sub>8</sub>(SO<sub>4</sub>)<sub>4</sub>(CO<sub>3</sub>)(OH)<sub>6</sub>·48H<sub>2</sub>O



**Origin:** Nakauri mine, near Shinshiro city, Aichi pref., Chubu Region, Honshu Island, Japan (type locality).

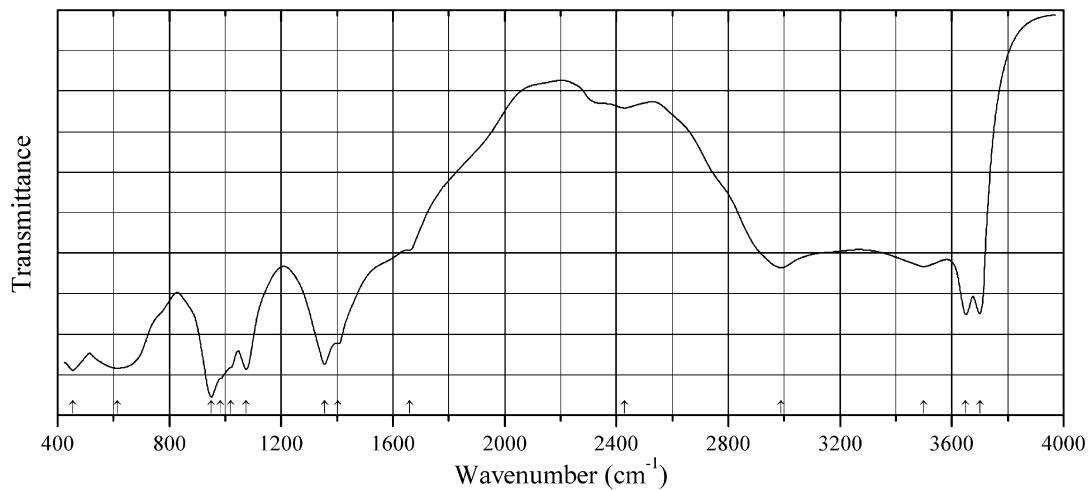
**Description:** Light blue crust consisting of radial aggregates. The associated minerals are chrysotile and brucite. Confirmed by the IR spectrum.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3686w, 3650, 3495, 3275sh, 2996, 2435w, 1650sh, 1600, 1361s, 1143w, 1066w, 959w, 864w, 760sh, 689s, 672s, 514, 423, 376s.

**Note:** The spectrum was obtained by N.V. Chukanov. The formula accepted for nakauriite is wrong and is to be revised: actually, nakauriite does not contain sulfate groups. The weak bands at 959 and 3686  $\text{cm}^{-1}$  correspond to chrysotile impurity.

### C363 Nakauriite Cu<sub>8</sub>(SO<sub>4</sub>)<sub>4</sub>(CO<sub>3</sub>)(OH)<sub>6</sub>·48H<sub>2</sub>O



**Origin:** Nakauri mine, near Shinshiro city, Aichi pref., Chubu Region, Honshu Island, Japan (type locality).

**Description:** Holotype sample with impurities (see [Sect. 1.3](#) in this book).

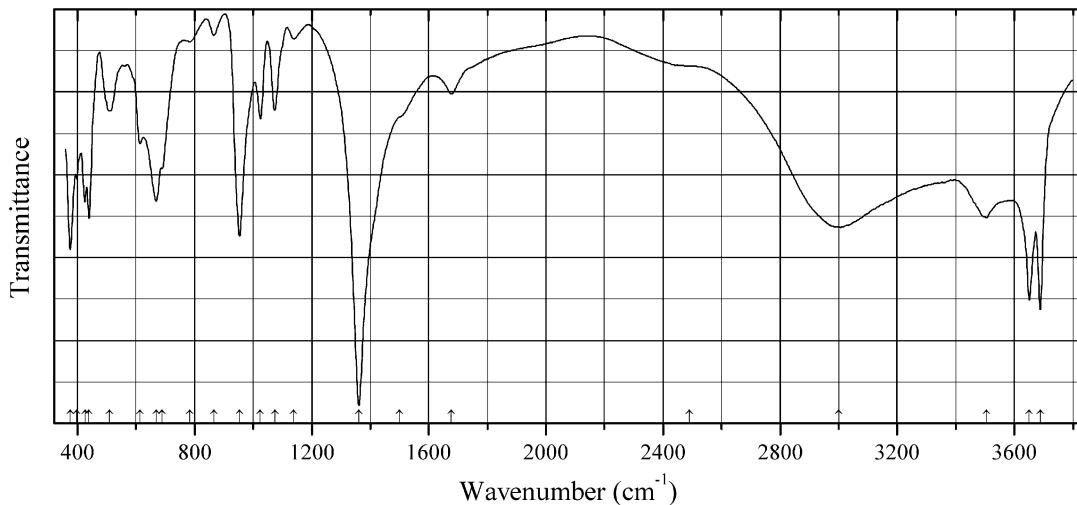
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Suzuki et al. (1976).

**Wavenumbers (cm<sup>-1</sup>):** 3700s, 3650s, 3500, 2990, 2430, 1660sh, 1404 (plateau), 1355s, 1075s, 1020sh, 983sh, 950s, 613s (broad), 454s.

**Note:** The strong bands at 3700, 1075, 950, 613, and 454 cm<sup>-1</sup> correspond to chrysotile impurity.

### C364 Nakauriite Cu<sub>8</sub>(SO<sub>4</sub>)<sub>4</sub>(CO<sub>3</sub>)(OH)<sub>6</sub>·48H<sub>2</sub>O



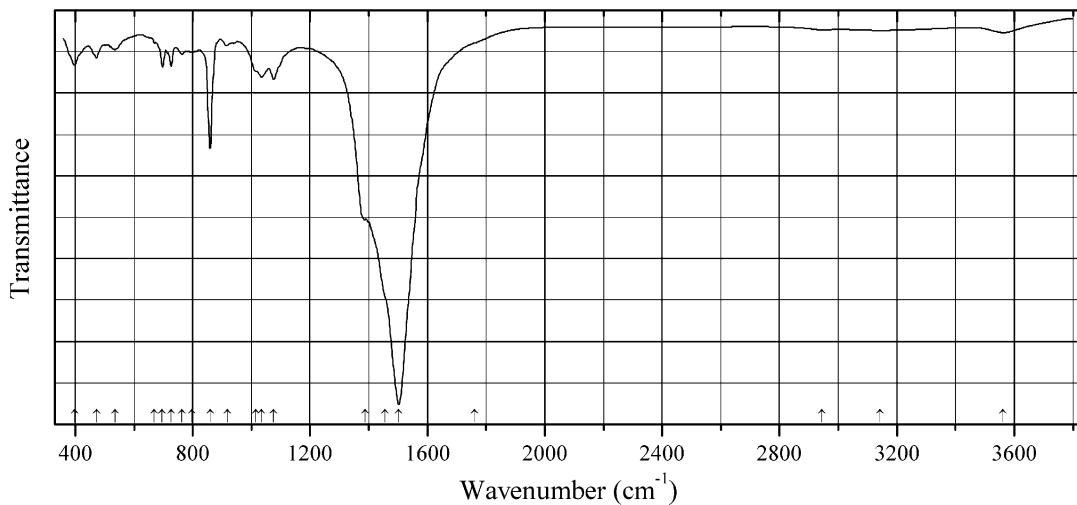
**Origin:** Chromite quarry near Karkodin railway station, Chelyabinsk region, South Urals.

**Description:** Blue crystalline crust on serpentine. Investigated by I.V. Pekov and N.V. Chukanov. For the description see [Sect. 1.3](#) in this book.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Wavenumbers (cm<sup>-1</sup>):** 3688s, 3651s, 3504, 3000s, 2490sh, 1678, 1500sh, 1361s, 1139w, 1074, 1025, 954s, 866w, 784w, 690sh, 669s, 614, 509, 440s, 426s, 398, 376s.

**Note:** The spectrum was obtained by N.V. Chukanov. The formula accepted for nakauriite is wrong and is to be revised: actually, nakauriite does not contain sulfate groups. The bands at 3688, 1074, 1025, 954, 614, and 376 cm<sup>-1</sup> correspond to serpentine.

**C365 Paratooite-(La)  $(\text{La,Ca,Na,Sr})_{12}\text{Cu}_2(\text{CO}_3)_{16}$** 

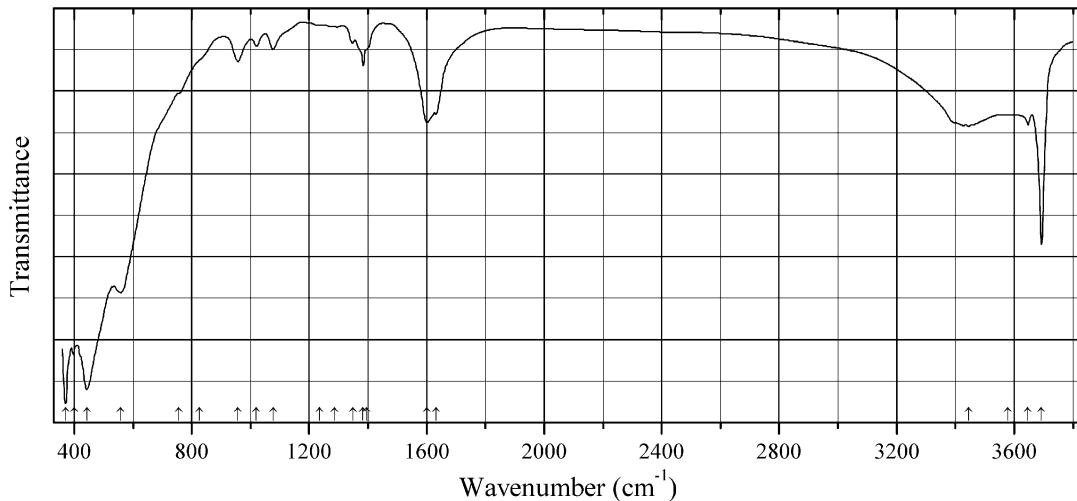
**Origin:** Paratoo copper mine, Yunta, Olary Province, South Australia, Australia (type locality).

**Description:** Light blue clusters. The sample was kindly provided by A. Pring, the author of the first description of paratooite.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3561w, 3142w, 2944w, 1760sh, 1502s, 1455sh, 1387, 1076, 1034, 1015sh, 917w, 859, 798w, 764w, 727, 697, 674w, 536w, 472, 397.

**Note:** The spectrum was obtained by N.V. Chukanov.

**C366 Coalingite  $\text{Mg}_{10}\text{Fe}^{3+}{}_2(\text{OH})_{24}(\text{CO}_3)\cdot 2\text{H}_2\text{O}$** 

**Origin:** Union Carbide Asbestos pit, New Idria district, Diablo Range, Fresno Co., California, USA (type locality).

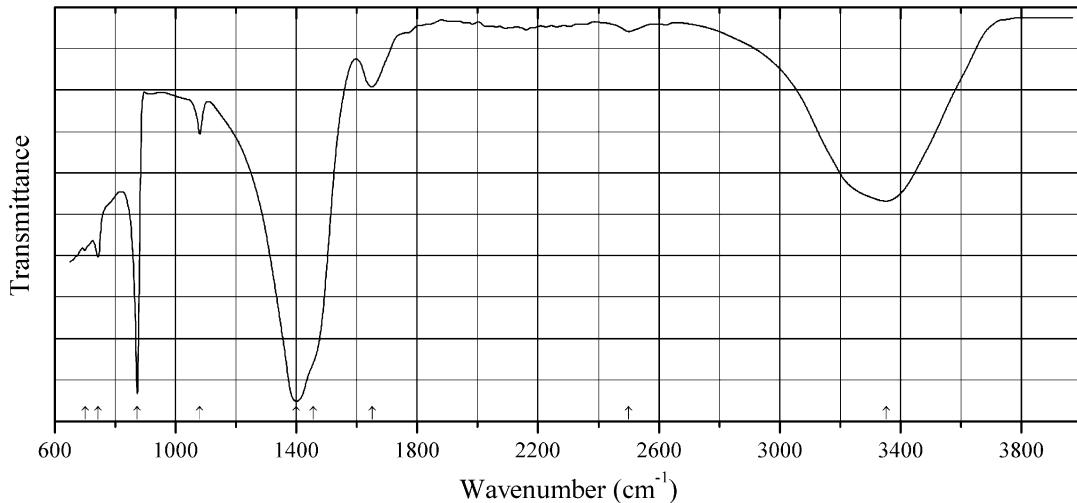
**Description:** Brown crust on serpentine. Identified by the IR spectrum.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3693s, 3647, 3445, 1632, 1601, 1395sh, 1384, 1349w, 1285w, 1235w, 1077, 1021w, 958, 825sh, 755sh, 558s, 443s, 399s, 371s.

**Note:** The spectrum was obtained by N.V. Chukanov.

### C369 Ikaite Ca(CO<sub>3</sub>)·6H<sub>2</sub>O



**Origin:** Artificial river bed in an alpine valley situated in the eastern part of Austria.

**Description:** Beige precipitate collected in February, 2014. Characterized by powder X-ray diffraction data.

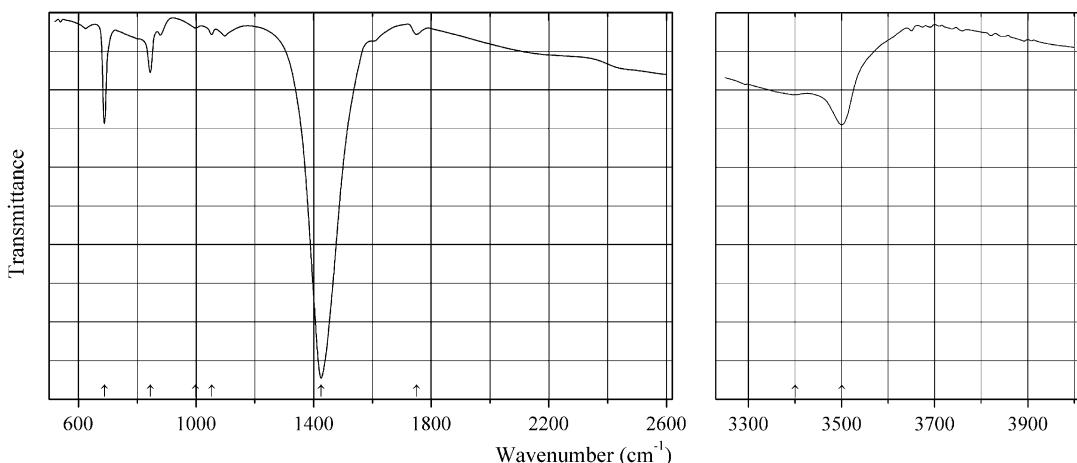
**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of powdered mineral.

**Source:** Boch et al. (2015).

**Wavenumbers (cm<sup>-1</sup>):** 3350s, 2000w, 1650, 1455sh, 1400s, 1080, 873s, 743, 700w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### C370 Abellaite NaPb<sub>2</sub>(CO<sub>3</sub>)<sub>2</sub>(OH)



**Origin:** Eureka mine, southern Pyrenees, Lleida province, Catalonia, Spain (type locality).

**Description:** White coating on the surface of the aggregate of primary minerals (roscoelite, pyrite, uraninite, sulfides, etc.). Holotype sample. Trigonal, space group  $P63mc$ ,  $a = 5.254(2)$ ,  $c = 13.450(5)$  Å,  $V = 321.5(2)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{calc}} = 5.93$  g/cm $^3$ . The empirical formula is  $\text{Na}_{0.96}\text{Ca}_{0.04}\text{Pb}_{1.98}(\text{CO}_3)_2(\text{OH})$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 3.193 (100) (013), 2.627 (84) (110), 2.275 (29) (020), 2.242 (65) (021, 006), 2.029 (95) (023).

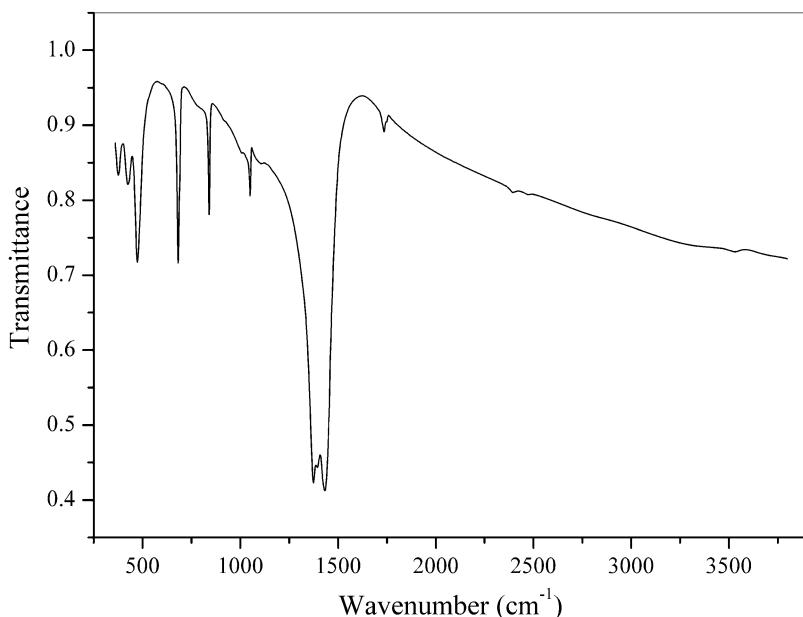
**Source:** Ibáñez-Insa et al. (2017).

**Wavenumbers (IR, cm $^{-1}$ ):** 3500, (3400), 1750w, (1600sh), 1425s, 1098w, 1053w, 998w, 878w, 844, 688s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 3504w, 1391, 1058s, 1038w, 868w, 683, 280, 202.

### C371 Shannonite Pb<sub>2</sub>O(CO<sub>3</sub>)



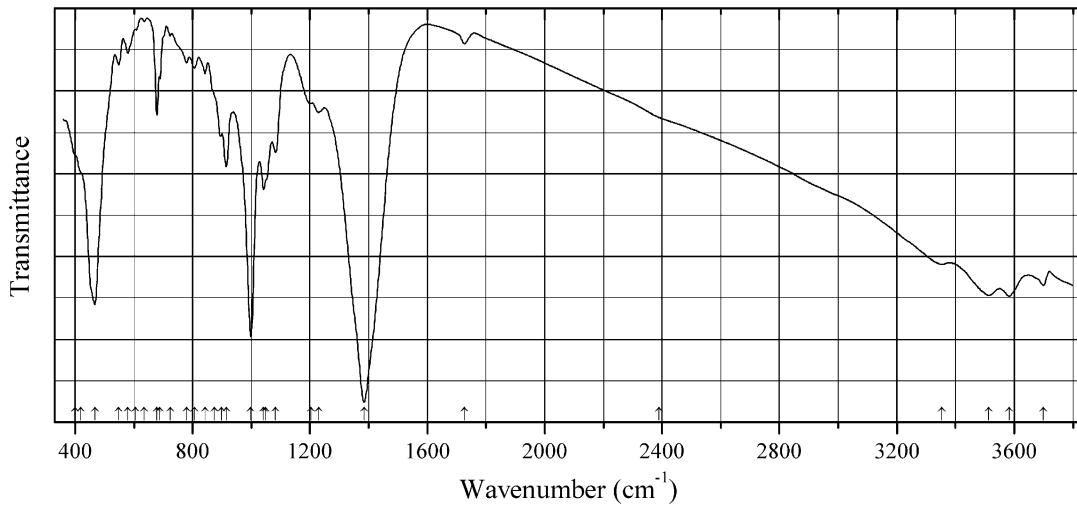
**Origin:** Tonopah-Belmont mine, Belmont Mt., Tonopah, Osborn district, Big Horn Mts., Maricopa Co., Arizona, USA.

**Description:** White masses from the association with plumbojarosite.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm $^{-1}$ ):** (3532w), 2470w, 2396w, 1745sh, 1735w, 1433s, 1392s, 1374s, 1102w, 1050, 1009w, 841, 682, 473, 425, 376.

**Note:** The spectrum was obtained by N.V. Chukanov.

**CSi30 Roymillerite**  $\text{Pb}_{24}\text{Mg}_9(\text{Si}_9\text{AlO}_{28})(\text{SiO}_4)(\text{BO}_3)(\text{CO}_3)_{10}(\text{OH})_{14}\text{O}_4$ 

**Origin:** Kombat Mine, Grootfontein district, Otjozondjupa region, Namibia (type locality).

**Description:** Colorless platy single-crystal grains from the association with jacobsite, cerussite, hausmannite, sahlinite, rhodochrosite, baryte, grootfonteinite, Mn-Fe-oxides, and melanotekite. Holotype sample. The crystal structure is solved. Triclinic, space group  $P-1$ ,  $a = 9.315(1)$ ,  $b = 9.316(1)$ ,  $c = 26.463(4)$  Å,  $\alpha = 83.295(3)^\circ$ ,  $\beta = 83.308(3)^\circ$ ,  $\gamma = 60.023(2)^\circ$ ,  $V = 1971.2(6)$  Å<sup>3</sup>,  $Z = 1$ .  $D_{\text{calc}} = 5.973$  g/cm<sup>3</sup>. Optically biaxial (−),  $\alpha = 1.86(1)$ ,  $\beta \approx \gamma = 1.94(1)$ ,  $2V = 5(5)^\circ$ . The empirical formula is  $\text{Pb}_{24.12}\text{Mg}_{8.74}\text{Mn}_{1.25}\text{Fe}_{0.94}\text{B}_{1.03}\text{Al}_{1.04}\text{C}_{9.46}\text{Si}_{9.39}\text{H}_{14.27}\text{O}_{83}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 25.9 (100) (001), 13.1 (11) (002), 3.480 (12) (017, 107, −115, 1−15), 3.378 (14) (126, 216), 3.282 (16) (−2−15, −1−25), 3.185 (12) (−116, 1−16), 2.684 (16) (031, 301, 030, 300, 332, −109, 0−19, 1−18), 2.382 (11) (0.0−11).

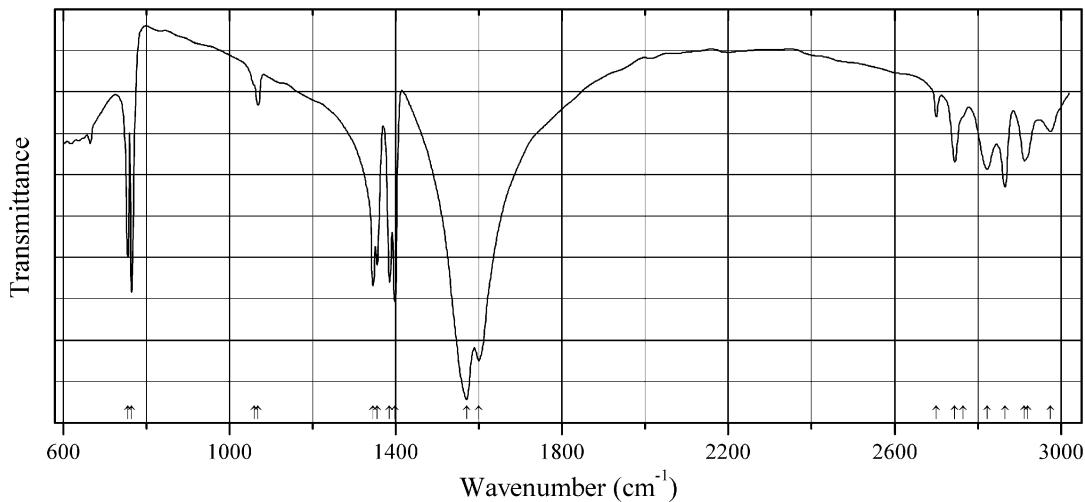
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>−1</sup>):** 3700, 3583, 3513, 3352, 1726w, 1385s, 1231, 1204, 1083, 1050sh, 1042, 999s, 915, 898, 875sh, 842w, 806w, 780w, 725w, 688, 679, 635w, 605w, 580w, 548w, 467s, 420sh, 400sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

## 2.3 Organic Compounds and Salts of Organic Acids

**Org70 Barium formate**  $\text{Ba}(\text{HCO}_2)_2$



**Origin:** Synthetic.

**Description:** Prepared from formic acid and barium carbonate. Orthorhombic, space group  $P2_12_12_1$ ,  $a = 6.81$ ,  $b = 8.91$ ,  $c = 7.67$  Å,  $Z = 4$ .

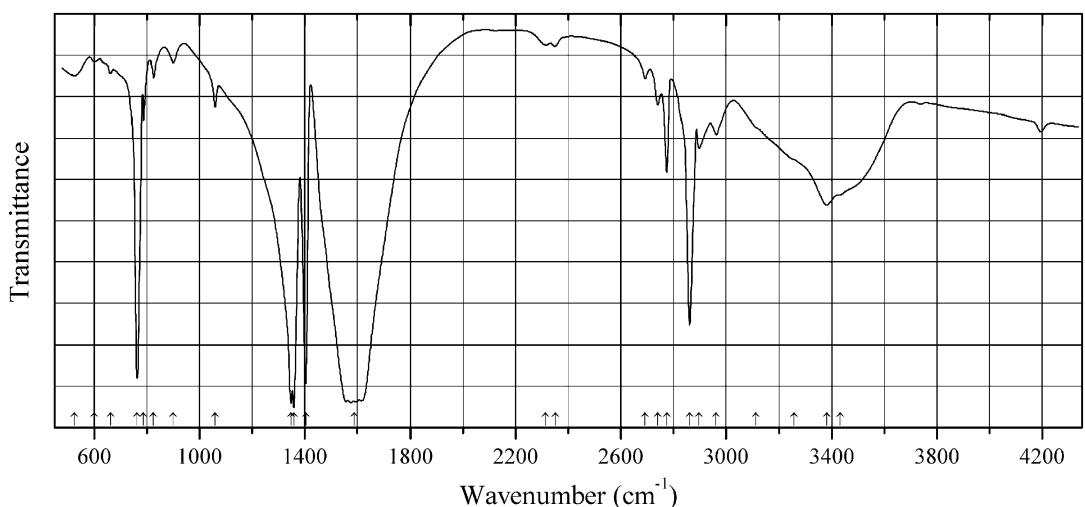
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Harvey et al. (1963).

**Wavenumbers (cm⁻¹):** 2975w, 2920sh, 2912, 2865, 2822, 2765sh, 2745, 2700w, 1600s, 1570s, 1398, 1385, 1355, 1345, 1069w, 1060sh, 765, 756.

**Note:** For the IR spectrum of barium formate see also Liu et al. (2001).

**Org71 Cadmium formatedihydrate**  $\text{Cd}(\text{HCOO})_2 \cdot 2\text{H}_2\text{O}$



**Origin:** Synthetic.

**Description:** Monolinic, space group  $P2_1/c$ ,  $Z = 4$ .

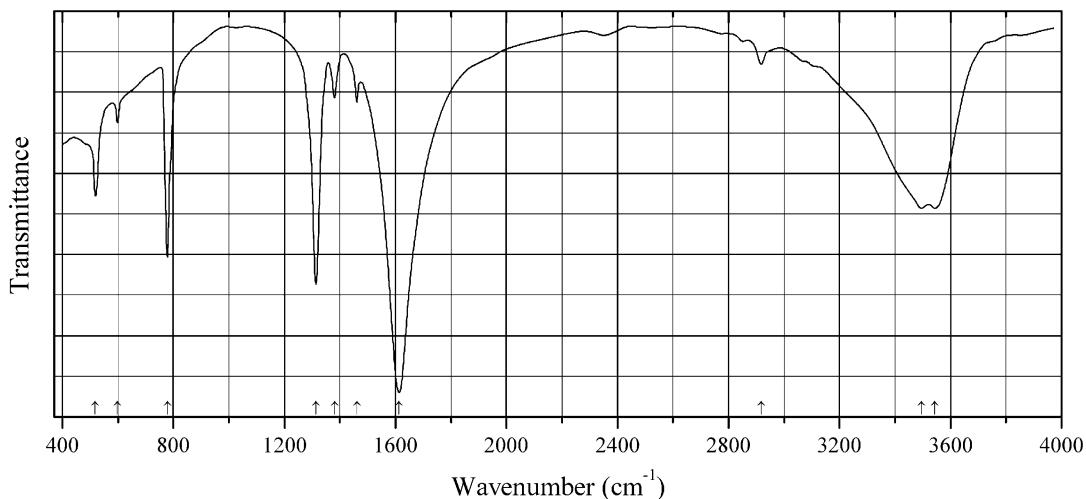
**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

**Source:** Abraham and Aruldas (1994).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3432sh, 3382, 3257sh, 3112sh, 2962w, 2896, 2862s, 2774, 2740w, 2690w, (2352w), (2314w), 1588s, 1405s, 1358s, 1348s, 1059w, 901w, 826w, 788w, 764s, 662w, 600w, 525w, 361, 299, 264, 231, 195, 154, 138, 121, 113, 103, 84, 68.

**Note:** Weak bands in the range from 2300 to 2400  $\text{cm}^{-1}$  may correspond to atmospheric  $\text{CO}_2$ .

### Org72 Cadmium oxalate trihydrate $\text{Cd}(\text{C}_2\text{O}_4) \cdot 3\text{H}_2\text{O}$



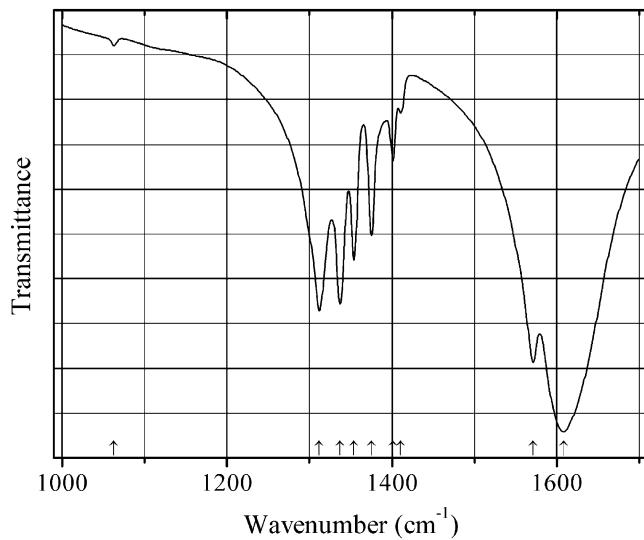
**Origin:** Synthetic.

**Description:** Colorless crystals grown at room temperature in silica gel, in the presence of  $\text{Cd}^{2+}$  ions impregnated with oxalic acid. Triclinic,  $a = 6.0059$ ,  $b = 6.66$ ,  $c = 8.49 \text{ \AA}$ ,  $\alpha = 105.71^\circ$ ,  $\beta = 98.99^\circ$ ,  $\gamma = 74.66^\circ$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Raj et al. (2008).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3542s, 3496s, 2919w, 1613s, 1461, 1381, 1314s, 778s, 599, 519.

**Org73 Copper strontium formate CuSr(HCOO)<sub>4</sub>**

**Origin:** Synthetic.

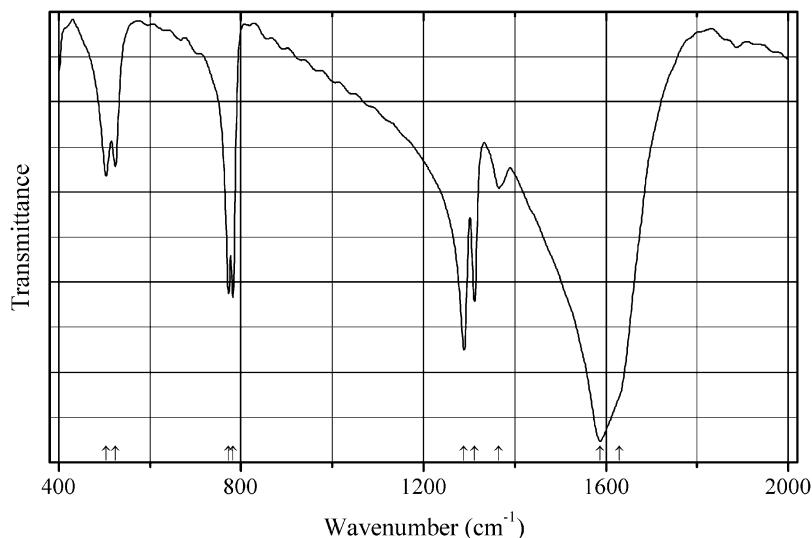
**Description:** Prepared by neutralization of the corresponding carbonates with dilute formic acid solution at 60–70 °C. Monoclinic, space group *P2/c*.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Stoilova and Vassileva (1999).

**Wavenumbers (cm<sup>-1</sup>):** 1608s, 1571s, 1411w, 1401, 1375, 1354, 1337, 1312, 1063.

**Note:** In the cited paper, the wavenumber 1401 cm<sup>-1</sup> is erroneously indicated as 1407 cm<sup>-1</sup>.

**Org74 Lead(II) oxalate Pb(C<sub>2</sub>O<sub>4</sub>)**

**Origin:** Synthetic.

**Description:** Prepared by reacting equimolecular amounts of 0.2 M solutions of lead nitrate and  $(\text{NH}_4)$   $(\text{HC}_2\text{O}_4)$ . Characterized by powder X-ray diffraction data. Triclinic, space group  $P-1$ ,  $Z = 2$  (see JCPDF 14–0803).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

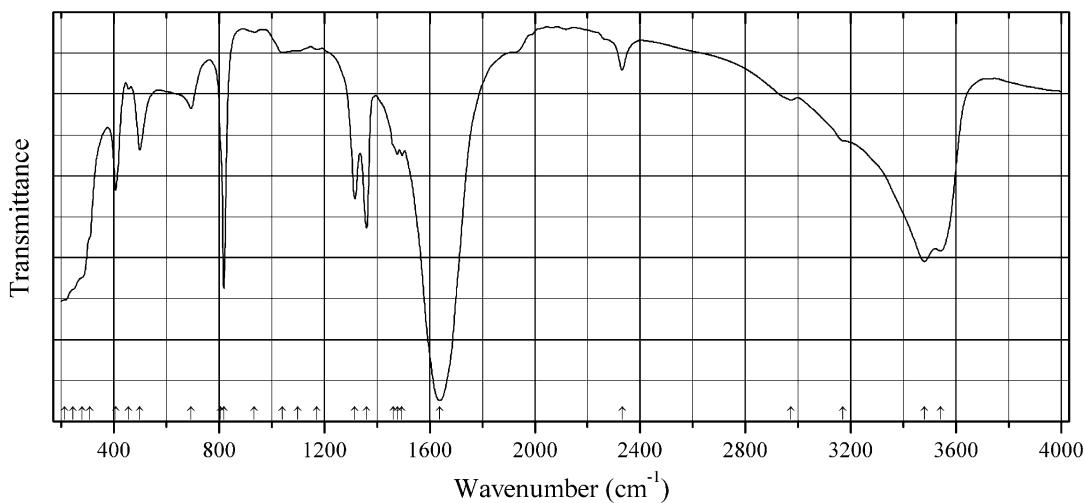
**Source:** Mancilla et al. (2009b).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1630sh, 1587s, 1365w, 1312, 1289s, 782, 773, 524, 504.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1707w, 1589s, 1476s, 1436s, 1400w, 1366w, 911w, 891, 854, 572w, 497s, 484s.

### Org75 Neptunium(IV) oxalate hexahydrate $\text{Np}(\text{C}_2\text{O}_4)_2 \cdot 6\text{H}_2\text{O}$



**Origin:** Synthetic.

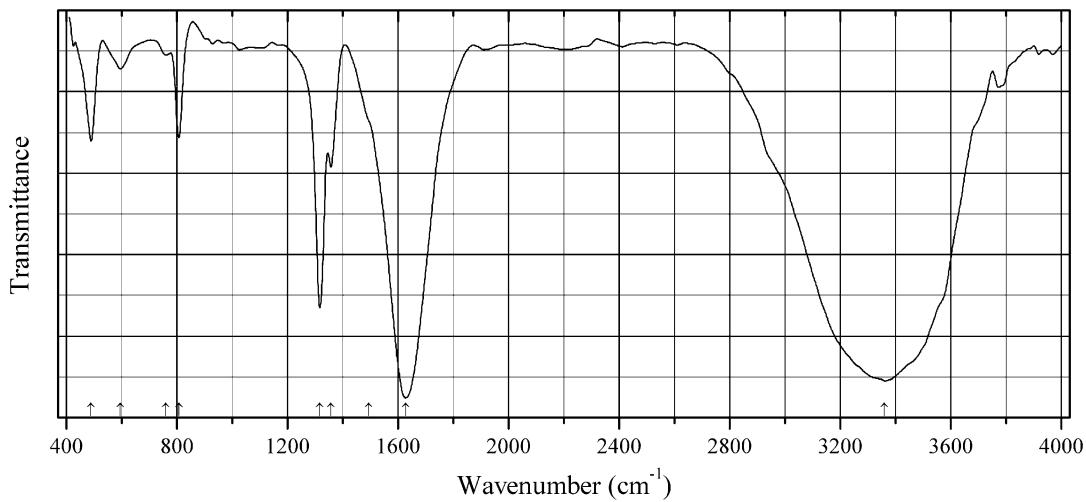
**Description:** Obtained by precipitation from aqueous solution. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %)] are: 7.88 (70), 6.36 (100), 5.04 (15), 4.91 (20), 3.93 (90), 3.18 (15).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Lindsay et al. (1970).

**Wavenumbers (cm<sup>-1</sup>):** 3542, 3480s, 3170sh, 2974w, 2332w, 1638s, 1495w, 1477w, 1461sh, 1360s, 1316, 1172w, 1098w, 1039w, 934w, 818s, 805sh, 694, 499, 456, 407, 309sh, 279sh, 245sh, 212sh.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**Org76 Samarium oxalate decahydrate**  $\text{Sm}_2(\text{C}_2\text{O}_4)_3 \cdot 10\text{H}_2\text{O}$ 

**Origin:** Synthetic.

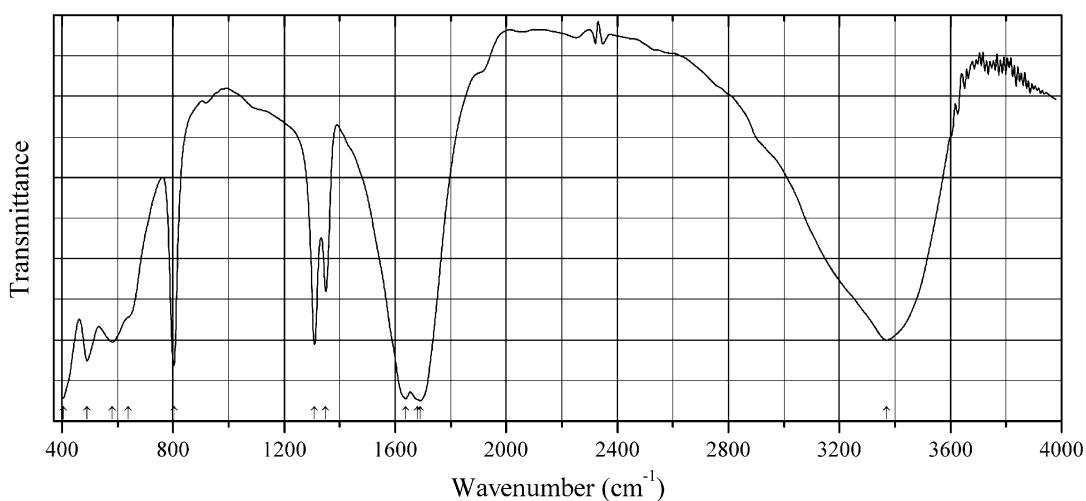
**Description:** Single crystals grown using diffusion gel technique from samarium nitrate hexahydrate and oxalic acid dihydrate in the presence of sodium silicate (meta)nonahydrate. Characterized by powder X-ray diffraction data and thermal analysis. Monoclinic, space group  $P2_1/c$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Vimal et al. (2014).

**Wavenumbers (cm⁻¹):** 3360s, 1628s, 1495sh, 1357, 1317s, 807, 761w, 595, 490.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Org77 Uranium(IV) oxalate fluoride hydrate**  $\text{U}_2(\text{C}_2\text{O}_4)\text{F}_6 \cdot 2\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Prepared hydrothermally from  $\text{UO}_2$ , HF, and oxalic acid dihydrate at 120 °C for 3 days.

Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $C2/c$ ,  $a = 17.246(3)$ ,  $b = 6.088(1)$  Å,  $c = 8.589(2)$  Å,  $\beta = 95.43(3)^\circ$ ,  $Z = 8$ .

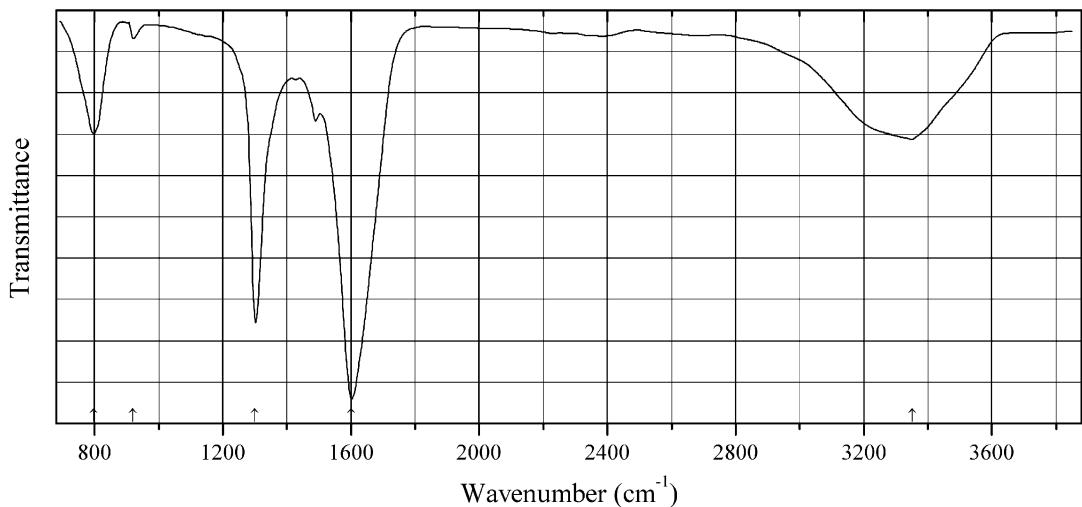
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Wang et al. (2006b).

**Wavenumbers (cm<sup>-1</sup>):** 3370 (broad), 1691s, 1680sh, 1638s, 1350, 1310, 804s, 638sh, 582s, 491, 405s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### Org78 Zirconium basic oxalate $\text{Zr}(\text{C}_2\text{O}_4)(\text{OH})_2 \cdot 0.5\text{H}_2\text{O}$



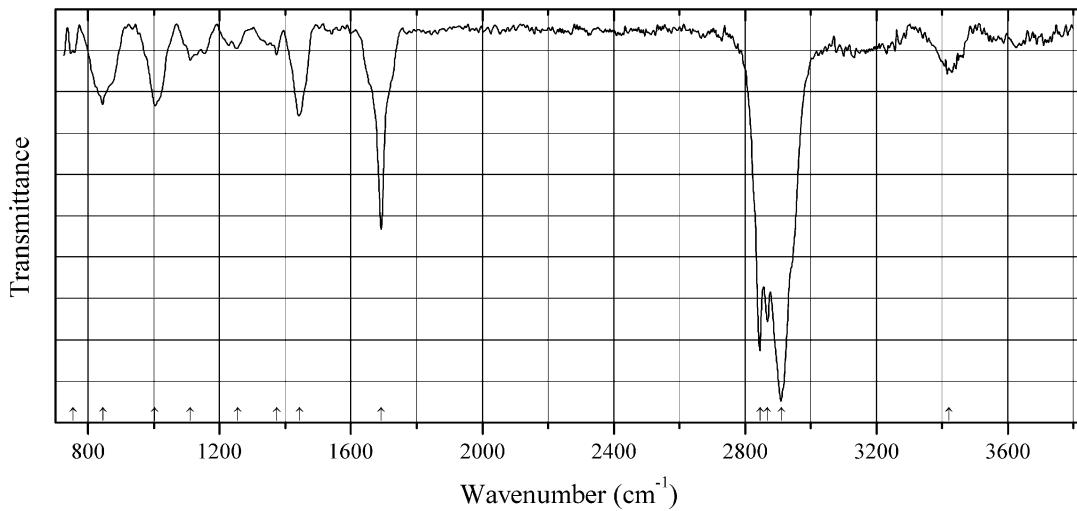
**Origin:** Synthetic.

**Description:** Obtained by interdiffusion of oxalic acid and  $\text{ZrO}(\text{NO}_3)_2$  in silicate gel. Characterized by TG analysis. The crystal structure is solved. Tetragonal, space group  $I4/m$ ,  $a = 12.799(5)$ ,  $c = 7.527$  (5) Å,  $V = 1233.0(1)$  Å<sup>3</sup>,  $Z = 8$ .  $D_{\text{calc}} = 2.35$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Hamdouni et al. (2013).

**Wavenumbers (cm<sup>-1</sup>):** 3350, 1600s, 1300s, 920w, 798.

**Org79 Bacalite**

**Origin:** El Gallo, near El Rosario, Late Cretaceous El Gallo Formation, Baja California, northwestern Mexico.

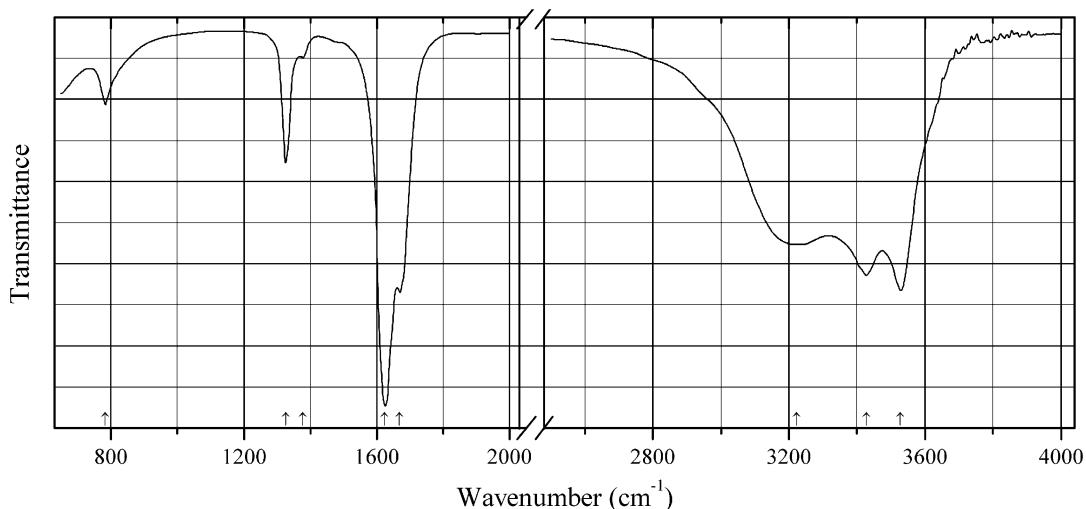
**Description:** Reddish to brownish yellow fossil resin forming lumps up to 5 cm in size from yellowish-brown mud and fine-grained sandstones.

**Kind of sample preparation and/or method of registration of the spectrum:** Synchrotron-based FTIR microspectroscopy.

**Source:** Riquelme et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 3420, 2910s, 2868s, 2845s, 1693s, 1444, 1375, 1255, 1110, 1002, 845, 755.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. For IR spectra of some other fossil resins (succinate, gedanite, gedano-succinate, rumanite, and retinite) see Golubev and Martirosyan (2012).

**Org80 Caoxite Ca(C<sub>2</sub>O<sub>4</sub>)·3H<sub>2</sub>O**

**Origin:** Synthetic.

**Description:** Obtained by the reaction between an aqueous solution of diethyl oxalate and calcite crystals. Characterized by powder X-ray diffraction data. Triclinic, space group  $P\bar{1}$ ,  $a = 6.1097(13)$ ,  $b = 7.1642(10)$ ,  $c = 8.4422(17)$  Å,  $\alpha = 76.43(1)^\circ$ ,  $\beta = 70.19(2)^\circ$ ,  $\gamma = 70.91(2)^\circ$ ,  $V = 325.3(1)$  Å<sup>3</sup>,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** A single crystal pressed in a diamond anvil cell. Transmission.

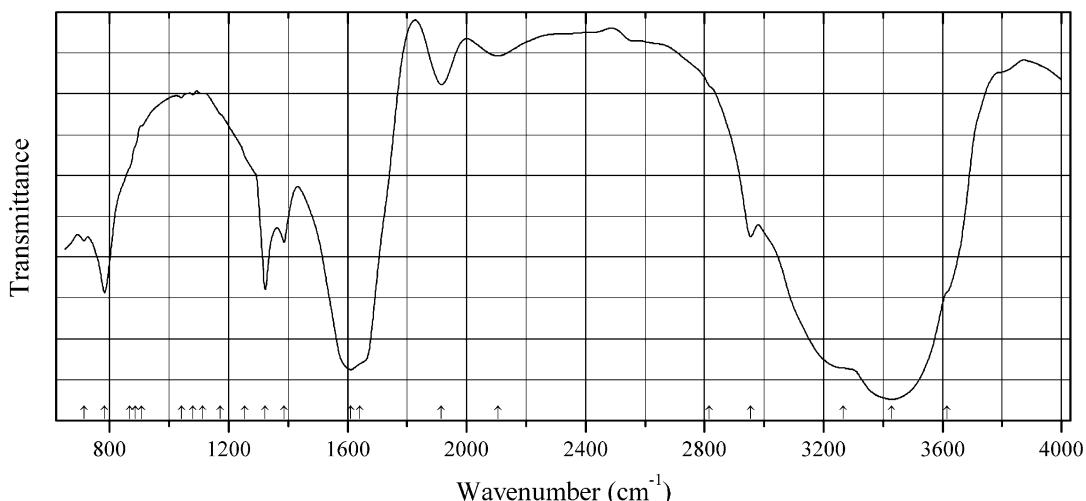
**Source:** Conti et al. (2015).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3528s, 3427s, 3222, 1668s, 1624s, 1377w, 1327, 783.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given. Raman bands at 2941 and 2882 cm<sup>-1</sup> may correspond to a compound with C–H bonds. Raman shifts above 3000 cm<sup>-1</sup> are not given in the cited paper.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 2941, 2882, 1472s, 912s, 507, 156.

### Org81 Caoxite Ca(C<sub>2</sub>O<sub>4</sub>)·3H<sub>2</sub>O



**Origin:** Synthetic.

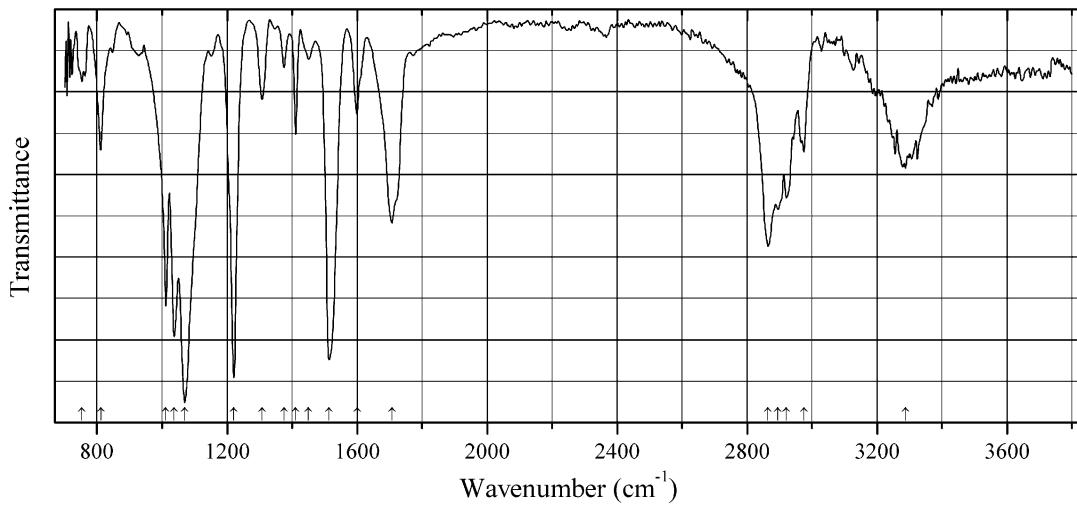
**Description:** Crystals synthesized at room temperature by reaction of aqueous solution of dimethyl oxalate with an aqueous solution of anhydrous calcium chloride in a stoichiometric proportion. Characterized by TG and DTA data.

**Kind of sample preparation and/or method of registration of the spectrum:** Single crystal placed on a KBr plate. Transmission.

**Source:** Echigo et al. (2005).

**Wavenumbers (cm<sup>-1</sup>):** 3615sh, 3429s, 3265sh, 2955, 2815sh, 2105, 1915, 1640sh, 1610s, 1386, 1323, 1254sh, 1173sh, 1114sh, 1080, 1041, 908sh, 887sh, 867sh, 783, 714.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The bands in the range from 2800 to 3000 cm<sup>-1</sup> correspond to the admixture of an organic substance with C–H bonds.

**Org82 Coahuilite**

**Origin:** El Gallo, near El Rosario, Late Cretaceous El Gallo Formation, Baja California, northwestern Mexico.

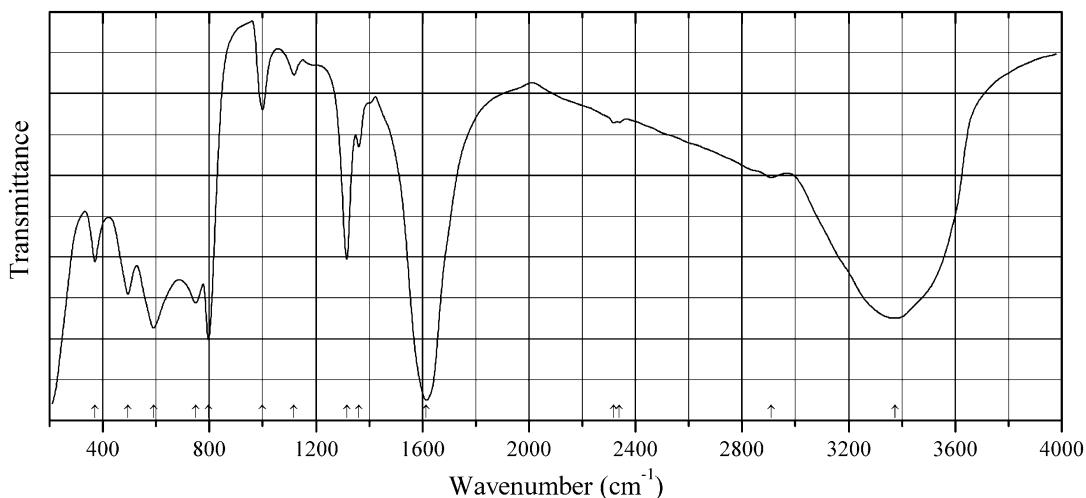
**Description:** Yellow to orange-brown fossil resin insoluble in alcohol and acetone, with a relatively high content of aromatic groups.

**Kind of sample preparation and/or method of registration of the spectrum:** Synchrotron-based FTIR microspectroscopy.

**Source:** Riquelme et al. (2014).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3287, 2975, 2921, 2895, 2865, 1707, 1600, 1513s, 1451, 1411, 1375, 1308w, 1220s, 1070s, 1038s, 1012, 812, 753.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. For IR spectra of some other fossil resins (succinate, gedanite, gedano-succinate, rumanite, and retinite) see Golubev and Martirosyan (2012).

**Org83 Deveroite-(Ce)  $\text{Ce}_2(\text{C}_2\text{O}_4)_3 \cdot 10\text{H}_2\text{O}$** 

**Origin:** Synthetic.

**Description:** Synthesized by mixing aqueous solutions of stoichiometric amounts of  $\text{CeCl}_3 \cdot 7\text{H}_2\text{O}$  and oxalic acid. Characterized by powder X-ray diffraction data, DTA-TG-DTG, and elemental analyses.

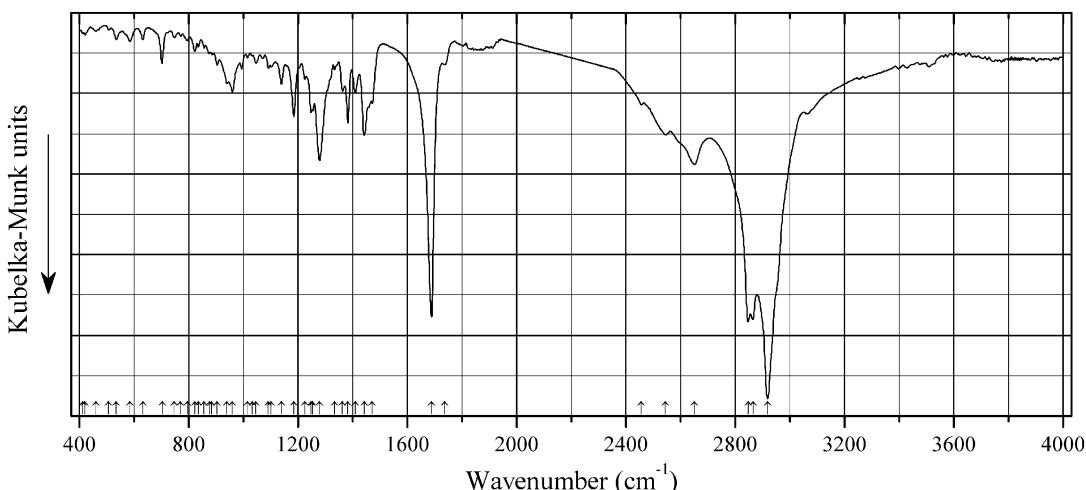
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Gabal et al. (2012).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3375, 2910w, 1615s, 1361, 1316, 1118w, 999, 797s, 749, 591s, 495, 371.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

#### Org84 Refikite $\text{C}_{20}\text{H}_{32}\text{O}_2$



**Origin:** Krásno, Slavkovský Les Mts., western Bohemia, Czech Republic.

**Description:** Polycrystalline crusts on pinetree bark and wood. The crystal structure is solved. Orthorhombic, space group  $P2_12_12$ ,  $a = 22.6520(7)$ ,  $b = 10.3328(3)$ ,  $c = 7.6711(2)$  Å,  $V = 1795.49(9)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 1.1334$  g/cm<sup>3</sup>. The empirical formula is  $\text{C}_{19}\text{H}_{33}\text{COOH}$ .

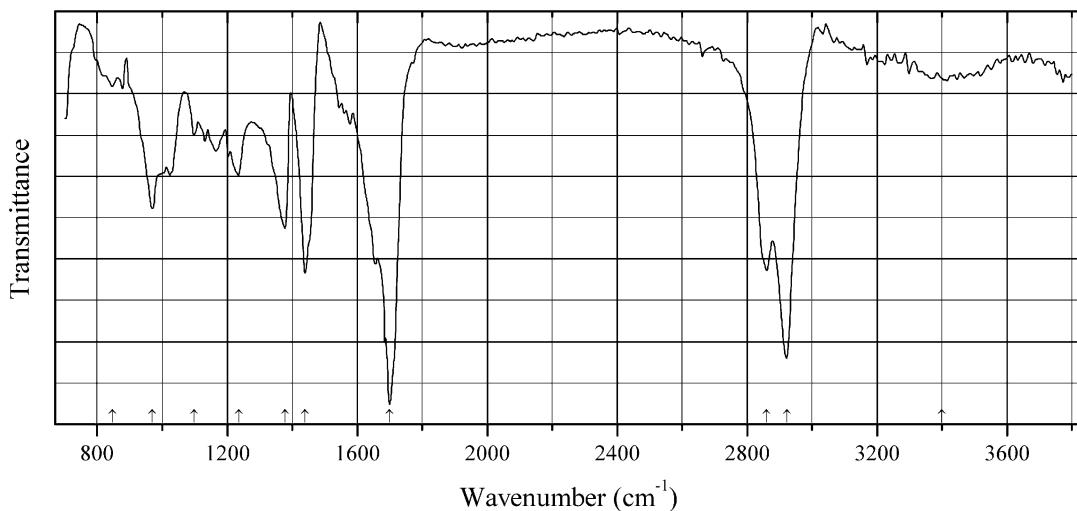
**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection.

**Source:** Pažout et al. (2015).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 2919s, 2865s, 2847s, 2651, 2545, 2456, 1737w, 1689s, 1472, 1442, 1410, 1383, 1363, 1334, 1279, 1254, 1248, 1225w, 1185, 1139, 1101w, 1092w, 1046w, 1032w, 1015w, 960, 940, 904w, 885w, 875w, 856w, 836w, 823w, 794w, 770w, 747w, 703, 633w, 586w, 535w, 507w, 461w, 420w, 412w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 3013, 2952s, 2935s, 2890s, 2844s, 1474s, 1452s, 1383, 1362, 1249, 1202, 739, 725s.

**Org85 Simojovelite**

**Origin:** La Pimienta, near Simojovel, Chiapas Highlands, Mexico.

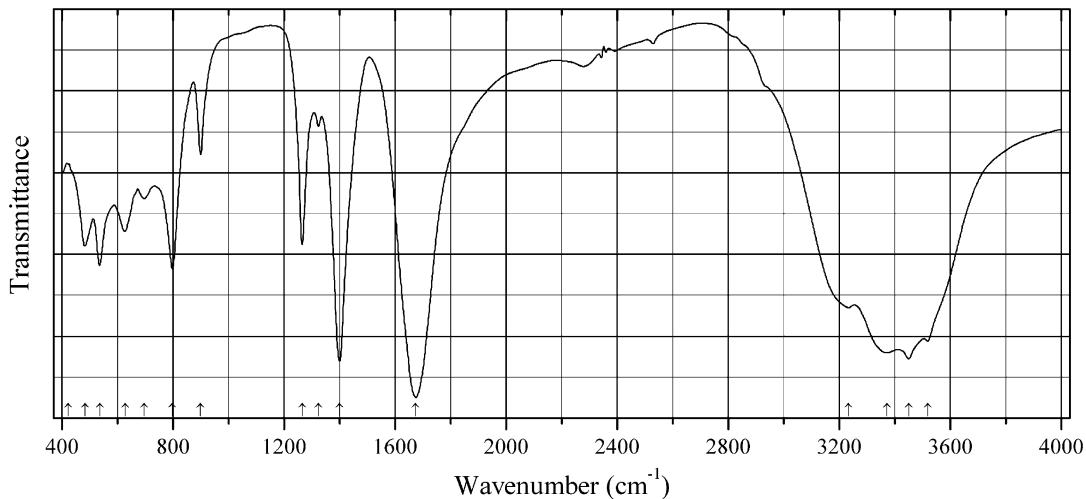
**Description:** Fossil resin.

**Kind of sample preparation and/or method of registration of the spectrum:** Synchrotron-based FTIR microspectroscopy.

**Source:** Riquelme et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 3400 (broad), 2923s, 2860s, 1700s, 1440, 1378, 1235, 1098, 970, 846.

**Note:** For IR spectra of some other fossil resins (succinate, gedanite, gedano-succinate, rumanite, and retinite) see Golubev and Martirosyan (2012).

**Org86 Stepanovite NaMgFe<sup>3+</sup>(C<sub>2</sub>O<sub>4</sub>)<sub>3</sub>·8–9H<sub>2</sub>O**

**Origin:** Synthetic.

**Description:** Obtained by the reaction of an aqueous solution of  $\text{Na}_3[\text{Fe}(\text{C}_2\text{O}_4)_3]\cdot 5\text{H}_2\text{O}$  (prepared by reaction of a suspension of freshly precipitated  $\text{Fe}(\text{OH})_3$  with an aqueous solution of  $\text{NaHC}_2\text{O}_4$ ) with a great excess of  $\text{MgCl}_2$ . The crystal structure is solved. Trigonal, space group  $P3c1$ ,  $a = 17.0483(4)$ ,  $c = 12.4218(4)$  Å,  $V = 3126.7(1)$  Å $^3$ ,  $Z = 6$ .  $D_{\text{calc}} = 1.687$  g/cm $^3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

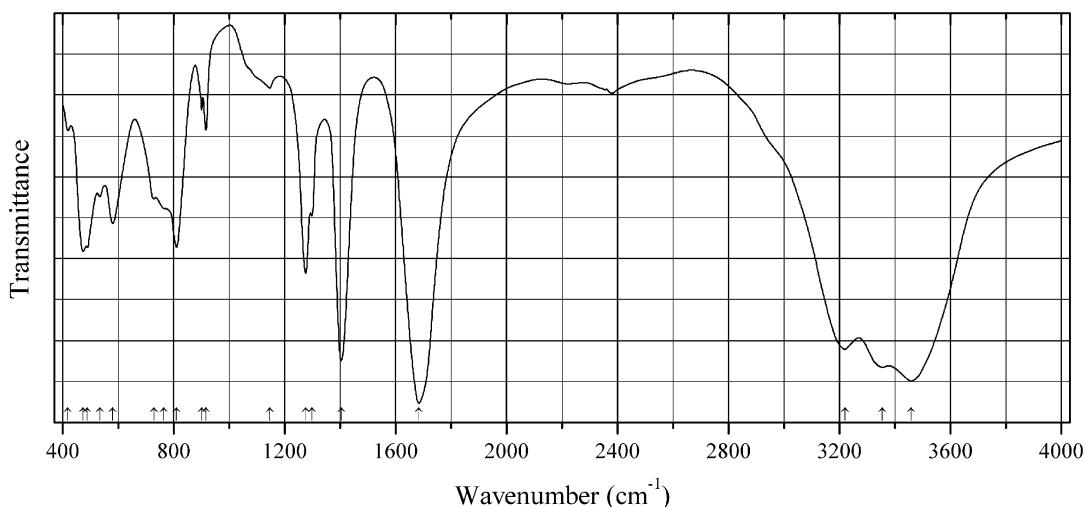
**Source:** Piro et al. (2016).

**Wavenumbers (IR, cm $^{-1}$ ):** 3518s, 3450s, 3371s, 3233, 1674s, 1400s, 1324w, 1265, 900, 798, 696, 627, 536, 483, 423.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 3450w, 3350w, 3275w, 1728s, 1666, 1478, 1460, 1523, 1398, 1267, 903, 599, 537, 480s.

### Org87 Zhemchuzhnikovite $\text{NaMgAl}(\text{C}_2\text{O}_4)_3\cdot 8\text{H}_2\text{O}$



**Origin:** Synthetic.

**Description:** Fe-rich variety,  $\text{NaMg}(\text{Al}_{0.55}\text{Fe}^{3+}_{0.45})(\text{C}_2\text{O}_4)_3\cdot n\text{H}_2\text{O}$ , obtained by the mixing aqueous solutions of  $\text{NaMg}[\text{Fe}(\text{C}_2\text{O}_4)_3]\cdot 9\text{H}_2\text{O}$  and  $\text{NaMg}[\text{Al}(\text{C}_2\text{O}_4)_3]\cdot 9\text{H}_2\text{O}$ . The crystal structure is solved. Trigonal, space group  $P3c1$ ,  $a = 16.8852(5)$ ,  $c = 12.5368(5)$  Å,  $V = 3095.5(2)$  Å $^3$ ,  $Z = 6$ .  $D_{\text{calc}} = 1.652$  g/cm $^3$ .

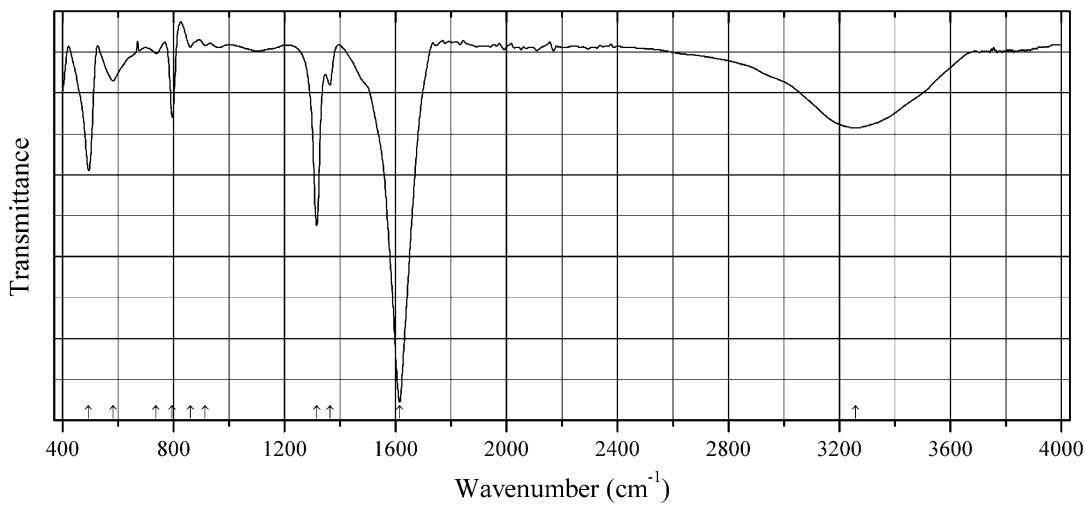
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Piro et al. (2016).

**Wavenumbers (IR, cm $^{-1}$ ):** 3458s, 3355s, 3219s, 1684s, 1404s, 1298, 1276, 1146w, 916, 901, 811, 765sh, 729, 581, 534, 490, 475, 419w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 3467, 3222, 1788s, 1688, 1520w, 1479, 1440s, 1266, 991, 923, 856, 565, 533, 479s.

**Org88 Deveroite-(Ce)  $\text{Ce}_2(\text{C}_2\text{O}_4)_3 \cdot 10\text{H}_2\text{O}$** 

**Origin:** Synthetic.

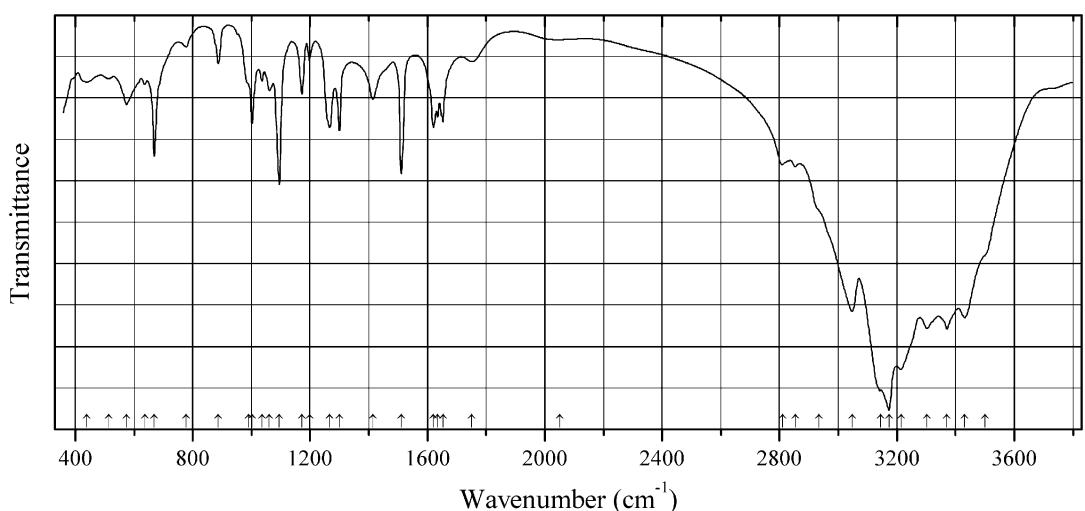
**Description:** Sm<sup>3+</sup> doped crystal synthesized using single diffusion gel technique. Characterized by powder X-ray diffraction data and EDS analysis. Monoclinic,  $a = 11.34$ ,  $b = 9.630$ ,  $c = 10.392 \text{ \AA}$ ,  $\beta = 114.5^\circ$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Unnikrishnan and Ittyachen (2016).

**Wavenumbers (cm<sup>-1</sup>):** 3257, 1615s, 1364, 1316s, 915w, 860w, 796, 582, 495.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Org89 Triazolite  $\text{NaCu}_2(\text{N}_3\text{C}_2\text{H}_2)_2(\text{NH}_3)_2\text{Cl}_3 \cdot 4\text{H}_2\text{O}$  where  $\text{N}_3\text{C}_2\text{H}_2^-$  is 1,2,4-triazolate anion**

**Origin:** Pabellón de Pica Mountain, 1.5 km south of Chanabaya village, Iquique Province, Tarapacá Region, Chile (type locality).

**Description:** Clusters and radiated aggregates of prismatic crystals from the association with salammoniac, halite, ammineite, joanneumite, chanabayaita, nitratine, natroxalate, and möhnite. Holotype sample. The crystal structure is solved. Orthorhombic, space group  $P2_12_12_1$ ,  $a = 19.3575(5)$ ,  $b = 7.15718(19)$ ,  $c = 12.5020(4)$  Å,  $V = 1732.09(8)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 2.028$  g/cm $^3$ . Optically biaxial (−),  $\alpha = 1.582(4)$ ,  $\beta = 1.625(3)$ ,  $\gamma = 1.625(3)$ ,  $2V = 5(3)^\circ$ . The empirical formula is  $\text{Na}_{1.14}(\text{Cu}_{1.86}\text{Fe}_{0.14})(\text{Cl}_{2.99}\text{S}_{0.23})\text{N}_{9.23}\text{C}_{3.43}\text{H}_{23.34}\text{O}_{4.29}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å (I, %) ( $hkl$ )] are: 10.22 (97) (101), 6.135 (40) (011), 5.696 (17) (301), 5.182 (59) (202), 5.119 (100) (211), 4.854 (19) (400), 3.752 (16) (312, 501), 3.294 (18) (221), 2.644 (17) (404), 2.202 (18) (324, 713).

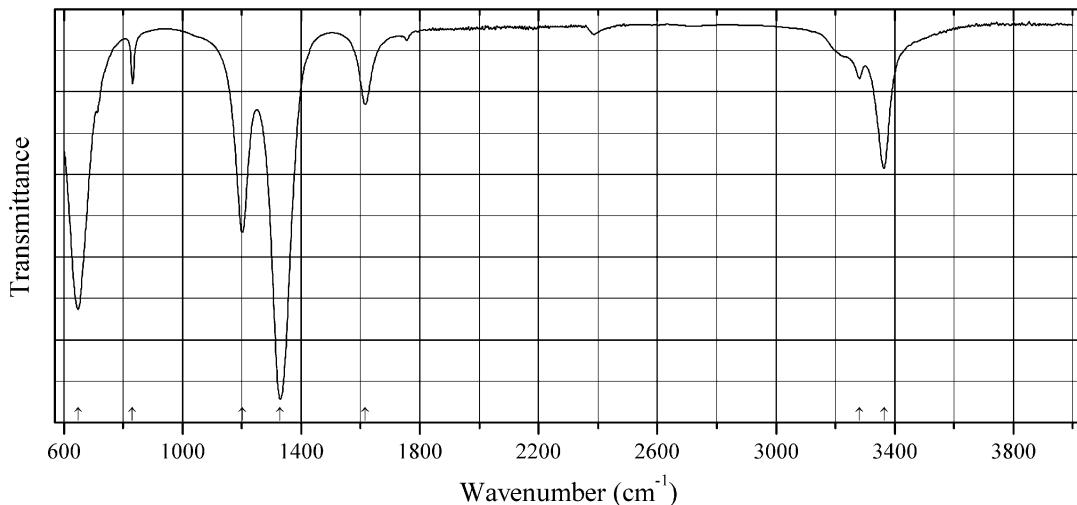
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm $^{-1}$ ):** 3500sh, 3431s, 3371s, 3302s, 3215s, 3173s, 3145sh, 3047s, 2935sh, 2855, 2812, 2050w, 1751, 1653, 1635, 1621, 1510, 1414, 1300, 1267, 1198w, 1172, 1095, 1062, 1036w, 1002, 990sh, 887, 778w, 669, 638w, 575, 513w, 440w.

**Note:** The spectrum was obtained by N.V. Chukanov.

## 2.4 Nitrides and Nitrates

### N20 Hexaamminenickel(II) nitrate [Ni(NH<sub>3</sub>)<sub>6</sub>](NO<sub>3</sub>)<sub>2</sub>



**Origin:** Synthetic.

**Description:** Prepared in the reaction between nickel nitrate hexahydrate and gaseous ammonia in the presence of silica gel. The crystal structure is solved. Cubic, space group  $Fm-3m$ ,  $a = 10.8738(6)$  Å,  $V = 1285.73(7)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 1.471(1)$  g/cm $^3$ .

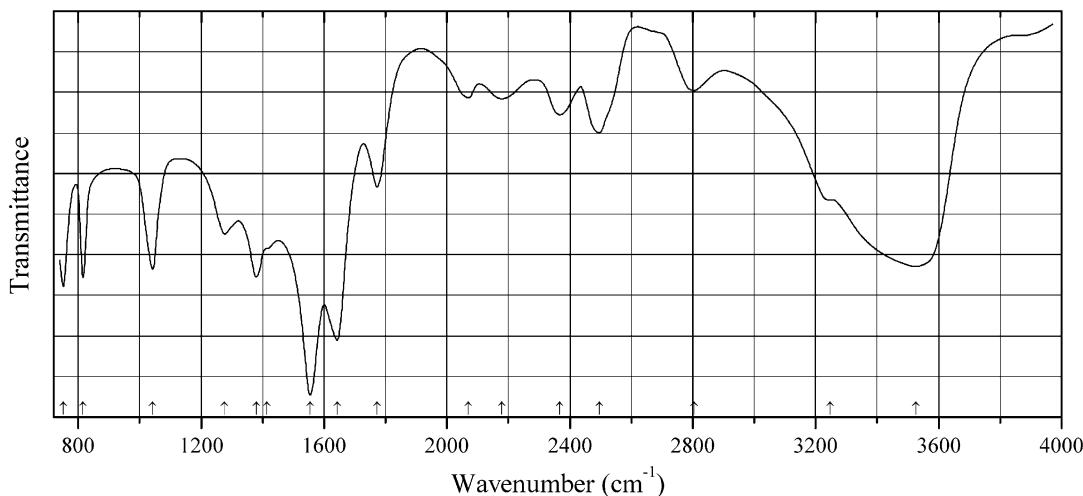
**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of a powdered sample.

**Source:** Breternitz et al. (2015).

**Wavenumbers (cm<sup>-1</sup>):** 3364, 3282w, 1616w, 1329, 1202s, 832, 648s.

**Note:** In the cited paper, the wavenumber 832 cm<sup>-1</sup> is erroneously indicated as 823 cm<sup>-1</sup>.

### N21 Lanthanum nitrate hexahydrate La(NO<sub>3</sub>)<sub>3</sub>·6H<sub>2</sub>O



**Origin:** Synthetic.

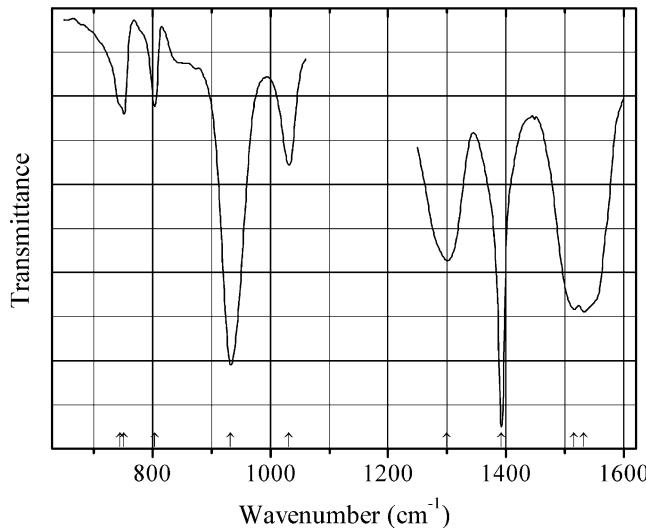
**Description:** Commercial reactant. Triclinic, space group  $P\bar{2}_1/c$ ,  $a = 7.386(3)$ ,  $b = 7.716(3)$ ,  $c = 11.345(4)$  Å,  $\alpha = 99.773(5)^\circ$ ,  $\beta = 91.141(6)^\circ$ ,  $\gamma = 115.58(5)^\circ$ ,  $V = 571.6(3)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{meas}} = 2.39(3)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 2.391$  g/cm<sup>3</sup>. Optically biaxial (-),  $\alpha = 1.554(2)$ ,  $\beta = 1.558(2)$ ,  $\gamma = 1.566(2)$ ,  $2V = 70(5)^\circ$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 11.089 (100) (001), 3.540 (81) (0–13, -1–12), 5.484 (79) (002, 101), 2.918 (60) (-122), 3.089 (33) (-113, 201), 4.022 (30) (102, -112), 6.826 (23) (010).

**Kind of sample preparation and/or method of registration of the spectrum:** Diffuse reflection of powdered sample mixed with KBr. The transformation into absorbance spectra was carried out by using background spectra collected under identical conditions with KBr powder in the holder.

**Source:** Klingenberg and Vannice (1996).

**Wavenumbers (cm<sup>-1</sup>):** 3525s, 3246sh, 2804w, 2495, 2366, 2108w, 2069w, 1772, 1643s, 1554s, 1415sh, 1379, 1276, 1042, 815, 752.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, the wavenumber 2178 cm<sup>-1</sup> is erroneously indicated as 2108 cm<sup>-1</sup>.

**N22 Uranyl nitrate hexahydrate  $\text{UO}_2(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$** 

**Origin:** Synthetic.

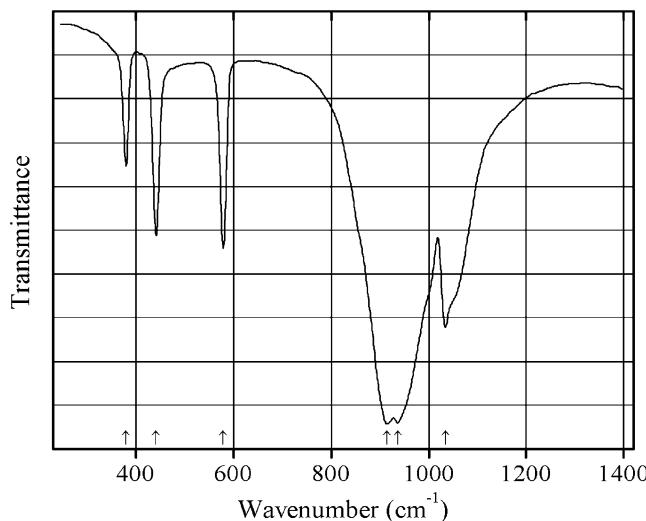
**Description:** Commercial reactant.

**Kind of sample preparation and/or method of registration of the spectrum:** A mixture with KBr. Transmission.

**Source:** Caldow et al. (1960).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1531s, 1515s, 1392s, 1300, 1032, 933s, 804, 752, 745sh.

**Note:** The band at 1392  $\text{cm}^{-1}$  may correspond to  $\text{KNO}_3$  formed in the reaction between  $\text{UO}_2(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$  and KBr. Consequently, the presence of uranyl bromide in the sample is not excluded.

**N23 Nierite  $\beta\text{-Si}_3\text{N}_4$** 

**Origin:** Synthetic.

**Description:** Prepared by reacting silicon powder with nitrogen at 1350 °C for 2 h followed by heating at 1500 °C for 16 h. Hexagonal, space group  $P6_3/m$ ,  $Z = 2$ .

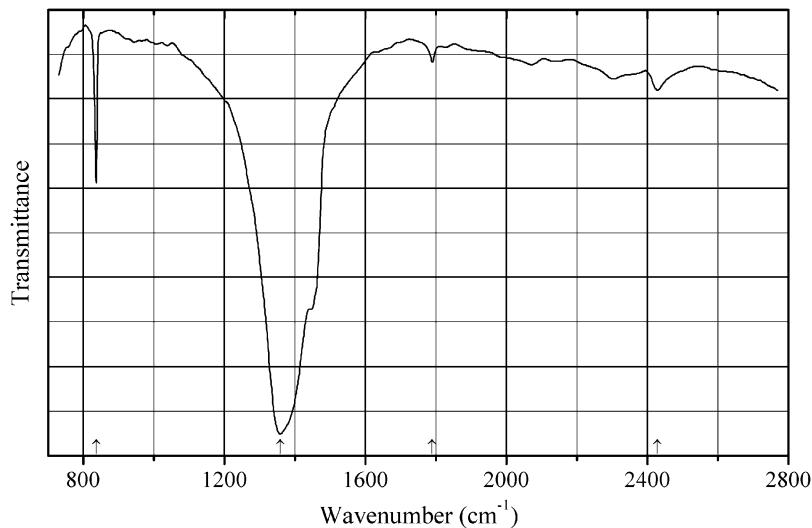
**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc. Transmission.

**Source:** Wild et al. (1978).

**Wavenumbers (cm<sup>-1</sup>):** 1035, 938s, 915s, 579, 441, 380.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

#### N24 Nitratine Na(NO<sub>3</sub>)



**Origin:** Synthetic.

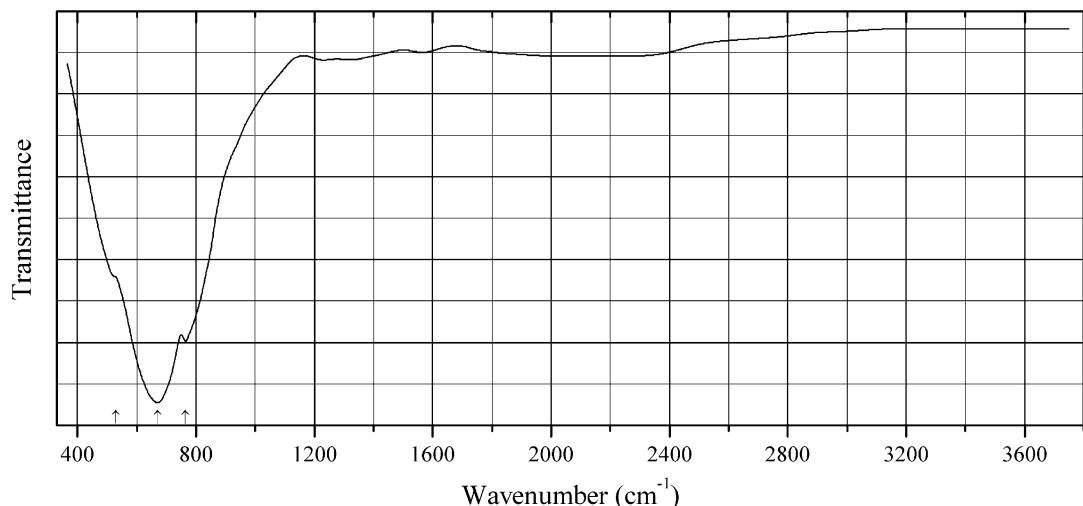
**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull. Transmission.

**Source:** Miller and Wilkins (1952).

**Wavenumbers (cm<sup>-1</sup>):** 2428w, 1790w, 1358s, 836.

**Note:** A shoulder near 1447 cm<sup>-1</sup> corresponds to Nujol.

#### N25 Osbornite TiN



**Origin:** Synthetic.

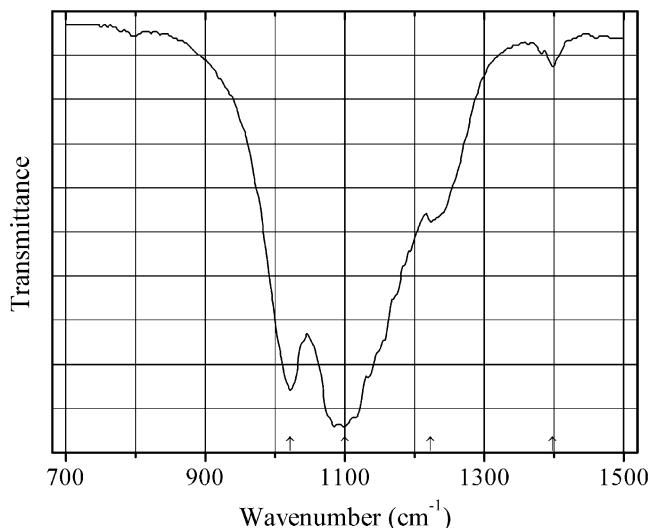
**Description:** A layer deposited using sequential additions of  $\text{TiCl}_4$  and  $\text{NH}_3$  on fumed silica powder.

**Kind of sample preparation and/or method of registration of the spectrum:** Diffuse reflection of a mixture with KBr powder.

**Source:** Snyder et al. (2006).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 765, 670s, 530sh.

### N26 Qingsongite BN



**Origin:** Synthetic.

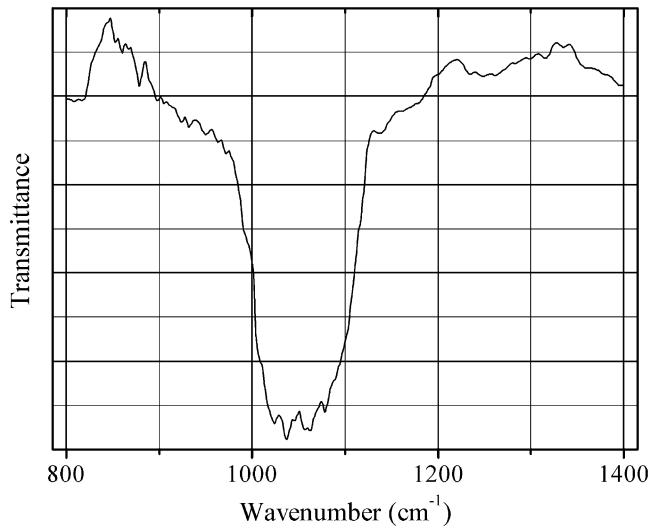
**Description:** Produced from hexagonal BN by spontaneous high pressure (5.5 GPa) and high temperature (1800–1900 K) nucleation using Mg as a solvent-catalyst.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Kutsay et al. (2010).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1398, 1223, 1100, 1022.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. The weak band at  $1398 \text{ cm}^{-1}$  corresponds to the admixture of hexagonal BN. In the cited paper, a figure of qingsongite Raman spectrum is given.

**N27 Qingsongite (C-bearing)  $\text{C}_{0.3}(\text{BN})_{0.7}$** 

**Origin:** Synthetic.

**Description:** Obtained from a mixture of hexagonal BN and graphite powders at 30 GPa and temperature between 2000 and 2500 K. Cubic,  $a = 3.613(3)$ . The observed lines of the powder X-ray diffraction pattern [ $d$ , Å ( $hkl$ )] are: 2.086 (111), 1.806 (200) (very weak), 1.276 (220).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Knittle et al. (1995).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** ~1045.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1323.

**N28 Sinoite  $\text{Si}_2\text{N}_2\text{O}$** 

**Origin:** Synthetic.

**Description:** Orthorhombic, space group  $Cmc2_1$ .

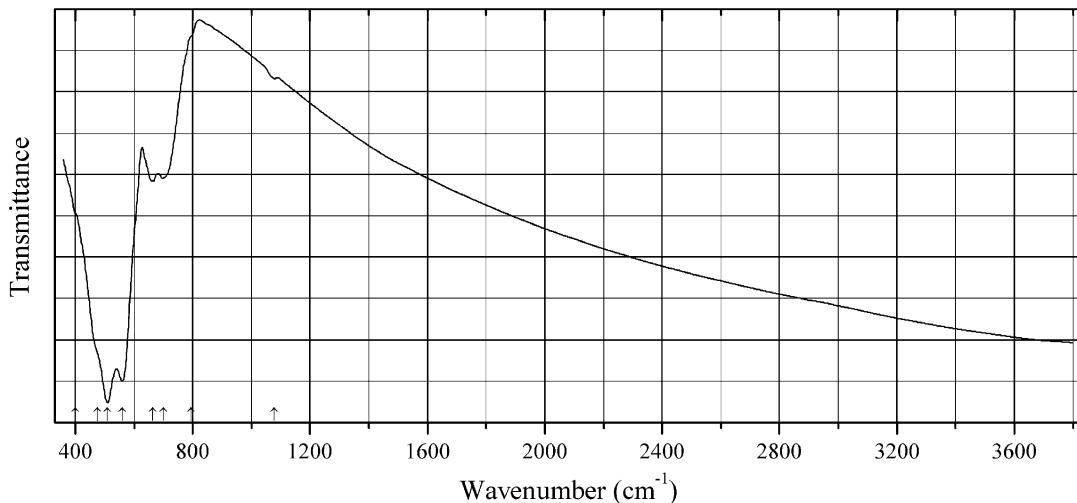
**Kind of sample preparation and/or method of registration of the spectrum:** No data.

**Source:** Mirgorodsky et al. (1989).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1130, 1070sh, 1030sh, 990, 953s, 906s, 730sh, 679, 648w, 542, 496, 448, 327, 252.

## 2.5 Oxides and Hydroxides

**O495 Ferricoronadite**  $\text{Pb}(\text{Mn}^{4+})_6\text{Fe}^{3+})_2\text{O}_{16}$



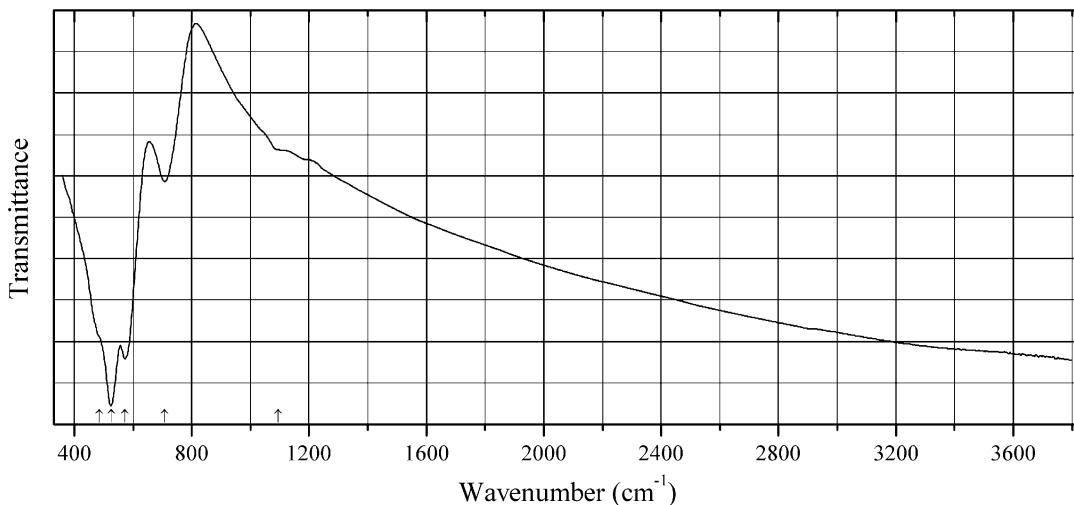
**Origin:** “Mixed Series” metamorphic complex near the Nežilovo village, Pelagonian massif, Republic of Macedonia (type locality).

**Description:** Veinlets in granular aggregate consisting of franklinite, gahnite, hetaerolite, roméite, almeidaite, Mn-analogue of plumboferrite, högbomite-group minerals, Zn-bearing talc, baryte, quartz, etc. Holotype sample. The crystal structure is solved. Tetragonal, space group  $I4/m$ ,  $a = 9.9043(7)$ ,  $c = 2.8986(9)$  Å,  $V = 284.34(9)$  Å<sup>3</sup>,  $Z = 1$ .  $D_{\text{calc}} = 5.538$  g/cm<sup>3</sup>. The empirical formula is (electron microprobe):  $\text{Pb}_{1.03}\text{Ba}_{0.32}(\text{Mn}^{4+})_{4.85}\text{Fe}^{3+}_{1.35}\text{Mn}^{3+}_{1.18}\text{Ti}_{0.49}\text{Al}_{0.09}\text{Zn}_{0.04})\text{O}_{16}$ . According to the Mössbauer spectrum, all iron is trivalent. The Mn  $K$ -edge XANES spectroscopy shows that Mn is predominantly tetravalent, with subordinate Mn<sup>3+</sup>. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 3.497 (33) (220), 3.128 (100) (-130, 130), 2.424 (27) (-121, 121), 2.214 (23) (240, -240), 2.178 (17) (031), 1.850 (15) (141, -141), 1.651 (16) (060), 1.554 (18) (-251, 251).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 1078w, 795sh, 700, 665, 560s, 510s, 475sh, 400sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**O496 Ferrihollandite**  $\text{Ba}(\text{Mn}^{4+}_6\text{Fe}^{3+}_2)\text{O}_{16}$ 

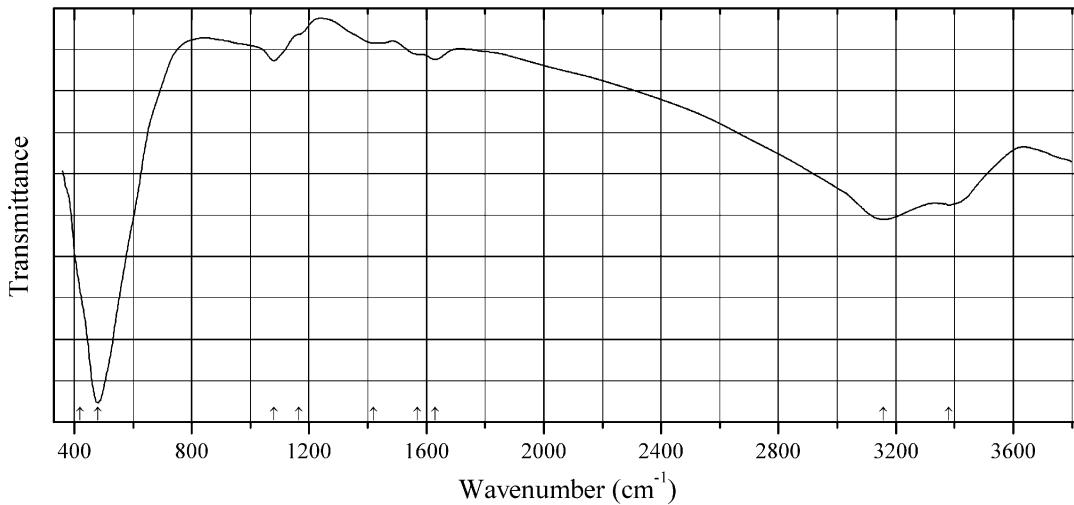
**Origin:** Sörhåras, Ultevis, Lappland, Sweden.

**Description:** Black prismatic crystals. The empirical formula is (electron microprobe):  $(\text{Ba}_{0.79}\text{K}_{0.17}\text{Pb}_{0.11}\text{Sr}_{0.07}\text{Na}_{0.07})(\text{Mn}_{6.22}\text{Fe}_{0.93}\text{Al}_{0.43}\text{Ti}_{0.32}\text{Mg}_{0.10}\text{Zn}_{0.02})\text{O}_8$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1095w, 708, 572s, 525s, 485sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**O497 Cesàrolite**  $\text{PbMn}^{4+}_3\text{O}_6(\text{OH})_2$ 

**Origin:** Belorechenskoe deposit, Adygea (Adygeya) Republic, Northern Caucasus, Russia.

**Description:** Black massive, with brown streak, from the association with baryte, dolomite, fluorite, galena, and gypsum. Investigated by A.V. Kasatkin. The empirical formula is (electron microprobe):  $\text{Pb}_{0.75}\text{Cu}_{0.2}\text{Zn}_{0.1}\text{Mn}_{3.0}(\text{O},\text{OH})_8$ . The strongest lines of the powder X-ray diffraction pattern are observed at 3.42, 3.13, 2.39, 2.21, 2.11, 1.88, 1.77, 1.69, 1.57, 1.48, and 1.41 Å.

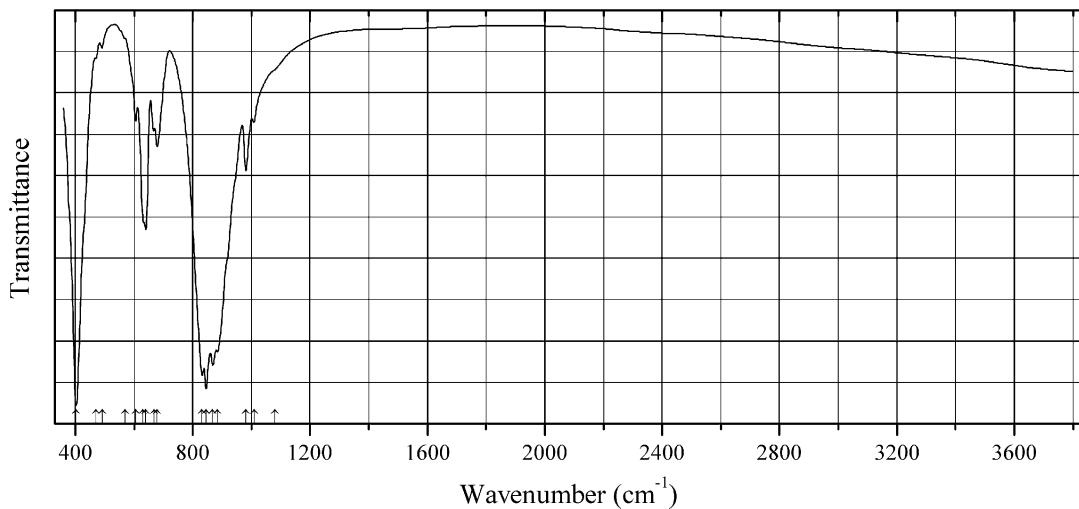
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3381, 3158s, 1630, 1570, 1420w, 1165sh, 1080, 480, (420sh).

**Note:** The band at 1630 cm<sup>-1</sup> may correspond to adsorbed water; the weak band at 1420 cm<sup>-1</sup> may be due to dolomite impurity.

**Note:** The spectrum was obtained by N.V. Chukanov.

#### O498 Sodalite Ca-Al-Mo-W-analogue $\text{Ca}_8(\text{Al}_{12}\text{O}_{24})[(\text{MoO}_4)_{1.5}(\text{WO}_4)_{0.5}]$



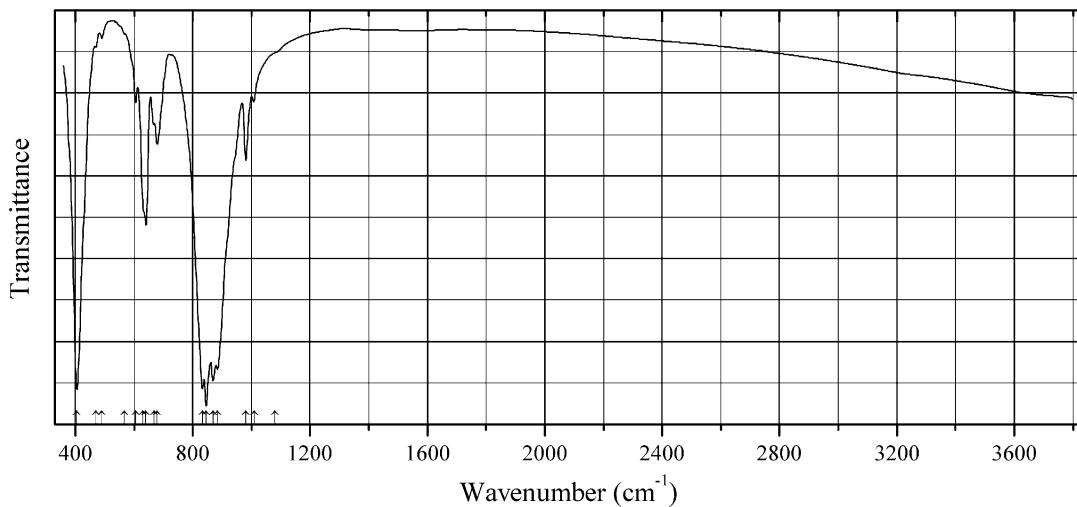
**Origin:** Synthetic.

**Description:** Synthesized in a solid-state reaction from the stoichiometric mixture of  $\gamma\text{-Al}_2\text{O}_3$ ,  $\text{CaCO}_3$ ,  $\text{MoO}_3$ , and  $\text{WO}_3$ . The sample was provided by Prof. W. Depmeier. Cubic or pseudocubic.  $\text{MoO}_4^{2-}$  and  $\text{WO}_4^{2-}$  are extra-framework anions. The composition is confirmed by electron microprobe analyses.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 1080sh, 1009, 982, 885s, 868s, 846s, 832s, 679, 668, 640, 630sh, 606, 570sh, 491w, 470w, 403s.

**Note:** The spectrum was obtained by N.V. Chukanov. The anions  $\text{MoO}_4^{2-}$  and  $\text{WO}_4^{2-}$  are almost indistinguishable by means of IR spectroscopy (compare powellite and scheelite).

**O499 Sodalite Ca-Al-Mo-W-analogue**  $\text{Ca}_8(\text{Al}_{12}\text{O}_{24})[(\text{MoO}_4)(\text{WO}_4)]$ 

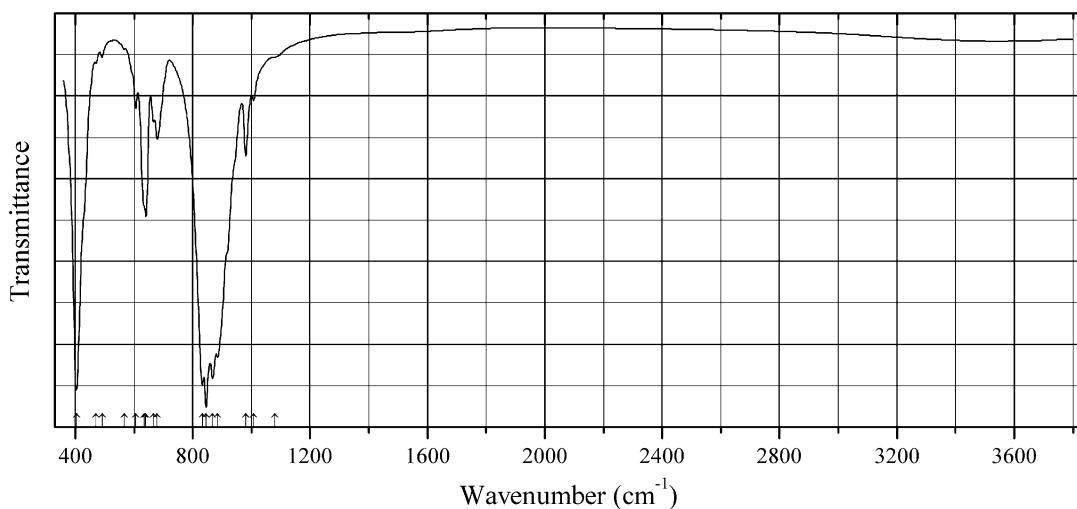
**Origin:** Synthetic.

**Description:** Synthesized in a solid-state reaction from the stoichiometric mixture of  $\gamma$ - $\text{Al}_2\text{O}_3$ ,  $\text{CaCO}_3$ ,  $\text{MoO}_3$ , and  $\text{WO}_3$ . The sample was provided by Prof. W. Depmeier. Cubic or pseudocubic.  $\text{MoO}_4^{2-}$  and  $\text{WO}_4^{2-}$  are extra-framework anions. The composition is confirmed by electron microprobe analyses.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1080sh, 1009, 981, 885s, 869s, 846s, 833s, 679, 668, 640, 630sh, 606, 568w, 490w, 470w, 406s.

**Note:** The spectrum was obtained by N.V. Chukanov. The anions  $\text{MoO}_4^{2-}$  and  $\text{WO}_4^{2-}$  are almost indistinguishable by means of IR spectroscopy (compare powellite and scheelite).

**O500 Sodalite Ca-Al-Mo-analogue**  $\text{Ca}_8(\text{Al}_{12}\text{O}_{24})[(\text{MoO}_4)(\text{WO}_4)]$ 

**Origin:** Synthetic.

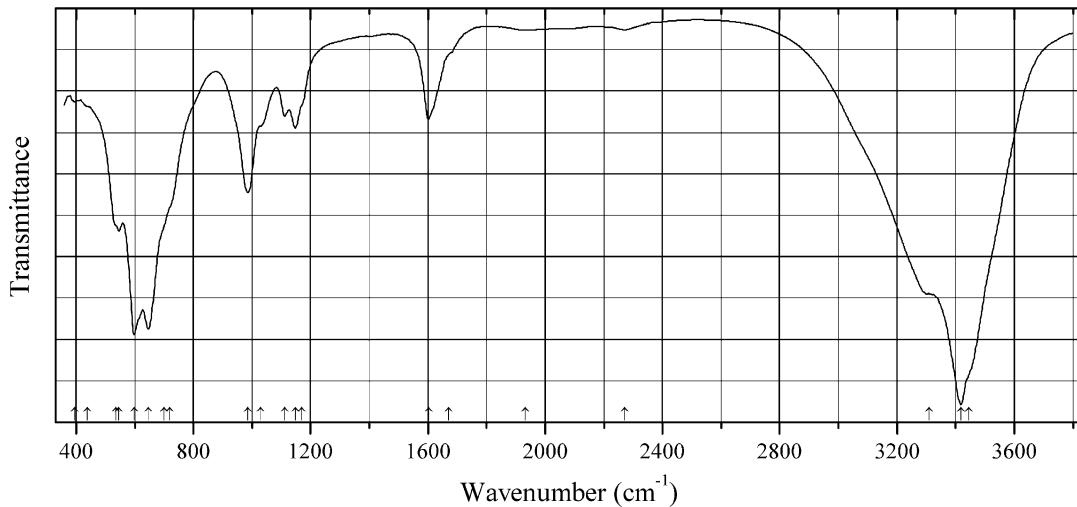
**Description:** Synthesized in a solid-state reaction from the stoichiometric mixture of  $\gamma\text{-Al}_2\text{O}_3$ ,  $\text{CaCO}_3$ , and  $\text{MoO}_3$ . The sample was provided by Prof. W. Depmeier. Cubic or pseudocubic.  $\text{MoO}_4^{2-}$  is extra-framework anion. The composition is confirmed by electron microprobe analyses.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1080, 1008, 981, 885s, 868s, 846s, 833s, 679, 667, 641, 635sh, 606, 568w, 491w, 470w, 404s.

**Note:** The spectrum was obtained by N.V. Chukanov.

### O501 Lesukite Cu-bearing variety $(\text{Al,Cu})_2(\text{OH})_{5-x}\text{Cl}\cdot n\text{H}_2\text{O}$ ( $n \approx 2$ )



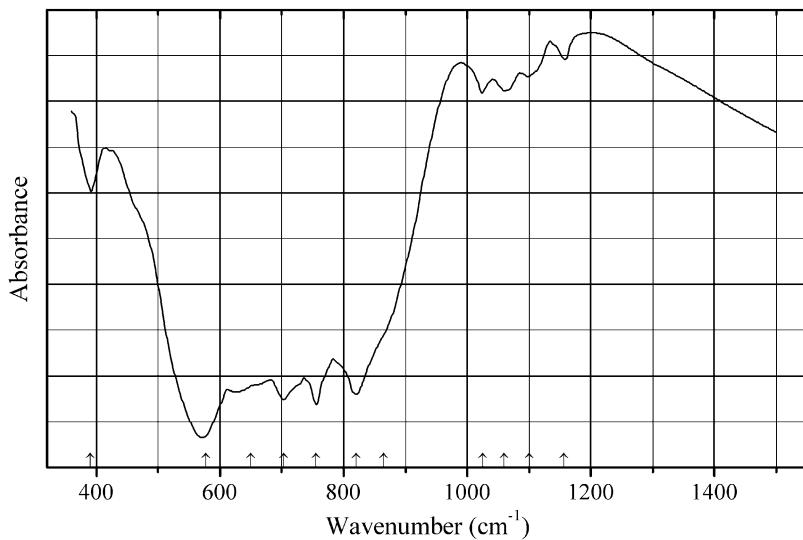
**Origin:** Cerro Mejillones, Mejillones Peninsula, Mejillones, Antofagasta, II Region, Chile.

**Description:** Lemon-yellow powdery aggregate consisting of microscopic cubic crystals from the association with gypsum, atacamite, and goethite. Investigated by I.V. Pekov. Characterized by powder X-ray diffraction data. The empirical formula is (electron microprobe):  $(\text{Al}_{1.85}\text{Cu}_{0.15})(\text{OH})_{4.85}\text{Cl}_{1.00}\cdot n\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3445sh, 3418s, 3310s, 2271w, 1933w, 1670sh, 1602, 1170sh, 1148, 1111, 1030sh, 986, 720sh, 700sh, 647s, 598s, 546, 535sh, 440w, 395w.

**Note:** The spectrum was obtained by N.V. Chukanov.

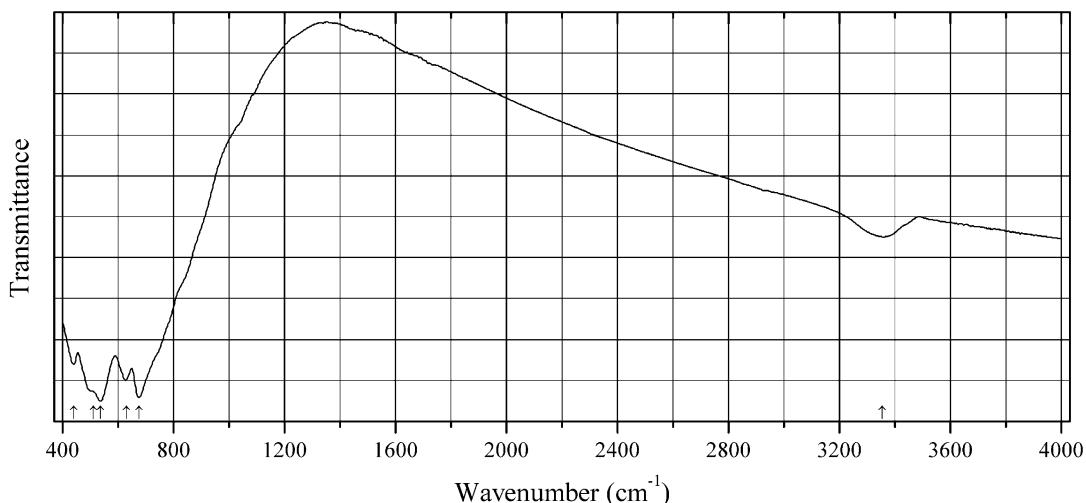
**O502 Deltalumite  $\delta\text{-Al}_2\text{O}_3$** 

**Origin:** Western lava flow of the 2012–2013 Tolbachik Fissure Eruption, Tolbachik volcano, Kamchatka Peninsula, Far-Eastern Region, Russia (type locality).

**Description:** Pale beige spherical clusters from the association with corundum and moissanite. Holotype sample. Tetragonal, space group  $P-4m2$ ,  $a = 5.608(1)$ ,  $c = 23.513(7)$  Å,  $V = 739.4(4)$  Å<sup>3</sup>,  $Z = 16$ .  $D_{\text{calc}} = 3.663$  g/cm<sup>3</sup>. Optically uniaxial (−),  $\omega = 1.654(2)$ ,  $\epsilon = 1.653(2)$ . The empirical formula is (electron microprobe):  $\text{Al}_{2.00}\text{O}_3$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 2.728 (61) (202), 2.424 (51) (212), 2.408 (49) (213), 2.281 (42) (206), 1.993 (81) (1.011, 220, 221), 1.954 (48) (0.012), 1.396 (100) (327, 3.011, 400, 401, 2.1.14, 2.2.12).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption. **Wavenumbers (cm<sup>-1</sup>):** 1157w, 1100w, 1063w, 1024w, 865sh, 820s, 755s, 703s, 628, 571s, 391.

**Note:** The spectrum was obtained by N.V. Chukanov.

**O503 Magnesiohögbonite-2N3S ( $\text{Mg,Fe,Zn,Ti}_4(\text{Al,Fe})_{10}\text{O}_{19}(\text{OH})$ )**

**Origin:** Sadok Lake, Chelyabinsk region, South Urals.

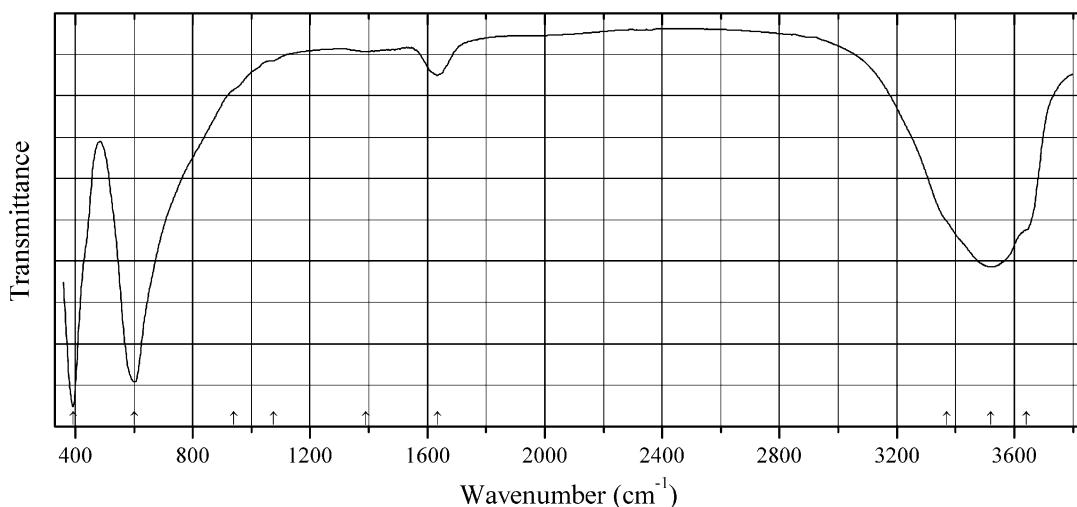
**Description:** Dark brown platy grains from clinopyroxenite. Characterized by powder X-ray diffraction data and Mössbauer spectroscopy. Hexagonal,  $a = 5.715(5)$ ,  $c = 23.931(2)$  Å,  $V = 677.01(4)$  Å<sup>3</sup>. The empirical formula is  $(\text{Mg}_{5.4-5.7}\text{Fe}^{3+}_{1.4-1.7}\text{Fe}^{2+}_{0.8-0.9})(\text{Al}_{18.0-18.6}\text{Ti}_{1.0-1.1}\text{Fe}^{3+}_{0.4-0.9}\text{Cr}_{0-0.1})\text{O}_{38}(\text{OH})_2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Korinevsky et al. (2016).

**Wavenumbers (cm<sup>-1</sup>):** 3355, 675s, 630s, 536s, 511sh, 440.

#### O504 Woodallite $\text{Mg}_6\text{Cr}_2(\text{OH})_{16}\text{Cl}_2 \cdot 4\text{H}_2\text{O}$



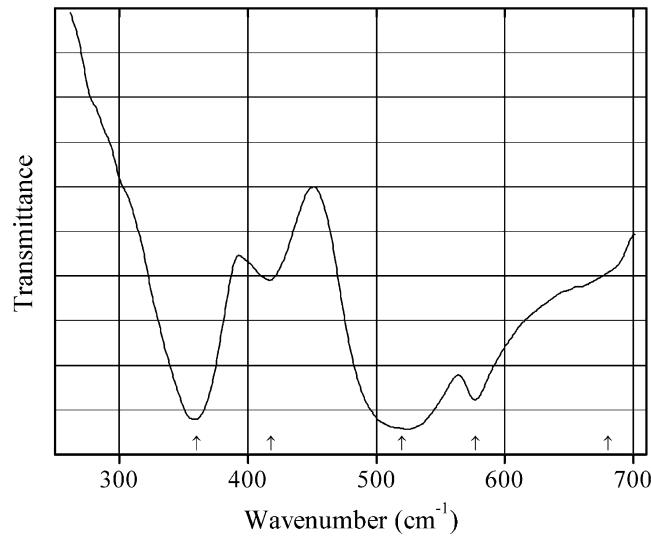
**Origin:** Kyzyl-Uyuk stream, Terektn ridge, Altai Mts., Siberia, Russia.

**Description:** Lilac crust on serpentine. Investigated by I.V. Pekov. The empirical formula is (electron microprobe):  $(\text{Mg}_{5.90}\text{Fe}_{0.10})(\text{Cr}_{0.94}\text{Fe}_{0.89}\text{Al}_{0.17})\text{Cl}_{1.92}(\text{SO}_4)_{0.02}(\text{CO}_3)_x(\text{OH})_{16} \cdot 4\text{H}_2\text{O}$  ( $x \ll 1$ ). The sample contains zones with  $\text{Fe:Cr} \approx 1:1$  in atomic units.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3640sh, 3520s, 3370sh, 1635, 1390w, 1076w, 940sh, 600s, 392s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**O505 Gallium(III) oxide  $\alpha\text{-Ga}_2\text{O}_3$** 

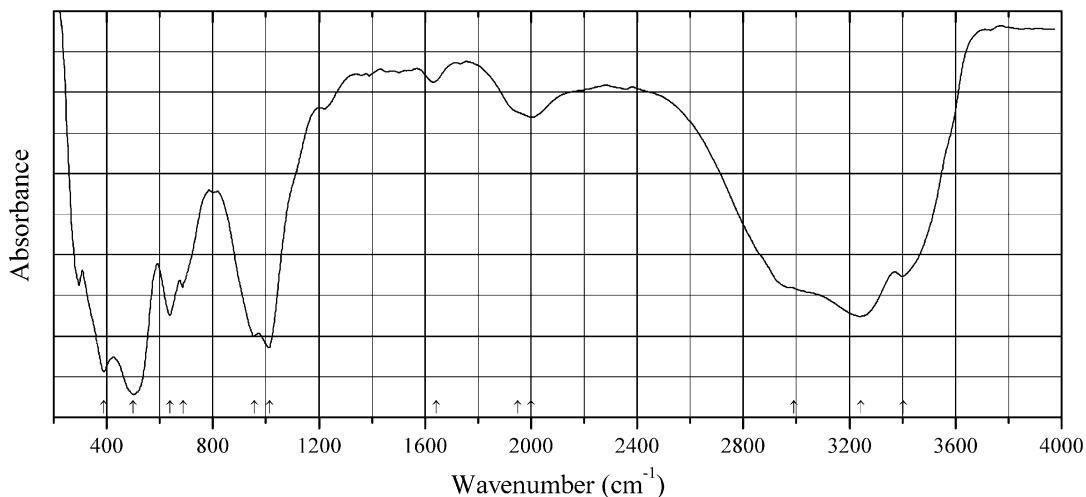
**Origin:** Synthetic.

**Description:** Prepared by the precipitation from  $\text{GaCl}_3$  aqueous solution, by adding aqueous solution of tetramethyl ammonium hydroxide up to pH 7.82. After 2 h of aging at room temperature the precipitate was dried and heated at 500 °C for 4 h in air. Confirmed by powder X-ray diffraction data. Trigonal, space group  $R\text{-}3c$ ,  $a = 4.982$ ,  $c = 13.433$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Ristić et al. (2005).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 680sh, 577, 520s, 418, 360s.

**O506 Gallium(III) oxyhydroxide  $\alpha\text{-GaOOH}$** 

**Origin:** Synthetic.

**Description:** Prepared by the precipitation from  $\text{GaCl}_3$  aqueous solution, by adding aqueous solution of tetramethyl ammonium hydroxide up to pH 7.82. Confirmed by powder X-ray diffraction data.

Isostructural with goethite. Orthorhombic, space group  $Pbnm$ ,  $a = 4.58$ ,  $b = 9.80$ ,  $c = 2.97 \text{ \AA}$ .

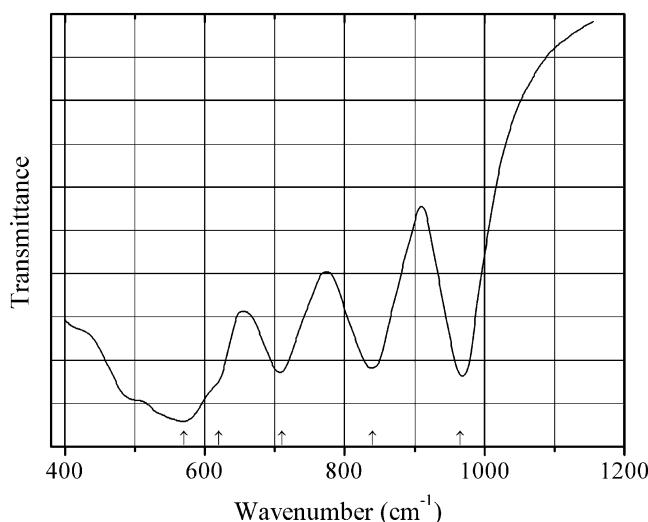
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Ristić et al. (2005).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3403, 3243s, 2990, 2000, 1950, 1642w, 1221w, 1015s, 958s, 688, 640, 500s, 388s, 295.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### O507 Aluminium niobate $\text{AlNbO}_4$



**Origin:** Synthetic.

**Description:** Prepared by firing intimate mixture of  $\text{Al(OH)}_3$  and  $\text{Nb}_2\text{O}_5$  in air at 1350 °C. Monoclinic.  
Characterized by powder X-ray diffraction data.

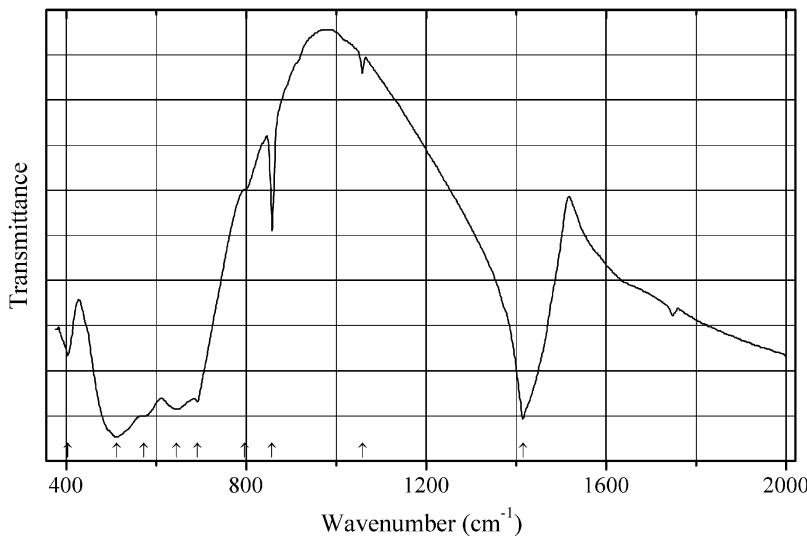
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Blasse and 'T Lam (1978).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 965, 840, 710, 620sh, 570.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 940sh, 800, 730, 690, 600, 400.

**O508 Barium cerium tantalite  $\text{Ba}_2\text{CeTaO}_6$** 

**Origin:** Synthetic.

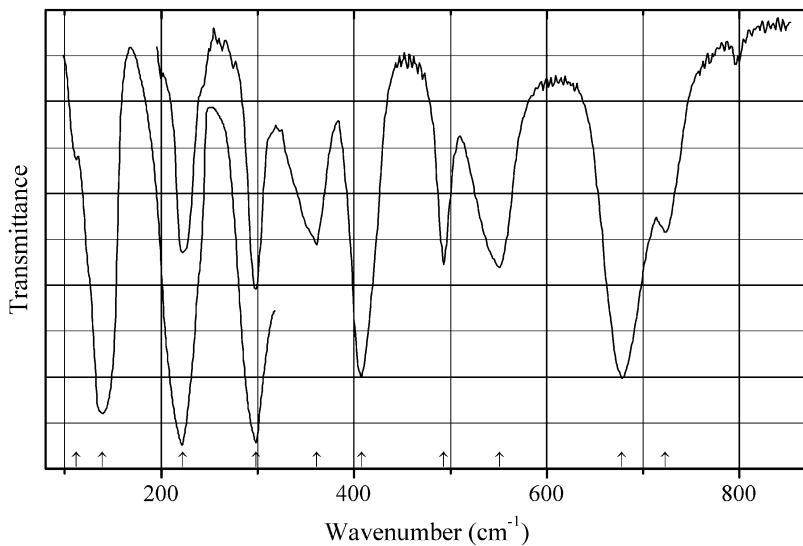
**Description:** Obtained in the solid-state reaction between  $\text{BaCO}_3$ ,  $\text{Ce}_2(\text{CO}_3)_3$ , and  $\text{Ta}_2\text{O}_5$ . The reactant mixture taken in stoichiometric ratio was calcined at 1350 °C for 15 h. The calcined sample was pelletized into a disk with polyvinyl alcohol as binder and sintered at 1370 °C for 5 h. Characterized by powder X-ray diffraction data. Monoclinic,  $a = 9.78$ ,  $b = 9.02$ ,  $c = 4.27 \text{ \AA}$ ,  $\beta = 93.8^\circ$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Bharti and Sinha (2011).

**Wavenumbers (cm<sup>-1</sup>):** 645, 573sh, 512s, 404.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. The bands at 1747, 1415, 1058, 857, 796(sh), and 691  $\text{cm}^{-1}$  correspond to the admixture of a carbonate. In the cited paper, the absorptions in the ranges 1700–1800 and 1400–1500  $\text{cm}^{-1}$  have been erroneously assigned to the presence of adsorbed moisture in KBr and symmetric stretching vibrations of  $\text{TaO}_6$  octahedra, respectively.

**O509 Barium cobalt antimonate**  $\text{Ba}_3\text{CoSb}_2\text{O}_9$ 

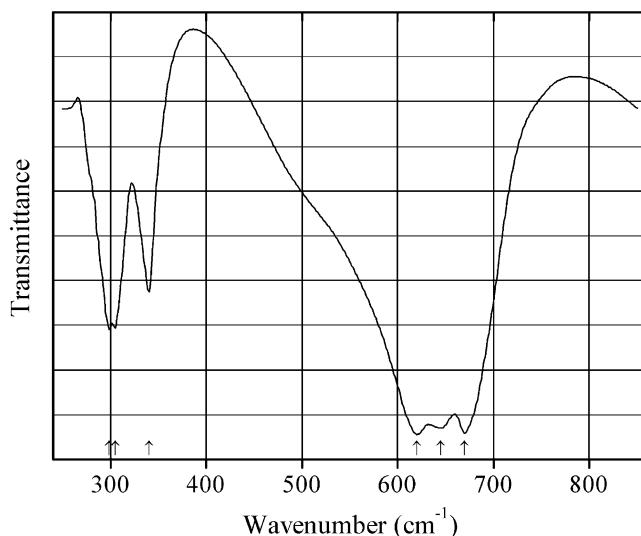
**Origin:** Synthetic.

**Description:** A compound with ordered hexagonal perovskite-type structure.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

**Source:** Liegeois-Duyckaerts (1985).

**Wavenumbers (cm⁻¹):** 723, 678s, 551, 493, 408s, 361, 298, 222, 139, 112.

**O510 Barium cobaltate**  $\text{Ba}_2\text{CoO}_4$ 

**Origin:** Synthetic.

**Description:** Synthesized from the mixture of barium and cobalt carbonates at 950 °C. Confirmed by chemical analyses and powder X-ray diffraction data.

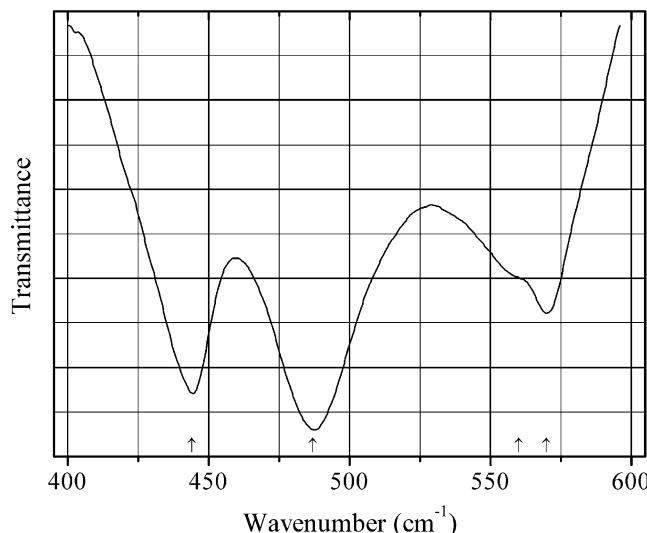
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Baran (1973).

**Wavenumbers (cm<sup>-1</sup>):** 670s, 645s, 620s, 340, 305, 299.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### O511 Barium nickel oxide BaNiO<sub>2</sub> BaNiO<sub>2</sub>



**Origin:** Synthetic.

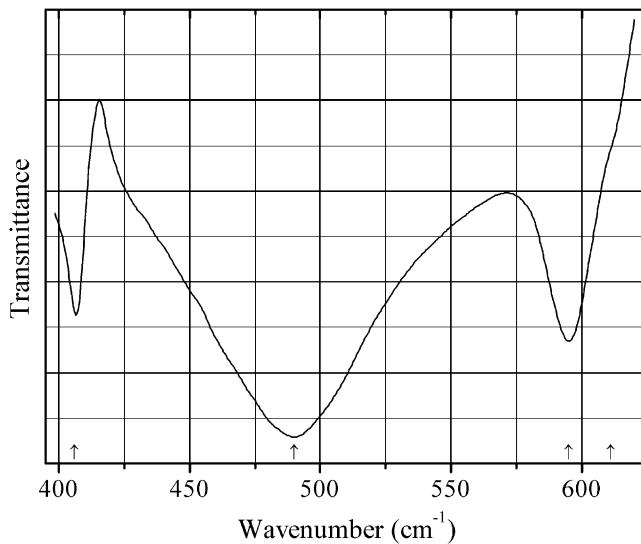
**Description:** Prepared by the conventional sintering process from NiO and BaCO<sub>3</sub>. Characterized by Mössbauer spectrum and powder X-ray diffraction data. Orthorhombic,  $a = 5.737$ ,  $b = 9.190$ ,  $c = 4.760$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Gottschall et al. (1998).

**Wavenumbers (cm<sup>-1</sup>):** 570, 560sh, 487s, 444s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**O512 Barium nickel oxide  $\text{BaNiO}_3$   $\text{BaNiO}_3$** 

**Origin:** Synthetic.

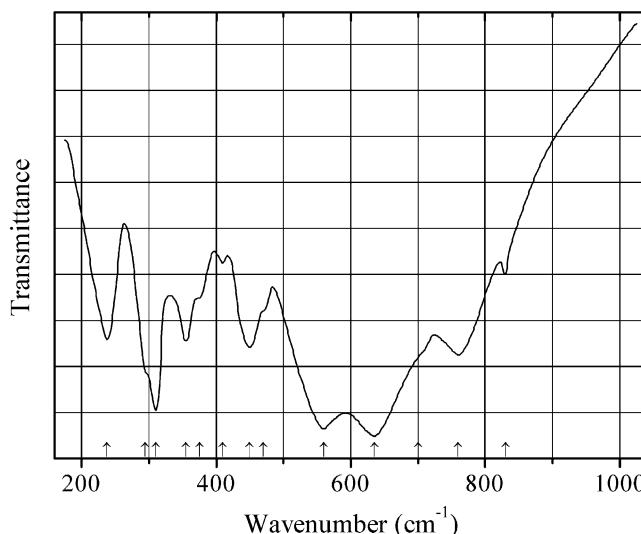
**Description:** Prepared by the conventional sintering process from  $\text{NiO}$  and  $\text{BaCO}_3$ . Characterized by Mössbauer spectrum and powder X-ray diffraction data. Hexagonal,  $a = 5.635$ ,  $c = 4.8041 \text{ \AA}$ . Hypothetically, Ni is trivalent and the formula is  $\text{Ba}^{2+}\text{Ni}^{3+}\text{O}^{2-}_2(\text{O}^{\cdot})^-$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Gottschall et al. (1998).

**Wavenumbers (cm<sup>-1</sup>):** 611sh, 595, 490s, 406.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**O513 Barium niobate  $\text{BaNb}_2\text{O}_6$** 

**Origin:** Synthetic.

**Description:** Prepared by heating stoichiometric mixture of  $\text{Nb}_2\text{O}_5$  and  $\text{BaCO}_3$  pressed in a pellet at 1200 °C for 60 h. Orthorhombic, space group  $Pbmm$ ,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission.

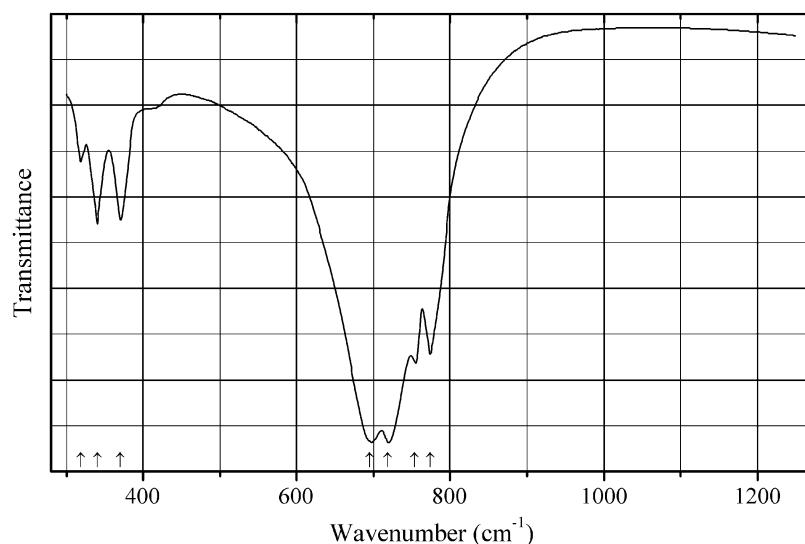
**Source:** Repelin et al. (1979).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 830w, 760, 700sh, 635s, 560s, 470sh, 450, 410w, 375sh, 355, 310s, 295sh, 238, 170, 151, 87.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 847, 712s, 633, 557s, 496, 379, 366, 306, 280, 230, 200, 190, 141, 120, 112, 100.

#### O514 Barium titanate $\text{Ba}_2\text{TiO}_4$



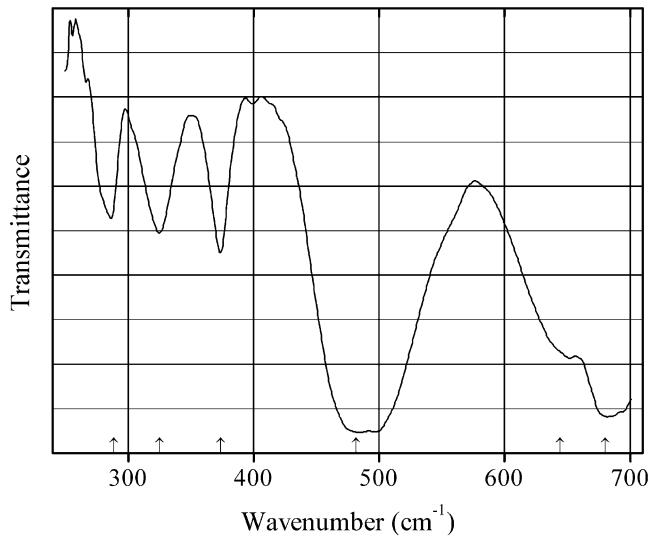
**Origin:** Synthetic.

**Description:** Obtained by heating a mixture of  $\text{TiO}_2$  and  $\text{BaCO}_3$  at 1200–1300 °C for 1–3 days.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Wijzen et al. (1994).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 774, 753, 719s, 695s, 370, 340, 319w.

**O515  $\beta$ -Gallium(III)-oxide  $\beta\text{-Ga}_2\text{O}_3$** 

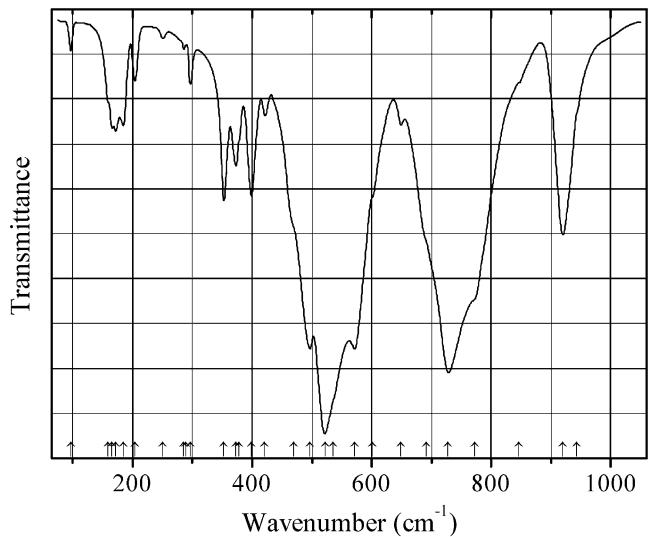
**Origin:** Synthetic.

**Description:** Monoclinic, space group  $C2/m$ ,  $a = 12.21$ ,  $b = 3.037$ ,  $c = 5.798 \text{ \AA}$ ,  $\beta = 103.838^\circ$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Ristić et al. (2005).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 680, 644, 482s, 374, 325, 289.

**O516 Bismuth(III) aluminate  $\text{Bi}_2\text{Al}_4\text{O}_9$   $\text{Bi}_2\text{Al}_4\text{O}_9$** 

**Origin:** Synthetic.

**Description:** Synthesized from a stoichiometric mixture of  $\text{Bi}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$  and  $\text{Al}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$  together with 10 wt.% of glycerine. The mixture was heated first at 353 K, then at 473 K for 2 h, and finally (after homogenization the powder) at 1210 K for 48 h. Structurally related to mullite.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Absorption.

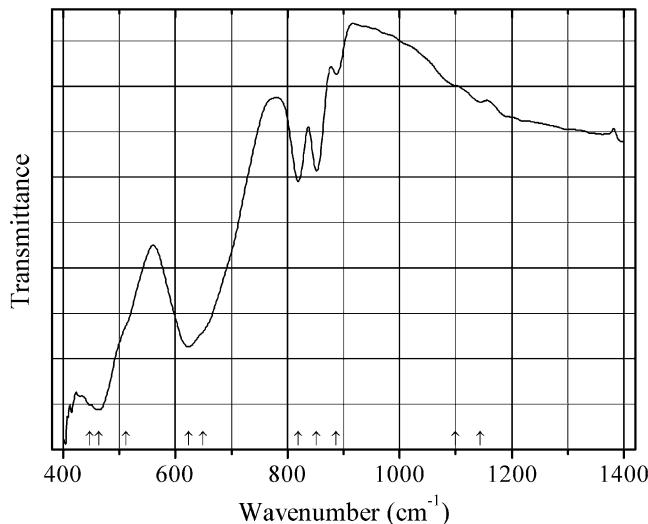
**Source:** Murshed et al. (2015).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** (943sh), 920, 846sh, 772sh, 728s, 691sh, 649, 601sh, 572s, 536sh, 522s, 497s, 470sh, 421w, 399, 378sh, 373, 353, 297w, 289sh, 286w, 251w, 204w, 185, 172, 166, 159, 97w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 840, 763, 691, 633, 615, 571, 509, 491, 478, 441, 406, 385, 373, 345, 322, 312, 281, 274s, 251, 184, 138, 120s, 103.

### O517 Bismuth(III) aluminoferrite $\text{Bi}_2\text{Fe}_3\text{AlO}_9$ , $\text{Bi}_2\text{Fe}_3\text{AlO}_9$



**Origin:** Synthetic.

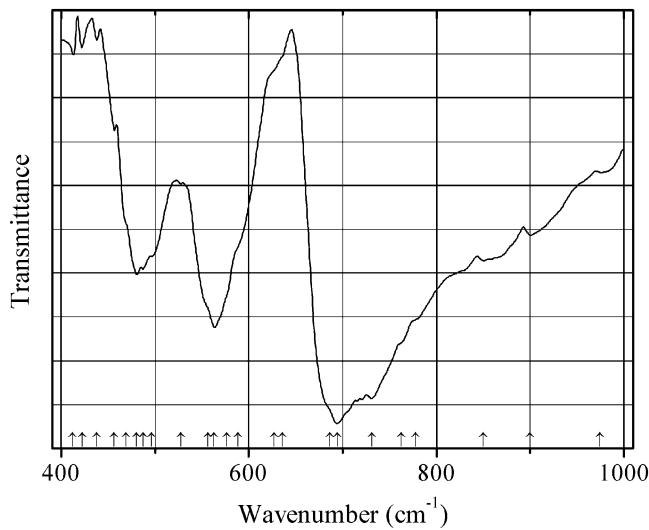
**Description:** Produced by thermal decomposition of a mixture of corresponding metal nitrates using a glycerine method. Structurally related to mullite.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Voll et al. (2006).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1144w, 1100sh, 887w, 852, 819, 650sh, 624s, 512sh, 464s, 448sh.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**O518 Bismuth(III) stannate pyrochlore-type  $\text{Bi}_2\text{Sn}_2\text{O}_7$** 

**Origin:** Synthetic.

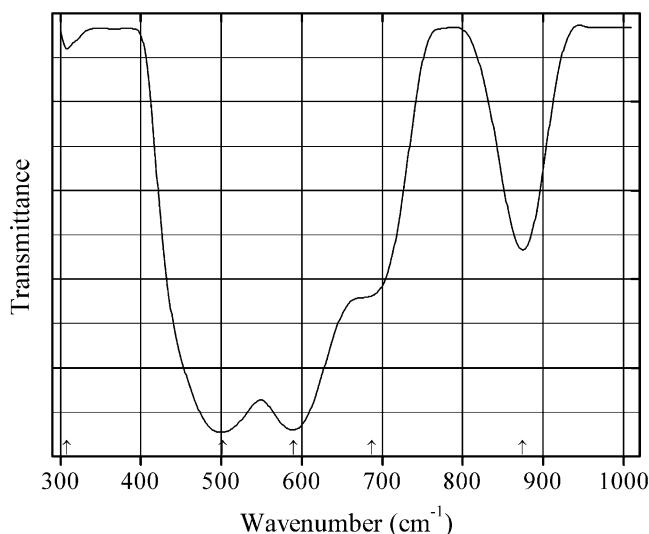
**Description:** Obtained by sintering at 1173 K of pelletized precipitate formed after adding ammonia solution to the 0.01 M solution containing bismuth chloride and stannous oxy chloride in stoichiometric ratio. Tetragonal,  $a = 21.328$ ,  $c = 21.4 \text{ \AA}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Ravi et al. (1999).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 731s, 694s, 686sh, 636sh, 627sh, 588sh, 576sh, 563, 556sh, 496sh, 487, 480, 469sh.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**O519 Bismuth(III) tantalate  $\text{Bi}_7\text{Ta}_3\text{O}_{18}$   $\text{Bi}_7\text{Ta}_3\text{O}_{18}$** 

**Origin:** Synthetic.

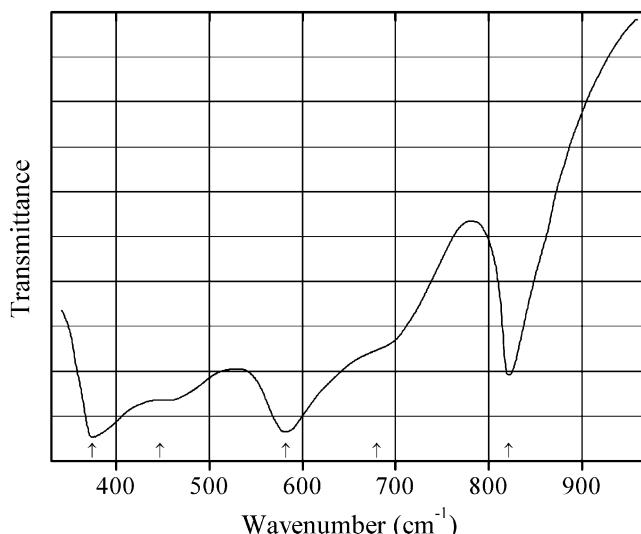
**Description:** Obtained from  $\text{Bi}_2\text{O}_3$  and  $\text{Ta}_2\text{O}_5$  by solid-state method at  $950\text{ }^\circ\text{C}$  for 18 h. Monoclinic, space group  $C2/m$ ,  $a = 34.060(3)$ ,  $b = 7.618(9)$ ,  $c = 6.647(6)\text{ \AA}$ ,  $\beta = 109.210(7)^\circ$ ,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Chon et al. (2014).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 874, 687sh, 590s, 502s, 308w.

#### O520 Bismuth(III) titanate $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ $\text{Bi}_4\text{Ti}_3\text{O}_{12}$



**Origin:** Synthetic.

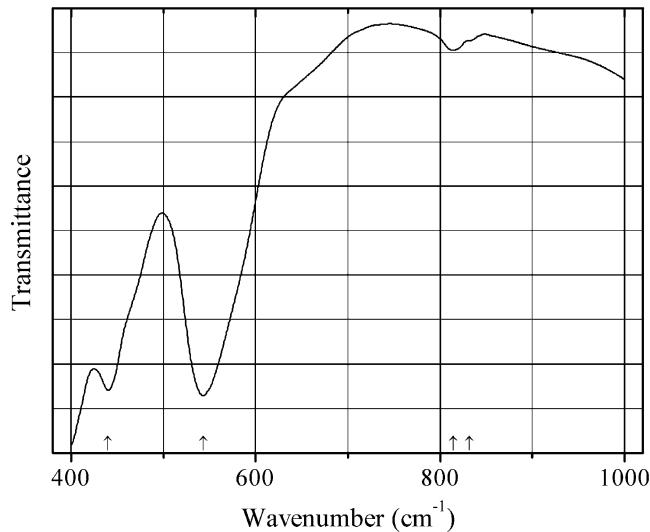
**Description:** Prepared hydrothermally. Structurally related to perovskite. The strongest lines of the powder X-ray diffraction pattern are observed at  $3.81$ ,  $2.95$ ,  $2.72$ ,  $2.26$ ,  $1.92$ , and  $1.61\text{ \AA}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Chen and Jiao (2001).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 822, 680sh, 582s, 447sh, 374s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**O521 Bismuth ferrite  $\text{BiFeO}_3$** 

**Origin:** Synthetic.

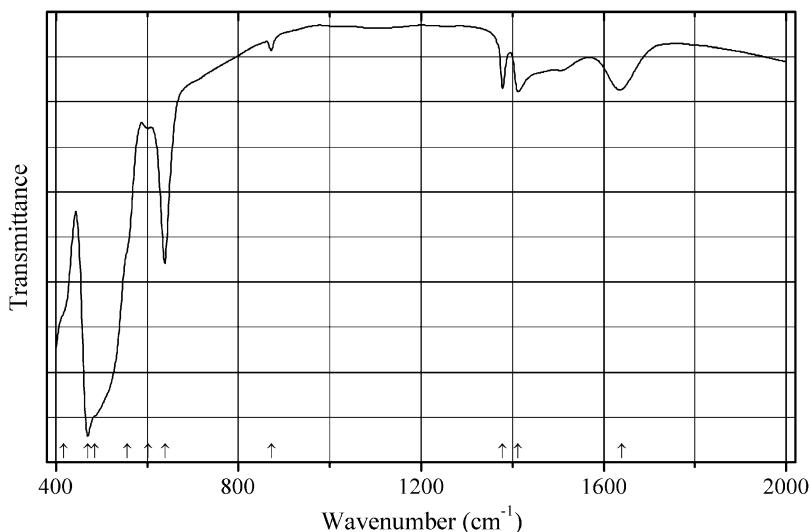
**Description:** Obtained by two-stage solid phase synthesis from  $\text{Bi}_2\text{O}_3$  and  $\text{Fe}_2\text{O}_3$ , first at 923 K for 1 h and thereafter (after re-grounding and pressing) at 1123 K for 2 h. The compound has rhombohedrally distorted perovskite structure, space group  $R\bar{3}c$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Bujakiewicz-Korońska et al. (2011).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 832sh, 814w, 543s, 440s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, also FIR spectrum for a sample suspended in Apiezon N grease is given.

**O522 Calcium indium oxide  $\text{Ca}_2\text{InO}_4$   $\text{Ca}_2\text{InO}_4$** 

**Origin:** Synthetic.

**Description:** Prepared from indium and calcium nitrates, in solid-state reaction at 1173 K for 2 h.

Characterized by powder X-ray diffraction data. Orthorhombic, space group  $Pca2_1$  or  $Pbcm$ ,  $Z = 4$  (see JCPDS 017-0643).

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

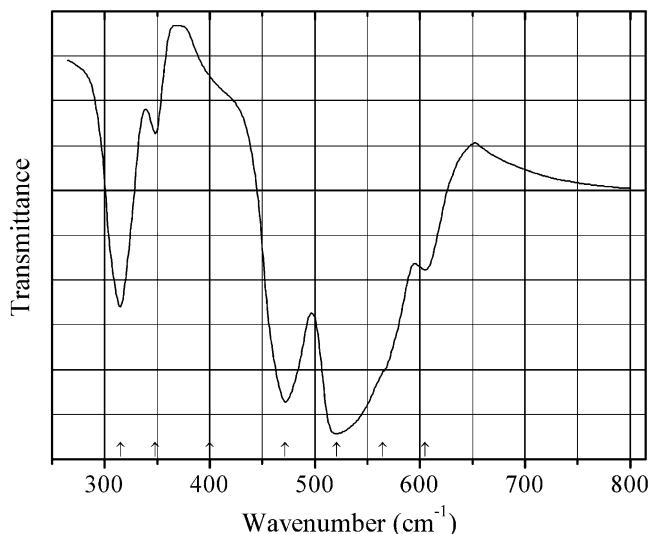
**Source:** Zheng et al. (2012).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1639w, 1412w, 1378w, 872w, 639, 602, 556sh, 485sh, 470s, 417sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The weak bands at 1639, 1412+872, and 1378  $\text{cm}^{-1}$  may correspond to  $\text{H}_2\text{O}$ ,  $\text{CO}_3^{2-}$ , and  $\text{NO}_3^-$  impurities, respectively. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 648w, 543s, 495, 455, 403, 370w, 336, 284w, 258, 199, 113s.

### O523 Cadmium stannate $\text{CdSnO}_3$



**Origin:** Synthetic.

**Description:** Obtained by thermal decomposition of  $\text{CdSn}(\text{OH})_6$  at 540 °C during 15 min.

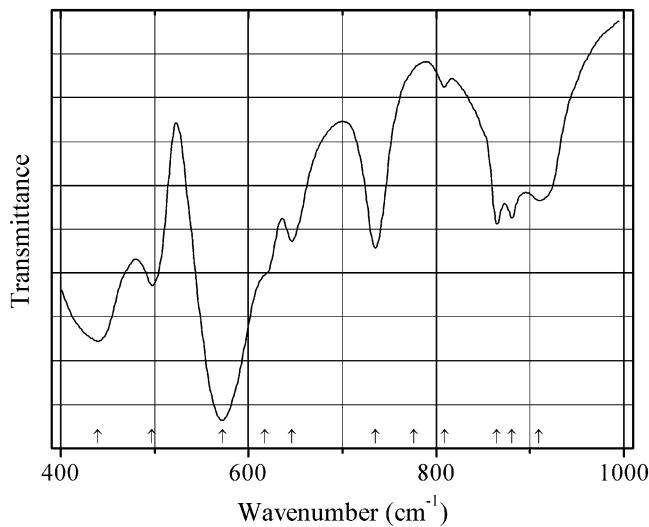
Characterized by powder X-ray diffraction data. Isostructural with ilmenite.

**Kind of sample preparation and/or method of registration of the spectrum:** CsIr disc. Transmission.

**Source:** Botto and Baran (1980).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 605, 565sh, 521s, 472s, 400sh, 348w, 315.

**Note:** The sample contains minor admixture of a spinel-type stannate.

**O524 Cesium uranyl niobate  $\text{Cs}_2(\text{UO}_2)_2(\text{Nb}_2\text{O}_8)$   $\text{Cs}_2(\text{UO}_2)_2(\text{Nb}_2\text{O}_8)$ , or  $\text{CsUNbO}_6$** 

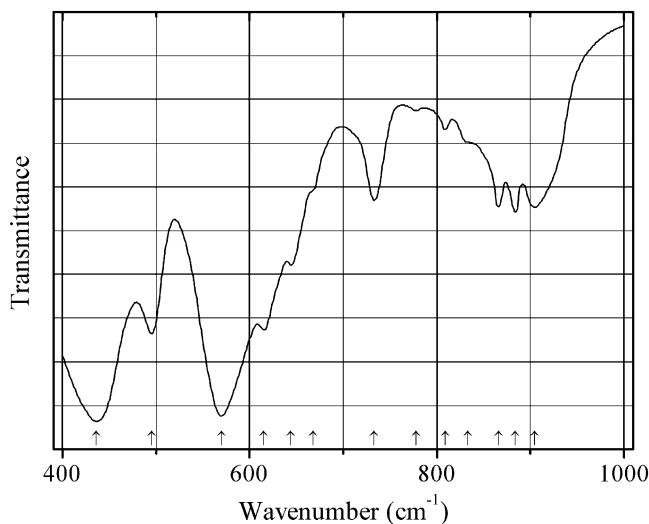
**Origin:** Synthetic.

**Description:** Carnotite-type niobate with  $\text{UNbO}_6$  layers.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Saad et al. (2008).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 910, 881, 865, 809w, 776sh, 735, 646, 617sh, 572s, 497, 439s.

**O525 Cesium uranyl niobate  $\text{Cs}_9[(\text{UO}_2)_8\text{O}_4(\text{NbO}_5)(\text{Nb}_2\text{O}_8)_2]$   $\text{Cs}_9[(\text{UO}_2)_8\text{O}_4(\text{NbO}_5)(\text{Nb}_2\text{O}_8)_2]$** 

**Origin:** Synthetic.

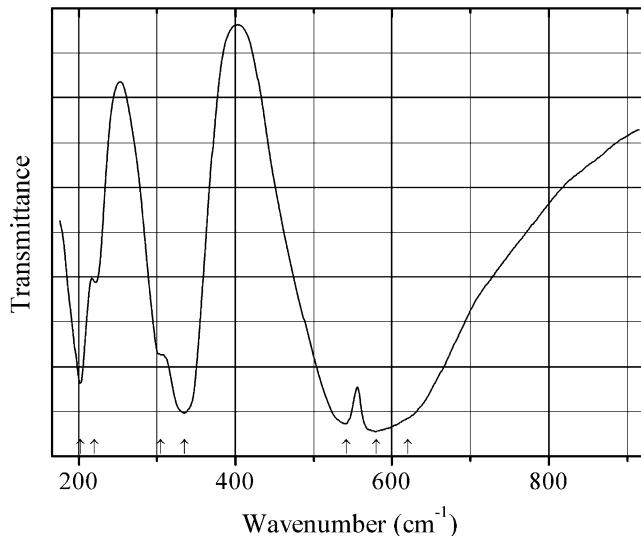
**Description:** Prepared from  $\text{CsNO}_3$ ,  $\text{U}_3\text{O}_8$ , and  $\text{Nb}_2\text{O}_5$  by solid-state reaction at 1000 °C in air. Monoclinic, space group  $P2_1/c$ ,  $a = 16.729(2)$ ,  $b = 14.933(2)$ ,  $c = 20.155(2)$  Å,  $\beta = 110.59(1)$ °,  $V = 4713.5(1)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{meas}} = 5.94(2)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 5.95(3)$  g/cm<sup>3</sup>. The crystal structure is based on the uranyl niobate layer containing  $\text{UO}_7$  pentagonal bipyramids and  $\text{NbO}_5$  square pyramids.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Saad et al. (2008).

**Wavenumbers (cm<sup>-1</sup>):** 905, 884, 866, 833sh, 809w, 778w, 733, 668sh, 644, 615, 570s, 495, 436s.

### O526 Calcium antimonite $\text{CaSb}_2\text{O}_6$



**Origin:** Synthetic.

**Description:** Obtained in a solid-state reaction between  $\text{CaCO}_3$  and  $\text{Sb}_2\text{O}_3$ . In the crystal structure,  $\text{SbO}_6$  octahedra are present. Trigonal, space group  $P-31/m$ ,  $a = 5.22$ ,  $c = 5.01$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc. Transmission.

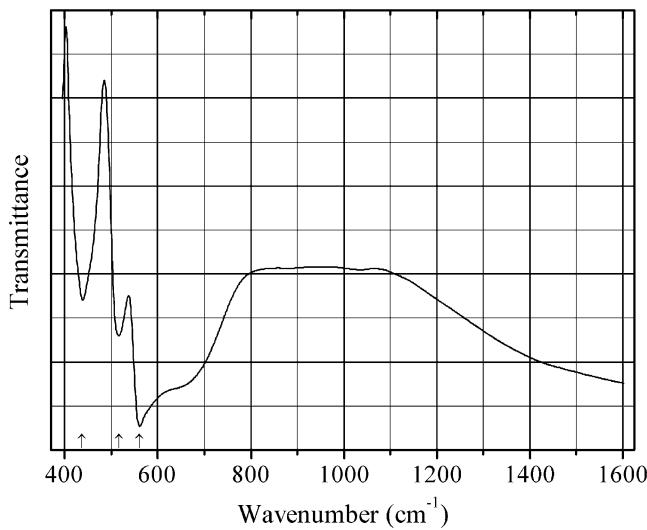
**Source:** Husson et al. (1984).

**Wavenumbers (IR, cm<sup>-1</sup>):** 620sh, 580s, 542s, 335s, 305sh, 220, 202.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 678s, 530, 498w, 345, 332, 243s.

**Note:** The wavenumbers of Sb–O stretching bands (at 580 and 542 cm<sup>-1</sup>) are anomalously low as compared with most other Sb(V) oxides.

**O527 Calcium copper titanate  $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$   $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$** 

**Origin:** Synthetic.

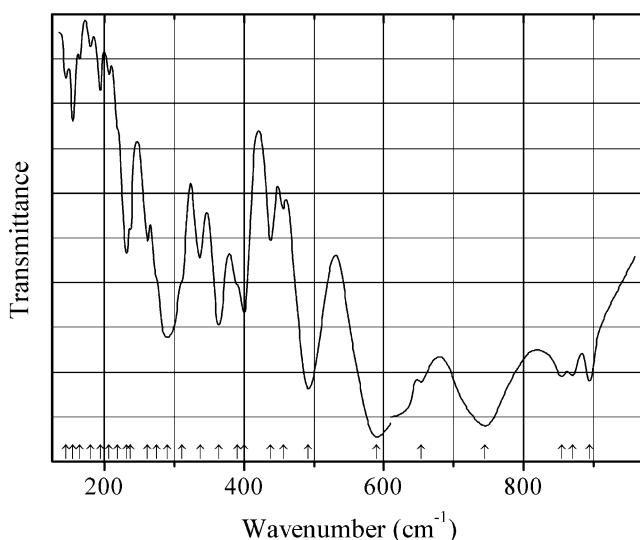
**Description:** Nano-sized powder synthesized by a polymerization-based complex method and calcined at 800 °C in air for 8 h. A perovskite-type compound. Characterized by powder X-ray diffraction data. Cubic,  $a = 7.398(2)$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Masingboon et al. (2008).

**Wavenumbers (cm⁻¹):** 561s, 516, 437.

**Note:** The sample exhibits a giant dielectric constant (Masingboon et al. 2009)

**O528 Calcium niobate columbite-type  $\text{CaNb}_2\text{O}_6$** 

**Origin:** Synthetic.

**Description:** White solid prepared from the mixture of  $\text{Nb}_2\text{O}_5$  and  $\text{CaCO}_3$  powders at 1300 °C for 48 h. Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** Powder spread on polyethylene film and on CsI plate. Transmission.

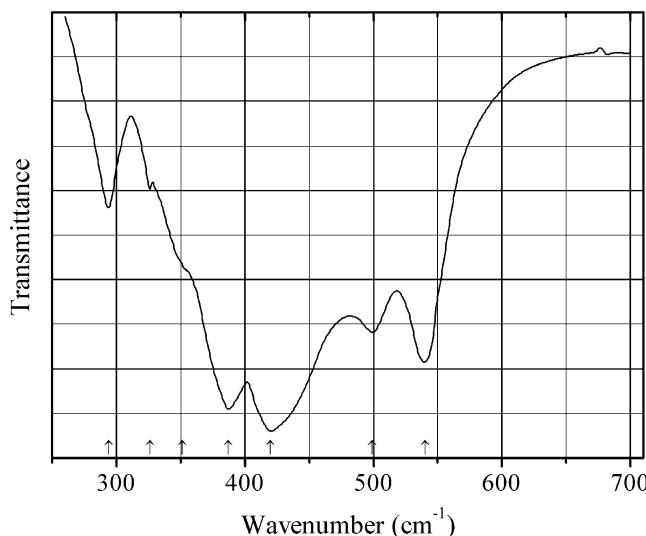
**Source:** Husson et al. (1977a).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 895, 870, 855, 745s, 653, 590s, 492s, 456, 438, 400, 390, 364, 337, 311sh, 290, 275sh, 262, 237, 232, 219sh, 207w, 194w, 180w, 165w, 155w, 145w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 904s, 849, 664, 627, 600, 540s, 495, 487, 462, 430, 385s, 379, 369, 344, 340, 314, 293s, 286, 264, 259, 239s, 223, 213w, 194s, 186, 162, 136s, 127, 108, 84, 63.

### O529 Calcium plumbate $\text{Ca}_2\text{PbO}_4$



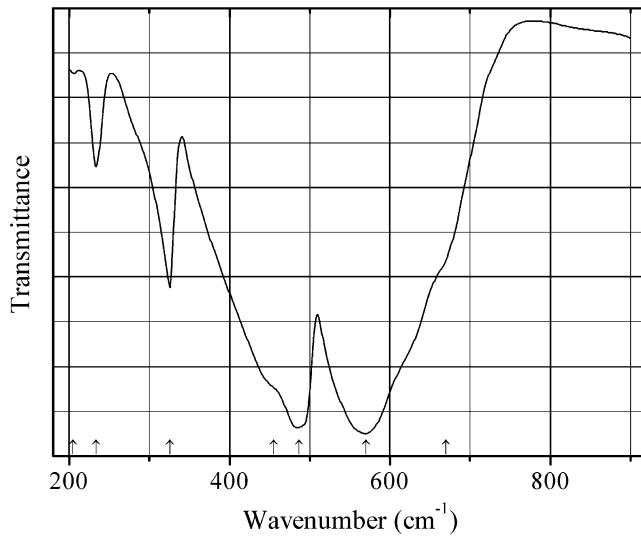
**Origin:** Synthetic.

**Description:** Obtained by standard solid-state reaction, starting with stoichiometric mixture of  $\text{PbO}_2/\text{CaCO}_3$ , heated between 850 and 900 °C, in the presence of a continuous air stream. Orthorhombic, space group  $Pbam$ ,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Diez et al. (1995).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 540, 499, 420s, 387s, 351sh, 326w, 294.

**O530 Chromium uranium oxide  $\text{Cr}_2\text{UO}_6$   $\text{Cr}_2\text{UO}_6$** 

**Origin:** Synthetic.

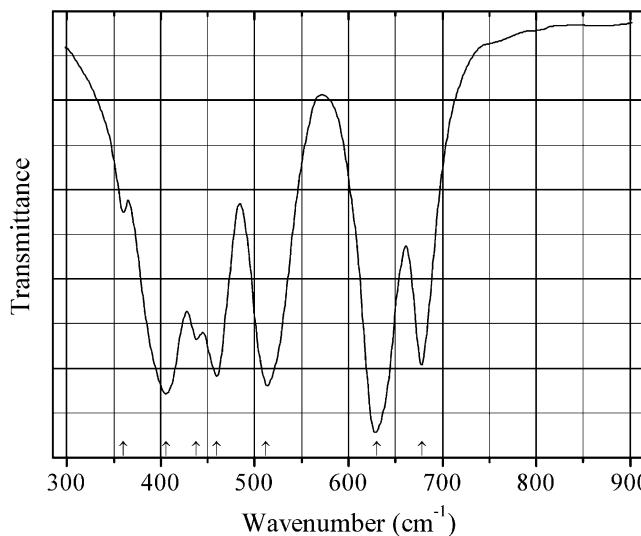
**Description:** Synthesized hydrothermally from  $\text{Cr}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$  and  $\gamma\text{-UO}_3$  at 325–425 °C. Characterized by powder X-ray diffraction data.

Hexagonal,  $a = 4.988(1)$ ,  $c = 4.620(1)$  Å.  $D_{\text{calc}} = 7.31$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc and Nujol mull. Absorption.

**Source:** Hoekstra and Siegel (1971).

**Wavenumbers (cm<sup>-1</sup>):** 670sh, 570s, 487s, 455sh, 326, 234, 205w.

**O531 Cobalt zinc tellurium oxide  $\text{Co}_3\text{Zn}_2\text{TeO}_8$** 

**Origin:** Synthetic.

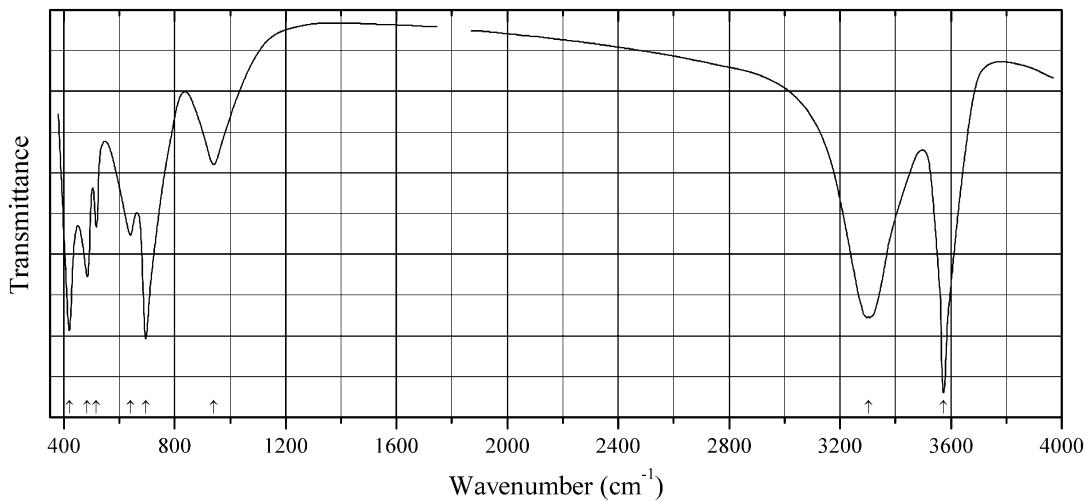
**Description:** Spinel-type compound obtained in the solid-state reaction between  $\text{TeO}_2$ ,  $\text{CoCO}_3$ , and  $\text{ZnCO}_3$  at 1050 °C.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Baran and Botto (1980).

**Wavenumbers (cm<sup>-1</sup>):** 678, 630s, 512s, 460, 438, 406s, 360w.

### O532 Copper(II) hydroxide Cu(OH)<sub>2</sub>



**Locality:** Synthetic.

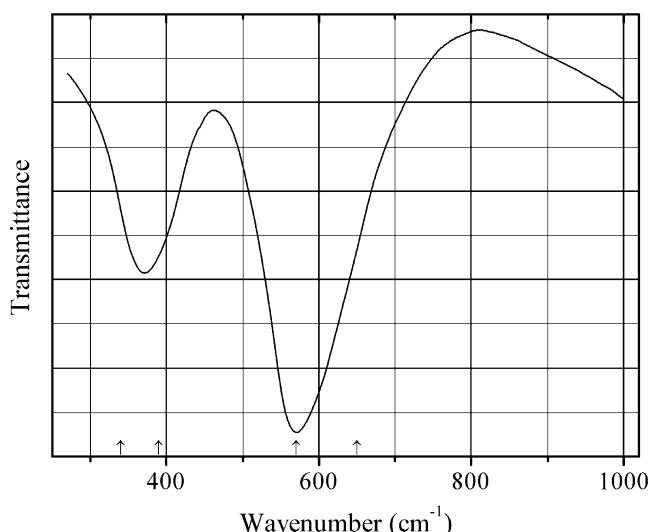
**Description:** Characterized by powder X-ray diffraction data. Orthorhombic, space group *Cmcm*,  $a = 2.936(5)$ ,  $b = 10.54(1)$ ,  $c = 5.238(8)$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Schönenberger et al. (1971).

**Wavenumbers (cm<sup>-1</sup>):** 3574s, 3304s, 940, 695s, 640, 517, 485, 420.

### O533 Cobalt ferrite spinel-type CoFe<sub>2</sub>O<sub>4</sub>



**Origin:** Synthetic.

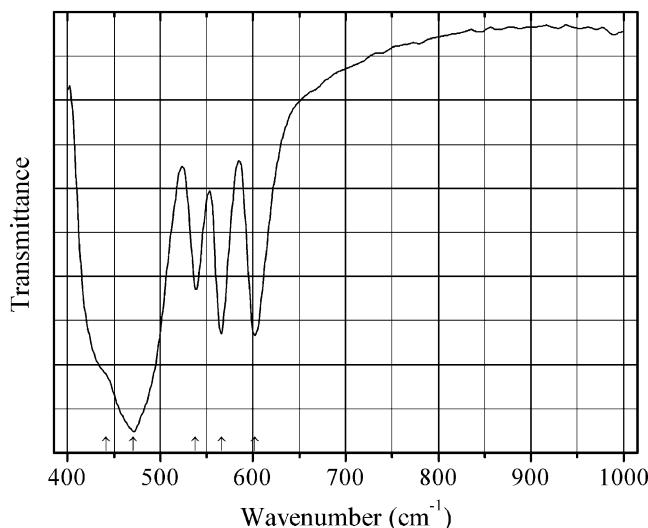
**Description:** Prepared using a conventional ceramic technique. The powder X-ray diffraction showed a single phase and a spinel structure.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Srinivasan et al. (1984).

**Wavenumbers (cm<sup>-1</sup>):** 650, 570, 390, 340.

#### O534 Indium oxide In<sub>2</sub>O<sub>3</sub>



**Origin:** Synthetic.

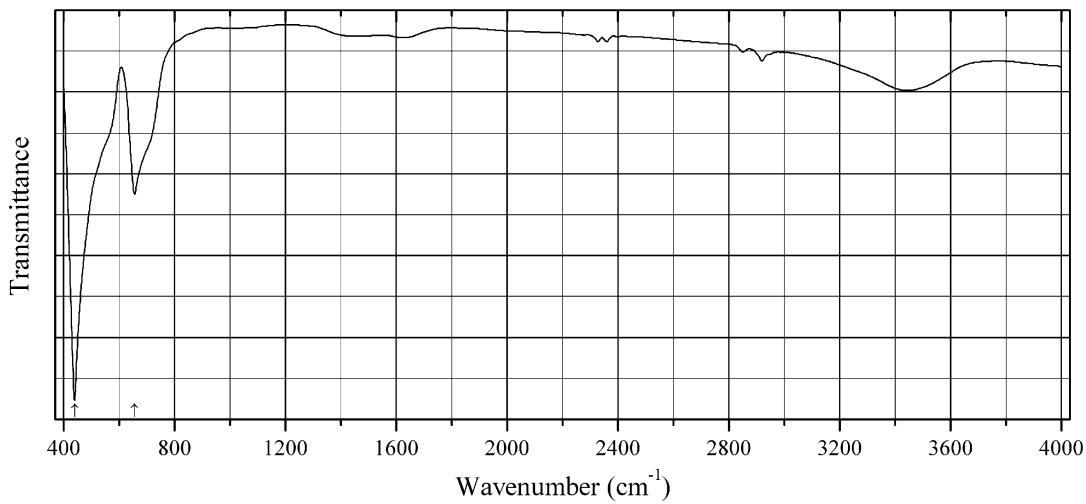
**Description:** Commercial reactant.

**Kind of sample preparation and/or method of registration of the spectrum:** Diffuse reflection of a powdery sample pressed into pellet with KBr. The absorption spectrum was calculated from reflection spectrum by using the Kubelka-Munk function.

**Source:** Jiang et al. (2011).

**Wavenumbers (cm<sup>-1</sup>):** 602, 566, 538, 471s, 441sh.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**O535 Lanthanum aluminum oxide  $\text{LaAlO}_3$** 

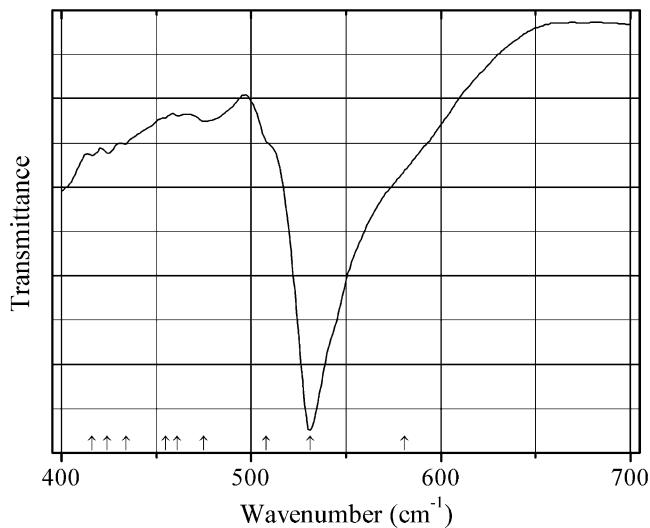
**Origin:** Synthetic.

**Description:** Cubic, with the perovskite-type structure (see JCPDS 85-848). Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Zhou et al. (2004).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 656, 440s.

**O536 Lanthanum iron(III) oxide  $\text{LaFeO}_3$** 

**Origin:** Synthetic.

**Description:** Prepared from stoichiometric mixture of  $\text{La}_2\text{O}_3$  and  $\text{Fe}_2\text{O}_3$  in the presence of excess of the eutectic mixture of NaCl and KCl at 900 °C for 6 h. Characterized by powder X-ray diffraction data. Orthorhombic, space group  $Pnma$ ,  $a = 5.5676(2)$ ,  $b = 7.8608(3)$ ,  $c = 5.5596(2)$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of a powdered sample.

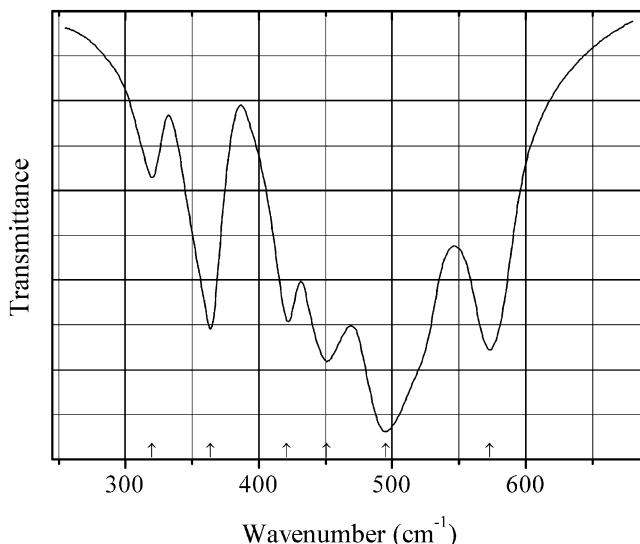
**Source:** Romero et al. (2014).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 581sh, 531s, 508sh, 475w, 461sh, 455w, 434w, 424w, 416w.

**Note:** In the cited paper, Raman spectrum is given. The Raman bands at 1310 and 1143  $\text{cm}^{-1}$  have been assigned to second-order excitations.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1310s, 1143, 650s, 500, 486, 433s, 431, 411, 288, 264, 173, 151, 101.

### O537 Lead(II) stannate $\text{Pb}_2\text{SnO}_4$ $\text{Pb}_2\text{SnO}_4$



**Origin:** Synthetic.

**Description:** Prepared from the stoichiometric mixture of  $\text{PbO}$  and  $\text{SnO}_2$  at 700 °C for 25 h in air. Tetragonal,  $a = 8.74$ ,  $c = 6.30$  Å (see JCPDS No. 24-0589).

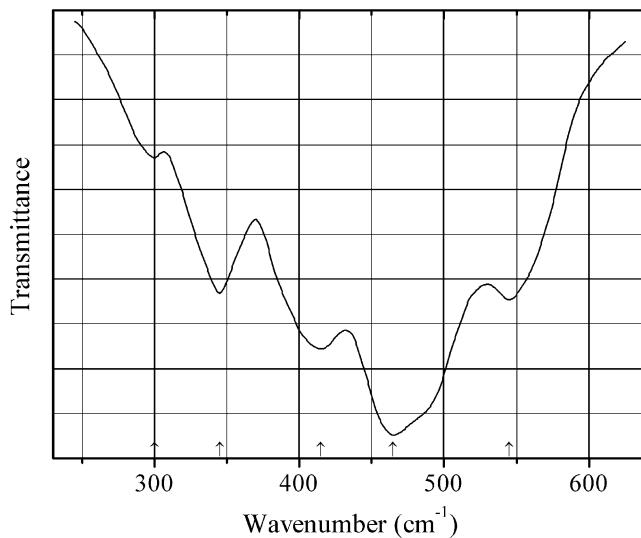
**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc. Transmission.

**Source:** Vigouroux et al. (1982).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 573, 495s, 451, 421, 364, 320w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 613w, 540, 457s, 379, 292s, 275, 196, 129s, 80, 35.

**O538 Lead tin oxide  $\text{Pb}^{2+}_4\text{Pb}^{4+}\text{Sn}^{4+}\text{O}_8$   $\text{Pb}^{2+}_4\text{Pb}^{4+}\text{Sn}^{4+}\text{O}_8$** 

**Origin:** Synthetic.

**Description:** Prepared from a mixture of  $\text{SnPb}_2\text{O}_4$  and  $\text{Pb}_3\text{O}_4$  powders at  $580^\circ\text{C}$  for several months.

The crystal structure is solved. Tetragonal, space group  $P4_2/m$ ,  $a = 8.77$ ,  $c = 6.43 \text{ \AA}$ .

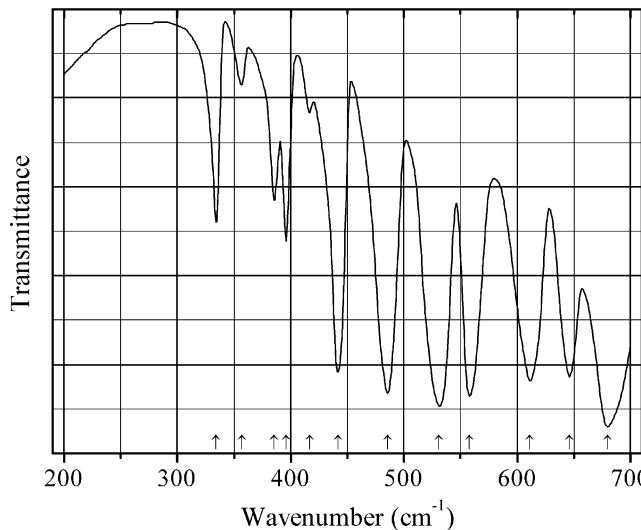
**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc. Absorption.

**Source:** Vigouroux et al. (1982).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 545, 465s, 415, 345, 300w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 550s, 260, 195, 152w, 125s.

**O539 Lithium aluminate  $\text{LiAl}_5\text{O}_8$   $\text{LiAl}_5\text{O}_8$** 

**Origin:** Synthetic.

**Description:** Prepared by sintering a mixture of  $\text{Li}_2\text{CO}_3$  and  $\text{Al}_2\text{O}_3$  at 1300 °C. A compound with ordered spinel-type structure. Characterized by powder X-ray diffraction data.

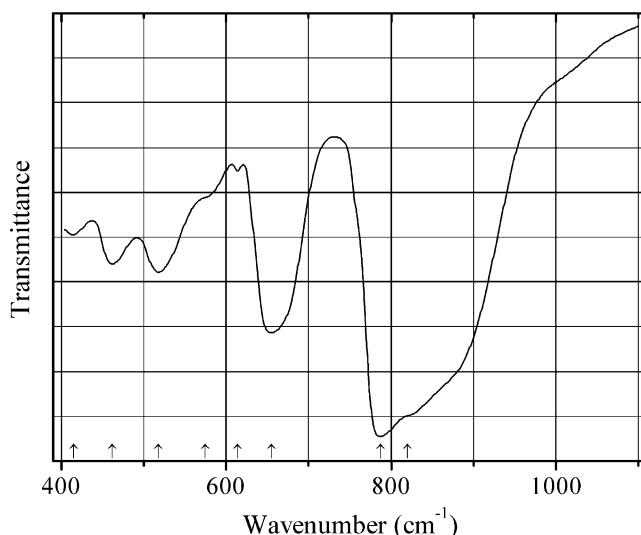
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Brabers (1976).

**Wavenumbers (cm<sup>-1</sup>):** 680s, 646s, 611s, 558s, 531s, 486s, 442s, 417w, 396, 385, 357w, 334.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

#### O540 Lithium aluminate $\text{LiAlO}_2$ -beta $\beta\text{-LiAlO}_2$



**Origin:** Synthetic.

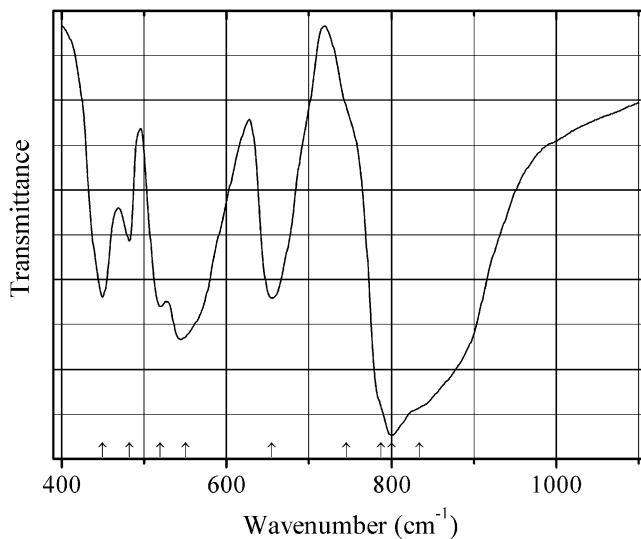
**Description:** Prepared from lithium ethoxide and aluminum methoxide with subsequent hydrolysis and heating to 600 °C. Characterized by powder X-ray diffraction data. Monoclinic.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Hirano et al. (1987).

**Wavenumbers (cm<sup>-1</sup>):** 820sh, 787s, 655, 614w, 575sh, 518, 462, 415w.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**O541 Lithium aluminate  $\text{LiAlO}_2$ -gamma  $\gamma\text{-LiAlO}_2$** 

**Origin:** Synthetic.

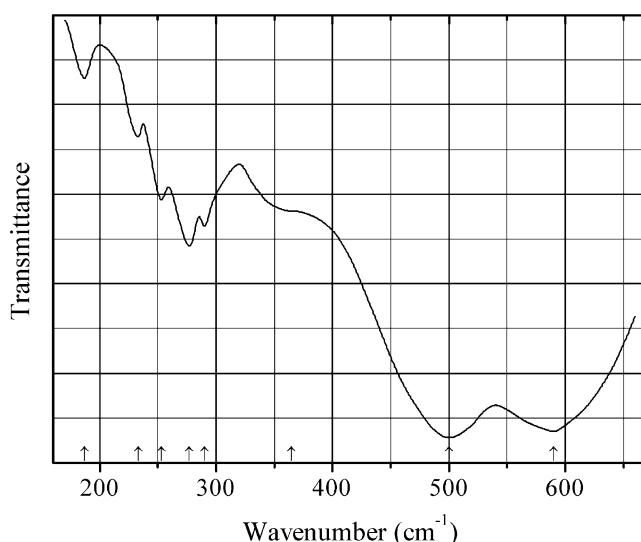
**Description:** Prepared from lithium ethoxide and aluminum ethoxide with subsequent hydrolysis and heating to 1000 °C. Characterized by powder X-ray diffraction data. Tetragonal.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Hirano et al. (1987).

**Wavenumbers (cm<sup>-1</sup>):** 834sh, 800s, 787sh, 745sh, 655, 550s, 520, 482, 450.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**O542 Lithium aluminium oxide-alpha  $\alpha\text{-LiAlO}_2$** 

**Origin:** Synthetic.

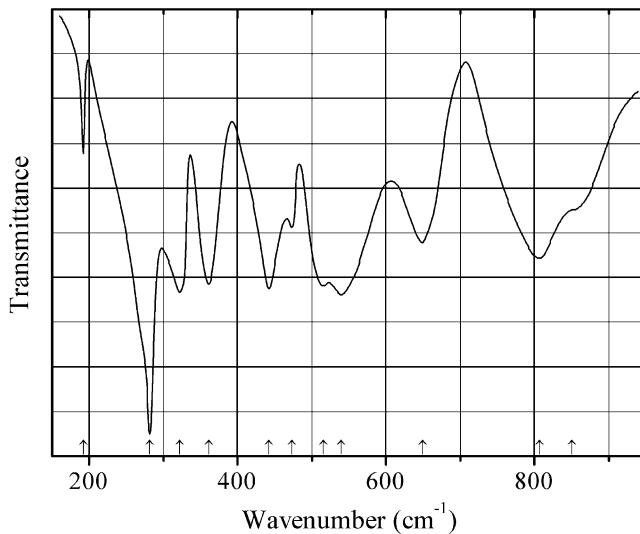
**Description:** The polymorph with trigonally distorted NaCl-type structure synthesized in a solid-state reaction from Al oxide and Li carbonate.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Moore and White (1970).

**Wavenumbers (cm<sup>-1</sup>):** 590s, 500s, 365sh, 290, 277, 253, 233w, 187w

**O543 Lithium aluminium oxide-gamma  $\gamma\text{-LiAlO}_2$**



**Origin:** Synthetic.

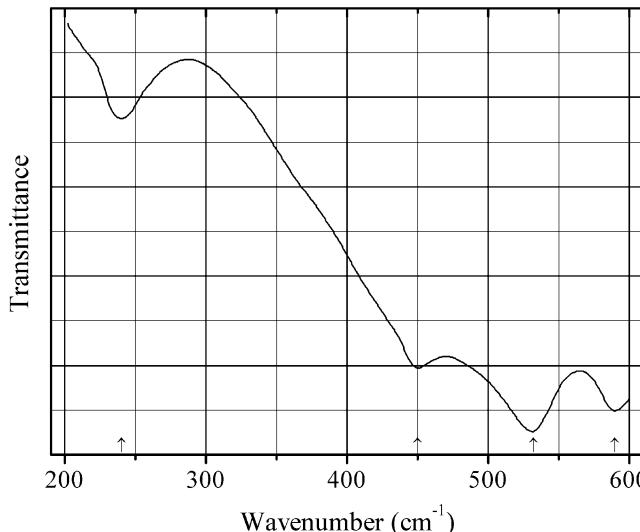
**Description:** Synthesized in a solid-state reaction from Al oxide and Li carbonate. The structure consists of corner-linked tetrahedra in which both Li and Al are four-coordinated. The space group is  $P4_12_12$ ,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Moore and White (1970).

**Wavenumbers (cm<sup>-1</sup>):** 850sh, 807, 649, 540, 516, 473w, 442, 361, 322, 282s, 192w.

**O544 Lithium cobalt(III) iron(III) oxide delafossite-type  $\text{LiCo}_{0.5}\text{Fe}_{0.5}\text{O}_2$**



**Origin:** Synthetic.

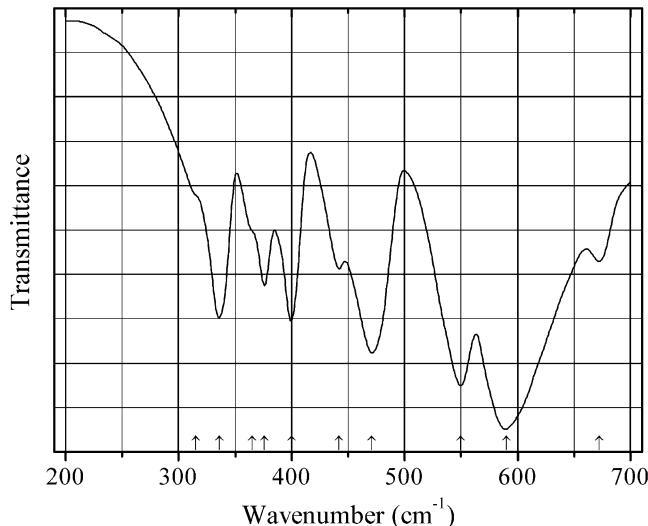
**Description:** Prepared by heating up to 600 °C a gel obtained from the stoichiometric mixture of Li, Co, and Fe nitrates and aqueous solution of maleic acid. Characterized by powder X-ray diffraction data. Trigonal, space group *R3m*.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Khosravi et al. (2013).

**Wavenumbers (cm<sup>-1</sup>):** 590s, 532s, 450, 240w.

### O545 Lithium ferrite $\text{LiFe}^{3+}\text{O}_8$ $\text{LiFe}^{3+}\text{O}_8$



**Origin:** Synthetic.

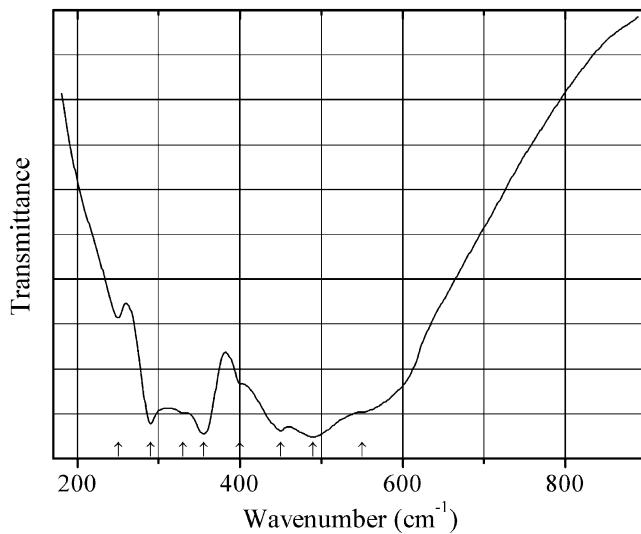
**Description:** Prepared by sintering a mixture of  $\text{Li}_2\text{CO}_3$  and  $\text{Fe}_2\text{O}_3$  at 1300 °C. A compound with ordered spinel-type structure. Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Brabers (1976).

**Wavenumbers (cm<sup>-1</sup>):** 672w, 590s, 550s, 471, 442, 400, 376, 365sh, 336, 315sh.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**O546 Lithium iron(III) oxide  $\gamma$ -LiFeO<sub>2</sub>**

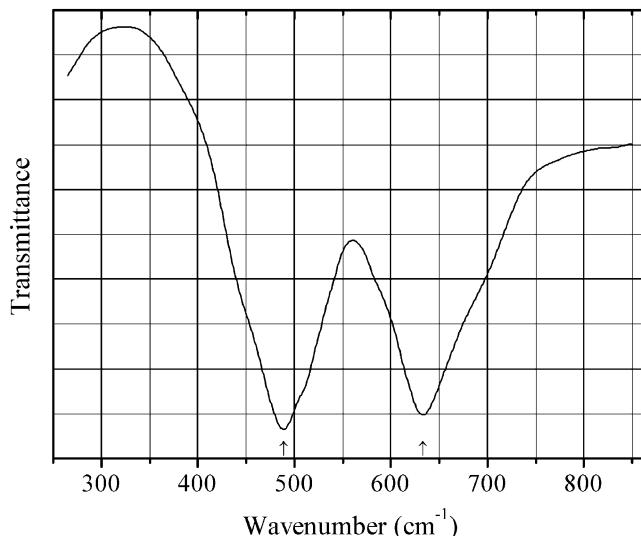
**Origin:** Synthetic.

**Description:** Synthesized in a solid-state reaction from Al oxide and Li carbonate. The structure consists of corner-linked tetrahedra in which both Li and Al are four-coordinated. The space group is P4<sub>1</sub>2<sub>1</sub>2, Z = 4.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Moore and White (1970).

**Wavenumbers (cm<sup>-1</sup>):** 550sh, 490s, 450s, 400sh, 355s, 330sh, 290s, 250.

**O547 Lithium magnesium manganese(IV) oxide spinel-type Li<sub>2</sub>MgMn<sub>3</sub>O<sub>8</sub>**

**Origin:** Synthetic.

**Description:** Prepared by solid-state reaction using  $\text{Li}_2\text{CO}_3$ ,  $\text{MnO}_2$ , and  $\text{MgO}$ . Characterized by powder X-ray diffraction data. Cubic, space group  $Fd\bar{3}m$ ,  $a = 8.2794(2)$  Å.

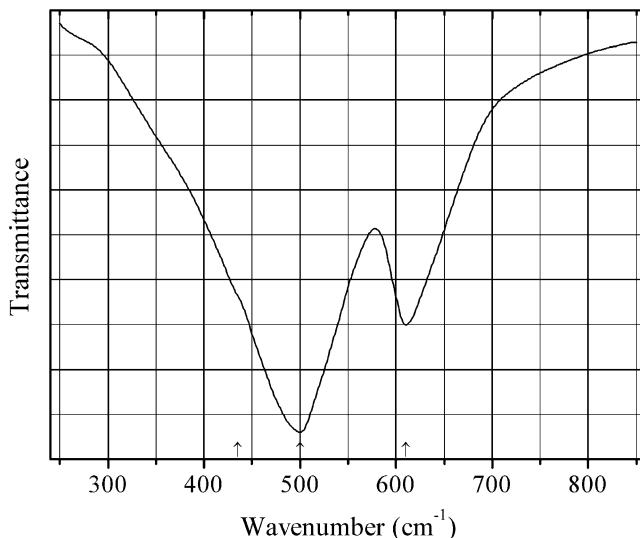
**Kind of sample preparation and/or method of registration of the spectrum:** TlBr disc. Absorption.

**Source:** Strobel et al. (2003).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 633s, 489s.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

### O548 Lithium manganese oxide spinel-type $\text{LiMn}^{3+}\text{Mn}^{4+}\text{O}_4$



**Origin:** Synthetic.

**Description:** Prepared by solid-state reaction. Cubic, space group  $Fd\bar{3}m$ ,  $a = 8.1967$  Å. A normal spinel containing Li at tetrahedral site and Mn at octahedral site.

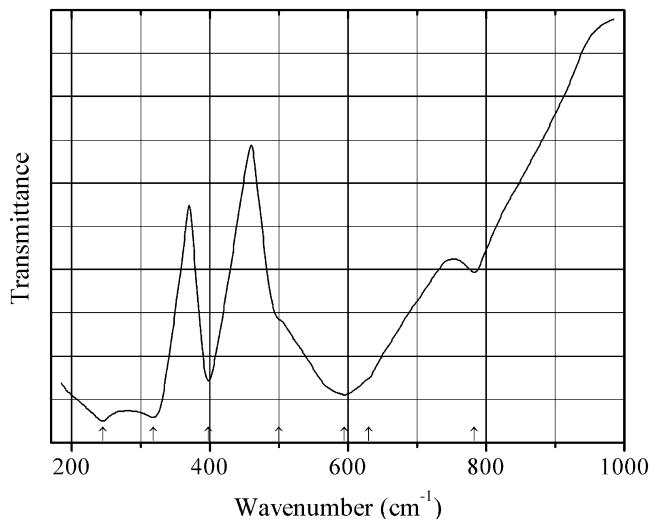
**Kind of sample preparation and/or method of registration of the spectrum:** TlBr disc. Absorption.

**Source:** Strobel et al. (2003).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 610, 500s, 435sh.

**Note:** For the vibrational spectra of  $\text{LiMn}^{3+}\text{Mn}^{4+}\text{O}_4$  see also Helan and Berchmans (2011) and Julien et al. (1998). In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 627s, 588s, 486, 421, 368w.

**O549 Lithium niobateilmenite-type  $\text{LiNbO}_3$** 

**Origin:** Synthetic.

**Description:** Obtained by hydrothermal synthesis. Metastable modification isostructural with ilmenite.

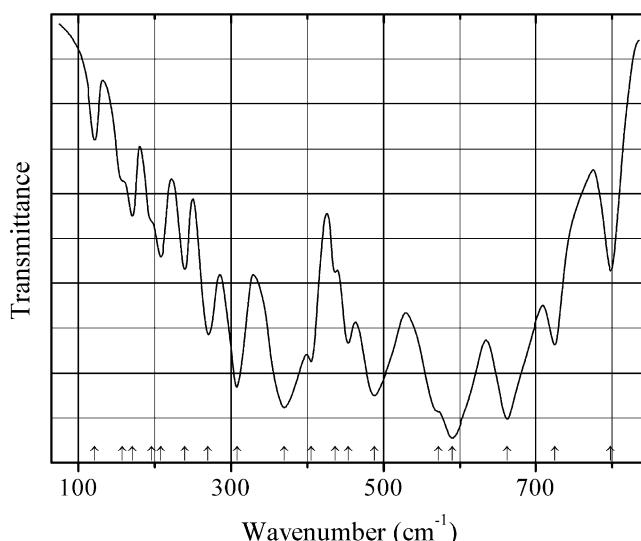
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Baran et al. (1986).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 783, 630sh, 595s, 500sh, 398, 318s, 245s.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 735s, 677w, 470, 381w, 291, 275, 214, 173w.

**O550 Lithium zinc niobium oxide spinel-type  $\text{LiZnNbO}_4$** 

**Origin:** Synthetic.

**Description:** Synthesized in the solid-state reaction between  $\text{Li}_2\text{CO}_3$ ,  $\text{ZnO}$ , and  $\text{Nb}_2\text{O}_5$  at 1000 °C for 10 h. Tetragonal, space group  $P4_122$ ,  $a = 6.079$ ,  $c = 8.401$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** Polyethylene disc. Transmission.

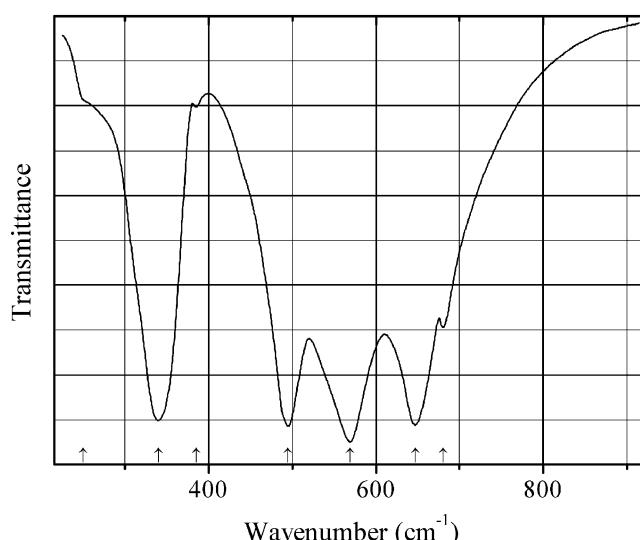
**Source:** Keramidas et al. (1975).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 798, 725, 662s, 590s, 572, 488s, 454, 437w, 405, 370s, 308s, 270, 240, 208, 196sh, 171, 158sh, 122w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 868w, 819s, 762w, 718, 684w, 616s, 589s, 582, 496, 460, 435, 366w, 335, 323, 300w, 266, 250s, 237s, 222s, 193, 155, 152, 134s, 120, 94s.

### O551 Manganese(II) antimony(III) oxide $\text{MnSb}_2\text{O}_4$



**Origin:** Synthetic.

**Description:** Synthesized hydrothermally from the stoichiometric mixture of  $\text{MnO}$  and  $\text{Sb}_2\text{O}_3$  in the presence of 5% HF, at 500 °C. Tetragonal, space group  $P4_2/mbc$ ,  $a = 8.7145$ ,  $c = 6.0011$  Å,  $Z = 4$ . Sb has tetrahedral  $\text{SbO}_3E$  coordination where  $E$  is a lone pair.

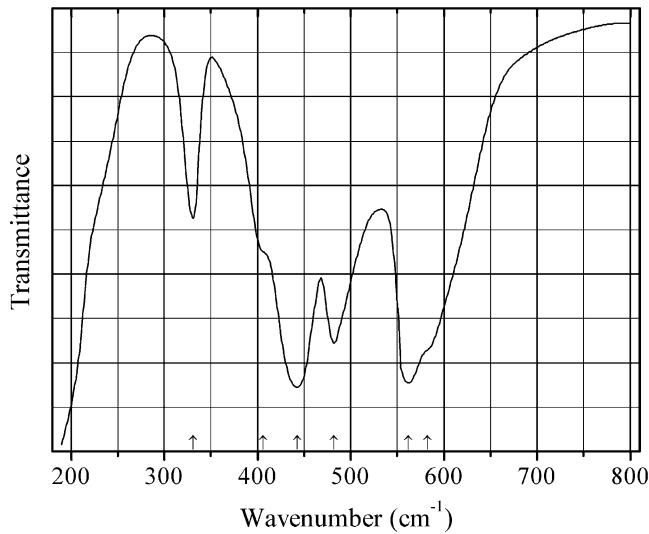
**Kind of sample preparation and/or method of registration of the spectrum:** KBr and CsI discs. Transmission.

**Source:** Chater et al. (1986).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 680, 647s, 569s, 495s, 385w, 340s, 250sh, 198, 170, 134, 96.5, 79.

**Note:** In the cited paper, Raman spectrum is given. For the vibrational spectra of  $\text{MnSb}_2\text{O}_4$  see also Gavarri et al. (1988).

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 670s, 620, 547w, 527, 473.5sh, 465, 398.5w, 350, 345sh, 292s, 254.5, 221, 215, 189, 155.5, 124s, 118w, 112w, 105s, 52, 47.

**O552 Nickel manganese(IV) oxide  $\text{Ni}_6\text{MnO}_8$** 

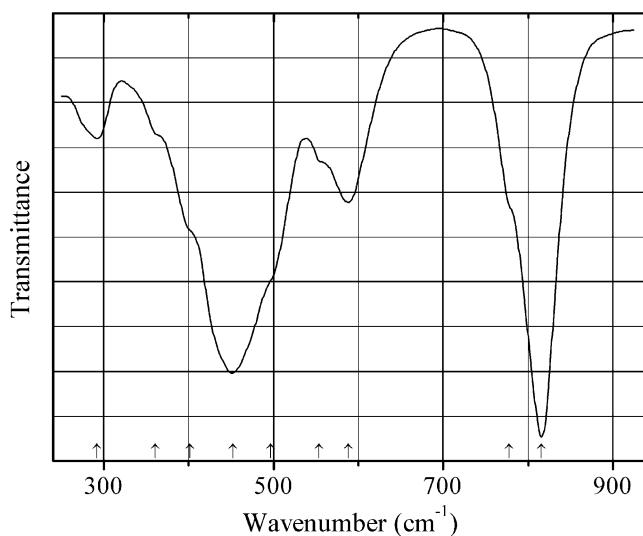
**Origin:** Synthetic.

**Description:** Prepared by addition of an excess of oxalic acid to boiled solution of Ni(II) and Mn (II) acetates in acetic acid (25%) with subsequent drying and calcination at 873 K for 3 h. Characterized by powder X-ray diffraction data. Cubic, space group  $Fm\bar{3}m$ ,  $a = 8.306(3)$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Porta et al. (1991).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 582sh, 562s, 482, 443s, 406sh, 331.

**O553 Potassium diuranate  $\text{K}_2\text{U}_2\text{O}_7$** 

**Origin:** Synthetic.

**Description:** Prepared by heating stoichiometric mixture of  $\text{U}_3\text{O}_8$  and  $\text{K}_2\text{CO}_3$  in air. Characterized by powder X-ray diffraction data. Orthorhombic,  $a = 6.95(2)$ ,  $b = 7.97(2)$ ,  $c = 22.16(2)$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

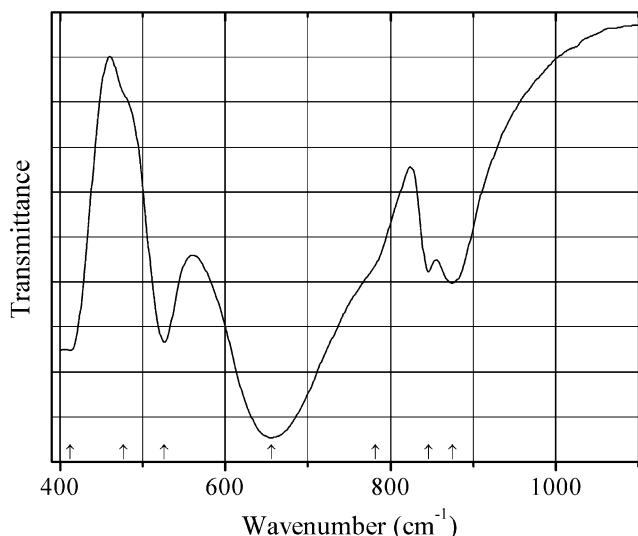
**Source:** Volkovich et al. (1998).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 816s, 778sh, 588, 554sh, 497sh, 452s, 401sh, 361sh, 292.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 778s, 562w, 491w, 434, 336, 287, 267w, 245w, 150sh, 133, 100w.

### O554 Potassium niobate $\text{KNbO}_3$



**Origin:** Synthetic.

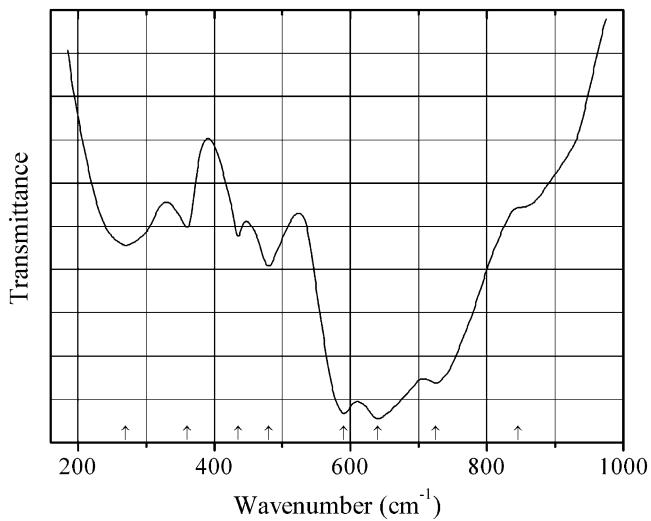
**Description:** Synthesized hydrothermally from  $\text{Nb}_2\text{O}_5$  and KOH at 200 °C. Characterized by powder X-ray diffraction data and electron microprobe analysis. Orthorhombic,  $a = 5.697$ ,  $b = 3.971$ ,  $c = 5.721$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Wang et al. (2007).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 875, 846, 782sh, 656s, 526s, 477sh, 412s.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**O555 Potassium niobate  $\text{KNb}_7\text{O}_{18}$   $\text{KNb}_7\text{O}_{18}$** 

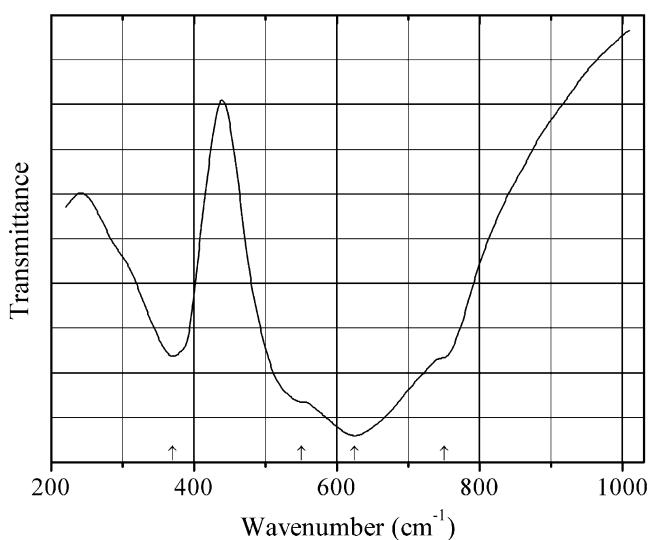
**Origin:** Synthetic.

**Description:** Structurally related to  $\text{TlNb}_7\text{O}_{18}$  (tetragonal, space group  $P4/mbm$ ,  $a = 27.50$ ,  $c = 3.94 \text{ \AA}$ ,  $Z = 8$ ).

**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc. Transmission.

**Source:** Bhide et al. (1980).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 845sh, 725s, 640s, 590s, 480, 435, 360, 270.

**O556 Potassium niobate perovskite-type  $\text{KNbO}_3$** 

**Origin:** Synthetic.

**Description:** Prepared in a solid-state reaction, by double-ply heating the stoichiometric mixture of  $\text{Nb}_2\text{O}_5$  and  $\text{KNO}_3$  at 1000 °C for 1 h with intermediate grinding. Structurally related to perovskite. Orthorhombic, space group  $Bmm2$ ,  $a = 5.697$ ,  $b = 3.971$ ,  $c = 5.721$  Å.

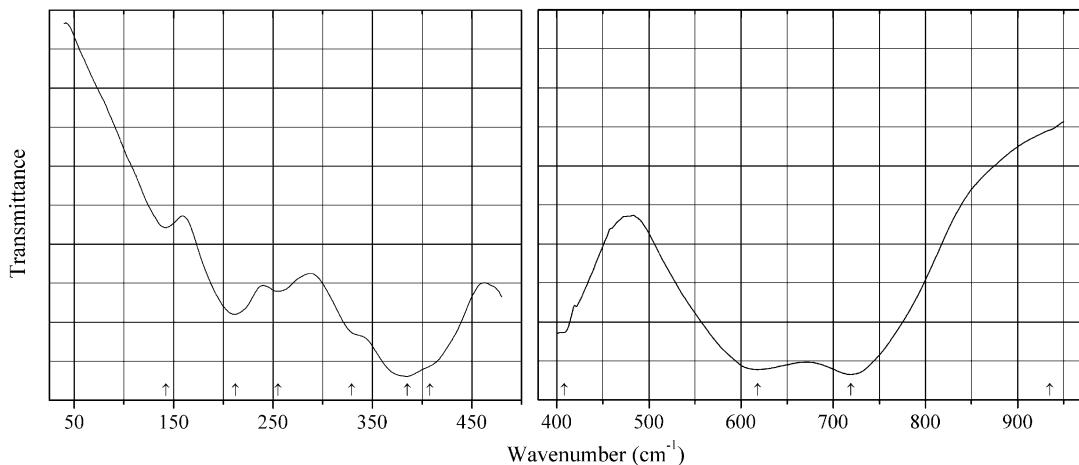
**Kind of sample preparation and/or method of registration of the spectrum:** KBr or CsI disc and polyethylene matrix. Transmission.

**Source:** Rocchiccioli-Deltcheff (1973).

**Wavenumbers (cm<sup>-1</sup>):** 750sh, 625s, 550sh, 370, 180.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### O557 Potassium niobate tungstate $\text{KNbWO}_6$



**Origin:** Synthetic.

**Description:** Prepared by the solid-state reaction between  $\text{WO}_3$ ,  $\text{Nb}_2\text{O}_5$ , and  $\text{KNO}_3$  at 973 K. The crystal structure solved by the Rietveld method is related to that of pyrochlore. Cubic, space group  $Fd\bar{3}m$ ,  $a = 10.5001(7)$ ,  $V = 1057.67(2)$  Å<sup>3</sup>,  $Z = 8$ .  $D_{\text{calc}} = 4.7529$  g/cm<sup>3</sup>.

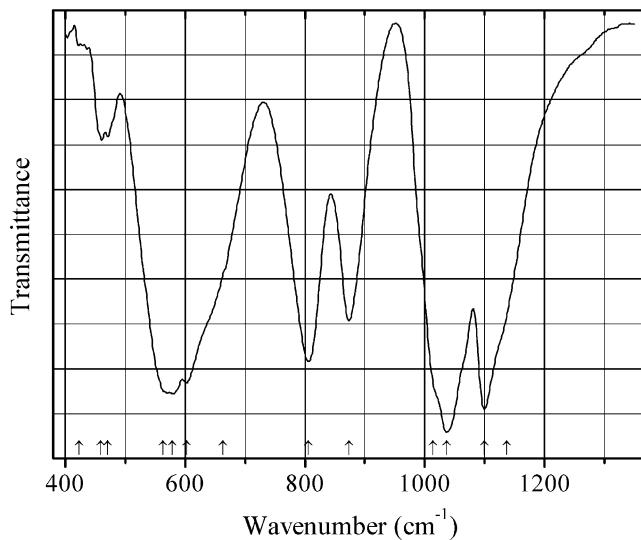
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc and Nujol suspension. Absorption.

**Source:** Knyazev et al. (2010).

**Wavenumbers (IR, cm<sup>-1</sup>):** 935sh, 719s, 618s, 408sh, 385s, 329sh, 255, 212, 142.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 934w, 861w, 664s, 576, 473w, 438w, 360w, 246sh, 196s, 152s.

**O558 Potassium tantalite perovskite-type  $\text{KTaO}_3$** 

**Origin:** Synthetic.

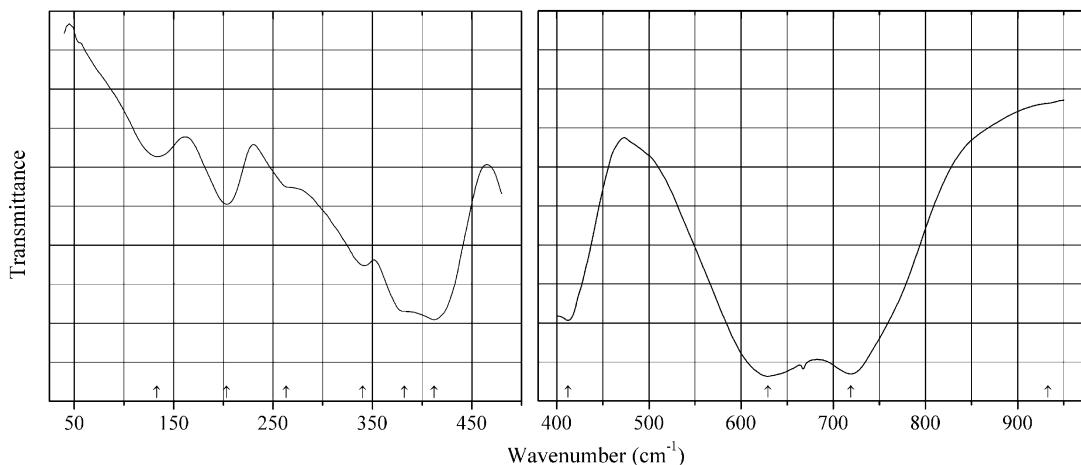
**Description:** Prepared in a solid-state reaction, by double-ply heating the stoichiometric mixture of  $\text{Nb}_2\text{O}_5$  and  $\text{KNO}_3$  at 1230 °C for 4 h with intermediate grinding. Structurally related to perovskite. Cubic,  $a = 3.989 \text{ \AA}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr or CsI disc and polyethylene matrix. Transmission.

**Source:** Rocchiccioli-Deltcheff (1973).

**Wavenumbers (cm<sup>-1</sup>):** 755sh, 605s, 340.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**O559 Potassium tantalate tungstate  $\text{KTaWO}_6$** 

**Origin:** Synthetic.

**Description:** Prepared by the solid-state reaction between  $\text{WO}_3$ ,  $\text{Nb}_2\text{O}_5$ , and  $\text{KNO}_3$  at 973 K. The crystal structure solved by the Rietveld method is related to that of pyrochlore. Cubic, space group  $Fd\bar{3}m$ ,  $a = 10.4695(1)$ ,  $V = 1147.57(3) \text{ \AA}^3$ ,  $Z = 8$ .  $D_{\text{calc}} = 5.8197 \text{ g/cm}^3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc and Nujol suspension. Absorption.

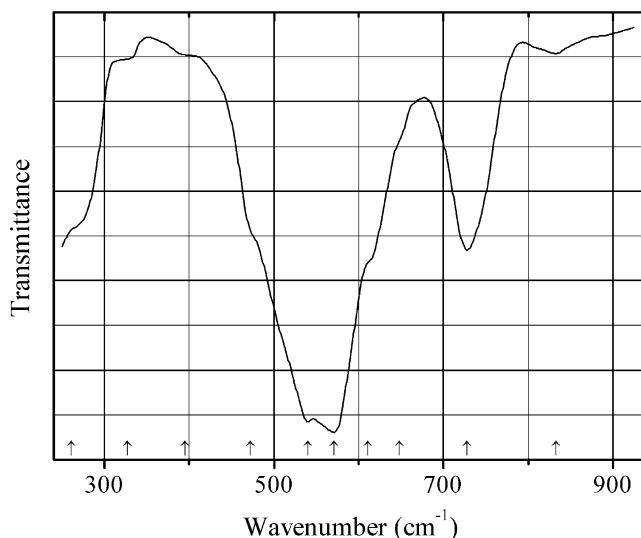
**Source:** Knyazev et al. (2010).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** (933sh), 719s, 629s, 412s, 382sh, 340, 263sh, 203, 133.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 937, 870, 664s, 580sh, 481w, 452w, 359w, 248s, 191s, 145s.

### O560 Potassium urinate $\text{K}_2\text{UO}_4$



**Origin:** Synthetic.

**Description:** Prepared by heating stoichiometric mixture of  $\text{U}_3\text{O}_8$  with  $\text{K}_2\text{CO}_3$  at 800 °C for several hours, with several intermediate grindings. Characterized by powder X-ray diffraction data. Tetragonal,  $a = 4.31(2)$ ,  $c = 13.09(2) \text{ \AA}$ .

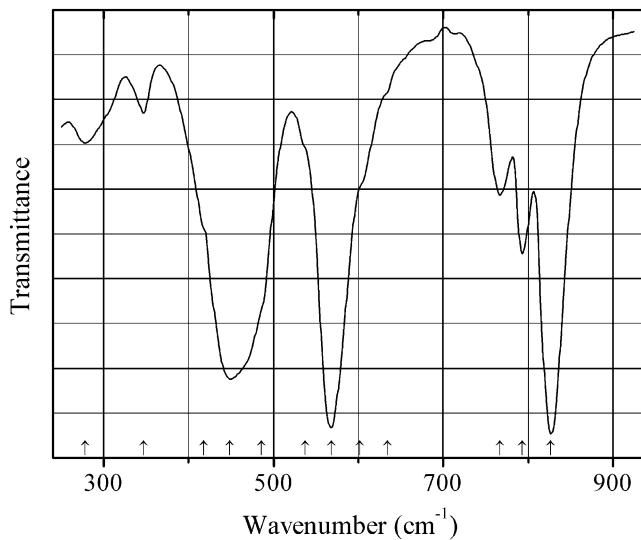
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Volkovich et al. (1998).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 833w, 728s, 648sh, 611sh, 571s, 540s, 472sh, 395sh, 327sh, 261sh.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 694s, 492, 439, 344w, 293w, 221, 168.

**O561 Sodium diuranate**  $\text{Na}_2\text{U}_2\text{O}_7$ 

**Origin:** Synthetic.

**Description:** Prepared by heating stoichiometric mixture of  $\text{U}_3\text{O}_8$  and  $\text{Na}_2\text{CO}_3$  in air. Characterized by powder X-ray diffraction data. Orthorhombic,  $a = 6.77(1)$ ,  $b = 7.97(1)$ ,  $c = 18.32(1)$  Å.

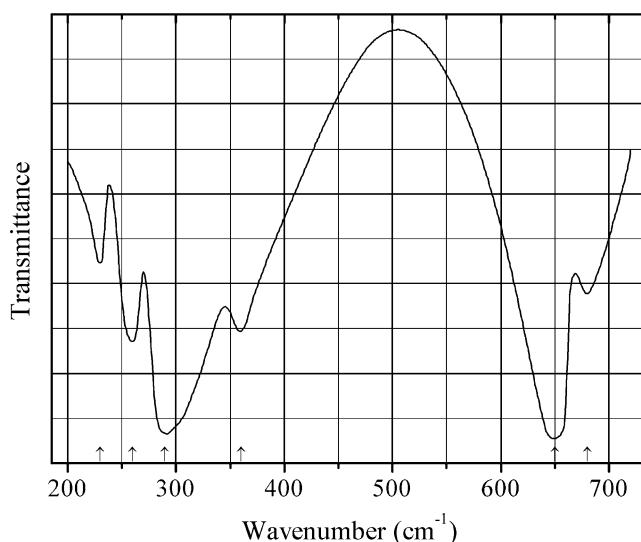
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Volkovich et al. (1998).

**Wavenumbers (IR, cm⁻¹):** 827s, 793, 767, 634sh, 602sh, 568s, 537sh, 486sh, 449s, 418sh, 347w, 278.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm⁻¹):** 826w, 788s, 779s, 752, 599sh, 584, 536w, 420s, 357w, 313s, 274, 233, 202, 146, 117s, 100w.

**O562 Sodium stannate**  $\text{Na}_4\text{SnO}_4$ 

**Origin:** Synthetic.

**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc. Transmission.

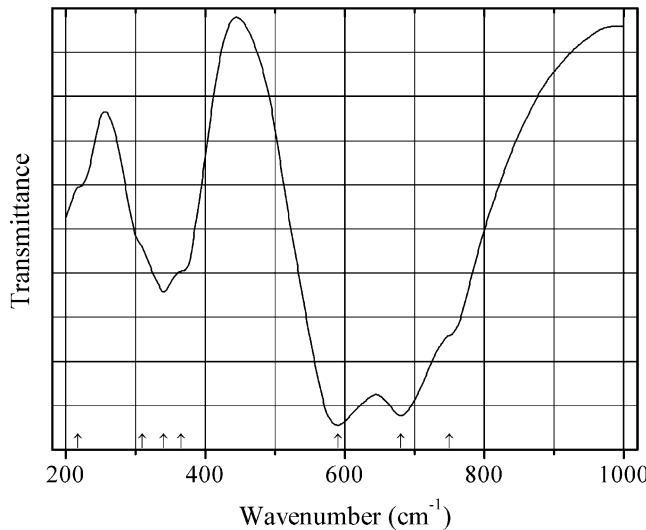
**Source:** Kessler et al. (1979).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 680, 650s, 360, 290s, 260, 230.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 679, 664s, 638, 612w, 310, 235, 212w, 180, 160, 145, 100.

### O563 Sodium tantalite perovskite-type $\text{NaTaO}_3$



**Origin:** Synthetic.

**Description:** Prepared in a solid-state reaction, by double-ply heating the stoichiometric mixture of  $\text{Ta}_2\text{O}_5$  and  $\text{NaNO}_3$  at 1200 °C for 6 h and for 12 h with intermediate grinding. Structurally related to perovskite. Orthorhombic, space group  $Pc2_1n$ ,  $a \approx 5.51\text{--}5.52$ ,  $b \approx 7.75\text{--}7.79$ ,  $c \approx 5.48\text{--}5.50$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr or CsI disc and polyethylene matrix. Transmission.

**Source:** Rocchiccioli-Deltcheff (1973).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 750sh, 680s, 590s, 365sh, 340, 310sh, 217sh, 173, 127.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**O564 Sodium uranate**  $\text{Na}_2\text{UO}_4$ 

**Origin:** Synthetic.

**Description:** Prepared by heating stoichiometric mixture of  $\text{U}_3\text{O}_8$  and  $\text{Na}_2\text{CO}_3$  at 800 °C for several hours, with several intermediate grindings. Characterized by powder X-ray diffraction data. Orthorhombic,  $a = 6.77(1)$ ,  $b = 7.97(1)$ ,  $c = 18.32(1)$  Å.

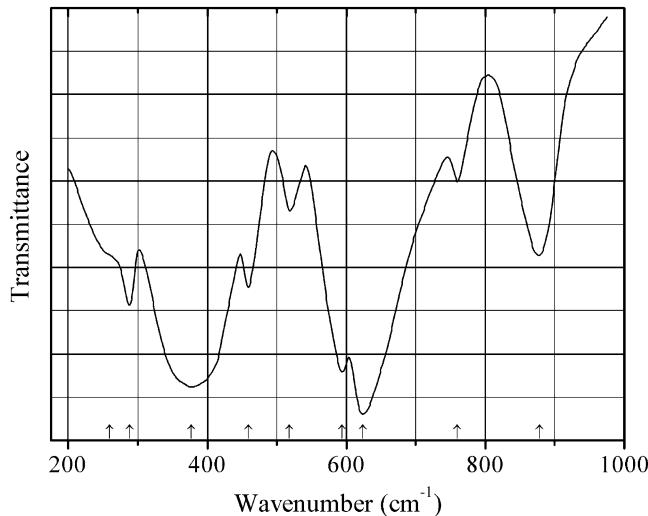
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Volkovich et al. (1998).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 809w, 774s, 732s, 706w, 518s, 488, 453s, 310, 257s.

**Note:** The IR data are taken from Volkovich et al. (1998). There are strong discrepancies between these data and the figure of the IR spectrum of  $\text{Na}_2\text{UO}_4$  given in this paper. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 736w, 712s, 547w, 506w, 442w, 362w, 329w, 238s, 177w, 140w.

**O565 Sodium yttrium titanate**  $\text{NaYTiO}_4$ 

**Origin:** Synthetic.

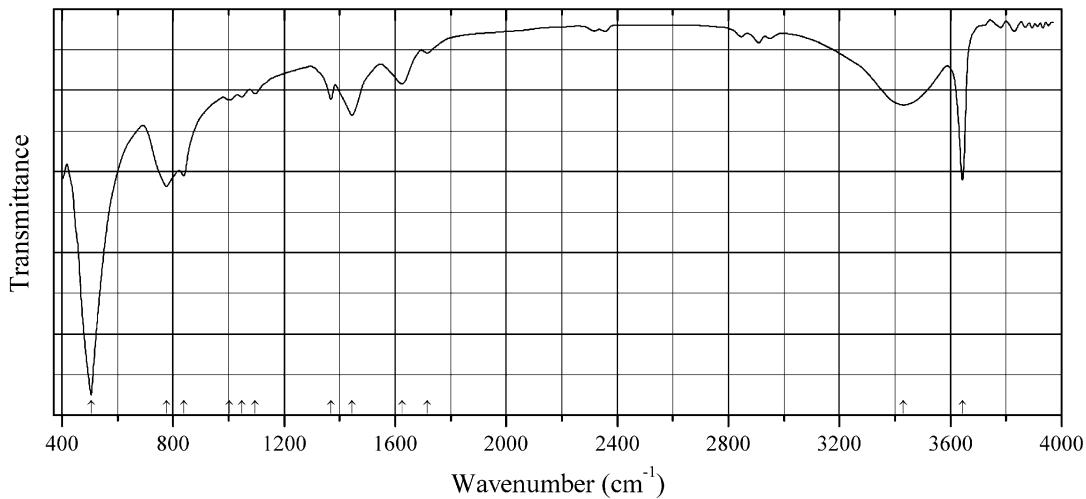
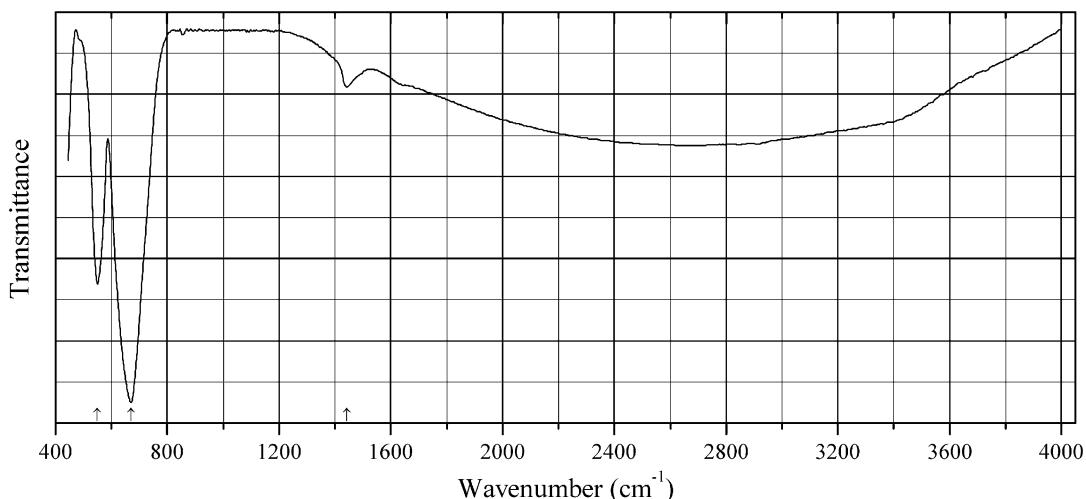
**Description:** Tetragonal, structurally related to perovskite. The structure based on double layers of  $\text{Y}^{3+}$  ions and double layers of  $\text{Na}^+$  ions perpendicular to the  $c$  axis.

**Kind of sample preparation and/or method of registration of the spectrum:** No data in the cited paper.

**Source:** Blasse and van den Heuvel (1974).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 878, 760w, 624s, 594s, 518w, 459, 377s, 288, 259sh.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. The band at  $878 \text{ cm}^{-1}$  is ascribed by the authors to stretching vibrations of the Ti–O bond directed towards the Na-layers. In the cited paper, a figure of the Raman spectrum is given.

**O566 Strontium aluminum hydroxide  $\text{Sr}_3\text{Al}_2(\text{OH})_{12}$** **Hydrogarnet  $\text{Sr}_3\text{Al}_2(\text{OH})_{12}$   $\text{Sr}_3\text{Al}_2(\text{OH})_{12}$** **Origin:** Synthetic.**Description:** Prepared hydrothermally. Characterized by powder X-ray diffraction data. Cubic, structurally related to garnet-group minerals.**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.**Source:** Li et al. (1997).**Wavenumbers (cm<sup>-1</sup>):** 3643s, 3430, 1715w, 1624, 1445, 1369, 1095w, 1048w, 1002w, 839, 776, 505s.**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.**O567 Strontium cerium antimonate perovskite-type  $\text{Sr}_2\text{CeSbO}_6$** 

**Origin:** Synthetic.

**Description:** A compound with ordered perovskite-type structure prepared by heating a mixture of  $\text{SrCO}_3$ ,  $\text{Ce}_2(\text{CO}_3)_3$ , and  $\text{Sb}_2\text{O}_5$ , taken in stoichiometric ratio, at  $1350^\circ\text{C}$  for 15 h. Characterized by powder X-ray diffraction data and energy dispersive X-ray spectrum. Orthorhombic,  $a = 8.84$ ,  $b = 6.22$ ,  $c = 5.83 \text{ \AA}$ .

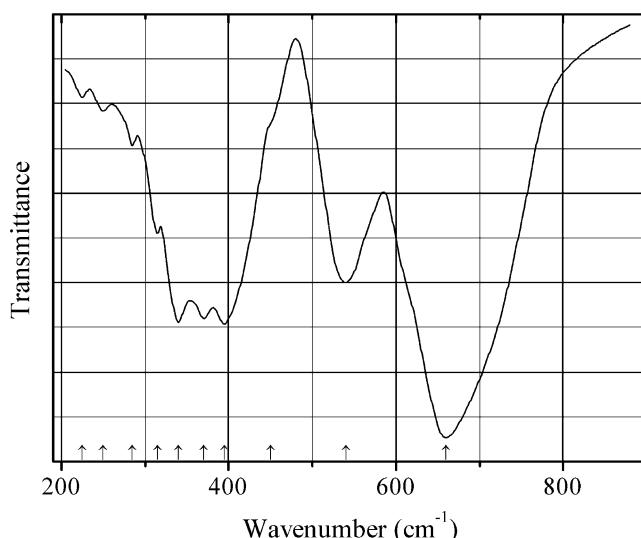
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Bharti, and Sinha (2010).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1443w, 670s, 550.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The weak band at  $1443 \text{ cm}^{-1}$  may correspond to the admixture of a carbonate.

### O568 Strontium magnesium niobate $\text{Sr}_3\text{MgNb}_2\text{O}_9$



**Origin:** Synthetic.

**Description:** A compound with ordered perovskite-type structure prepared by a solid-state reaction technique. Characterized by powder X-ray diffraction data.

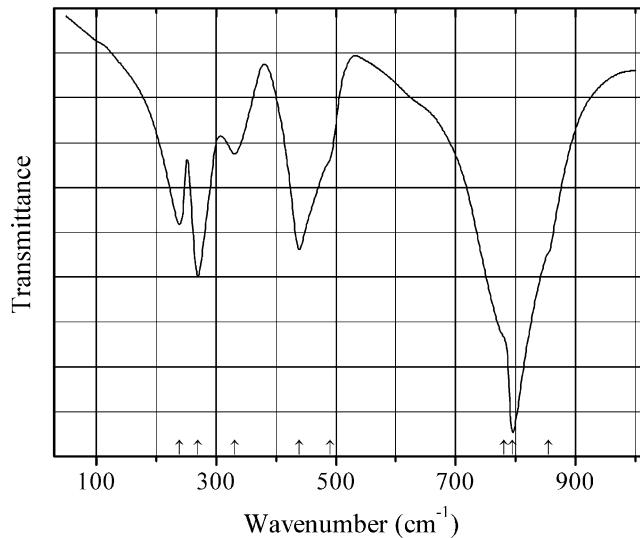
**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc (?). Transmission.

**Source:** Blasse, and Corsmit (1974).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 660s, 540, 450sh, 395s, 370s, 340s, 315, 285w, 250w, 225w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 830s, 535w, 455, 400, 310w, 240w.

**O569 Tellurite rhombohedral polymorph  $\text{TeO}_3$** 

**Origin:** Synthetic.

**Description:** Prepared by stepwise heating a mixture of  $\alpha\text{-TeO}_2$  and  $\text{I}_2\text{O}_5$  (with the molar ratio 1:2) at 250, 280, and 310 °C (for 2 h at each temperature) and 340 °C for 24 h. Characterized by powder X-ray diffraction data. Rhombohedral,  $a = 5.00383$ ,  $c = 13.22429 \text{ \AA}$ .

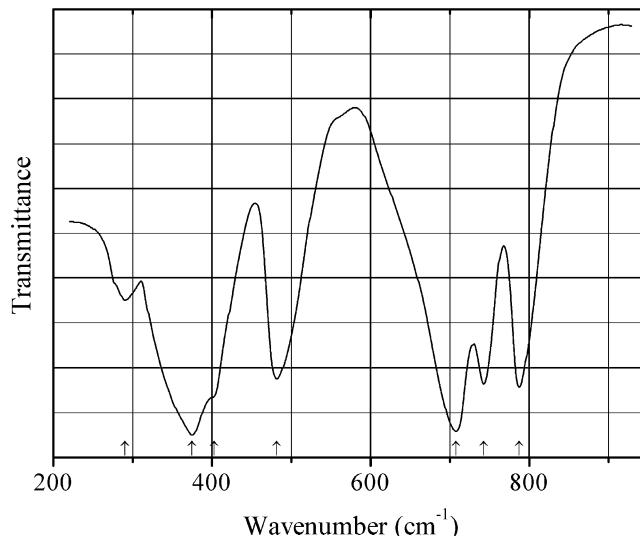
**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

**Source:** Cornette et al. (2011).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 855sh, 794s, 780sh, 490sh, 439s, 331, 270s, 239.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 844, 663w, 487, 333s, 261.

**O570 Tellurium(IV) tin oxide  $\text{Te}_3\text{SnO}_8$   $\text{Te}_3\text{SnO}_8$** 

**Origin:** Synthetic.

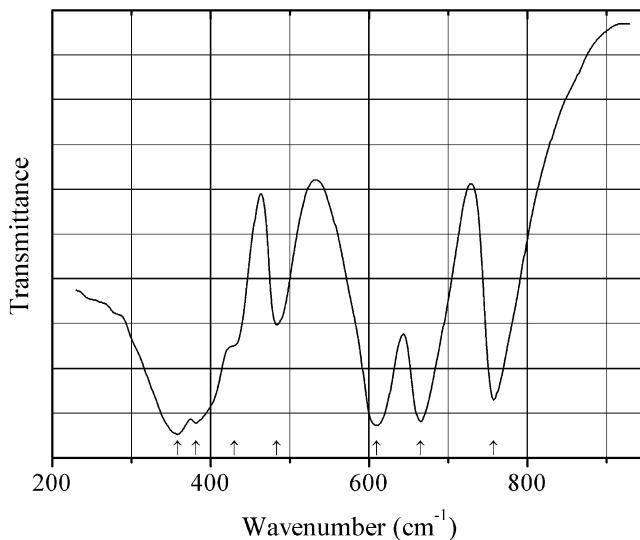
**Description:** Prepared by heating a mixture of  $\text{TeO}_2$  and  $\text{SnO}_2$  taken in stoichiometric amounts, at 700–750 °C for 12–15 h with several intermediate grindings. Cubic, space group  $Ia\bar{3}$ ,  $Z = 8$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Botto and Baran (1981).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 788, 743, 708s, 482, 403sh, 375s, 290w.

### O571 Tellurium(IV) titanium oxide $\text{Te}_3\text{TiO}_8$ $\text{Te}_3\text{TiO}_8$



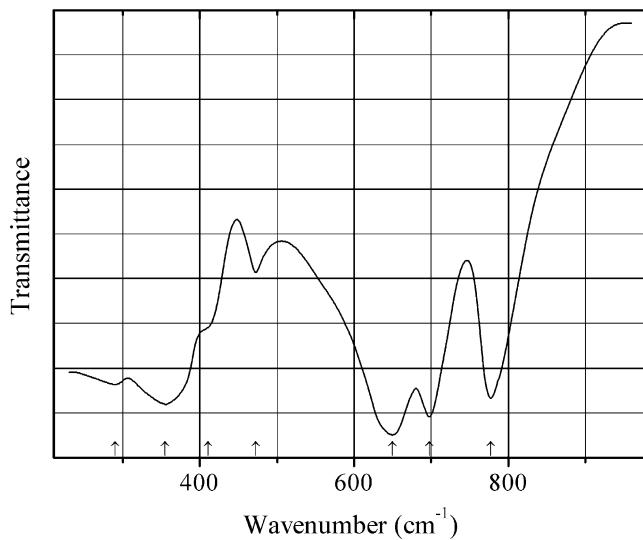
**Origin:** Synthetic.

**Description:** Prepared by heating a mixture of  $\text{TeO}_2$  and  $\text{TiO}_2$  taken in stoichiometric amounts, at 700–750 °C for 12–15 h with several intermediate grindings. Cubic, space group  $Ia\bar{3}$ ,  $Z = 8$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Botto and Baran (1981).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 758, 665s, 610s, 484, 430sh, 382sh, 358s.

**O572 Tellurium(IV) zirconium oxide  $\text{Te}_3\text{ZrO}_8$   $\text{Te}_3\text{ZrO}_8$** 

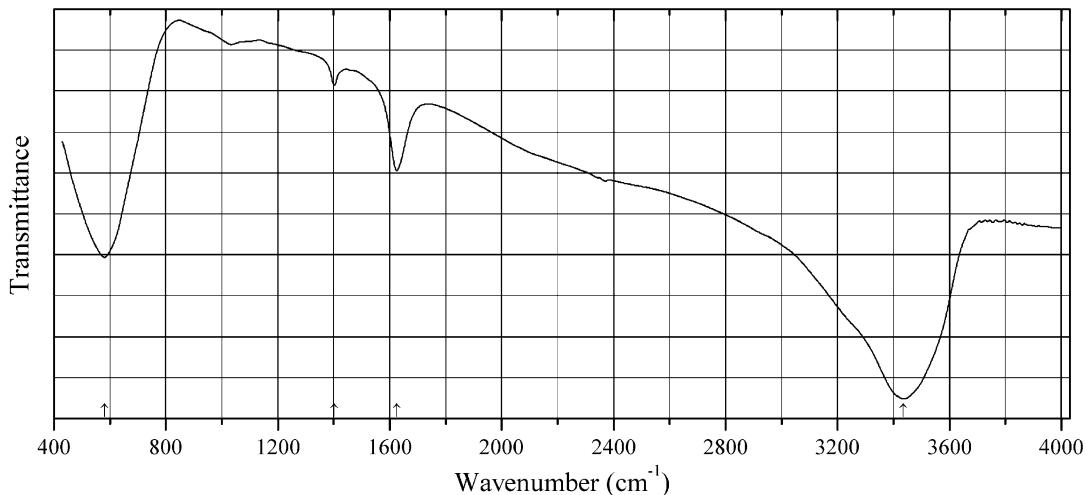
**Origin:** Synthetic.

**Description:** Prepared by heating a mixture of  $\text{TeO}_2$  and  $\text{ZrO}_2$  taken in stoichiometric amounts, at 700–750 °C for 12–15 h with several intermediate grindings. Cubic, space group *Ia3*,  $Z = 8$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Botto and Baran (1981).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 778, 698, 650s, 472w, 410sh, 355, 290.

**O573 Tin(IV) hydroxide  $\text{Sn}(\text{OH})_4$** 

**Origin:** Synthetic.

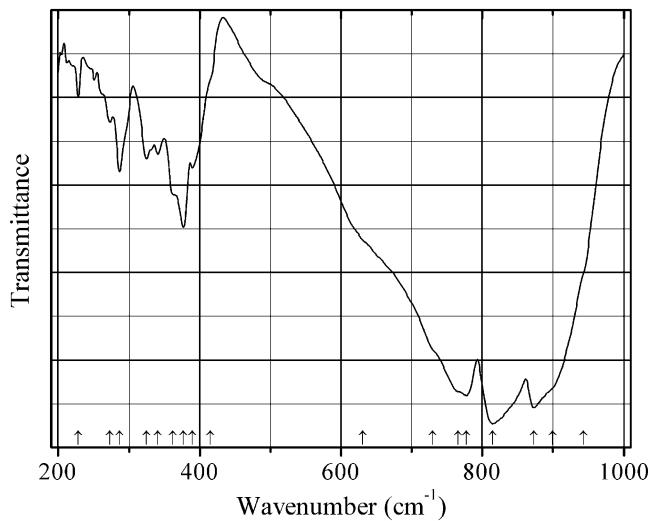
**Description:** Synthesized by dissolving tin metal in concentrated HCl followed by addition of concentrated NH<sub>4</sub>OH.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Prodjosantoso et al. (2015).

**Wavenumbers (cm<sup>-1</sup>):** 3436s, 1625, 1402w, 580s.

#### O574 Tungsten trioxide monoclinic WO<sub>3</sub>



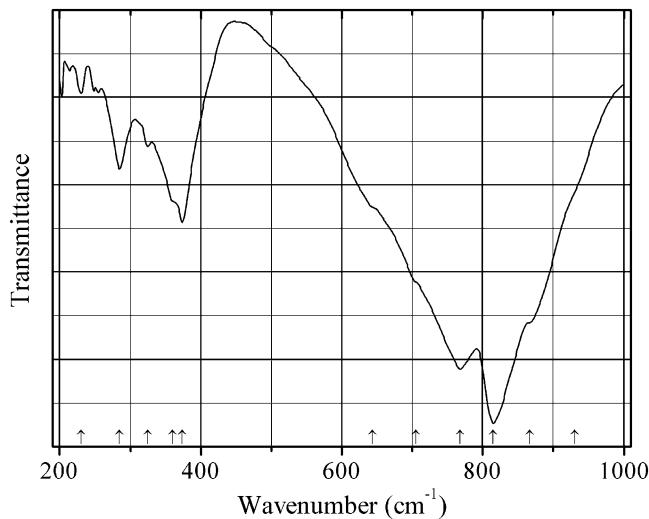
**Origin:** Synthetic.

**Description:** Obtained as a result of thermal decomposition of (NH<sub>4</sub>)<sub>10</sub>W<sub>12</sub>O<sub>41</sub>·nH<sub>2</sub>O at 1223 K for 5 h. Characterized by powder X-ray diffraction data. Monoclinic, space group *P2<sub>1</sub>/n*, *a* = 7.319, *b* = 7.556, *c* = 7.722 Å,  $\beta$  = 90.48° (see JCPDS card 43-1035).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Kustova et al. (2011).

**Wavenumbers (cm<sup>-1</sup>):** 943sh, 900sh, 873s, 815s, 777s, 766sh, 730sh, 631sh, 415sh, 390, 377, 362sh, 341, 325, 287, 273w, 228w.

**O575 Tungsten trioxide orthorhombic  $\text{WO}_3$** 

**Origin:** Synthetic.

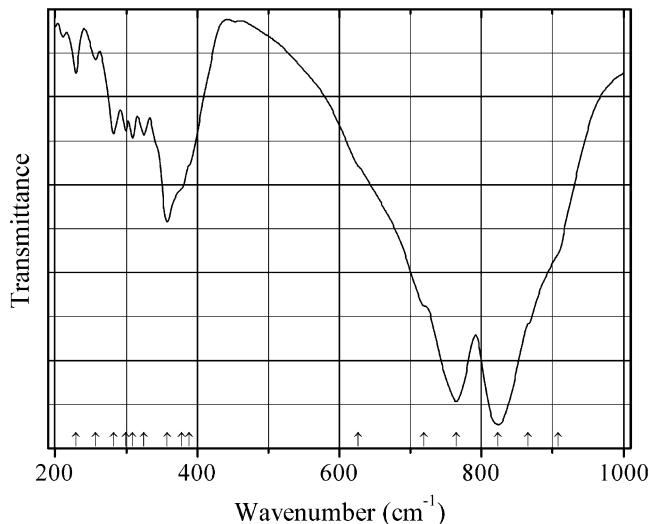
**Description:** Obtained as a result of thermal decomposition of  $(\text{NH}_4)_{10}\text{W}_{12}\text{O}_{41} \cdot n\text{H}_2\text{O}$  at 873 K for 6 h.

Characterized by powder X-ray diffraction data. Orthorhombic, space group  $Pcnb$ ,  $a = 7.339$ ,  $b = 7.574$ ,  $c = 7.742$  Å (see JCPDS card 20-1324).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Kustova et al. (2011).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 930sh, 867sh, 815s, 768s, 705sh, 644sh, 374, 360sh, 325, 285, 230w.

**O576 Tungsten trioxide triclinic  $\text{WO}_3$** 

**Origin:** Synthetic.

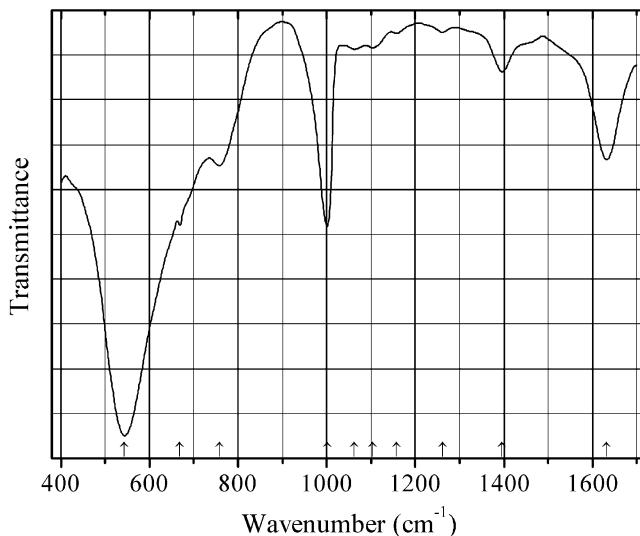
**Description:** Obtained by mechanical treatment (grinding and pressing) of monoclinic  $\text{WO}_3$ . Characterized by powder X-ray diffraction data. Orthorhombic, space group  $P-1$ ,  $a = 7.309$ ,  $b = 7.522$ ,  $c = 7.671 \text{ \AA}$ ,  $\alpha = 88.8^\circ$ ,  $\beta = 90.93^\circ$ ,  $\gamma = 90.93^\circ$  (see JCPDS card 32-1395).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Kustova et al. (2011).

**Wavenumbers (cm<sup>-1</sup>):** 908sh, 866sh, 823s, 765s, 719sh, 627sh, 389sh, 378sh, 358, 325, 309, 299, 282w, 257, 229w.

### O577 Vanadium oxide bariandite-type $\text{V}_{10}\text{O}_{24} \cdot 9\text{H}_2\text{O}$



**Origin:** Synthetic.

**Description:** Mixed valence vanadium(IV)/(V) nanostructured oxide with a bariandite-like structure prepared by sol-gel processing of the molecular vanadium(IV) alkoxide  $[\text{V}_2(\text{OPr}^i)_8]$  ( $\text{OPr}^i$  = isopropoxide).

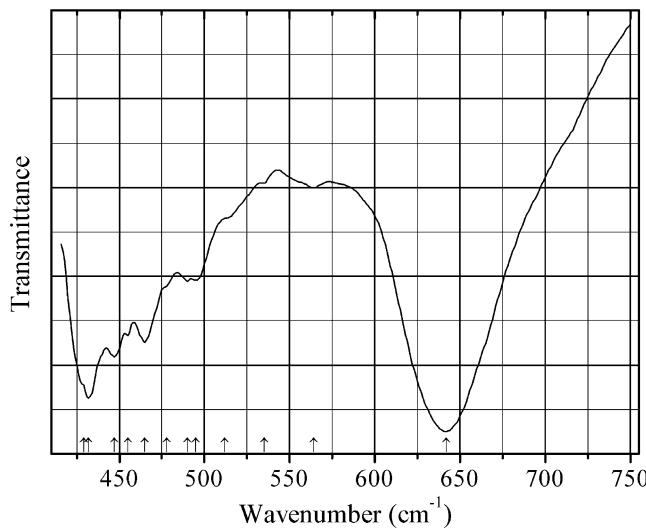
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Menezes et al. (2009).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1632, 1396, 1261w, 1158w, 1104w, 1062w, 1001, 758, 669, 544s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1022, 908s, 518s, 429w, 409w, 270s.

**O578 Yttrium iron antimony(V) oxide pyrochlore-type  $\text{Y}_2\text{FeSbO}_7$** 

**Origin:** Synthetic.

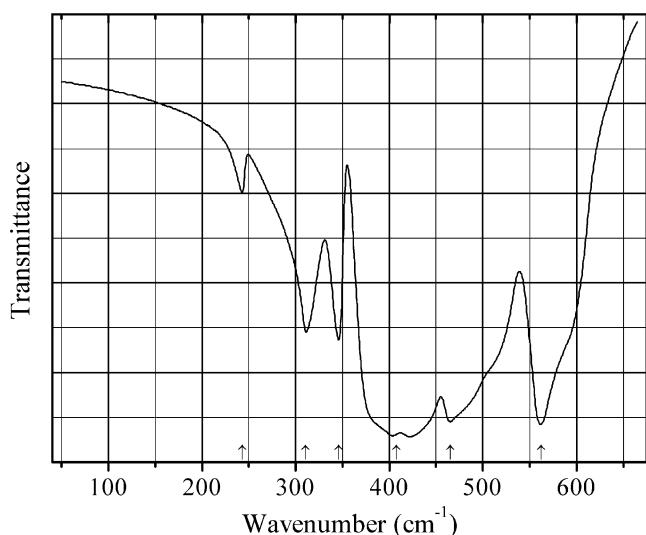
**Description:** Prepared by heating a mixture of  $\text{Y}_2\text{O}_3$ ,  $\text{Fe}_2\text{O}_3$ , and  $\text{Sb}_2\text{O}_3$ , taken in stoichiometric amounts, at 1150 °C for 4.5 h. Characterized by powder X-ray diffraction data. Cubic,  $a = 10.223 \text{ \AA}$ .  $D_{\text{calc}} = 5.811 \text{ g/cm}^3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Jana et al. (2016).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 642s, 564w, 535sh, 512sh, 495, 490, 478sh, 465, 455, 447, 432s, 429sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**O579 Yttrium oxide  $\text{Y}_2\text{O}_3$** 

**Origin:** Synthetic.

**Description:** Commercial reactant. Characterized by powder X-ray diffraction data. Cubic, space group *Ia3*.

**Kind of sample preparation and/or method of registration of the spectrum:** Thin powdery film on polyethylene sheet. Transmission.

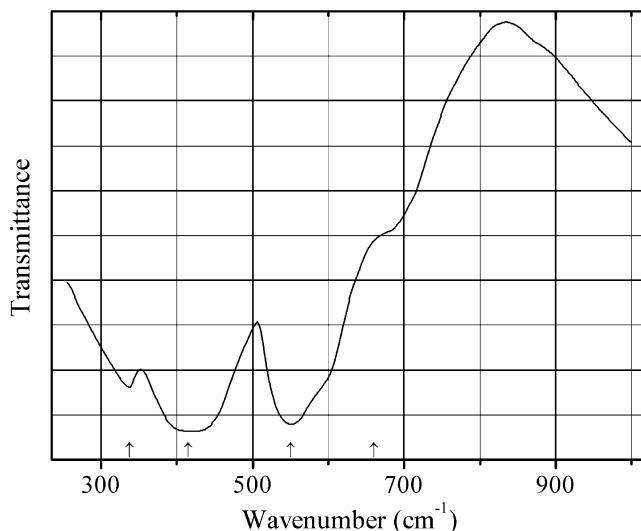
**Source:** White and Keramidas (1972).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 562s, 465s, 408s, 346, 311, 243.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 603, 576w, 480s, 440, 389s, 337, 325, 236w, 162.

### O580 Franklinite $\text{ZnFe}_2\text{O}_4$



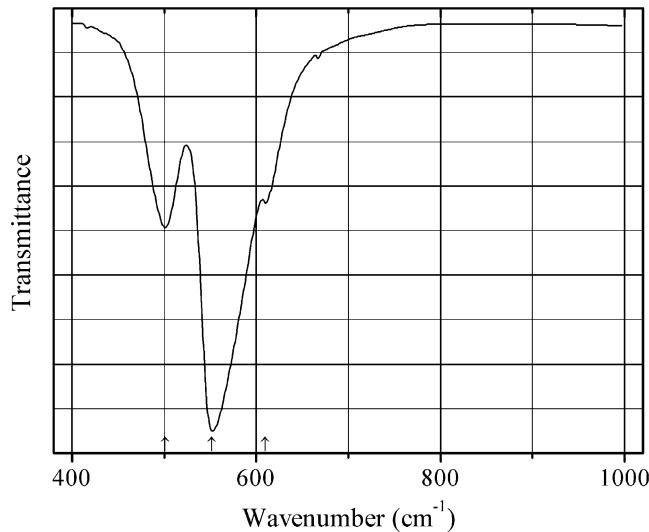
**Origin:** Synthetic.

**Description:** Prepared using a conventional ceramic technique. Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Srinivasan et al. (1984).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 660sh, 550s, 415s, 338.

**O581 Zinc stannate  $ZnSnO_3$** 

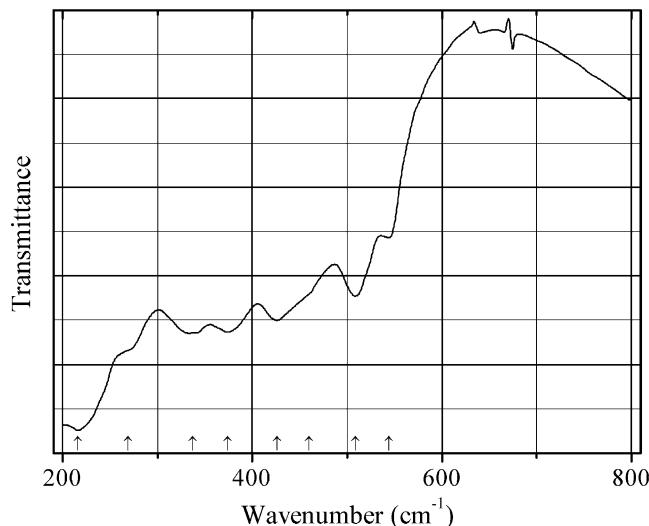
**Origin:** Synthetic.

**Description:** Prepared in the reaction between solid  $Li_2SnO_3$  and  $ZnCl_2$  melt. Characterized by powder X-ray diffraction data and electron probe microanalysis. Isostructural with ilmenite. Trigonal, space group  $R\bar{3}$ ,  $a = 5.2835$ ,  $c = 14.0913$  Å,  $Z = 6$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 3.84 (20) (102), 2.79 (100) (104), 2.64 (88) (110), 1.918 (26) (204), 1.755 (45) (116), 1.553 (32) (214), 1.526 (25) (300).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Kovacheva and Petrov (1998).

**Wavenumbers (cm<sup>-1</sup>):** 610, 552s, 501.

**O583 Bismite  $\alpha\text{-}Bi_2O_3$** 

**Origin:** Synthetic.

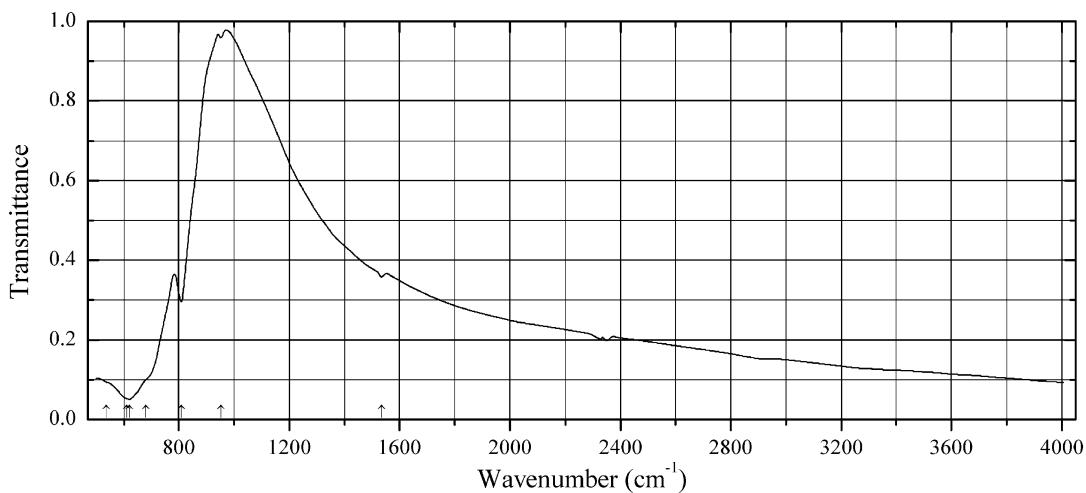
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Cahen et al. (1980).

**Wavenumbers (cm<sup>-1</sup>):** 544w, 509, 460sh, 426, 374, 337, 269sh, 216s.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

#### O584 Bismutocolumbite BiNbO<sub>4</sub>



**Origin:** Synthetic.

**Description:** Prepared by stepwise heating of stoichiometric mixture of Bi<sub>2</sub>O<sub>3</sub> and Nb<sub>2</sub>O<sub>5</sub> at 700, 800, and 900 °C for 6 h at each temperature. Characterized by powder X-ray diffraction data. Orthorhombic.

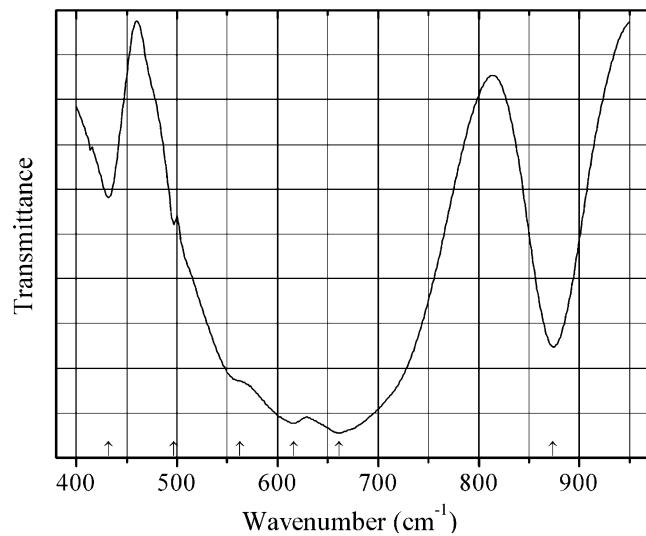
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Rao and Buddhudu (2010).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1534w, 952w, 809, 680sh, 620s, 610sh, 538sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 984w, 840s, 746w, 621, 540, 474w, 422, 242s, 196s.

**O585 Bismutotantalite triclinic dimorph BiTaO<sub>4</sub>**

**Origin:** Synthetic.

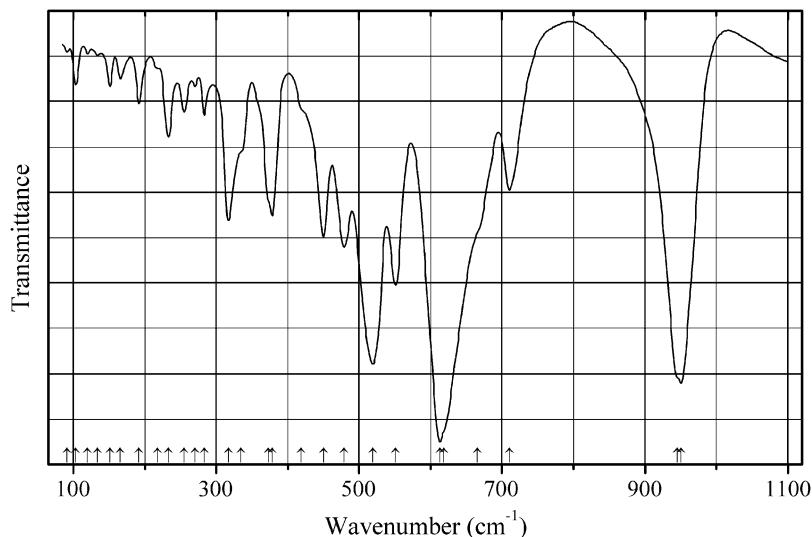
**Description:** Prepared from a mixture of oxides at 1373 K for 2 days. Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Zhang et al. (2009b).

**Wavenumbers (cm<sup>-1</sup>):** 874, 661s, 616s, 563sh, 497w, 432.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**O586 Braunite Mn<sup>2+</sup>Mn<sup>3+</sup><sub>6</sub>O<sub>8</sub>(SiO<sub>4</sub>)**

**Origin:** Synthetic.

**Description:** Prepared from  $\text{MnO}_2$ ,  $\text{MnCl}_2$ , and  $\text{SiO}_2$  above  $615^\circ\text{C}$  (i.e. above the  $\text{MnCl}_2$  melting point). Characterized by powder X-ray diffraction data. The crystal structure is solved. Tetragonal, space group  $I4_1/acd$ ,  $a = 9.371(2)$ ,  $c = 18.847(8)$  Å,  $V = 571.6(3)$  Å $^3$ ,  $Z = 8$ .

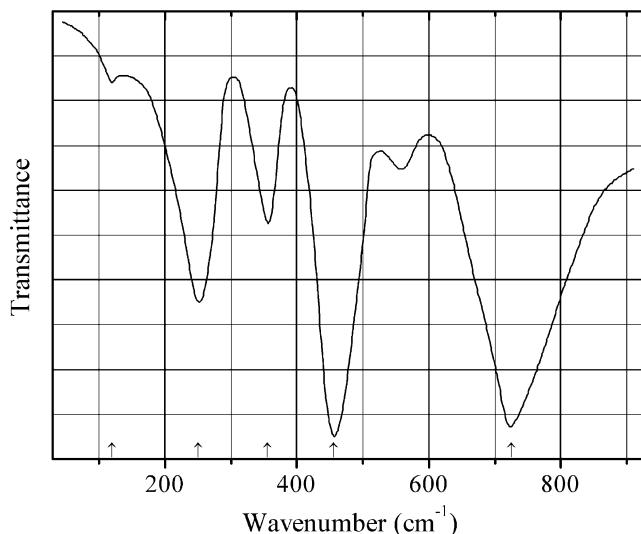
**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull between polyethylene plates. Absorption.

**Source:** Palvadeau et al. (1991).

**Wavenumbers (cm $^{-1}$ ):** 951s, 945sh, 710, 666sh, 619sh, 613s, 551, 519s, 479, 450, 419sh, 378, 373sh, 335sh, 317, 283w, 270w, 255w, 233, 218sh, 192w, 166w, 151w, 134w, 120w, 103w, 91w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### O587 Brizzite polymorph $\text{Na}_2\text{Sb}_2\text{O}_6$



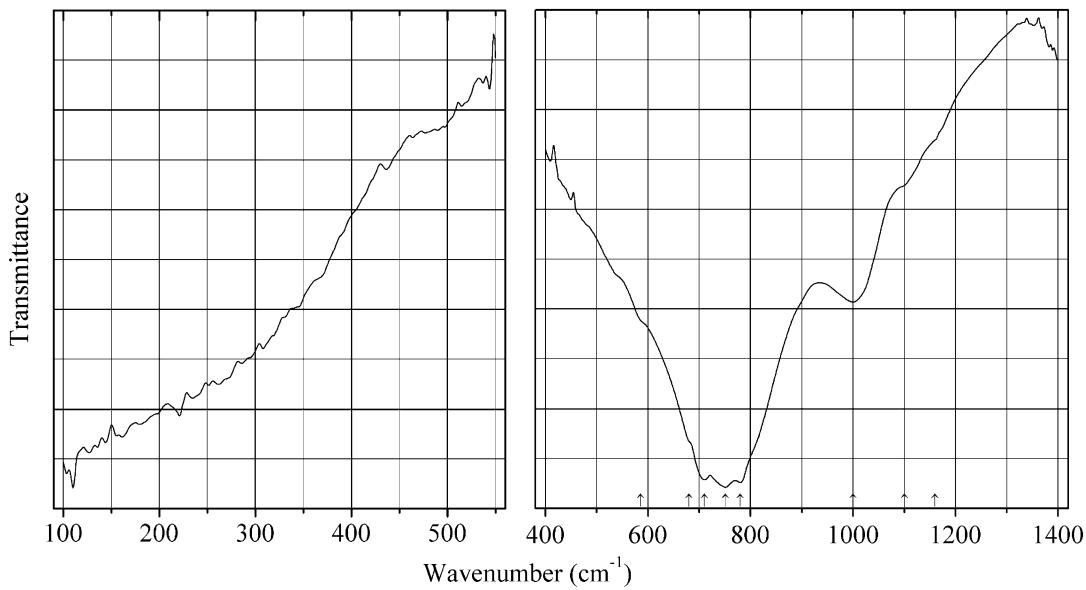
**Origin:** Synthetic.

**Description:** Structurally related to pyrochlore.

**Source:** Vandeborre et al. (1982).

**Wavenumbers (cm $^{-1}$ ):** 725s, 455s, 355, 250, 120w.

**Note:** A weak band between 500 and 600 cm $^{-1}$  corresponds to  $\text{H}_2\text{O}$  impurity.

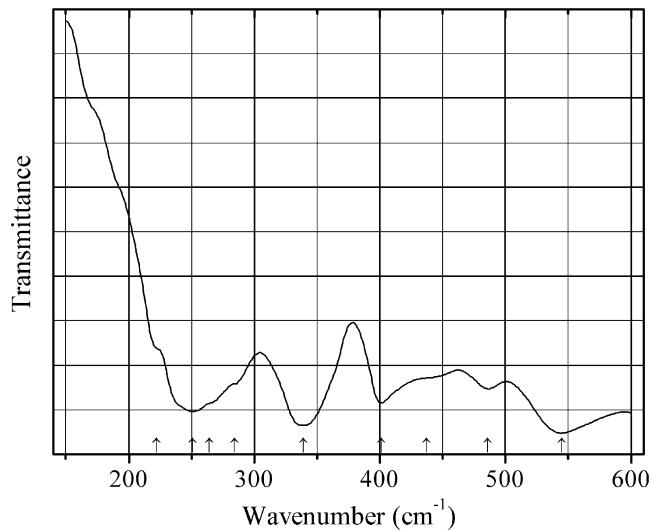
**O588 Bromellite BeO**

**Origin:** Synthetic.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Hofmeister et al. (1987).

**Wavenumbers (cm<sup>-1</sup>):** (1160sh), (1100sh), 1000, 780s, 751s, 710s, (680sh), (585sh).

**O589 Brookite TiO<sub>2</sub>**

**Origin:** Synthetic.

**Description:** Nanocrystals prepared hydrothermally. Characterized by powder X-ray diffraction data.

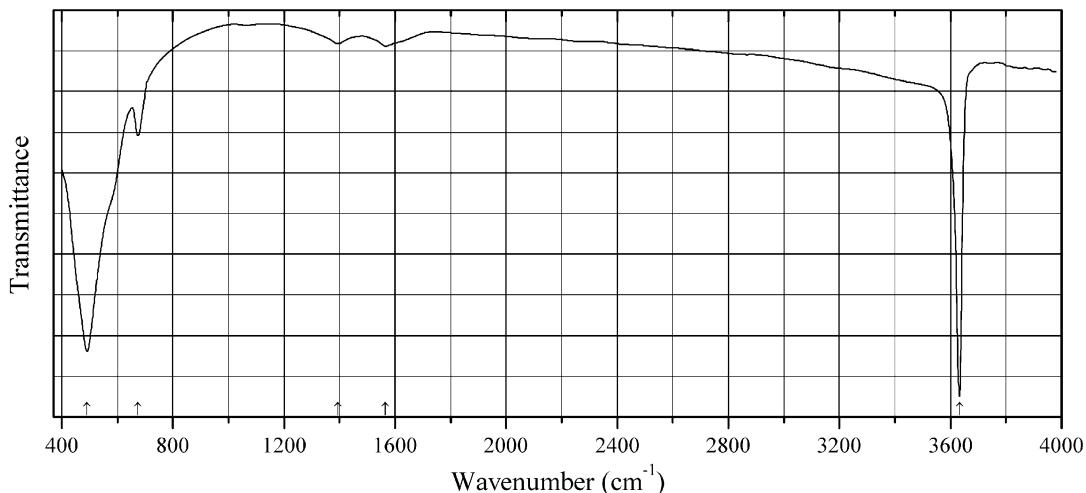
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Yanqing et al. (2000).

**Wavenumbers (cm<sup>-1</sup>):** 545s, 486, 437sh, 401s, 339s, 284sh, 264sh, 251s, 222sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### O590 Brucite Co-analogue $\beta\text{-Co(OH)}_2$



**Origin:** Synthetic.

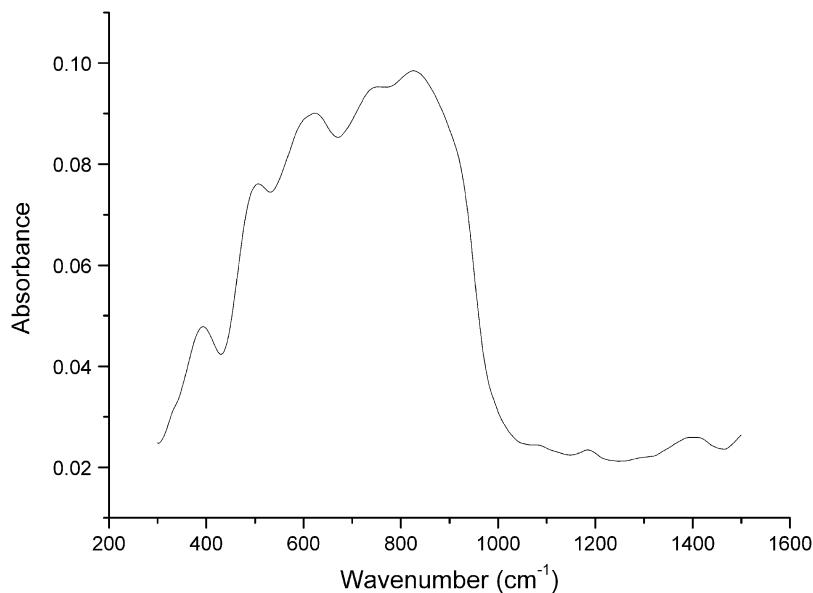
**Description:** Nanoplates prepared hydrothermally from  $\text{CoCl}_2$  and  $\text{NaOH}$  at 120 °C for 3 h.  
Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Zhan (2009).

**Wavenumbers (cm<sup>-1</sup>):** 3633s, 1566w, 1394w, 675, 490s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The bands in the range of 600–1600  $\text{cm}^{-1}$  may correspond to impurities.

**O591 Gamma-alumina  $\gamma\text{-Al}_2\text{O}_3$** 

**Origin:** Synthetic.

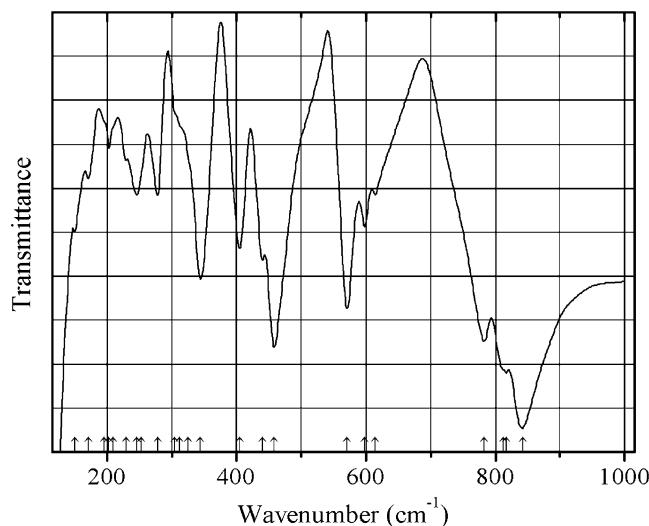
**Description:** Obtained by calcining commercial boehmite at 550 °C for 5 h. Characterized by powder X-ray diffraction data.  $\gamma\text{-Al}_2\text{O}_3$  has tetragonally deformed defect spinel-type structure.

**Kind of sample preparation and/or method of registration of the spectrum:** Thin powdery layer between two KBr windows. Absorption.

**Source:** Saniger (1995).

**Wavenumbers (cm⁻¹):** 1403w, 1184w, 1085w, 826s, 764sh, 634s, 506, 393.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**O592 Chlormayenite  $\text{Ca}_{12}\text{Al}_{14}\text{O}_{32}(\square_4\text{Cl}_2)$** 

**Origin:** Synthetic.

**Description:** Synthesized by heating of a stoichiometric mixture of  $\text{CaCO}_3$ ,  $\text{Al}_2\text{O}_3$ , and  $\text{CaCl}_2$  first at 1323 K for 16 h and thereafter at 1473 K for 24 h with intermediate grinding. Characterized by powder X-ray diffraction data, neutron powder diffraction, and EDX analysis. The crystal structure is solved. Cubic.

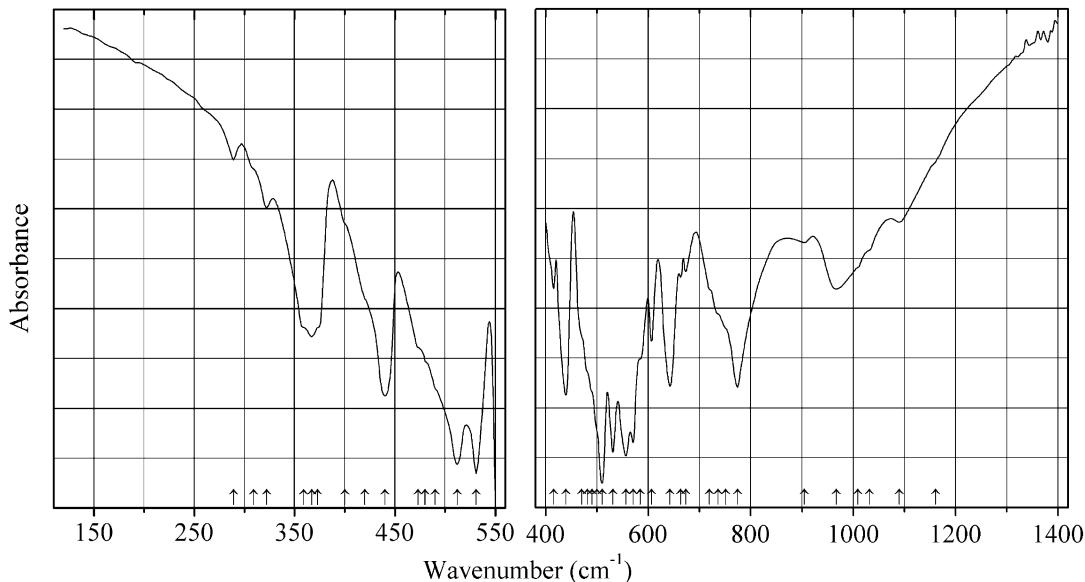
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Schmidt et al. (2014).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 842s, 817s, 812sh, 783s, 614, 598, 571, 458s, 440, 405, 344s, 325sh, 312sh, 304sh, 278, 253sh, 246, 229, 209sh, 203w, 195sh, 171w, 150.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, the wavenumber  $783 \text{ cm}^{-1}$  is erroneously indicated as  $738 \text{ cm}^{-1}$ .

### O593 Chrysoberyl $\text{BeAl}_2\text{O}_4$



**Origin:** Colatine, Espirito Santo, Brazil.

**Description:** The sample contains 3.1 wt%  $\text{Fe}_2\text{O}_3$ , which corresponds to 2.5 mol%  $\text{BeFe}_2\text{O}_4$ .

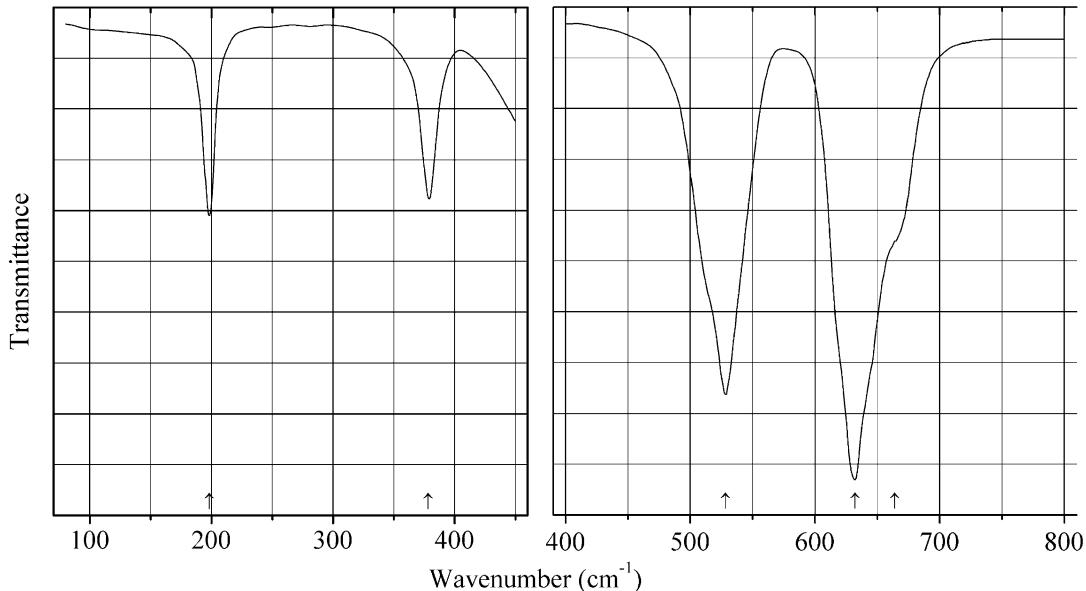
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc and powder dispersed in petroleum jelly. Absorption.

**Source:** Hofmeister et al. (1987).

**Wavenumbers (cm<sup>-1</sup>):** 1161sh, 1090, 1032sh, 1009sh, 967, 904, 774, 751sh, 736sh, 719sh, 673, 663, 642, 606, 584, 570s, 556s, 531s, 510s, 500sh, 490sh, 481sh, 470sh, 439, 415 (for a sample pressed in a disc with KBr); 531s, 512s, 490sh, 480sh, 473, 440, 420sh, 400sh, 373sh, 367, 359sh, 322, 309w, 289w.

**Note:** In the cited paper, the wavenumber 531 cm<sup>-1</sup> is erroneously indicated as 538 cm<sup>-1</sup>.

### O594 Cochromite Ni-bearing Co<sub>0.9</sub>Ni<sub>0.1</sub>Cr<sub>2</sub>O<sub>4</sub>



**Origin:** Synthetic.

**Description:** Spinel-type compound obtained by annealing a mixture of Co(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O, Ni(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O, and Cr(NO<sub>3</sub>)<sub>3</sub>·9H<sub>2</sub>O (taken in stoichiometric amounts and preheated at 400 °C) at 1000 °C for 24 h. Characterized by powder X-ray diffraction data. Cubic,  $a = 8.3323 \text{ \AA}$ .

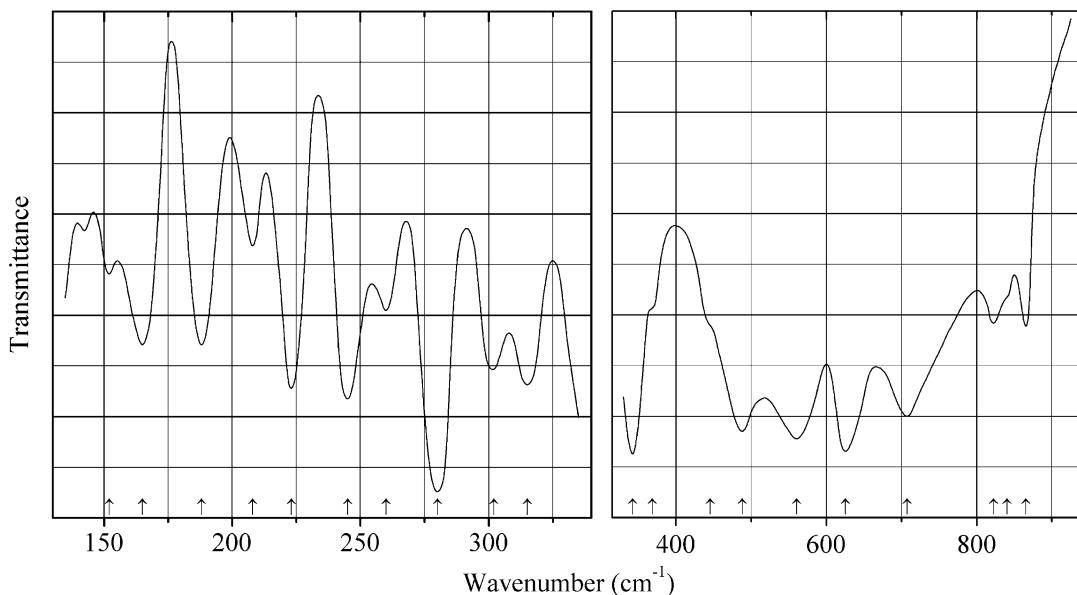
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc and Nujol mull. Transmission.

**Source:** Ptak et al. (2014).

**Wavenumbers (IR, cm<sup>-1</sup>):** 664sh, 632s, 528s, 378, 198.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. For the vibration spectra of synthetic cochromite analogue see also Mączka et al. (2013). In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 683, 601w, 514, 450, 195s.

**O595 Columbite-(Mn)  $Mn^{2+}Nb_2O_6$** 

**Origin:** Synthetic.

**Description:** Prepared using conventional solid-state reaction techniques. Characterized by powder X-ray diffraction data. Orthorhombic,  $a = 14.413(17)$ ,  $b = 5.759(5)$ ,  $c = 5.083(7)$  Å.

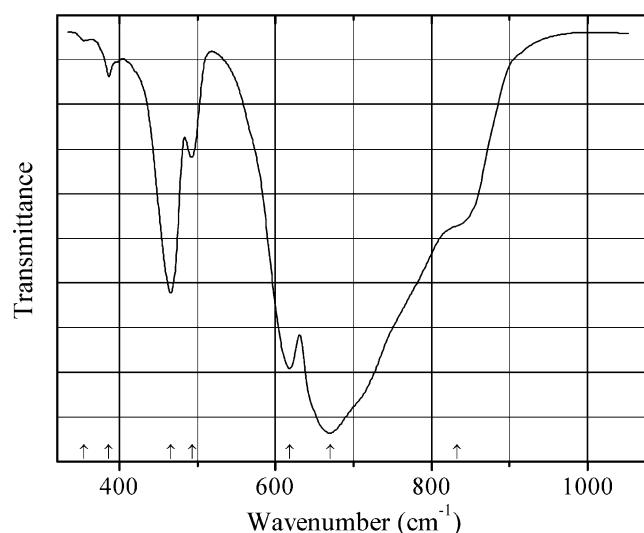
**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc (above 340  $\text{cm}^{-1}$ ) and polyethylene film (below 340  $\text{cm}^{-1}$ ). Transmission.

**Source:** Husson et al. (1977a, b).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 865, 840sh, 822, 707s, 625s, 560s, 488s, 445sh, 368sh, 342s, 315, 302, 280s, 260, 245, 223, 208w, 188, 165, 152w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 877s, 823, 707w, 634w, 624w, 606, 531s, 487, 440w, 399, 386, 361, 315s, 298w, 288, 275, 264w, 245s, 215, 207, 179, 160w, 140s, 127, 113, 89s.

**O596 Corundum  $\alpha\text{-Al}_2\text{O}_3$** 

**Origin:** Synthetic.

**Description:** Irregular grains from 1 to 3  $\mu\text{m}$  across.

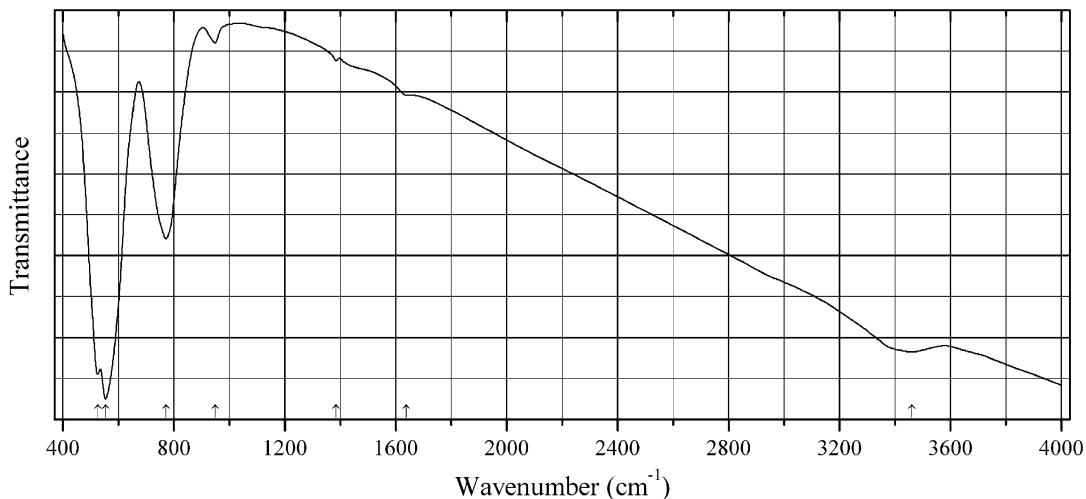
**Kind of sample preparation and/or method of registration of the spectrum:** Free particles dispersed in air. Absorption.

**Source:** Mutschke et al. (2013).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 833sh, 670s, 618s, 493, 466, 386w, 354w.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

### O597 Delafossite Al analogue $\text{Cu}^{1+}\text{AlO}_2$



**Origin:** Synthetic.

**Description:** Synthesized from  $\text{CuO}$  and  $\text{Al}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$  by a sol-gel method using ethylene glycol as solvent. Characterized by powder X-ray diffraction data. Trigonal, space group  $R-3m$ ,  $a = 2.852$ ,  $c = 16.830 \text{ \AA}$ .

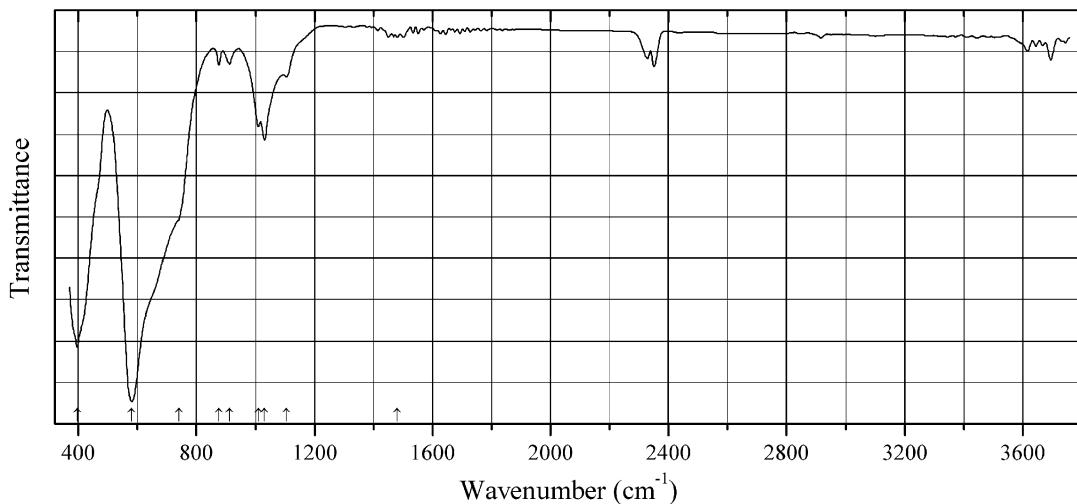
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Benreguia et al. (2015).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** (3460), 1637sh, 1385w, 949w, 772, 554s, 526s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The bands above  $1600 \text{ cm}^{-1}$  may correspond to adsorbed water. In the cited paper, Raman spectrum is given. The band at  $1385 \text{ cm}^{-1}$  may correspond to the admixture of potassium nitrate in KBr.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 773s, 417s, 255, 214.

**O598 Fluorcalciomicrolite**  $(\text{Ca},\text{Na},\square)_2\text{Ta}_2\text{O}_6\text{F}$ 

**Origin:** No data.

**Description:** The empirical formula is (electron microprobe):  $(\text{Ca}_{1.23}\text{Na}_{0.745}\text{REE}_{0.01}\text{Sr}_{0.01})(\text{Ta}_{1.78}\text{Nb}_{0.08}\text{Ti}_{0.08}\text{Si}_{0.06})\text{O}_6[\text{F}_{0.57}(\text{OH},\text{O},\square)_{0.43}]$ .

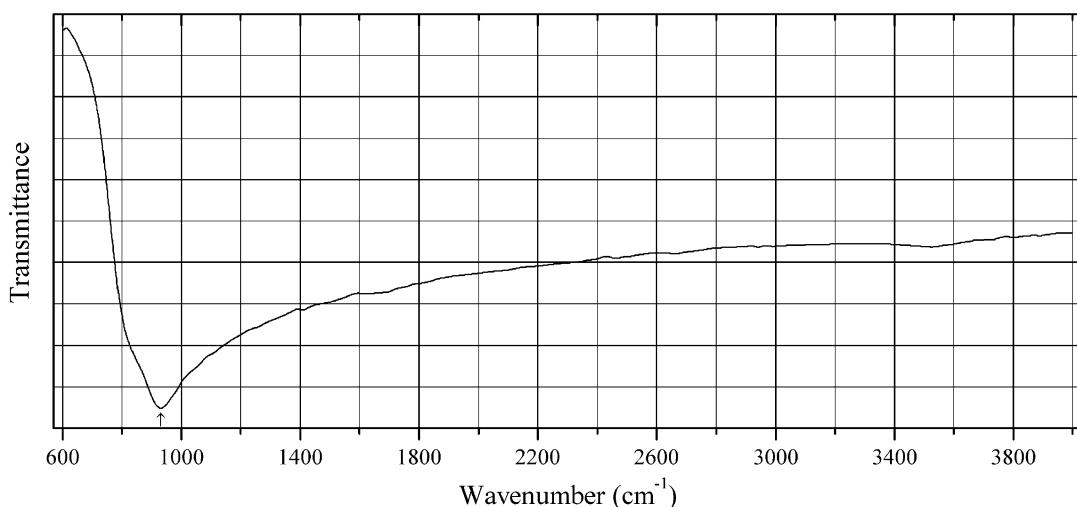
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Geisler et al. (2004).

**Wavenumbers (IR, cm<sup>-1</sup>):** (1480w), 1105w, 1031, 1010, 912w, 876w, 740sh, 580s, 396s.

**Note:** Weak bands in the range from 2300 to 2400 cm<sup>-1</sup> correspond to atmospheric CO<sub>2</sub>. The weak band at 1480 cm<sup>-1</sup> may correspond to the admixture of a carbonate. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 835, 690s, 504s, 341, 295, 155.

**O599 Fluornatropyrochlore**  $(\text{Na},\text{Pb},\text{Ca},\text{REE},\text{U})_2\text{Nb}_2\text{O}_6\text{F}$ 

**Origin:** Boziguuer REE deposit, Baicheng County, Akesu, Xinjiang, China (type locality).

**Description:** A grain from the holotype specimen.

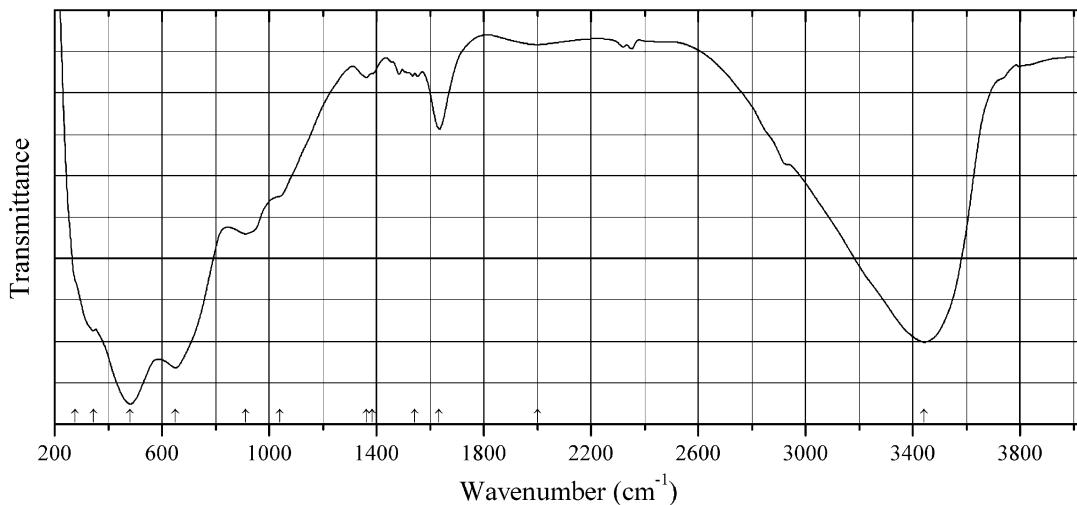
**Kind of sample preparation and/or method of registration of the spectrum:** Reflection.

**Source:** Yin et al. (2015).

**Wavenumbers (cm<sup>-1</sup>):** 932.

**Note:** The spectrum is wrong. The main broad band at 932 cm<sup>-1</sup> may correspond to an anhydrous metamict silicate [possibly, thorite or chevkinite-(Ce)] that are present in the association with fluornatropyrochlore.

### O601 Gallium hydroxyde hydrate $\text{Ga(OH)}_3 \cdot n\text{H}_2\text{O}$ $\text{Ga(OH)}_3 \cdot n\text{H}_2\text{O}$



**Origin:** Synthetic.

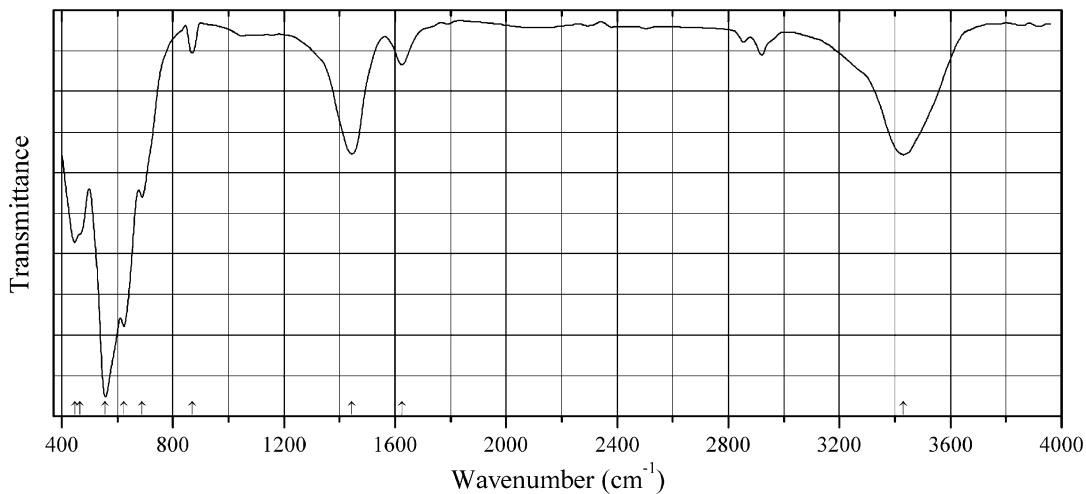
**Description:** Obtained by addition of hot water and tetramethylammonium hydroxide solution to the solution of gallium(III)-isopropoxide dissolved in 2-propanol. X-ray amorphous.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Ristić et al. (2005).

**Wavenumbers (cm<sup>-1</sup>):** 3443s, 2000w, 1634, 1542w, 1383sh, 1362, 1040sh, 912, 650s, 482s, 345s, 278sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**O602 Harmunite cubic polymorph  $\text{CaFe}_2\text{O}_4$** 

**Origin:** Synthetic.

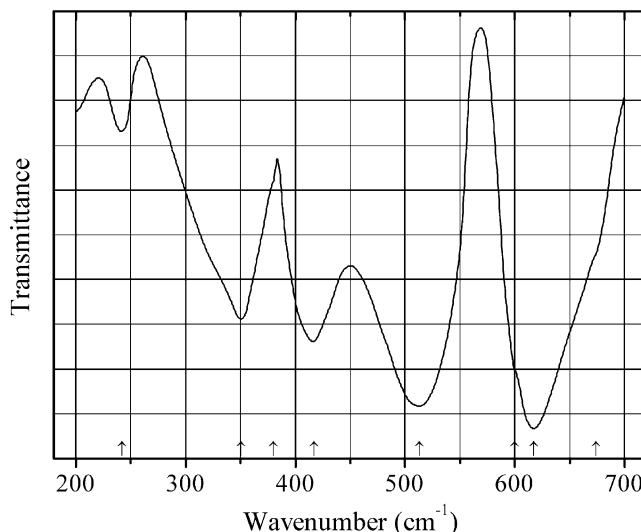
**Description:** Nanoparticles synthesized from a stoichiometric mixture of calcium chloride and iron (III) nitrate by a sol-gel technique with subsequent annealing. Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** An et al. (2015).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3431, 1625w, 1445, 869w, 690, 624s, 557s, 466sh, 447.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. The bands at 3431 and 1625  $\text{cm}^{-1}$  may correspond to water molecules adsorbed on the surface of the nanoparticles. The bands at 1445 and 869  $\text{cm}^{-1}$  may correspond to the admixture of a carbonate. The assignment of the band at 1445  $\text{cm}^{-1}$  given in the cited paper is erroneous.

**O603 Hausmannite  $\text{Mn}^{2+}\text{Mn}^{3+}_2\text{O}_4$** 

**Origin:** Synthetic.

**Description:** Prepared by heating  $\text{MnCO}_3$  at 1185 °C for 5 h. Characterized by powder X-ray diffraction data. Tetragonal.

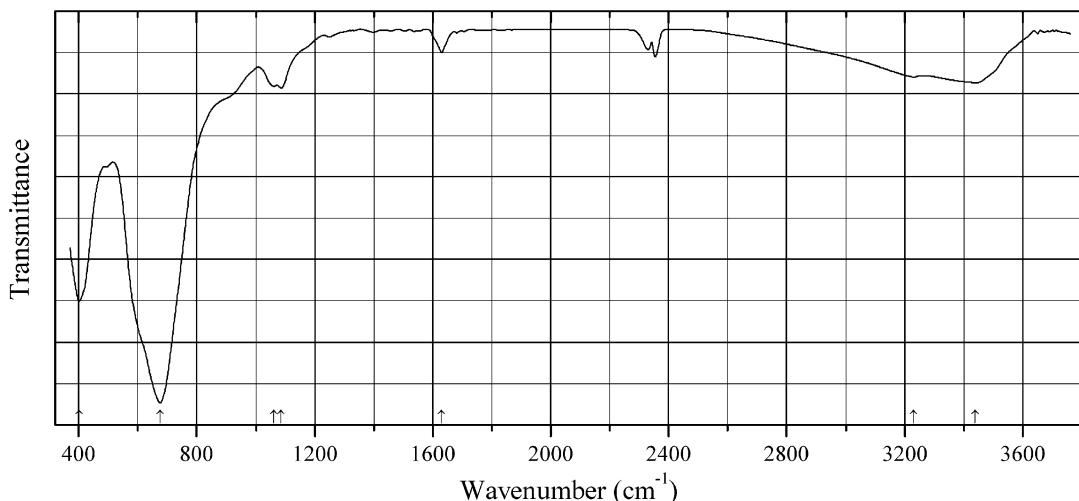
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Brabers (1969).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 674sh, 617s, 600sh, 513s, 417, 380sh, 351, 242w

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

#### O604 Hydrokenomicrolite ( $\square, \text{H}_2\text{O})_2\text{Ta}_2(\text{O},\text{OH})_6(\text{H}_2\text{O})$



**Origin:** Artificial.

**Description:** Prepared by treating natural fluorcalciomicrolite at 175 °C in a 1 M HCl-CaCl<sub>2</sub> solution for 14 days. The grains are heterogeneous, with fluorcalciomicrolite core and hydrokenomicrolite outer zones.

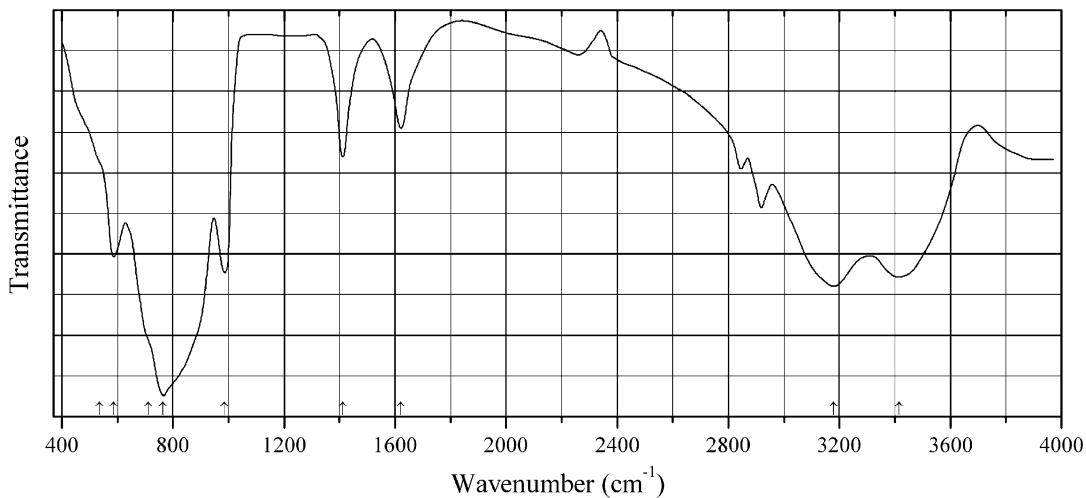
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Geisler et al. (2004).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3440, 3230w, 1630w, 1086, 1061, 676s, 402s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. Weak bands in the range from 2300 to 2400  $\text{cm}^{-1}$  correspond to atmospheric CO<sub>2</sub>. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1115w, 800, 637, 549, 515, 338s, 302, 248sh, 159, 138, 120.

**O605 Ilsemannite  $\text{Mo}_3\text{O}_8 \cdot n\text{H}_2\text{O}$  (?)**

**Origin:** Synthetic.

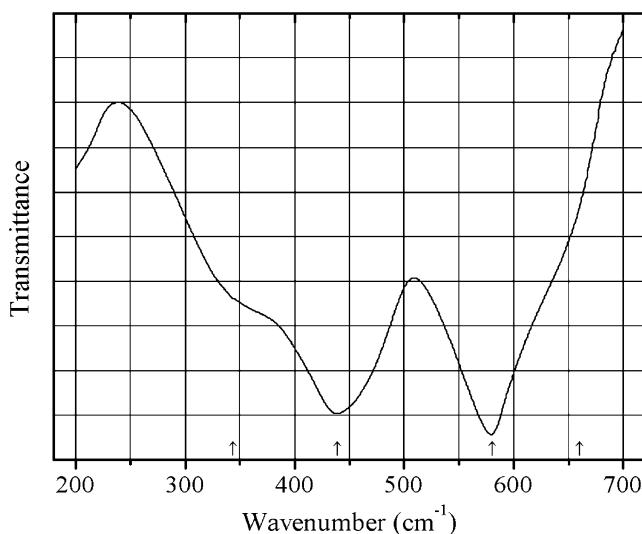
**Description:** Blue amorphous product of ultrasound irradiation of a slurry of molybdenum hexacarbonyl. Characterized by DSC and TG data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Dhas and Gedanken (1997).

**Wavenumbers (cm⁻¹):** 3415, 3180, 1621, 1412, 986, 765s, 712sh, 587, 535sh.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. The assignment of the band at  $1412\text{ cm}^{-1}$  made by the authors of the cited paper is questionable. Weak bands in the range from  $2800$  to  $3000\text{ cm}^{-1}$  correspond to the admixture of an organic substance.

**O606 Iwakiite-hausmannite intermediate member  $\text{Mn}^{2+}(\text{Mn}^{3+}\text{Fe}^{3+})\text{O}_4$** 

**Origin:** Synthetic.

**Description:** Prepared by heating  $\text{MnCO}_3$  at 1360 °C for 5 h in air. Characterized by powder X-ray diffraction data. Tetragonal.

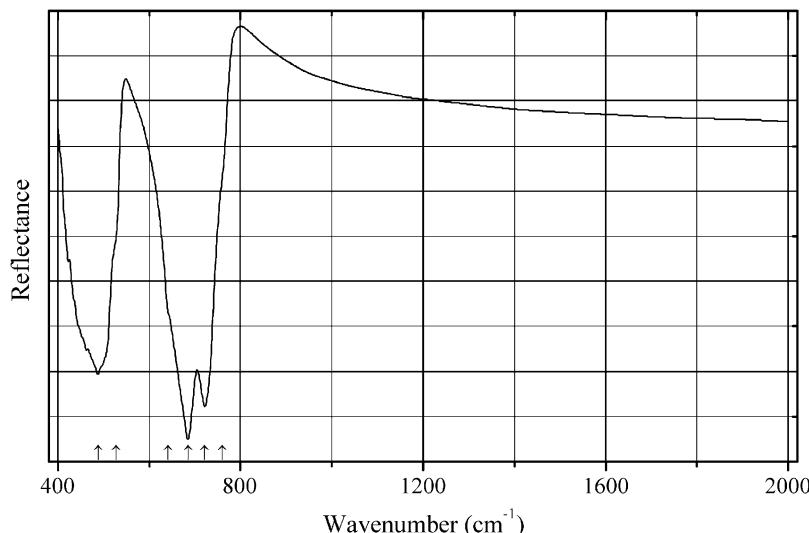
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Brabers (1969).

**Wavenumbers (cm<sup>-1</sup>):** 660sh, 580s, 439s, 344sh.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

### O607 Kyawthuite $\text{Bi}^{3+}\text{Sb}^{5+}\text{O}_4$



**Origin:** Chaung-gyi-ah-le-ywa, Chaung-gyi valley, 5 km north-northeast of the town of Mogok, Pyin-Oo-Lwin district, Myanmar (type locality).

**Description:** Reddish orange faceted waterworn crystal of gem quality from alluvium. Holotype (and the only known) sample. The crystal structure is solved. Monoclinic, space group  $I2/c$ ,  $a = 5.4624(4)$ ,  $b = 4.88519(17)$ ,  $c = 11.8520(8)$  Å,  $\beta = 101.195(7)^\circ$ ,  $V = 310.25(3)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{meas}} = 8.256(5)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 8.127$  g/cm<sup>3</sup>. The empirical formula is  $(\text{Bi}^{3+}_{0.83}\text{Sb}^{3+}_{0.18})(\text{Sb}^{5+}_{0.99}\text{Ta}^{5+}_{0.01})\text{O}_4$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å (I, %) ( $hkl$ )] are: 3.266 (100) (-112), 2.900 (66) (112), 2.678 (24) (200), 2.437 (22) (020, -114), 1.8663 (21) (024), 1.8026 (43) (-116, 220, 204), 1.6264 (23) (-224, 116), 1.5288 (28) (312, -132).

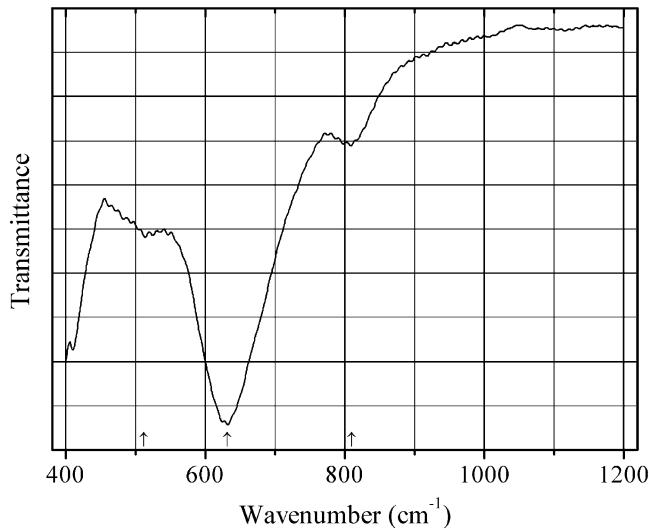
**Kind of sample preparation and/or method of registration of the spectrum:** Specular reflection.

**Source:** Kampf et al. (2016i).

**Wavenumbers (IR, cm<sup>-1</sup>):** 760sh, 722s, 685s, 641sh, 527sh, 510–430 (broad, with an extremum at 488 cm<sup>-1</sup>).

**Note:** Natural origin of kyawthuite is questionable and is to be confirmed by independent finds. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 793, 736, 453s, 396s, 322, 258, 173s.

**O608 Layered perovskite  $\text{BaBi}_2\text{Ta}_2\text{O}_9$ ,  $\text{BaBi}_2\text{Ta}_2\text{O}_9$** 

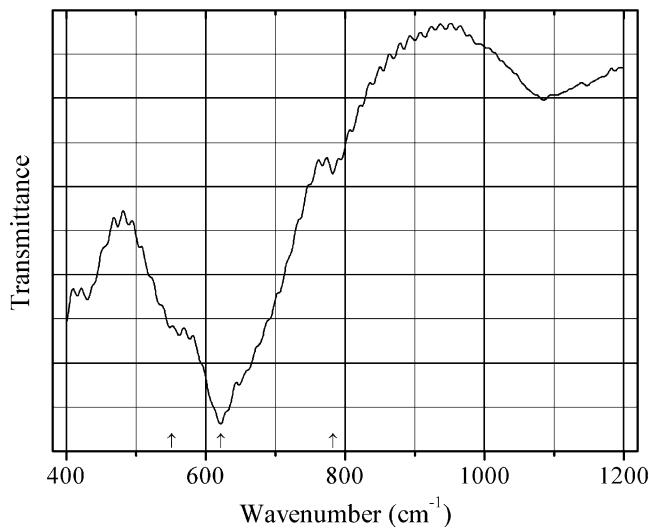
**Origin:** Synthetic.

**Description:** Prepared by solid-state reaction of  $\text{BaCO}_3$ ,  $\text{Bi}_2\text{O}_3$ , and  $\text{Ta}_2\text{O}_5$  at  $1000\text{ }^\circ\text{C}$  for 72 h with intermediate grindings. Characterized by powder X-ray diffraction data. Tetragonal, space group  $I4/mmm$ ,  $a = 3.954$ ,  $c = 25.487\text{ \AA}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Li et al. (2008).

**Wavenumbers (cm⁻¹):** 809.5, 631s, 512.

**O609 Layered perovskite  $\text{CaBi}_2\text{Ta}_2\text{O}_9$ ,  $\text{CaBi}_2\text{Ta}_2\text{O}_9$** 

**Origin:** Synthetic.

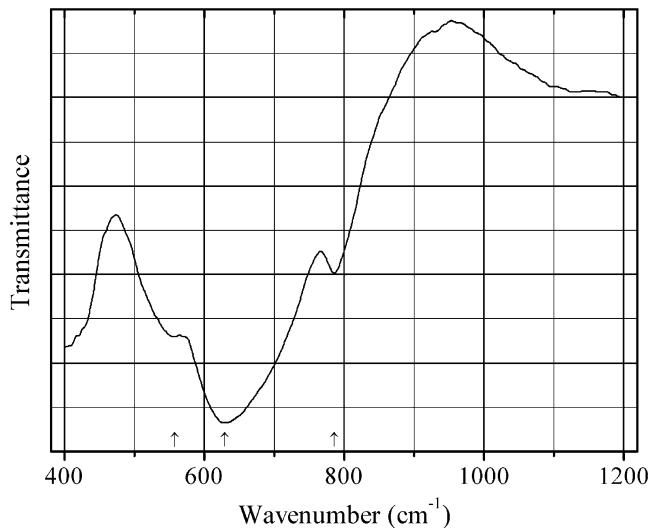
**Description:** Prepared by stepwise heating of a stoichiometric mixture of  $\text{CaCO}_3$ ,  $\text{Bi}_2\text{O}_3$ , and  $\text{Ta}_2\text{O}_5$ , first at 900 °C for 15 h, thereafter at 1000 °C for 15 h, and finally at 1200 °C for 24 h with intermediate grindings. Characterized by powder X-ray diffraction data. Orthorhombic, space group  $A2_1am$ ,  $a = 5.467$ ,  $b = 5.427$ ,  $c = 24.931$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Li et al. (2008).

**Wavenumbers (cm<sup>-1</sup>):** 782, 622s, 551.

### O610 Layered perovskite $\text{SrBi}_2\text{Ta}_2\text{O}_9$ $\text{SrBi}_2\text{Ta}_2\text{O}_9$



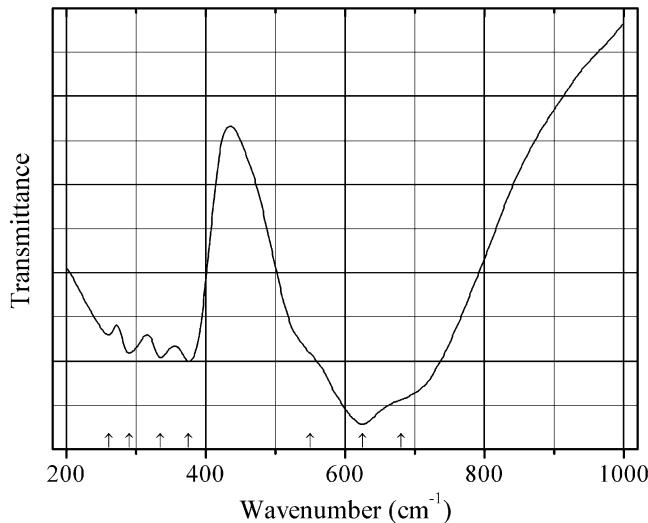
**Origin:** Synthetic.

**Description:** Prepared by stepwise heating of a stoichiometric mixture of  $\text{SrCO}_3$ ,  $\text{Bi}_2\text{O}_3$ , and  $\text{Ta}_2\text{O}_5$ , first at 900 °C for 15 h, thereafter at 1000 °C for 15 h, and finally at 1200 °C for 24 h with intermediate grindings. Characterized by powder X-ray diffraction data. Orthorhombic, space group  $A2_1am$ ,  $a = 5.473$ ,  $b = 5.527$ ,  $c = 25.031$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Li et al. (2008).

**Wavenumbers (cm<sup>-1</sup>):** 786, 629s, 558.

**O611 Lueshite**  $\text{NaNbO}_3$ 

**Origin:** Synthetic.

**Description:** Prepared by heating a stoichiometric mixture of  $\text{NaNO}_3$  and  $\text{Nb}_2\text{O}_5$  at 1000 °C for 1 h.

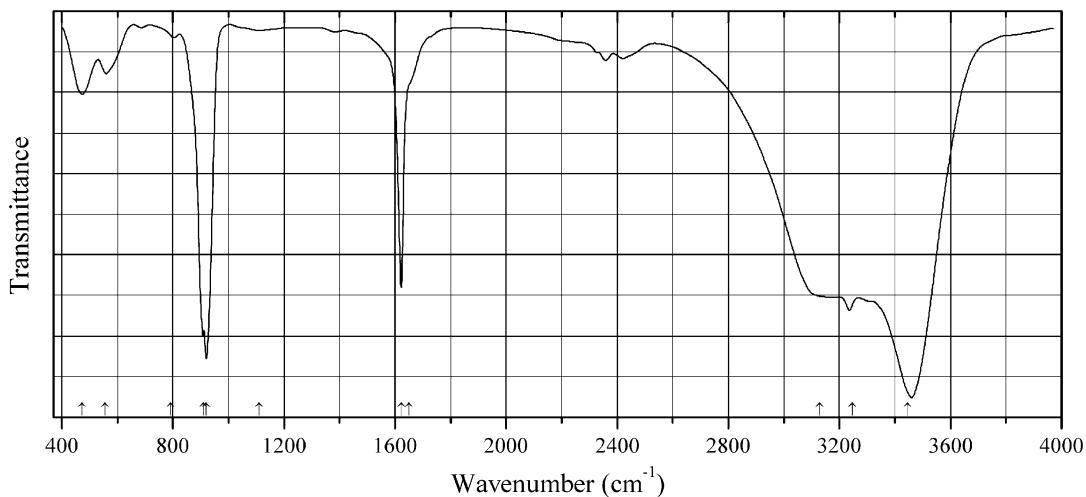
Characterized by powder X-ray diffraction data. Orthorhombic, space group  $Pbma$ ,  $a = 5.666$ ,  $b = 15.520$ ,  $c = 5.506 \text{ \AA}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc. Transmission.

**Source:** Rocchiccioli-Deltcheff (1973).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 680sh, 625s, 550sh, 375, 335, 290, 260.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**O612 Metastudtite**  $\text{UO}_3 \cdot 2\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Obtained by dehydrating synthetic studtite at 90 °C for 48 h. Characterized by powder X-ray diffraction and thermoanalytical data. Orthorhombic, space group *Pnma*,  $a = 8.4184(4)$ ,  $b = 8.7671(4)$ ,  $c = 6.4943(3)$  Å,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Guo et al. (2014a).

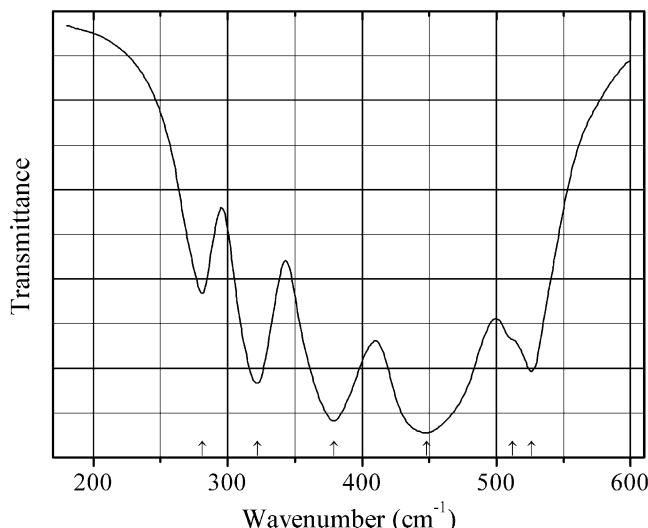
**Wavenumbers (IR, cm<sup>-1</sup>):** 3153.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1725, 1652, 869s, 829s, 478w, 356, 280, 190, 156.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

### O613 Minium Pb<sup>2+</sup><sub>2</sub>Pb<sup>4+</sup>O<sub>4</sub>



**Origin:** Synthetic.

**Description:** Commercial reactant. Tetragonal, space group *P4<sub>2</sub>/m*.

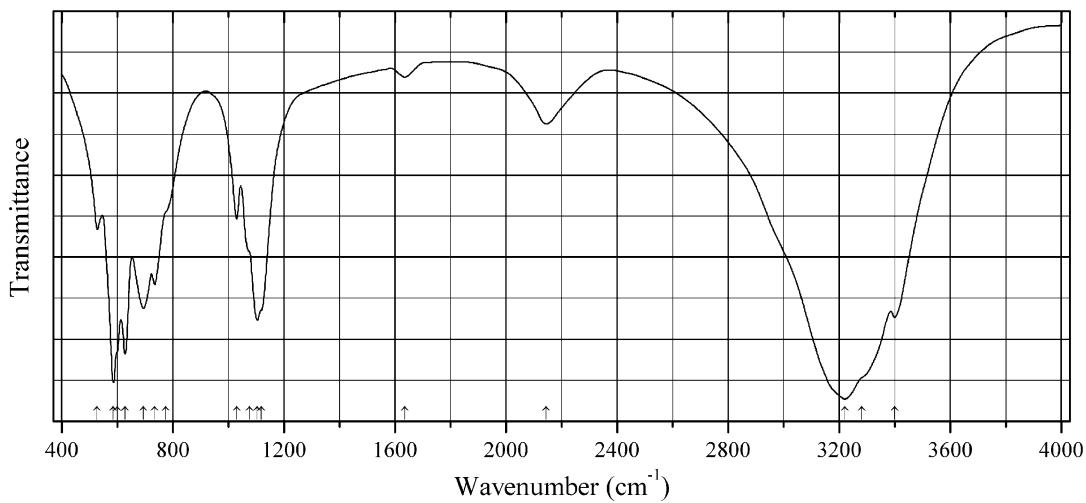
**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc.  
Transmission.

**Source:** Vigouroux et al. (1982).

**Wavenumbers (IR, cm<sup>-1</sup>):** 526, 512sh, 448s, 379s, 322s, 281.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 549s, 477, 391s, 313, 232, 152w, 121s, 76, 34w.

**O614 Mopungite  $\text{NaSb}(\text{OH})_6$** 

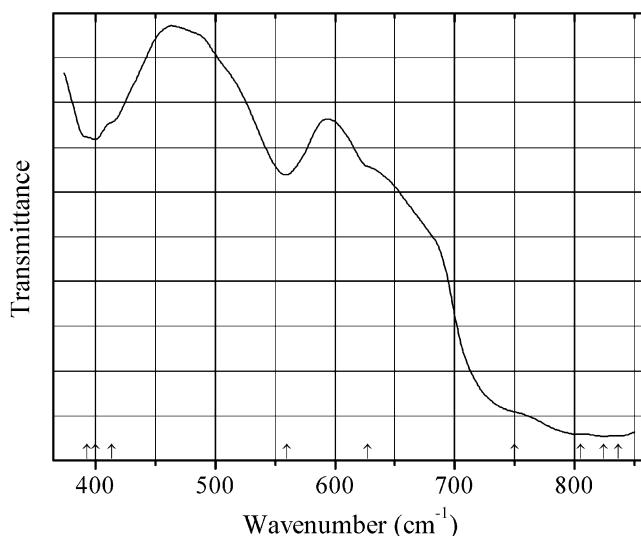
**Origin:** Synthetic.

**Description:** Obtained by boiling aqueous solution of  $\text{NaCl}$  with potassium antimonate.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Siebert (1959).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3400, 3280sh, 3220s, 2145, 1635w, 1120sh, 1105s, 1075sh, 1030, 775, 735, 695, 628s, 600sh, 586s, 528.

**O615 Nichromite  $\text{Ni}_2\text{CrO}_4$** 

**Origin:** Synthetic.

**Description:** Synthesized by heating a mixture of corresponding nitrates. Characterized by powder X-ray diffraction data. Cubic. Contains ~25% admixture of tetragonal (pseudocubic), phase, space group  $I4_1/\text{amd}$ . For the main phase,  $a = 8.3186(2)$ .

**Kind of sample preparation and/or method of registration of the spectrum:** A spectrometer fitted with a photoacoustic detector was used.

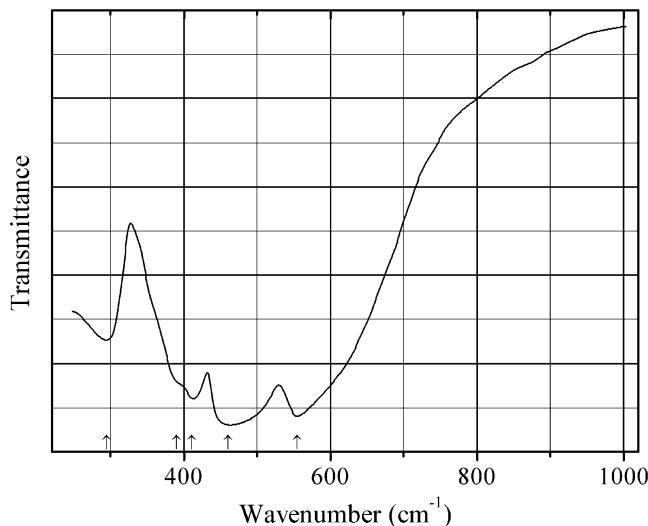
**Source:** Hosterman et al. (2013).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** No quantitative data (only a figure of the IR spectrum is given).

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 678, 508, 427, 190.

### O616 Oxybetafite-(Gd) $\text{Gd}_2\text{Ti}_2\text{O}_7$



**Origin:** Synthetic.

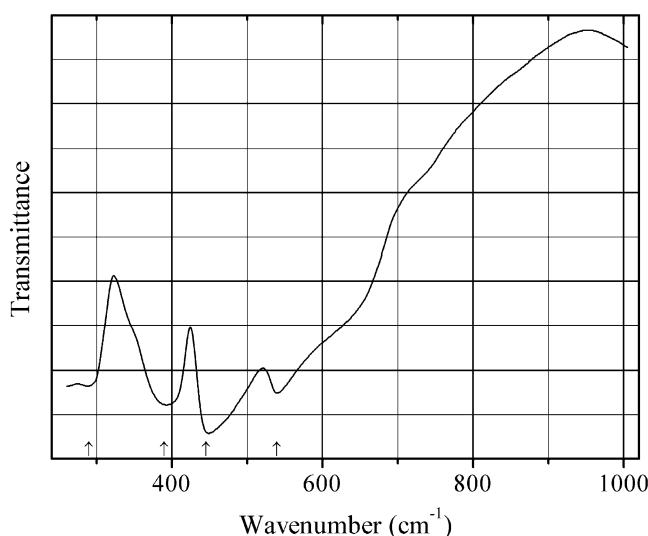
**Description:** Obtained using a solid-state reaction technique. Characterized by powder X-ray diffraction data. Cubic.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Knop et al. (1969).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 555s, 460s, 411, 390sh, 295.

### O617 Oxybetafite-(Sm) $\text{Sm}_2\text{Ti}_2\text{O}_7$



**Origin:** Synthetic.

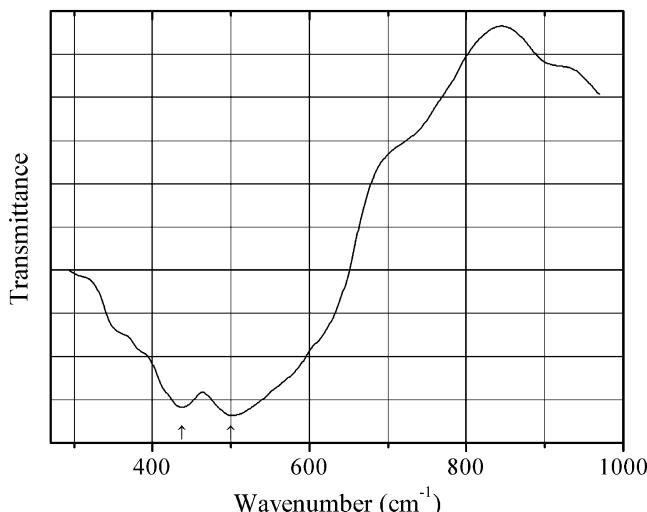
**Description:** Obtained using a solid-state reaction technique. Characterized by powder X-ray diffraction data. Cubic.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Knop et al. (1969).

**Wavenumbers (cm<sup>-1</sup>):** 539, 445s, 390s, 290.

### O618 Oxybismuthobetafite Bi<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>



**Origin:** Synthetic.

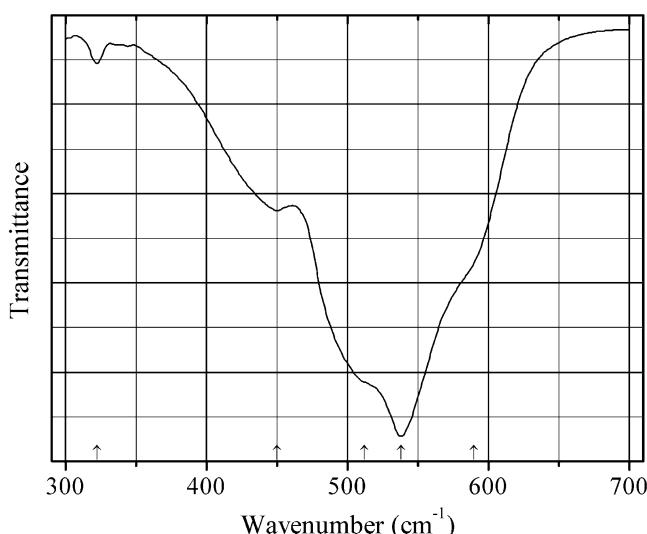
**Description:** Obtained using a solid-state reaction technique. Characterized by powder X-ray diffraction data. The symmetry is not cubic.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Knop et al. (1969).

**Wavenumbers (cm<sup>-1</sup>):** 500s, 437s.

### O619 Paramelaconite Cu<sup>1+</sup><sub>2</sub>Cu<sup>2+</sup><sub>2</sub>O<sub>3</sub>



**Origin:** Synthetic.

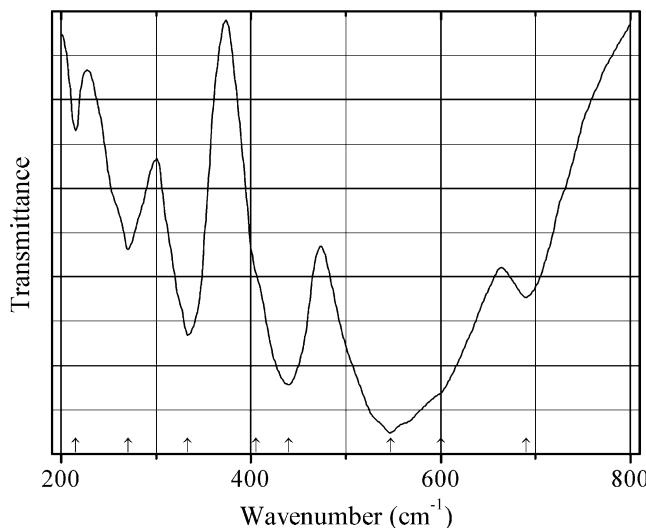
**Description:** Prepared by oxidation of  $\text{Cu}_2\text{O}$  or reduction of  $\text{CuO}$ . Trtragonal,  $a \approx 5.84$ ,  $c \approx 9.93 \text{ \AA}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Absorption. Kind of sample preparation is not indicated.

**Source:** Djurek et al. (2015).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 590sh, 538s, 512sh, 450, 322w.

### O620 Pyrophanite $\text{MnTiO}_3$



**Origin:** Synthetic.

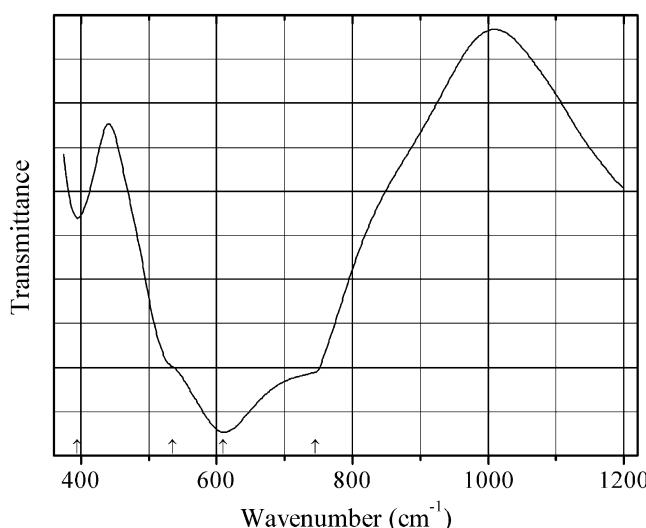
**Description:** Prepared using solid-state reaction techniques. Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc. Transmission.

**Source:** Baran and Botto (1978).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 690, 600sh, 547s, 440s, 405, 333, 270, 215w.

### O621 Rutile $\text{TiO}_2$



**Origin:** Unknown.

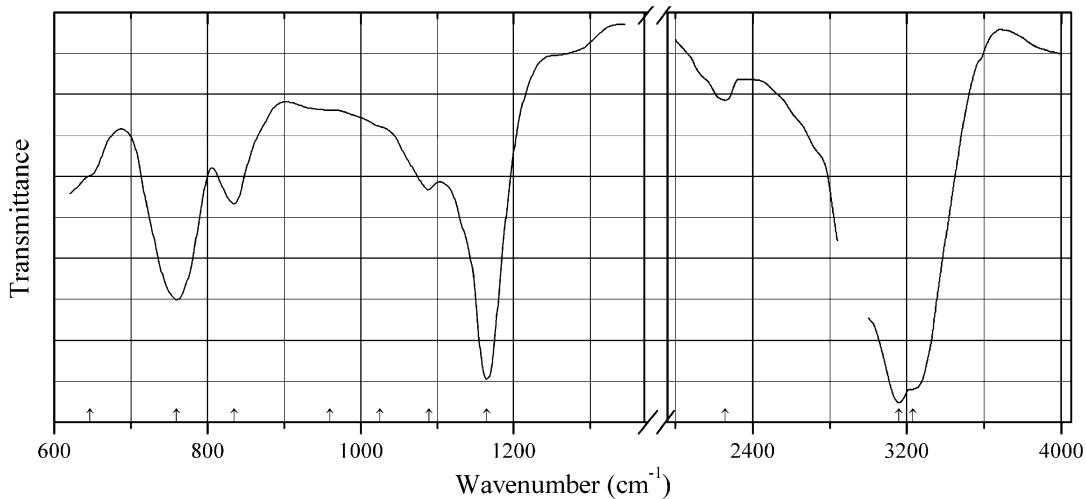
**Description:** Natural fibrous crystals included in quartz.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Peng et al. (1995).

**Wavenumbers (cm<sup>-1</sup>):** 745sh, 610s, 535sh, 395.

### O622 Schoenfliesite MgSn(OH)<sub>6</sub>



**Origin:** Pitkäranta, Karelia, Russia.

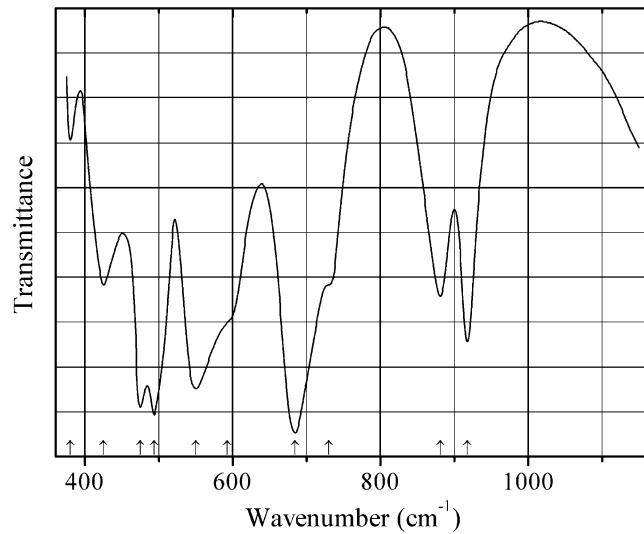
**Description:** Fibrous aggregate from the association with serpentine, chlorite, chondrodite, diopside, fluorite, calcite, dolomite, magnetite, and cassiterite. Cubic,  $a = 7.77(1)$ .  $D_{\text{meas}} = 3.32 \text{ g/cm}^3$ ,  $D_{\text{calc}} = 3.49 \text{ g/cm}^3$ . The empirical formula is  $(\text{Mg}_{0.94}\text{Mn}_{0.13})\text{Sn}_{0.97}(\text{OH})_{6.00}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 4.495 (60) (111), 3.898 (100) (200), 2.758 (60) (220), 2.349 (40) (311), 1.741 (50) (420).

**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull. Transmission.

**Source:** Nefedov et al. (1977).

**Wavenumbers (cm<sup>-1</sup>):** 3230sh, 3160s, 2260w, 1165s, 1089, 1025sh, 960sh, 835, 760s, 647sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**O623 Sodium titanate  $\text{Na}_2\text{Ti}_3\text{O}_7$   $\text{Na}_2\text{Ti}_3\text{O}_7$** 

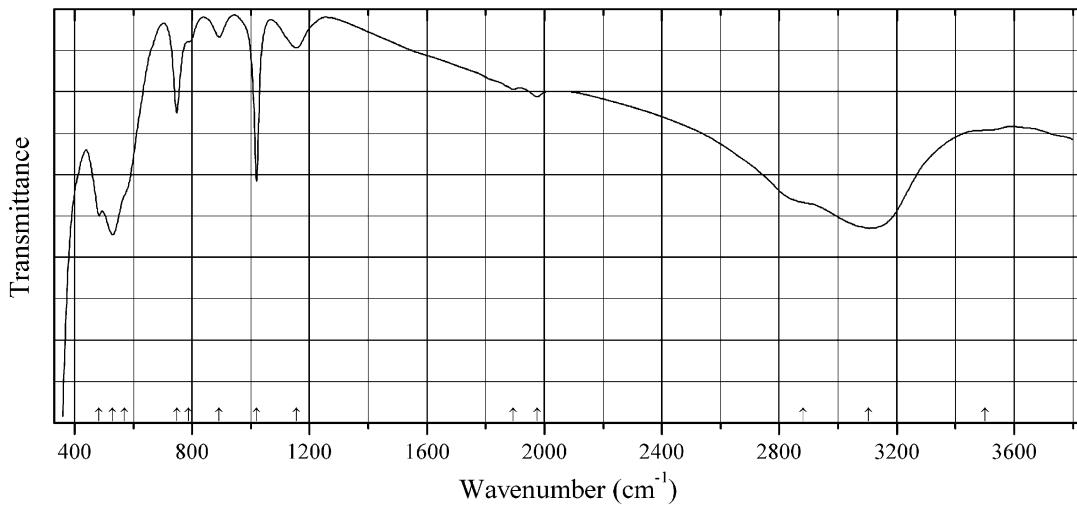
**Origin:** Synthetic.

**Description:** Prepared by using a stoichiometric molar ratio of  $\text{Na}_2\text{CO}_3$  and  $\text{TiO}_2$  (rutile) at  $1250^\circ\text{C}$  for 4 h. Characterized by powder X-ray diffraction data. Monoclinic. The crystal structure contains distorted  $\text{TiO}_5$  pyramid.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Peng et al. (1995).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 918, 881, 730sh, 684s, 593sh, 550s, 493s, 475s, 425, 380w.

**O624 Lepidocrocite  $\text{Fe}^{3+}\text{O(OH)}$** 

**Origin:** Hilarion mine, Agios Konstantinos, Lavrion mining District, Attikí (Attika, Attica) Prefecture, Greece.

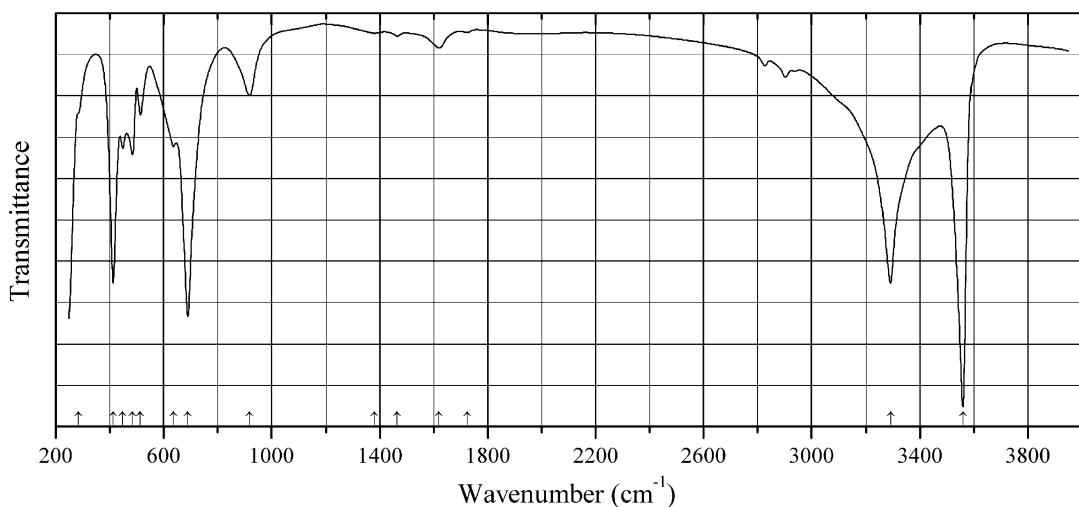
**Description:** Yellowish-brown columnar aggregate from the association with goethite and hematite. Pseudomorph after rail. The sample was kindly granted by I.V. Pekov. Confirmed by the IR spectrum.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** (3500sh), 3105s, 2880sh, 1976w, 1894w, 1155, 1020s, 892, 788, 748, 570sh, 528s, 483s.

**Note:** The spectrum was obtained by N.V. Chukanov.

### O625 Spertiniite Cu(OH)<sub>2</sub>



**Origin:** Synthetic.

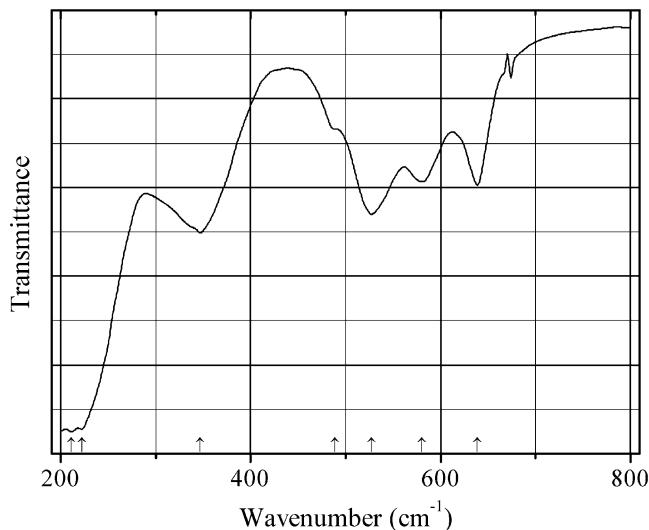
**Description:** Acicular crystals. Confirmed by powder X-ray diffraction data and electron microdiffraction pattern.

**Kind of sample preparation and/or method of registration of the spectrum:** Absorption. Kind of sample preparation is not indicated.

**Source:** Rodríguez-Clemente et al. (1994).

**Wavenumbers (cm<sup>-1</sup>):** 3560s, 3292s, 1725, 1620w, 1465w, 1380w, 917, 689s, 636, 514, 484, 448, 412s, 284sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The band at 1620 cm<sup>-1</sup> corresponds to adsorbed water. Weak bands in the range from 2800 to 3000 cm<sup>-1</sup> correspond to the admixture of an organic substance.

**O626 Sphaerobismoite  $\beta\text{-Bi}_2\text{O}_3$** 

**Origin:** Synthetic.

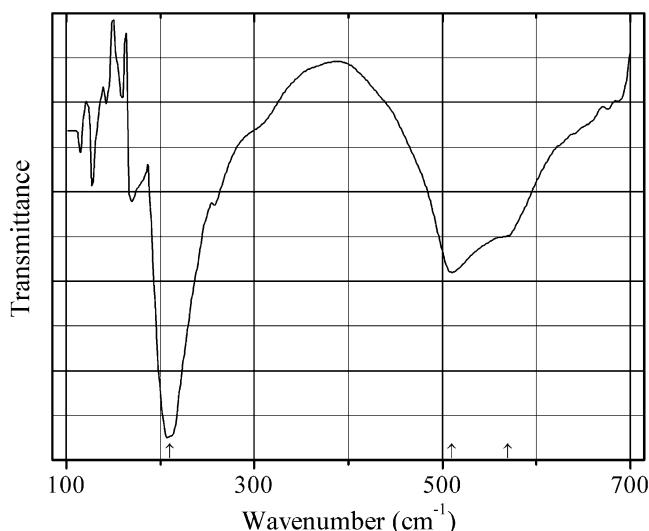
**Description:** Orange crystals obtained by rapid pouring an aqueous solution of  $\text{Bi}_2(\text{NO}_3)_3$  into a boiling solution of NaOH, followed by immediate filtration of the precipitate. Characterized by powder X-ray diffraction data. Tetragonal,  $a = 7.72$ ,  $c = 5.63 \text{ \AA}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Cahen et al. (1980).

**Wavenumbers (cm⁻¹):** 639, 580, 527, 489sh, 347, 222s, 211s.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**O627 Tantite  $\text{Ta}_2\text{O}_5$** 

**Origin:** Synthetic.

**Description:** A crystalline film deposited on Si substrate by using CVD at 430 °C and annealed at 800 °C for 10 min. Surface SiO<sub>2</sub> was removed by using a diluted HF solution.

**Kind of sample preparation and/or method of registration of the spectrum:** A film 100 nm thick.

Absorption.

**Source:** Ono et al. (2001).

**Wavenumbers (cm<sup>-1</sup>):** 570sh, 510, 210s.

### O628 Tistarite Ti<sub>2</sub>O<sub>3</sub>

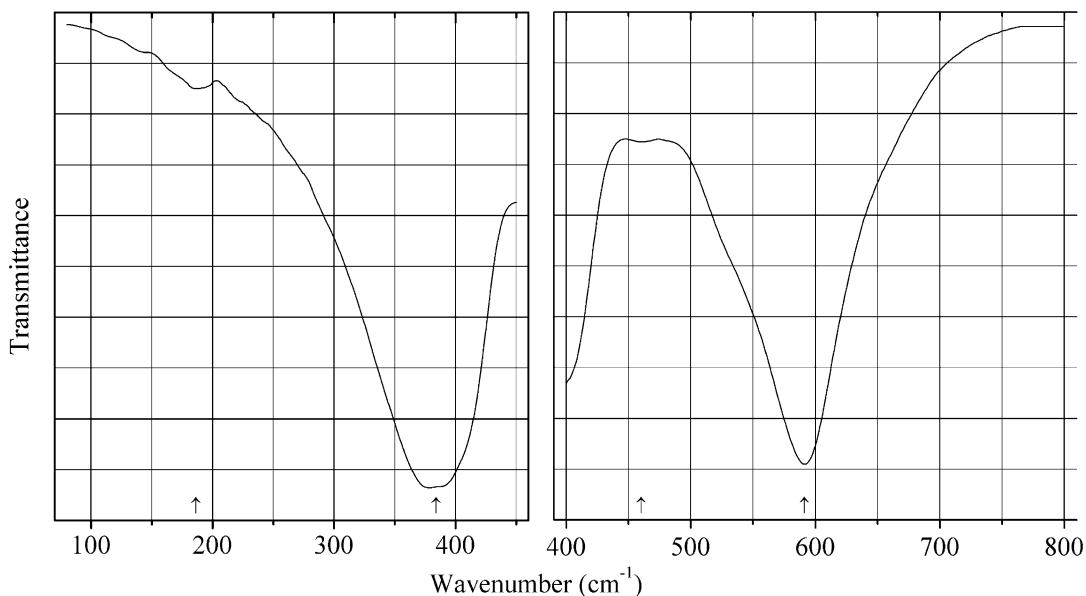
**Origin:** Synthetic.

**Kind of sample preparation and/or method of registration of the spectrum:** Reflectance of a single crystal.

**Source:** Lucovsky et al. (1977).

**Wavenumbers (cm<sup>-1</sup>):** 448s, 343 (for  $E \parallel c$ ); 511, 451s, 376s, 280w (for  $E \perp c$ ).

### O629 Trevorite Co-analogue CoFe<sub>2</sub>O<sub>4</sub>



**Origin:** Synthetic.

**Description:** Synthesized from corresponding nitrates by a solid-state reaction technique at 1000 °C for 24 h. Characterized by powder X-ray diffraction data. Cubic, space group *Fd-3m*.

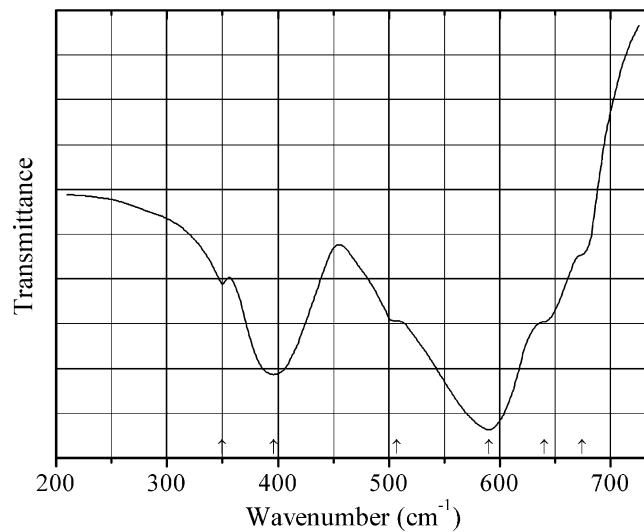
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc and Nujol mull. Absorption.

**Source:** Ptak et al. (2014).

**Wavenumbers (IR, cm<sup>-1</sup>):** 591, 460w, 384, 186w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 470.

**O630 Ulvöspinel Zn-analogue  $TiZn_2O_4$** 

**Origin:** Synthetic.

**Description:** Synthesized from corresponding oxides by a solid-state reaction technique at 1000 °C for 25 h. Characterized by powder X-ray diffraction data.

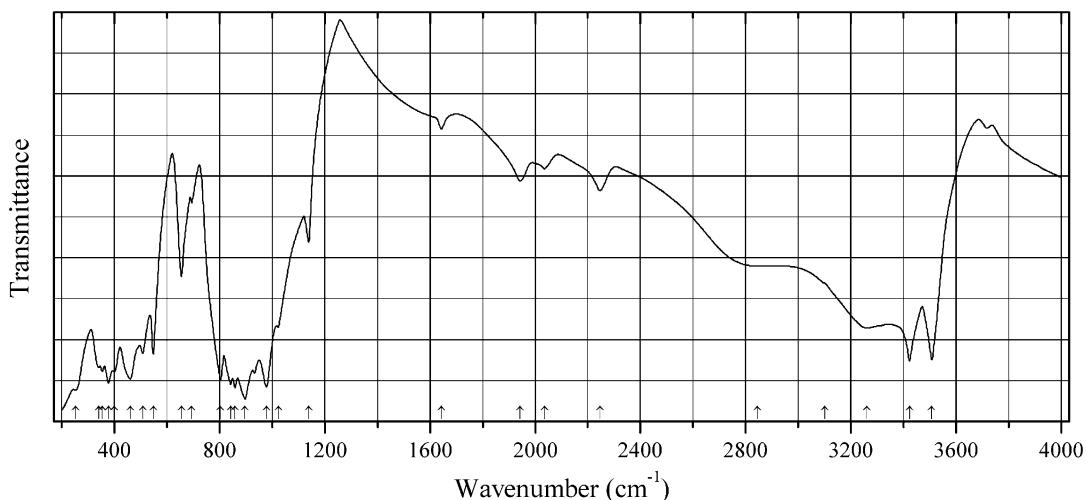
**Kind of sample preparation and/or method of registration of the spectrum:** Powder spread uniformly over the surface of a polyethylene plate. Transmission.

**Source:** Keramidas et al. (1975).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 674sh, 640sh, 590s, 50sh, 396s, 350.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 780, 722s, 567w, 541w, 478, 441w, 351, 344, 313s, 256, 156, 136, 117, 101.

**O631 Vandenbrandeite  $Cu(UO_2)(OH)_4$** 

**Origin:** Kalongwe deposit, Shaba, province, Zaire (type locality).

**Description:** Green tabular crystals from the association with kasolite. Characterized by powder X-ray diffraction data and electron microprobe analyses.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

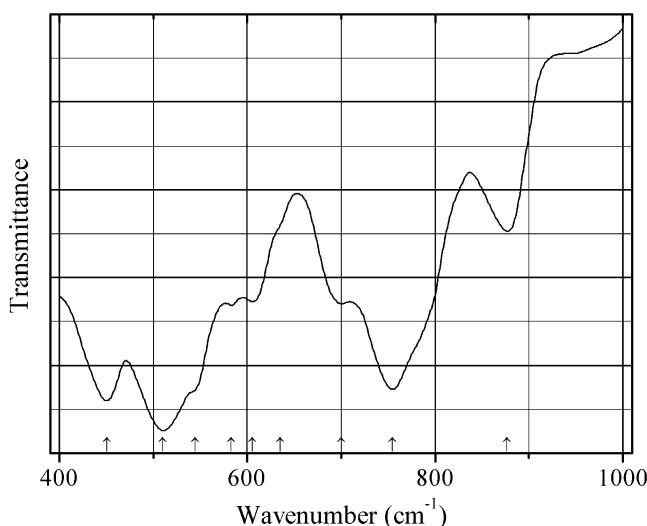
**Source:** Botto et al. (2002).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3508s, 3423s, 3262, 2845, 3100sh, 2247, 2035, 1943, 1643w, 1139, 1024, 978s, 897s, 859s, 842s, 803s, 694, 655, 548s, 508s, 460s, 400s, 377s, 354s, 340s, 252s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 2233, 2018, 1946, 862, 805s, 474, 186.

### O632 Vandenbrandeite hydrogen-free analogue $\text{CuUO}_4$



**Origin:** Synthetic.

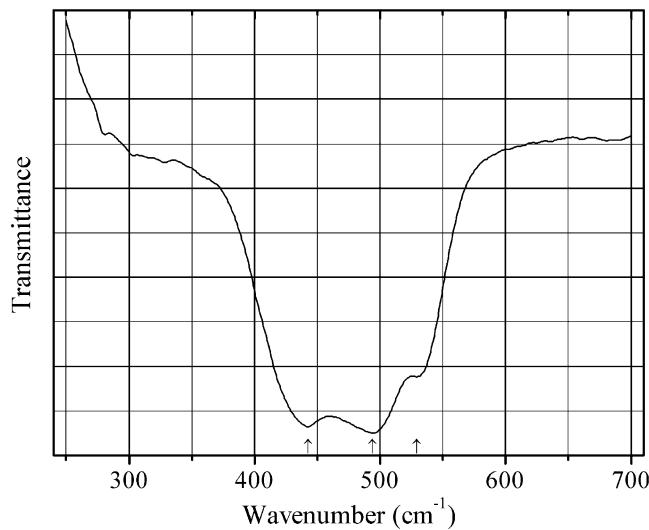
**Description:** Prepared in a solid-state reaction between  $\text{CuO}$  and  $\text{UO}_3$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %)] are: 5.08 (50), 4.15 (90), 3.76 (50), 3.44 (100), 3.26 (50), 2.71 (90).

**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull. Transmission.

**Source:** Jakeš et al. (1968).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 877, 755s, ~700, 635sh, ~605, 583, ~544sh, ~510s, ~450s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, also IR spectra of  $\text{MnUO}_4$ ,  $\text{MnU}_3\text{O}_{10}$ ,  $\text{CoUO}_4$ ,  $\text{CoU}_3\text{O}_{10}$ ,  $\text{NiUO}_4$ ,  $\text{NiU}_3\text{O}_{10}$ ,  $\text{CuU}_3\text{O}_{10}$ ,  $\text{AgUO}_4$ , and  $\text{HgUO}_4$  are given.

**O633 Zincite ZnO**

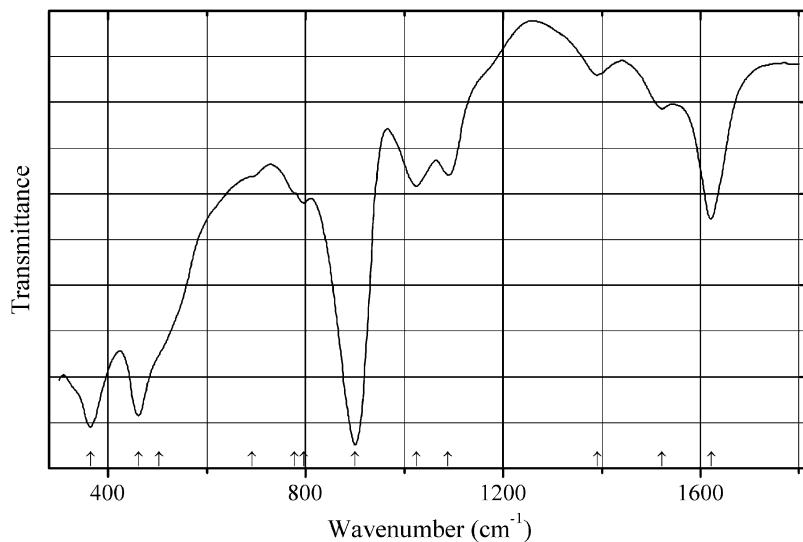
**Origin:** Synthetic.

**Description:** Commercial reactant.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Musić et al. (2003).

**Wavenumbers (cm<sup>-1</sup>):** 529, 494s, 443s.

**O634 Masuyite Pb(UO<sub>2</sub>)<sub>3</sub>O<sub>3</sub>(OH)<sub>2</sub>·3H<sub>2</sub>O**

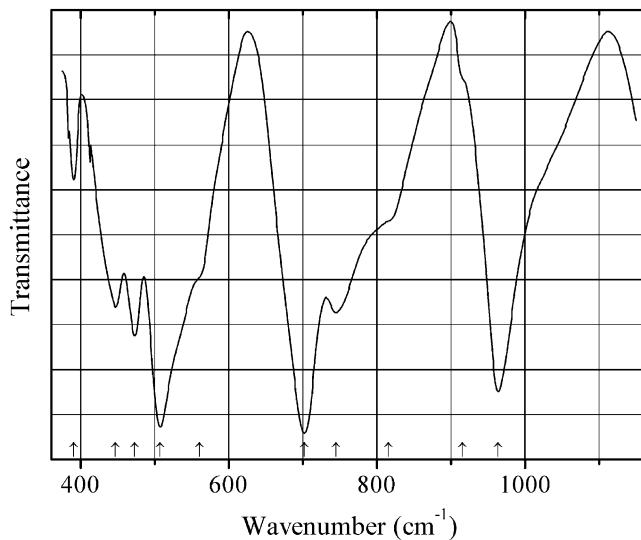
**Origin:** Rum Jungle (?), northern Australia.

**Description:** Specimen No. 26494 from the collections of the Department of Geology and Mineralogy, University of Queensland. Confirmed by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission.

**Source:** Wilkins (1971).

**Wavenumbers (cm<sup>-1</sup>):** 1622, 1522w, 1391w, 1089, 1024, 900s, 796w, 778sh, 692sh, 503sh, 462s, 364s.

**O635 Sodium titanate  $\text{Na}_2\text{Ti}_6\text{O}_{13}$   $\text{Na}_2\text{Ti}_6\text{O}_{13}$** 

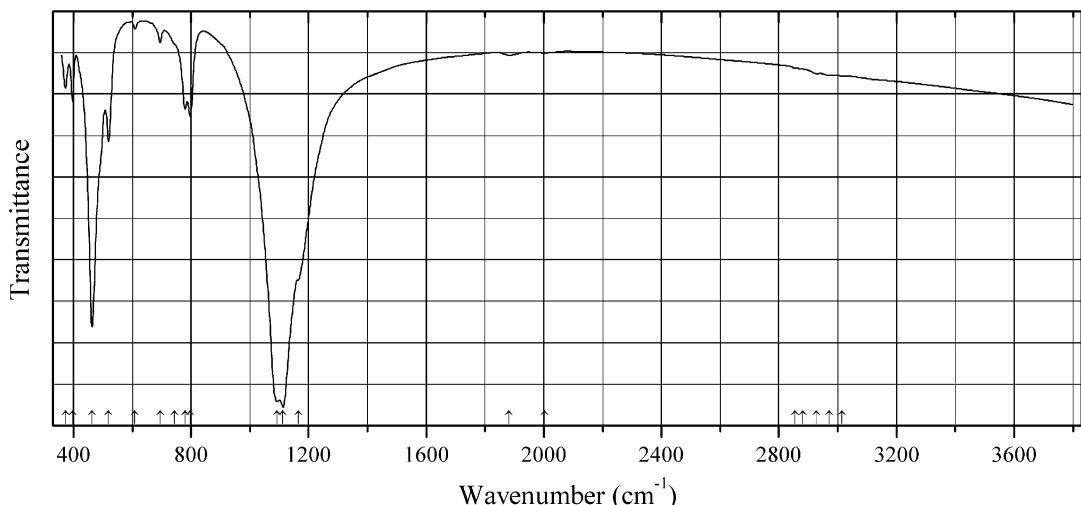
**Origin:** Synthetic.

**Description:** Prepared by using a stoichiometric mixture of  $\text{Na}_2\text{CO}_3$  and  $\text{TiO}_2$  (rutile) at  $1250^\circ\text{C}$  for 4 h. Characterized by powder X-ray diffraction data. Monoclinic, with distorted  $\text{TiO}_6$  octahedra.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Peng et al. (1995).

**Wavenumbers (cm⁻¹):** 964s, 916sh, 816sh, 745, 702s, 560sh, 507s, 473, 447, 390w.

**O640 Chibaite  $\text{SiO}_2 \cdot n(\text{CH}_4, \text{C}_2\text{H}_6, \text{C}_3\text{H}_8, \text{C}_4\text{H}_{10})$  ( $n_{\max} = 3/17$ )**

**Origin:** Arakawa, Minamiboso city, Chiba prefecture, Kanto region, Honshu Island, Japan (type locality).

**Description:** White semitransparent crystals. Intergrowths with quartz.

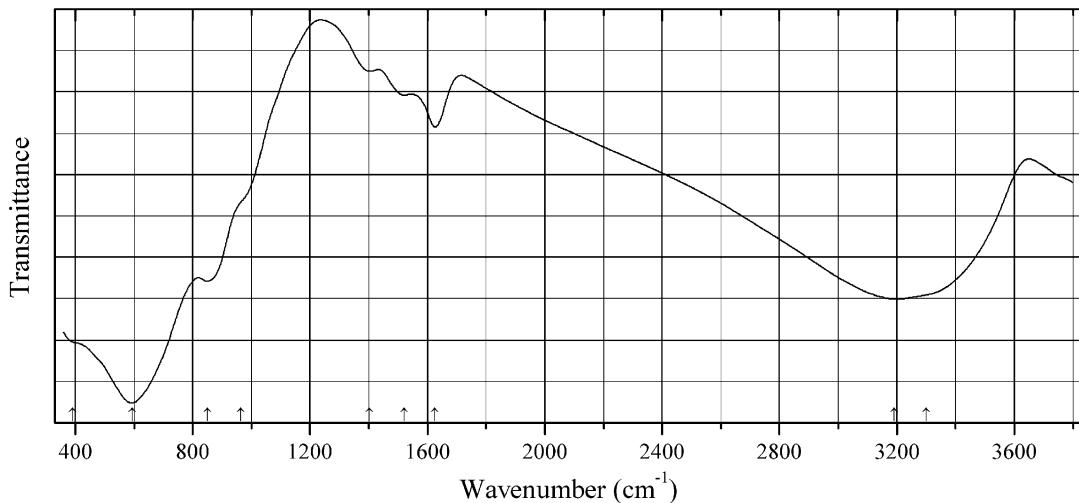
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3014w, 2970w, 2928w, 2880w, 2854w, 2003w, 1882w, 1165sh, 1113s, 1093s, 797, 780, 745sh, 695, 609w, 519, 464s, 398, 374.

**Note:** The bands at 1165, 797, 780, 695, 464s 398, and 374 cm<sup>-1</sup> are partly due to quartz.

**Note:** The spectrum was obtained by N.V. Chukanov.

#### O641 Samarskite-(Y) (Y,Ce,U,Fe,Nb)(Nb,Ta,Ti)O<sub>4</sub>



**Origin:** Herrebøkasa, Aspedammen, Idd, Halden, Østfold, Norway.

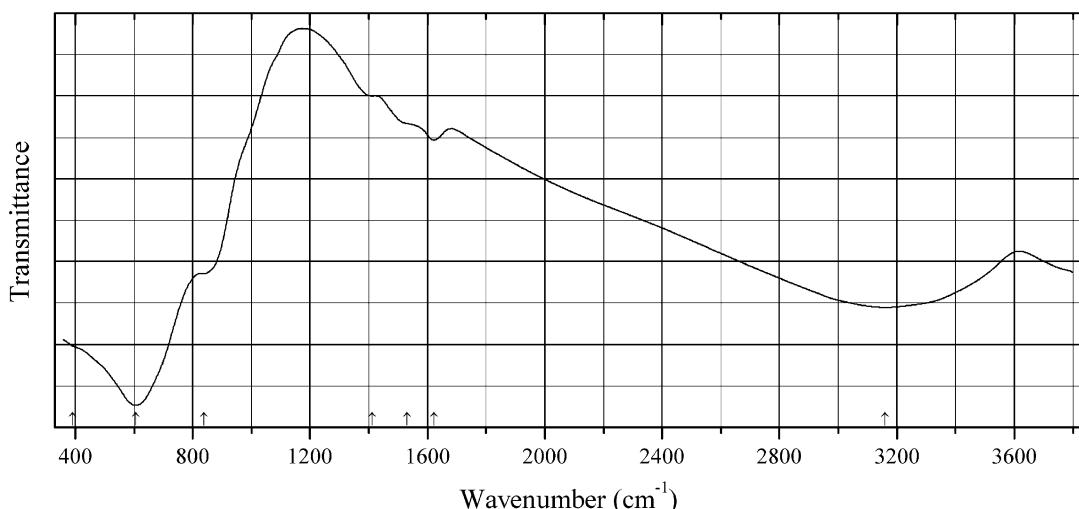
**Description:** Black grains. X-ray amorphous, metamict. The empirical formula is (electron microprobe):  $(Y_{0.25}U_{0.2}Ca_{0.2}Fe_{0.2}Ln_{0.1})(Nb_{0.85}Ti_{0.1}Ta_{0.05})O_9 \cdot nH_2O$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3300sh, 3192s (broad), 1626, 1520, 1403w, 965sh, 851, 593s, 390sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

#### O642 Samarskite-(Yb) YbNbO<sub>4</sub>



**Origin:** Little Patsy pegmatite (Patsy pegmatite), South Platte Pegmatite District, Jefferson Co., Colorado, USA (type locality).

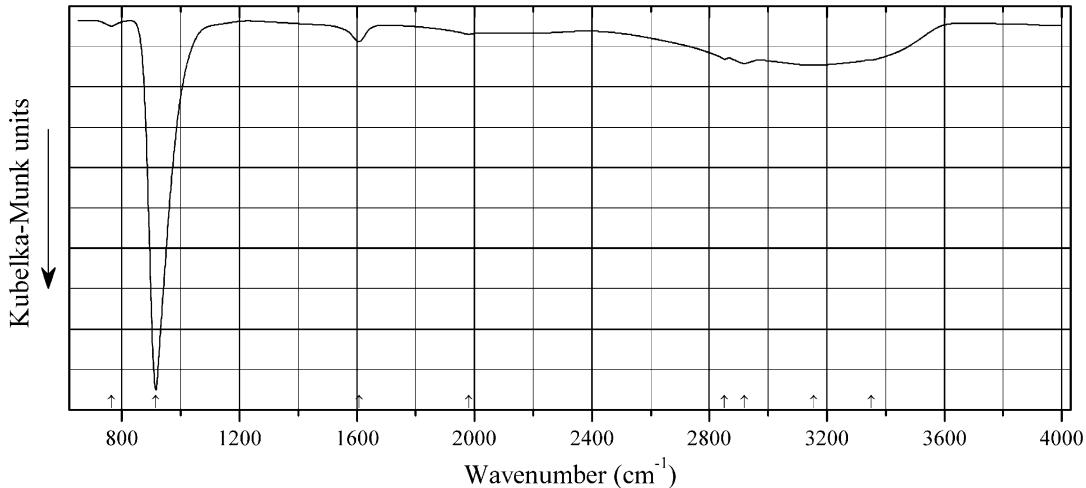
**Description:** Black grains in pegmatite. X-ray amorphous, metamict. The empirical formula is (electron microprobe):  $(\text{Yb}_{0.13}\text{Dy}_{0.07}\text{Er}_{0.04}\text{Y}_{0.01}\text{La}_{0.01})\text{Ca}_{0.24}\text{U}_{0.12}\text{Th}_{0.08}\text{Fe}_{0.18}\text{Mn}_{0.02}(\text{Nb}_{0.93}\text{Ta}_{0.11}\text{Ti}_{0.01}) \cdot n\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3160s (broad), 1623, 1530sh, 1412w, 838, 607s, (390sh).

**Note:** The spectrum was obtained by N.V. Chukanov.

### O643 Gauthierite $\text{KPb}[(\text{UO}_2)_7\text{O}_5(\text{OH})_7] \cdot 8\text{H}_2\text{O}$



**Origin:** Shinkolobwe mine, Shinkolobwe, Katanga province, Democratic Republic of Congo (type locality).

**Description:** Yellowish orange crystals from the association with soddyite and a metazeunerite–metatorbernite series mineral. Holotype sample. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 29.844(2)$ ,  $b = 14.5368(8)$  Å,  $c = 14.0406(7)$  Å,  $\beta = 103.708(6)^\circ$ ,  $V = 5917.8(6)$  Å<sup>3</sup>,  $Z = 8$ .  $D_{\text{calc}} = 5.437$  g/cm<sup>3</sup>. Optically biaxial (−),  $\alpha = 1.780(5)$ ,  $\beta = 1.815(5)$ ,  $\gamma = 1.825(5)$ ,  $2V = 70(5)^\circ$ . The empirical formula is  $\text{K}_{0.67}\text{Pb}_{0.78}\text{U}_7\text{O}_{34}\text{H}_{23.77}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å (I, %) ( $hkl$ )] are: 7.28 (49) (020, 400), 3.566 (67) (040, -802, -204), 3.192 (100) (622, -224), 2.541 (18) (-842, -244), 2.043 (14) (406), 2.001 (23) (662, -264, 14.2.0), 1.962 (14) (426, -146), 1.783 (17) (12.0.4, -10.4.6).

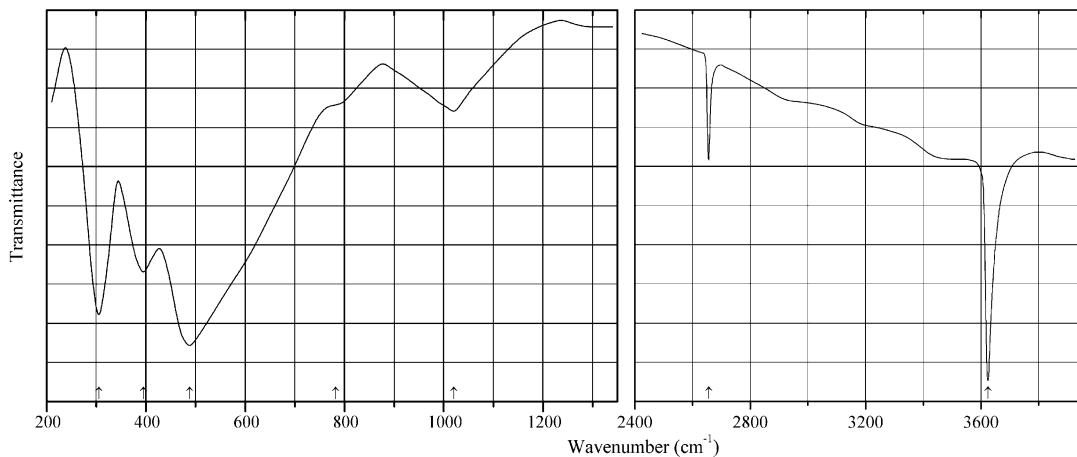
**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of a polycrystalline sample.

**Source:** Olds et al. (2016a).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3350sh, 3154 (broad), 2919, 2852, 1980w, 1607, 915s, 764w.

**Note:** The bands in the range from 2800 to 3000 cm<sup>-1</sup> correspond to the admixture of an organic substance. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 833s, 821s, 696, 558, 539, 464, 454, 403, 355, 328, 260, 204, 160, 128.

**O645 Amakinite ( $\text{Fe}^{2+},\text{Mg})(\text{OH})_2$ )**

**Origin:** Synthetic.

**Description:** Mg-free, partly deuterated sample. The empirical formula is  $\text{Fe}^{2+}(\text{OH})_{1.7}(\text{OD})_{0.3}$ . Characterized by powder X-ray and neutron diffraction data. Trigonal, space group  $P-3m1$ ,  $a = 3.2628(1)$ ,  $c = 4.604(1)$  Å.

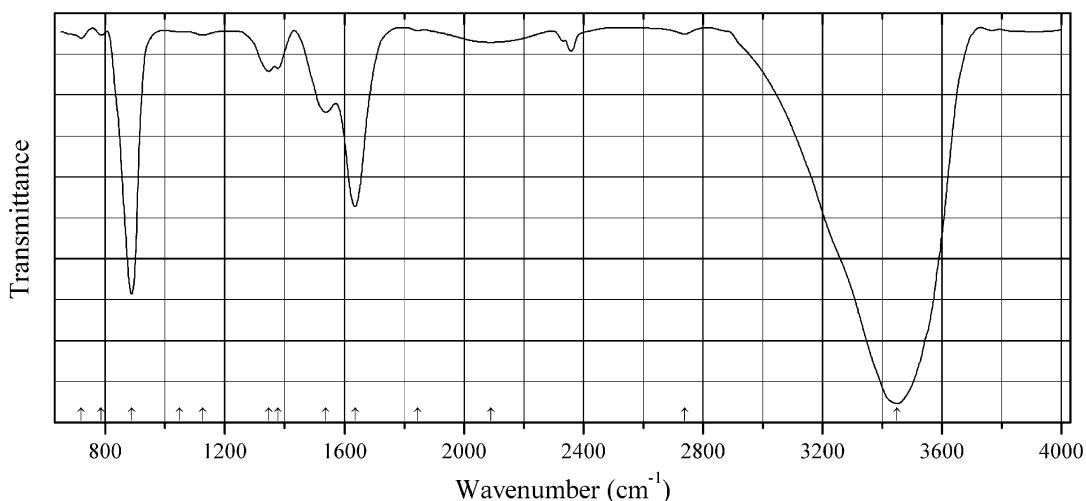
**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc. Transmission.

**Source:** Lutz et al. (1994).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3624s, 2656, 1020w, 782sh, 488s, 395, 305s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The band at 2656  $\text{cm}^{-1}$  corresponds to D–O-stretching vibrations. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 3573s, 407, 260.

**O646 Clarkeite  $\text{Na}(\text{UO}_2)\text{O}(\text{OH}) \cdot n\text{H}_2\text{O}$** 

**Origin:** Synthetic.

**Description:** Obtained by precipitation generated in a uranyl peroxy carbonato complex solution at pH 14 controlled by NaOH, with subsequent drying in vacuum at 100 °C for 3 h.

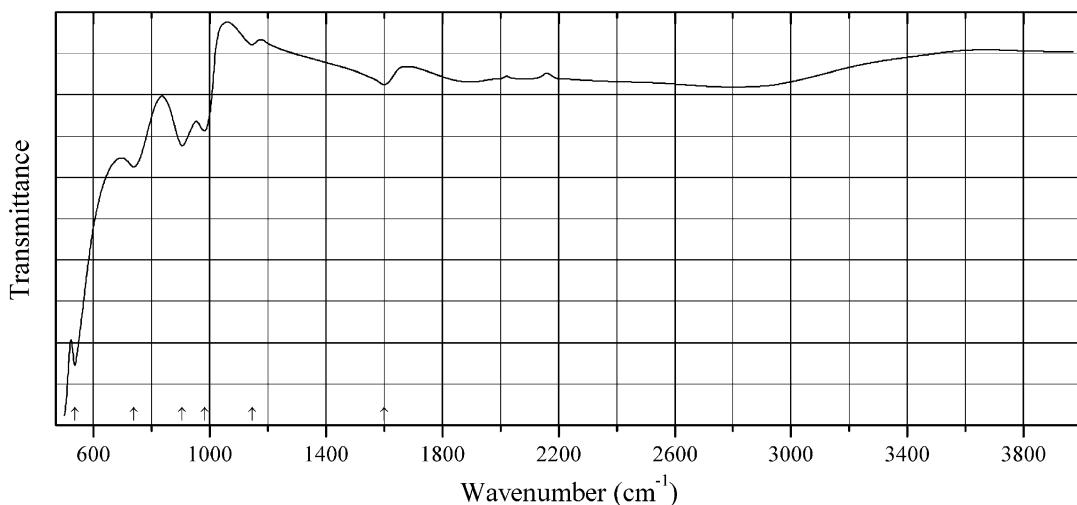
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Kim et al. (2009).

**Wavenumbers (cm<sup>-1</sup>):** 3450s (broad), 2738w, 2090w (broad), 1845, 1636s, 1537, 1378, 1347, 1126w, 1048sh, 888s, 786w, 720w.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

### O647 Duttonite V<sup>4+</sup>O(OH)<sub>2</sub>



**Origin:** Synthetic.

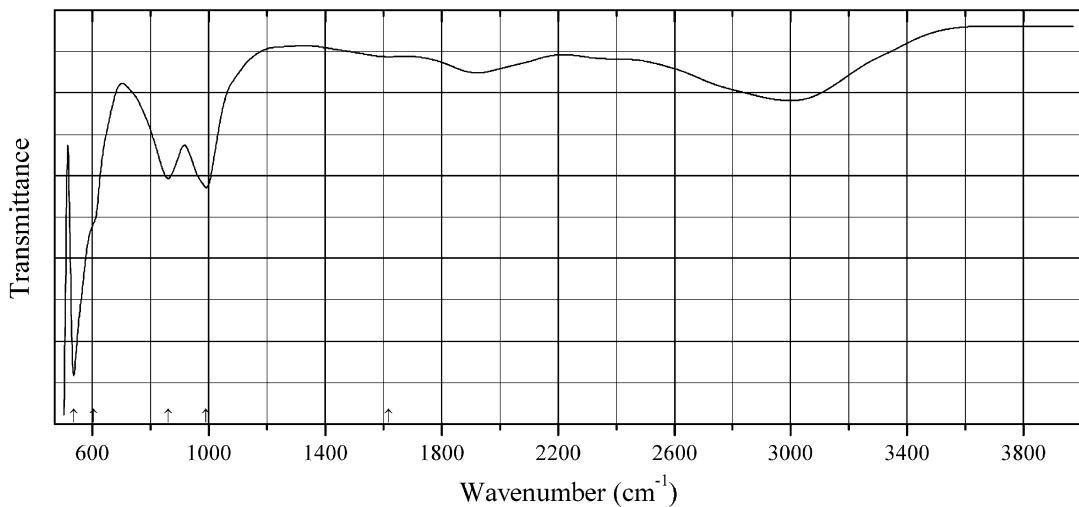
**Description:** Nanorods obtained by aqueous precipitation at pH 4.0 in the presence of hydrazine at 95 °C during 4.5 days. Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of a powdered sample.

**Source:** Besnardiere et al. (2016).

**Wavenumbers (cm<sup>-1</sup>):** 1600, 1145w, 982, 905, 738, 536s, and broad bands near 2800 and 1900 cm<sup>-1</sup>.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**O648 Häggite  $V^{3+}V^{4+}O_2(OH)_3$** 

**Origin:** Synthetic.

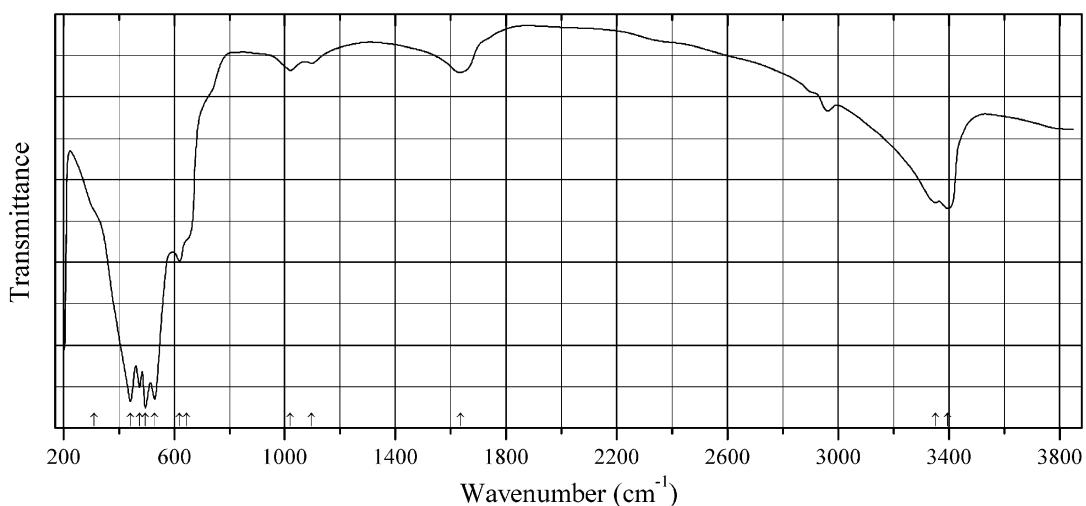
**Description:** Nanorods obtained by aqueous precipitation at pH 3.6–3.8 in the presence of hydrazine at 95 °C during 4.5 days. Characterized by powder X-ray diffraction data. Monoclinic,  $a = 12.208$ ,  $b = 2.997$ ,  $c = 4.840 \text{ \AA}$ ,  $\beta = 98.29^\circ$

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of powdered sample.

**Source:** Besnardiere et al. (2016).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1618w, 991, 860, 604sh, 536s.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**O649 Jianshuiite  $MgMn^{4+}_3O_7 \cdot 3H_2O$** 

**Origin:** Luzhai Mn deposit, Jianshui Co., Honghe Autonomous Prefecture, Yunnan, China (type locality).

**Description:** Aggregate of dark brown microcrystals. Holotype sample. Characterized by powder X-ray diffraction data. Triclinic, space group  $P-1$ ,  $a = 7.534(4)$ ,  $b = 7.525(6)$ ,  $c = 8.204(8)$  Å,  $\alpha = 89.753(8)^\circ$ ,  $\beta = 117.375(6)^\circ$ ,  $\gamma = 120.000(6)^\circ$ .  $D_{\text{meas}} = 3.50\text{--}3.60$  g/cm<sup>3</sup>. The empirical formula is  $(\text{Mg}_{0.85}\text{Mn}^{2+}_{0.05})\text{Mn}^{4+}_{3.15}\text{O}_{7.20}\cdot 2.80\text{H}_2\text{O}$ .

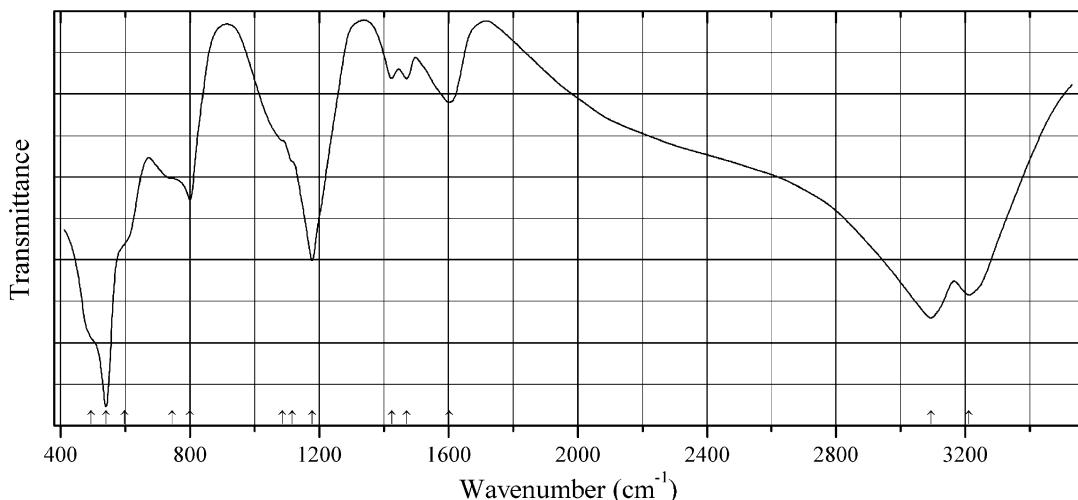
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission.

**Source:** Yan et al. (1992).

**Wavenumbers (cm<sup>-1</sup>):** 3396, 3352, 1635, 1096w, 1020w, 645sh, 620, 530s, 496s, 475s, 442s, 312sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. Weak bands in the range from 2800 to 3000 cm<sup>-1</sup> correspond to the admixture of an organic substance.

### O650 Mushistonite $\text{Cu}^{2+}\text{Sn}^{4+}(\text{OH})_6$



**Origin:** Mushiston Sn deposit, Kaznok valley, Penjikent, Zeravshan range, Tajikistan (type locality).

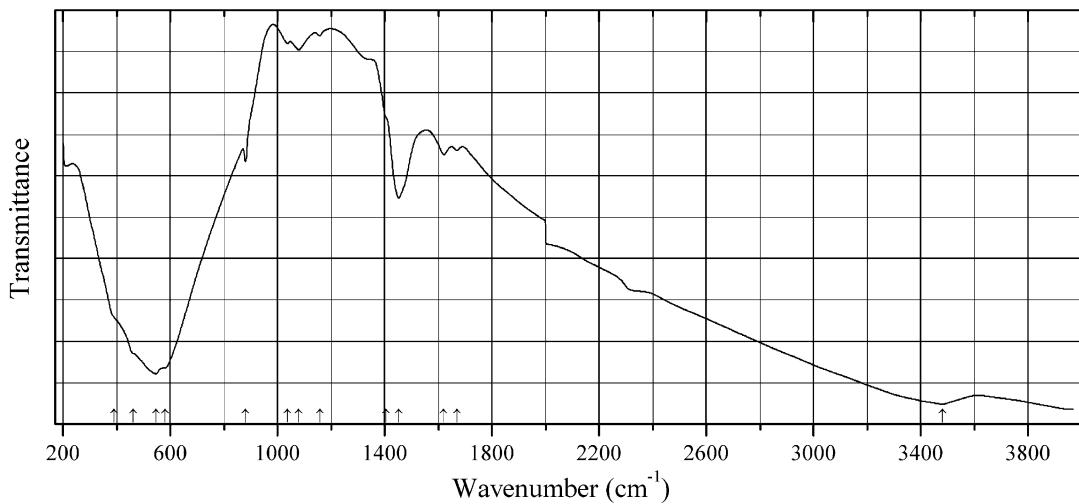
**Description:** Pseudomorphs after stannite. Holotype sample. Cubic,  $a = 7.735$  Å. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 3.88 (100) (111), 2.740 (50) (220), 2.230 (20) (222), 1.932 (16) (400), 1.729 (35) (420), 1.578 (23) (422).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Marshukova et al. (1984).

**Wavenumbers (cm<sup>-1</sup>):** 3211s, 3093s, 1603, 1471, 1424, 1178s, 1117sh, 1087sh, 800, 745sh, 597sh, 540s, 495sh.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**O651 Orthobrannerite  $\text{U}^{4+}\text{U}^{6+}\text{Ti}_4\text{O}_{12}(\text{OH})_2$** 


**Origin:** Dengzhong Co., Baoshan prefecture, Yunnan, China (type locality).

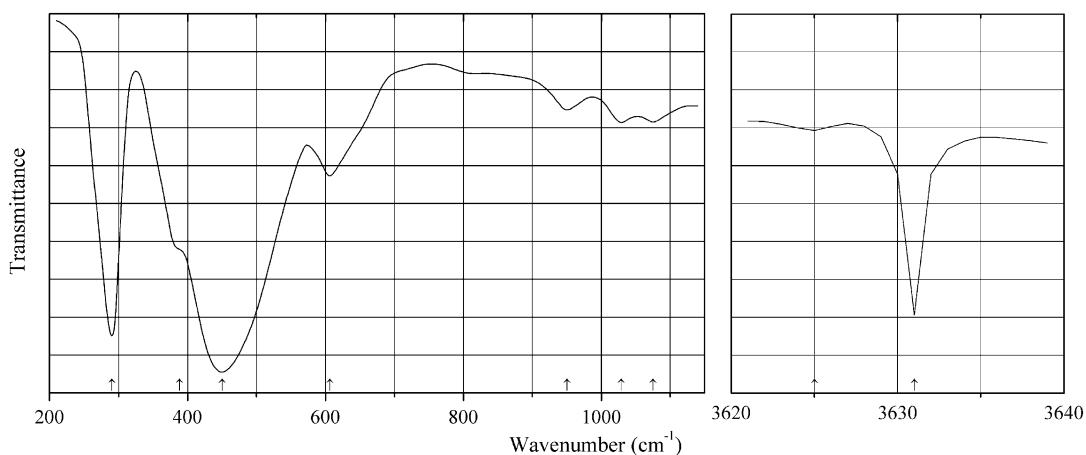
**Description:** Black crystals. Holotype sample. Metamict, X-ray amorphous. The strongest lines of the powder X-ray diffraction pattern of a heated sample [ $d$ ,  $\text{\AA}$  ( $I$ , %)] are: 4.87 (70), 3.89 (80), 3.17 (100), 2.45 (90), 1.659 (90).

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission.

**Source:** X-ray Laboratory, Peking Institute of Uranium Geology, Wuhan Geological College (1978).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3480, 1669w, 1620w, 1451, 1405sh, 1157w, 1078w, 1036w, 880, 581sh, 546s, 461sh, 391sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**O652 Pyrochroite  $\text{Mn}^{2+}(\text{OH})_2$** 


**Origin:** Synthetic.

**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc. Transmission.

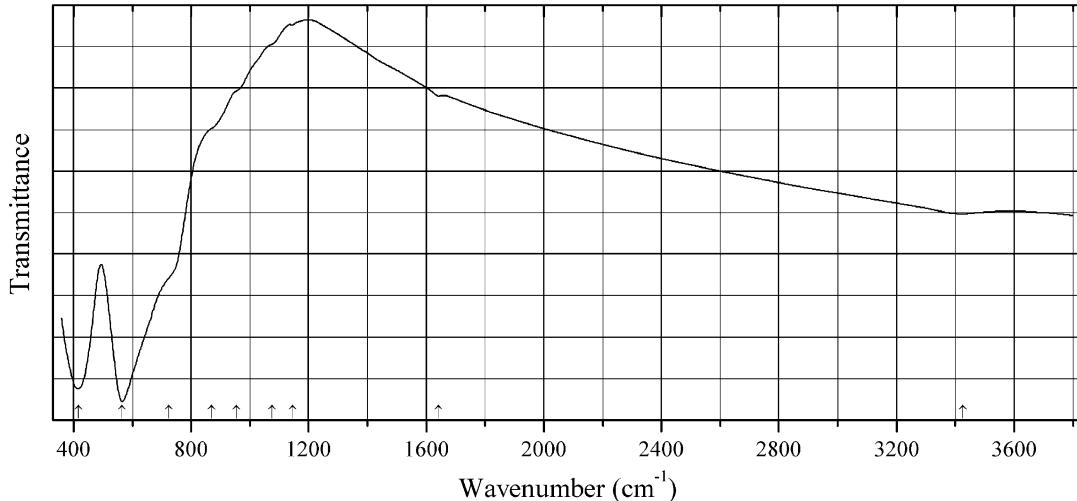
**Source:** Lutz et al. (1994).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3631s, 1075w, 1029w, 950w, 606, 450s, 388sh, 290s.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 3578s, 401, 234.

### O653 Fluorcalciopyrochlore $(\text{Ca},\text{Na})_2(\text{Nb},\text{Ti})_2\text{O}_6\text{F}$



**Origin:** Tatarka River, Krasnoyarskiy Kray, Siberia, Russia.

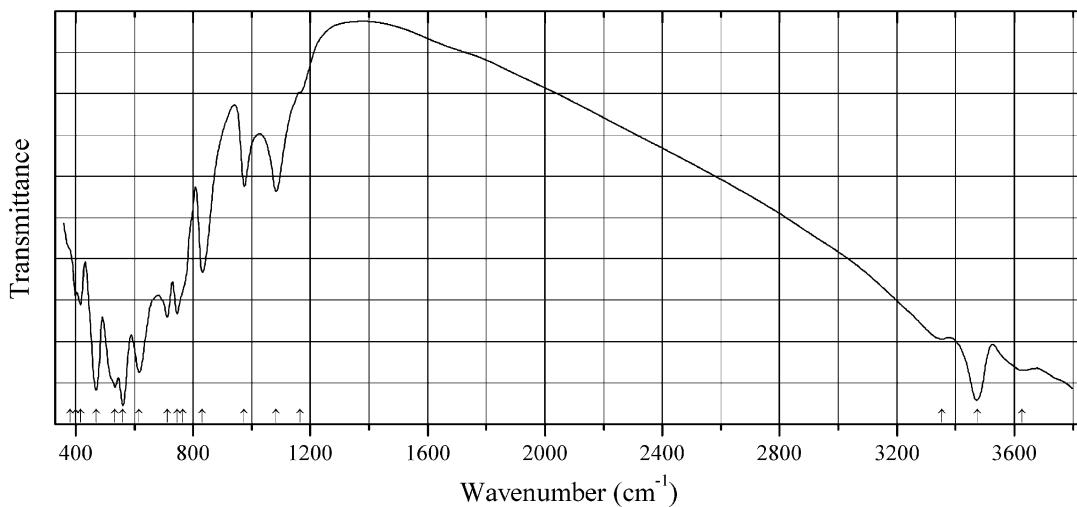
**Description:** Yellow-brown octahedral crystal. The empirical formula is (electron microprobe):  $(\text{Ca}_{0.85}\text{Na}_{0.19}\text{REE}_{0.02})(\text{Nb}_{1.91}\text{Ti}_{0.04}\text{Fe}_{0.03}\text{Re}_{0.02})(\text{O},\text{OH})_{6.36}\text{F}_{0.64} \cdot n\text{H}_2\text{O}$  ( $n \ll 1$ ).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3426w, 1643w, 1145w, 1075sh, 955sh, 870sh, 725sh, 565s, 416s.

**Note:** The spectrum was obtained by N.V. Chukanov.

### O654 Ferronigerite-2N1S $(\text{Al},\text{Fe},\text{Zn})_2(\text{Al},\text{Sn})_6\text{O}_{11}(\text{OH})$



**Origin:** Three Aloes Mine, Uis, Damaraland District, Kunene Region, Namibia.

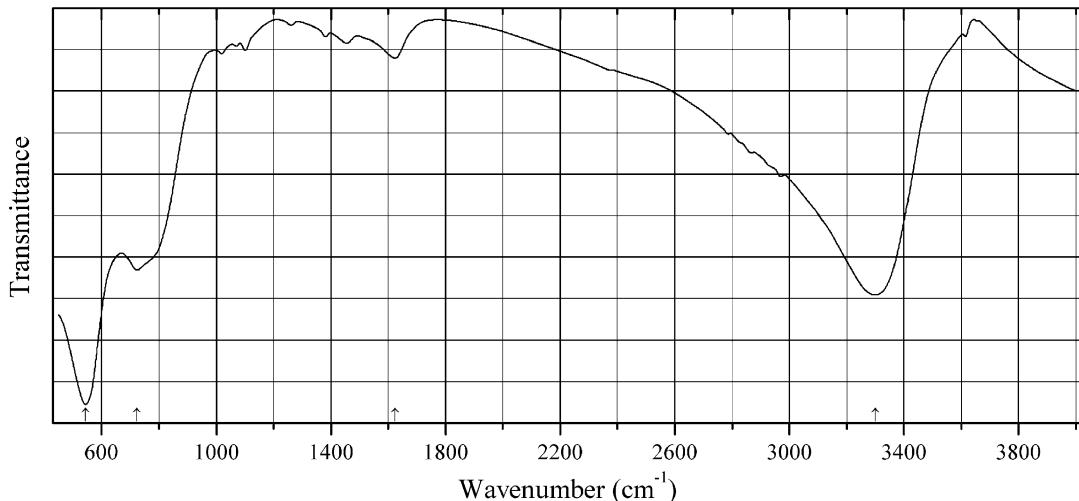
**Description:** Orange-brown tabular crystal. The empirical formula is (electron microprobe):  $\text{Al}_{5.97}\text{Fe}_{0.79}\text{Zn}_{0.15}\text{Mg}_{0.07}\text{Cr}_{0.02}(\text{Sn}_{0.93}\text{Ti}_{0.07})\text{O}_{11}(\text{OH})$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3627w, 3473, 3352w, 1165sh, 1083, 975, 832, 765sh, 746, 712, 616s, 561s, 534s, 470s, 417, 399, 380sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

### O655 Hydroromarchite $\text{Sn}^{2+}_3\text{O}_2(\text{OH})_2$



**Origin:** Synthetic.

**Description:** Yellow precipitate obtained by addition of water to diethylether solution of  $\text{Sn}(\text{NMe}_2)_2$ . Characterized by TG and powder X-ray diffraction data.

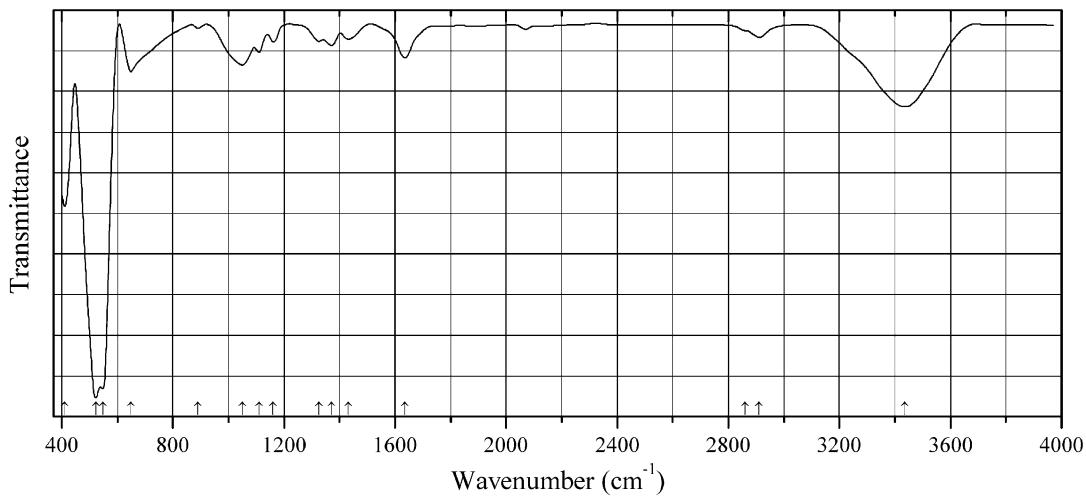
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Khanderi et al. (2015).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3300s, (1623), 724, 544s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. Weak bands in the ranges 1000–1500 and 2800–3000 cm<sup>-1</sup> correspond to the admixture of an organic substance. The band at 1623 cm<sup>-1</sup> may correspond to adsorbed water molecules. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 264, 229s, 186, 132s.

**O656 Kusachiite  $\text{Cu}^{2+}\text{Bi}^{3+}_2\text{O}_4$** 

**Origin:** Synthetic.

**Description:** Prepared hydrothermally from bismuth acetate and copper nitrate in the presence of NaOH at 140 °C for 12 h. Characterized by powder X-ray diffraction data. Tetragonal, space group  $P4/ncc$ ,  $a = 8.567$ ,  $c = 5.791$  Å,  $V = 425.17$  Å<sup>3</sup>.

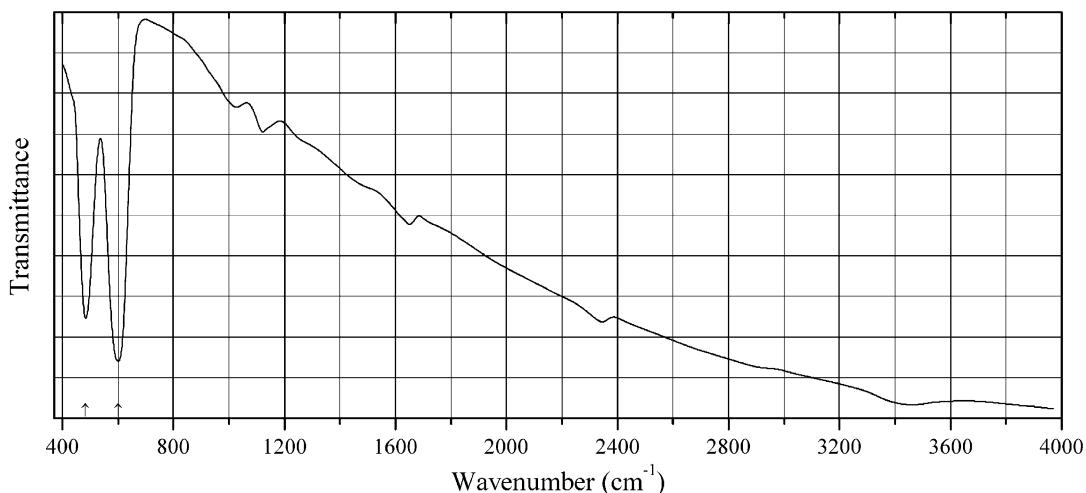
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Yuvaraj et al. (2016).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 890w, 648, 547s, 522s, 410.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. Bands above 1000  $\text{cm}^{-1}$  correspond to impurities. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 575w, 399, 257s, 187w, 123s, 84w.

**O657 Montroydite HgO**

**Origin:** Synthetic.

**Description:** Commercial reactant. Characterized by powder X-ray diffraction data.

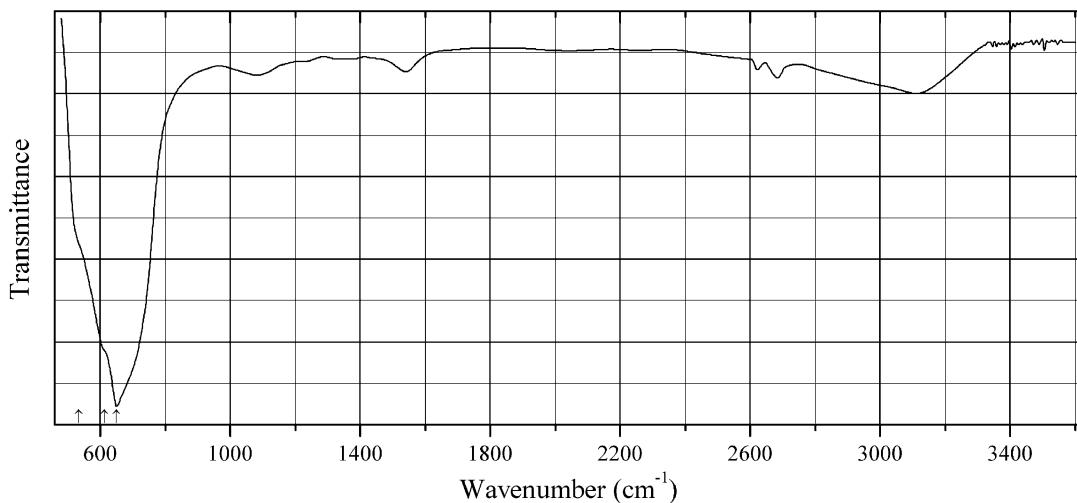
**Kind of sample preparation and/or method of registration of the spectrum:** No data.

**Source:** Xhaxhiu et al. (2013).

**Wavenumbers (cm<sup>-1</sup>):** 1122w, 600, 484.

**Note:** Bands above 1400 cm<sup>-1</sup> correspond to impurities. For the IR spectrum of montroydite see also Godelitsas et al. (2003).

### O658 Romarchite SnO



**Origin:** Synthetic.

**Description:** Nanoparticles. Characterized by powder X-ray diffraction data.

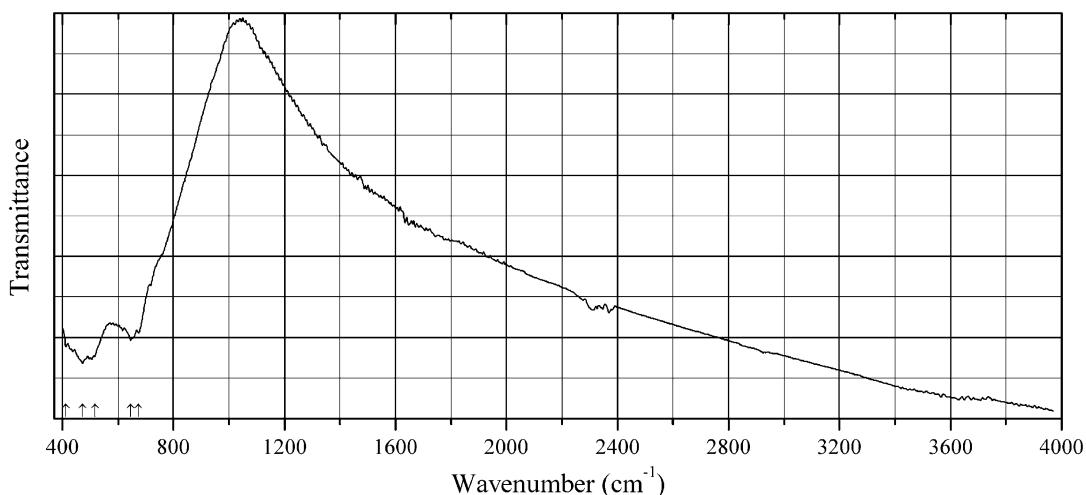
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Krishnakumar et al. (2008).

**Wavenumbers (cm<sup>-1</sup>):** 651s, 613sh, 535sh.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

### O659 Zirconolite-2M (Ca,Y)Zr(Ti,Mg,Al)<sub>2</sub>O<sub>7</sub>



**Origin:** Synthetic.

**Description:** Synthesized by a solid-state reaction method at 1400 °C for 16 h. Characterized by powder X-ray diffraction data. Monoclinic,  $a = 12.441$ ,  $b = 7.239$ ,  $c = 11.341$  Å,  $\beta = 100.694^\circ$ .

The empirical formula is  $\text{Ca}_{0.83}\text{Ce}_{0.17}\text{ZrTi}_{1.66}\text{Al}_{0.34}\text{O}_7$ .

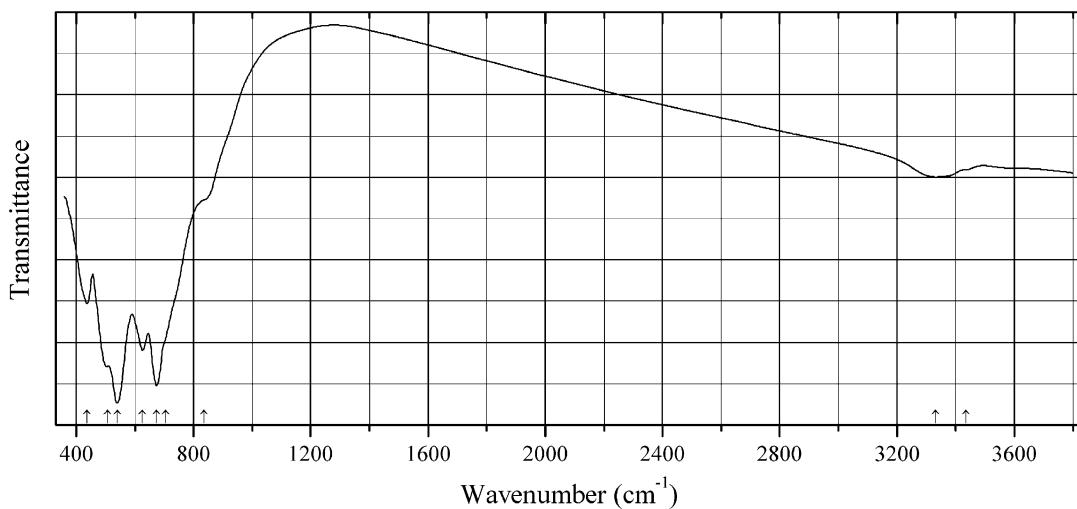
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Souag et al. (2015).

**Wavenumbers (cm<sup>-1</sup>):** 685, 646, 517s, 473s, 413sh.

**Note:** The band position denoted by Souag et al. (2015) as 685 cm<sup>-1</sup> was determined by us at 675 cm<sup>-1</sup>.

### O660 Magnesiohögbonite-2N3S ( $\text{Mg},\text{Fe},\text{Zn},\text{Ti})_4(\text{Al},\text{Fe})_{10}\text{O}_{19}(\text{OH})$



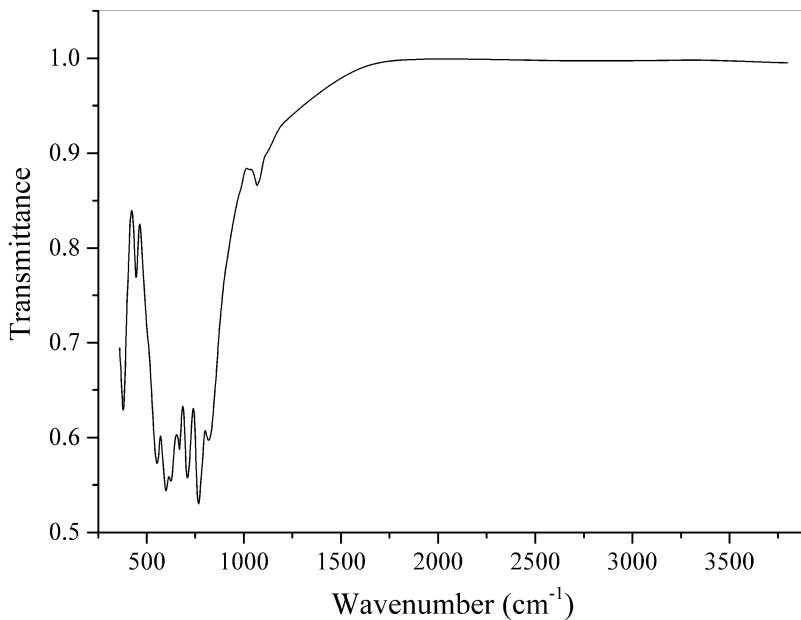
**Origin:** Zelentsovskaya pit, near Zlatoust, Chelyabinsk region, Southern Urals, Russia.

**Description:** Crystals from the association with clinochlore, magnetite, and spinel. Investigated by I.V. Pekov. Characterized by single-crystal X-ray diffraction data. Hexagonal,  $a = 5.743(3)$ ,  $c = 23.10(2)$  Å,  $V = 659.7(8)$  Å<sup>3</sup>. The empirical formula is (electron microprobe):  $(\text{Mg}_{2.04}\text{Fe}_{1.89}\text{Zn}_{0.06}\text{Mn}_{0.02})(\text{Al}_{9.52}\text{Ti}_{0.77})\text{O}_{19}(\text{OH})$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3435sh, 3332, 835sh, 705sh, 674s, 626s, 540s, 507s, 437.

**Note:** The spectrum was obtained by N.V. Chukanov.

**O661 Diaoyudaoite**  $\text{NaAl}_{11}\text{O}_{17}$ 

**Origin:** Technogenetic, from the slag of the Klyuchevskoi ferroalloy factory, Sverdlovsk region, Russia.

**Description:** Brown platy crystals from the association with corundum. Investigated by I.V. Pekov.

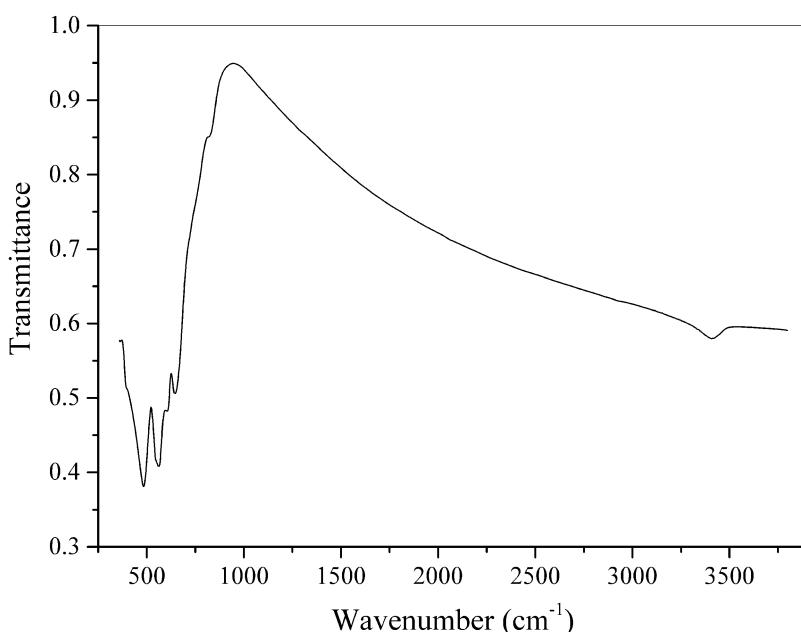
Characterized by single-crystal X-ray diffraction data. Hexagonal,  $a = 5.618(10)$ ,  $c = 22.62(3)$  Å,

$V = 618(2)$  Å<sup>3</sup>. The composition is close to that of diaoyudaoite end-member.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 1120sh, 1069w, 819, 768s, 709s, 668, 624s, 599s, 553, 445, 380.

**Note:** The spectrum was obtained by N.V. Chukanov.

**O662 Zincovelesite-6N6S**  $\text{Zn}_3(\text{Fe}^{3+},\text{Mn}^{3+},\text{Al,Ti})_8\text{O}_{15}(\text{OH})$ 

**Origin:** “Mixed Series” metamorphic complex near the Nežilovo village, Jacupica Mountains, Pelagonia mountain range, Macedonia (type locality).

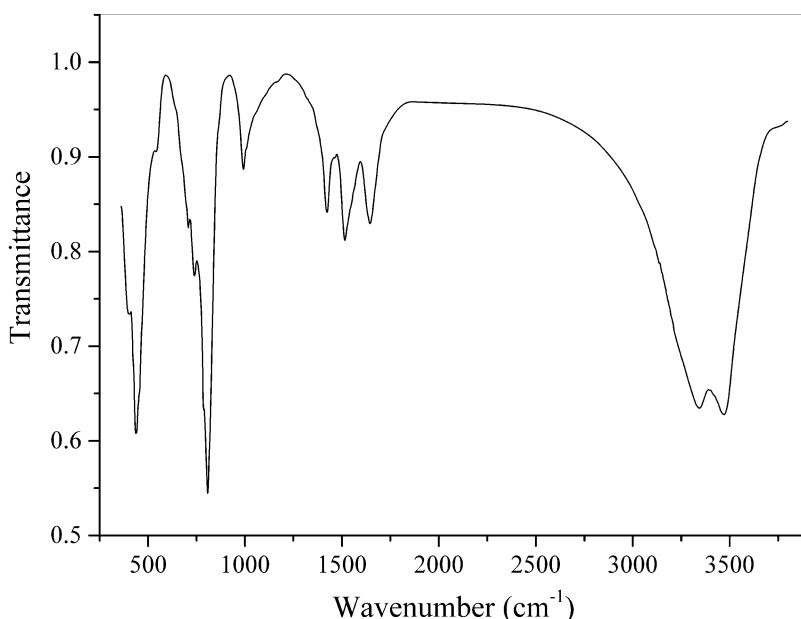
**Description:** Black lenticular aggregates from the association with franklinite, gahnite, hetaerolite, zincochromite, ferricoronadite, baryte, As-rich fluorapatite, dolomite, Zn-bearing talc, almeidaite, etc. Holotype sample. The crystal structure is refined by the Rietveld technique. Trigonal, probable space group  $P-3m1$ ,  $a = 5.902(2)$  Å,  $c = 55.86(1)$  Å,  $V = 1684.8(9)$  Å $^3$ ,  $Z = 6$ .  $D_{\text{calc}} = 5.158$  g/cm $^3$ . The empirical formula is  $\text{H}_{1.05}\text{Zn}_{3.26}\text{Mg}_{0.21}\text{Cu}_{0.05}\text{Fe}^{3+}_{3.18}\text{Mn}^{3+}_{2.32}\text{Al}_{1.38}\text{Ti}_{0.57}\text{Sb}_{0.20}\text{O}_{16}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 2.952 (62) (110), 2.881 (61) (1.0.16), 2.515 (100) (204), 2.493 (88) (1.1.12), 2.451 (39) (1.0.20), 1.690 (19) (304, 2.1.16), 1.572 (19) (2.0.28), 1.475 (29) (221).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm $^{-1}$ ):** 3407w, 817sh, 647, 605, 563s, 550sh, 484s, 400sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

### O663 Wölsendorfite $\text{Pb}_7(\text{UO}_2)_{14}\text{O}_{19}(\text{OH})_4 \cdot 12\text{H}_2\text{O}$



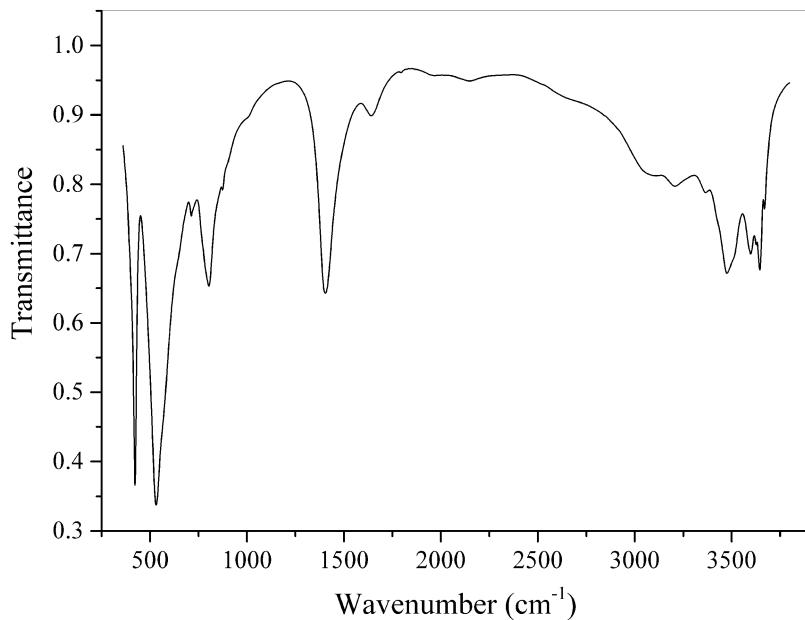
**Origin:** Shinkolobwe, Katanga (Shaba), Democratic Republic of Congo.

**Description:** Orange-red grains. Investigated by A.V. Kasatkin. The empirical formula based on semiquantitative electron microprobe analysis is  $\text{Pb}_{5.3}\text{Ca}_{1.0}\text{As}_{0.4}(\text{UO}_2)_{14.35}(\text{O},\text{OH})_x \cdot n\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm $^{-1}$ ):** 3470s, 3344s, 1645, 1515, 1423, 992, 808s, 739, 707, 542w, 437s, 402.

**Note:** The spectrum was obtained by N.V. Chukanov.

**O664 Hydrocalumite**  $\text{Ca}_2\text{Al}(\text{OH})_6(\text{Cl},\text{OH}) \cdot 3\text{H}_2\text{O}$ 

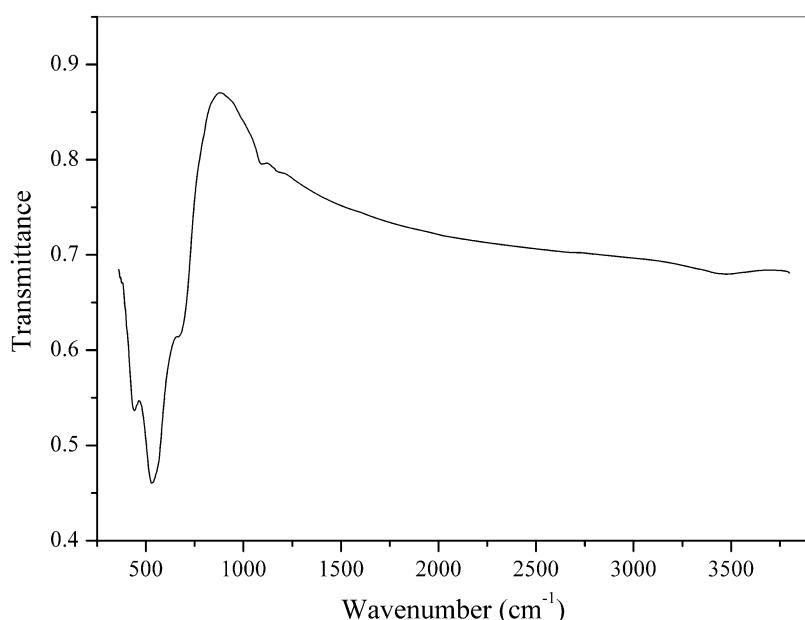
**Origin:** Bellerberg, near Ettringen, Eifel Mts., Rhineland-Palatinate (Rheinland-Pfalz), Germany.

**Description:** Colorless platy crystal from the association with ettringite. Confirmed by qualitative electron microprobe analyses.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3670, 3645s, 3629, 3598, 3500sh, 3475s, 3368, 3207, 3108, 2700sh, 2149w, 1973w, 1795w, 1641, 1404s, 990sh, 874, 804s, 713, 531s, 422s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**O665 Magnesiohögbonite-2N4S**  $(\text{Mg},\text{Fe}^{2+})_{10}\text{Al}_{22}\text{Ti}^{4+}_2\text{O}_{46}(\text{OH})_2$ 

**Origin:** Kastor, Kirkkjokk, Sweden.

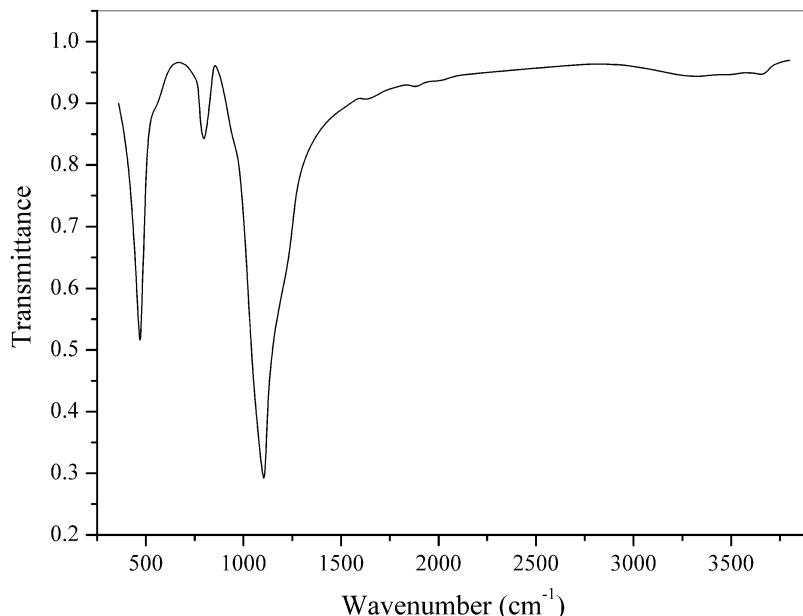
**Description:** Black grains. The empirical formula is (electron microprobe):  $(\text{Mg}_{5.64}\text{Fe}_{4.26}\text{Mn}_{0.12})(\text{Al}_{23.2}\text{Fe}_{0.80})(\text{Ti}_{1.87}\text{Fe}_{0.13})\text{O}_{44}(\text{OH})_2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3490sh, 3475, 1185sh, 1100sh, 667, 530s, 442, 370sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

### O667 Hyalite $\text{SiO}_2 \cdot \text{H}_2\text{O}$



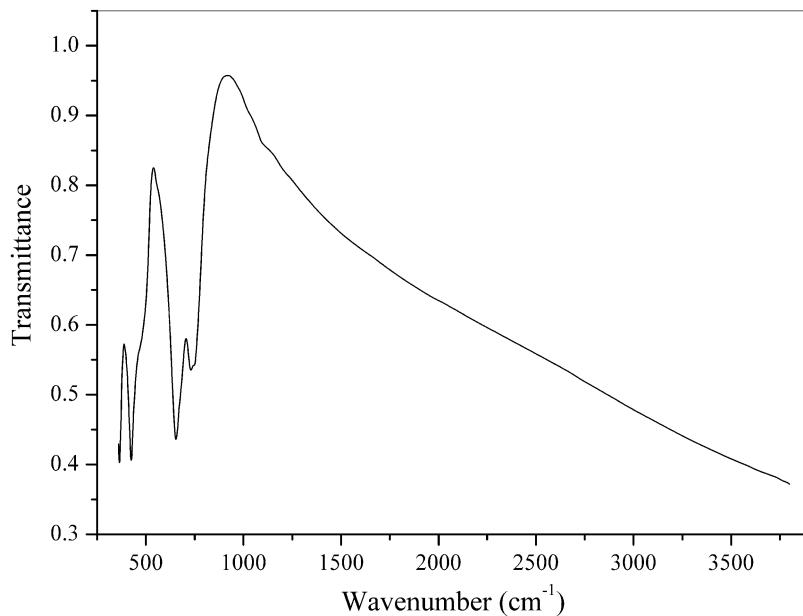
**Origin:** Tarcal, Borsod-Abaúj-Zemplén Hungary.

**Description:** Colorless sinter aggregate.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3652w, 3471sh, 3324w, 2000w, 1879w, 1625w, 1185sh, 1104s, 797, 540sh, 470s.

**Note:** The spectrum was obtained by N.V. Chukanov. The spectrum is very close to that of quartz glass but contains weak bands of  $\text{H}_2\text{O}$  molecules.

**O668 Clinocervantite  $\text{Sb}^{3+}\text{Sb}^{5+}\text{O}_4$** 

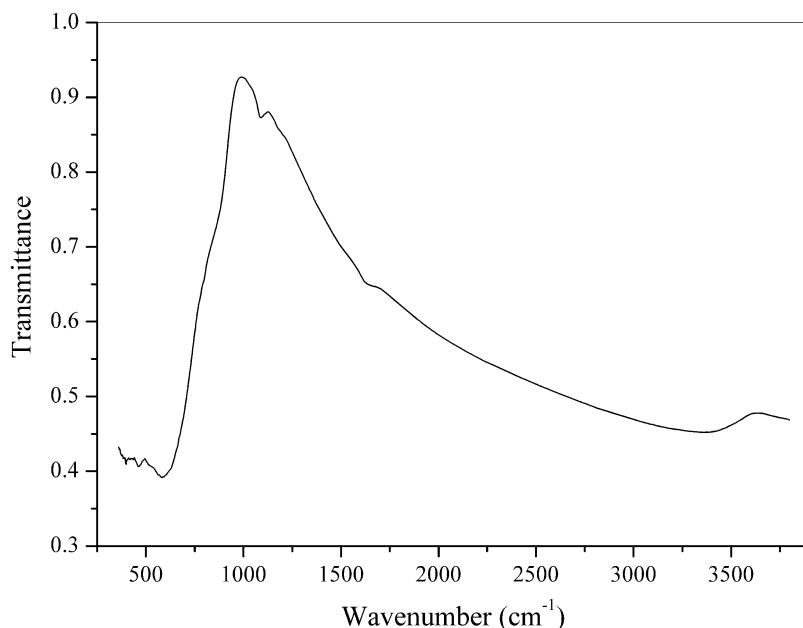
**Origin:** Le Cetine di Cotorniano Mine, Chiusdino, Siena Province, Tuscany, Italy.

**Description:** Colorless acicular crystals.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 1105sh, 1025sh, 745sh, 731, 654s, 470sh, 425s, 364s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**O669 Ishikawaite  $\text{U}_{1-x}\text{FeNb}_2\text{O}_8$** 

**Origin:** Pit No. 298, Ilmenskiy Natural Reserve, Ilmeny Mts., Chelyabinsk region, Southern Urals, Russia.

**Description:** Black prismatic crystal from the association with corundum. X-ray amorphous, metamict.

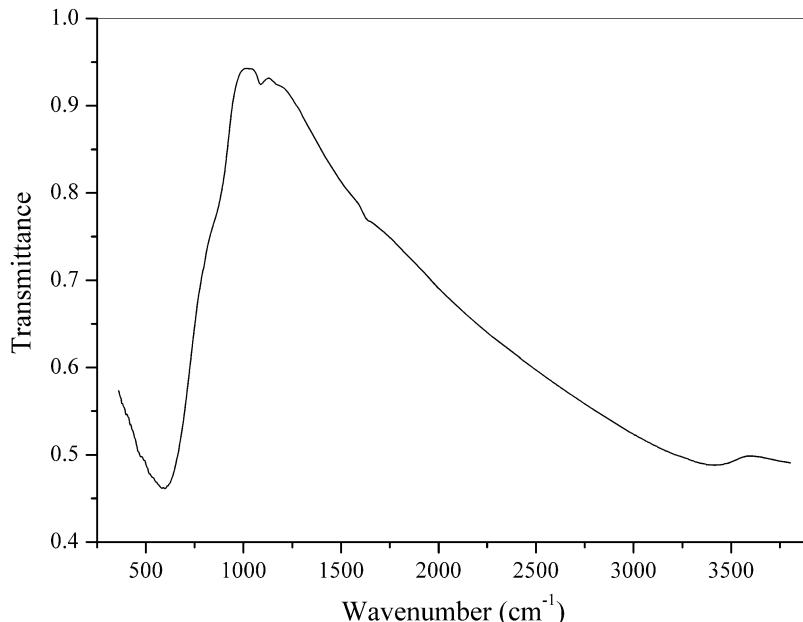
The empirical formula is (electron microprobe):  $U_{0.42}Th_{0.18}REE_{0.11}Fe_{0.88}Nb_{1.91}Ti_{0.09}O_8 \cdot nH_2O$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3364 (broad), 1645w, 1088w, 825sh, 583s (broad), 463s, 400s.

**Note:** The spectrum was obtained by N.V. Chukanov.

#### O670 Samarskite-(Y) $YFe^{3+}Nb_2O_8$



**Origin:** Blyumovskaya Pit (Pit No. 50), Ilmenskiy Natural Reserve, Ilmeny Mts., Chelyabinsk region, Southern Urals, Russia (type locality).

**Description:** Black prismatic crystal. X-ray amorphous, metamict. Confirmed by qualitative electron microprobe analyses.

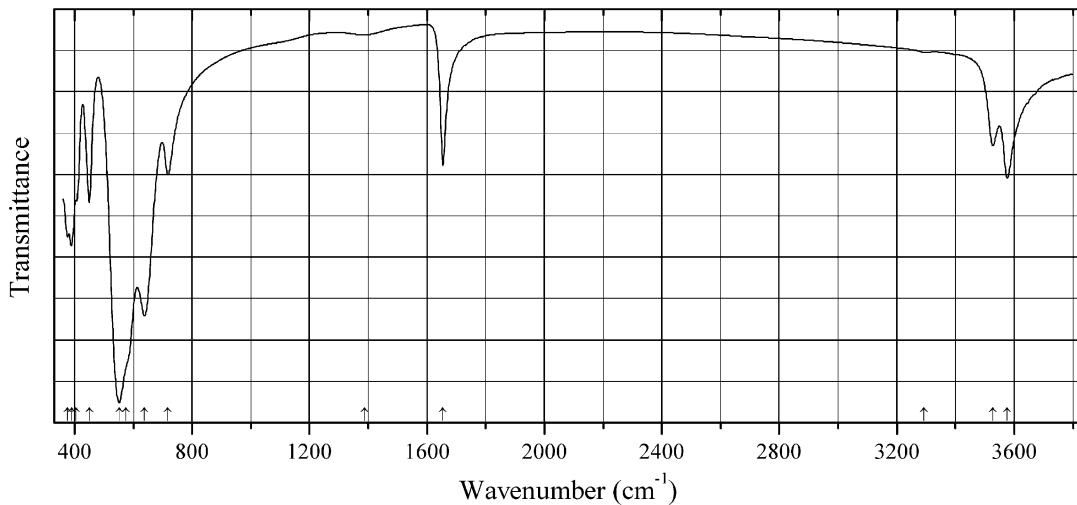
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3418 (broad), 1655w, 1088w, 850sh, 599s, 530sh, 475sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

## 2.6 Fluorides and Fluorochlorides

**F76 Carlhintzeite**  $\text{Ca}_2\text{AlF}_7 \cdot \text{H}_2\text{O}$



**Origin:** Synthetic.

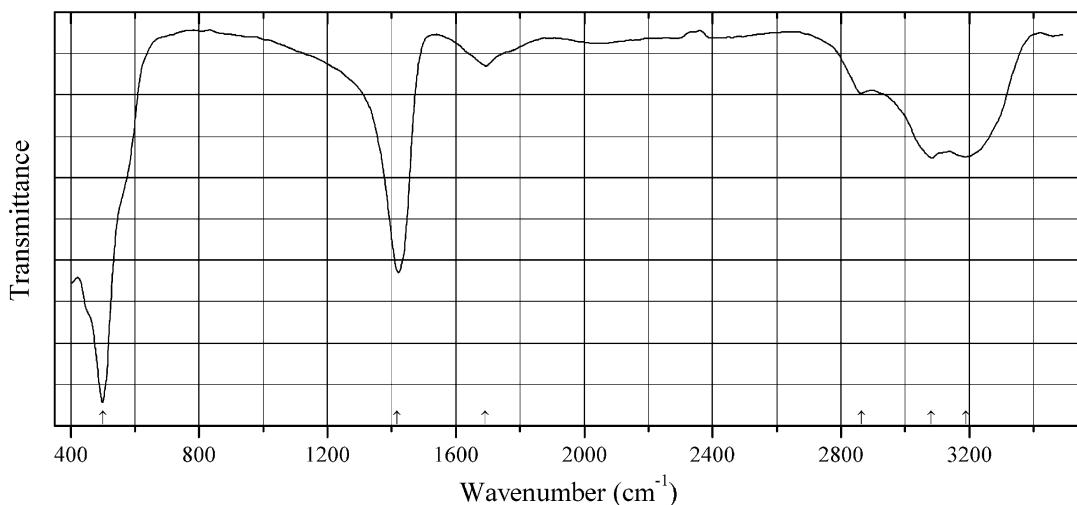
**Description:** Aggregate of colorless crystals from the association with pachnolite, strengite, and tobermorite. Confirmed by qualitative electron microprobe analyses.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3577, 3528, 1655, 1387w, 718, 638s, 575sh, 552s, 450, 405sh, 390, 380.

**Note:** The spectrum was obtained by N.V. Chukanov.

**F77 Ammonium zirconofluoride**  $(\text{NH}_4)_2\text{ZrF}_6$



**Origin:** Synthetic.

**Description:** Prepared by dissolving stoichiometric quantities of zirconium chloride and ammonium fluoride in concentrated hydrofluoric acid. Orthorhombic, space group  $Pca2_1$ ,  $Z = 8$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

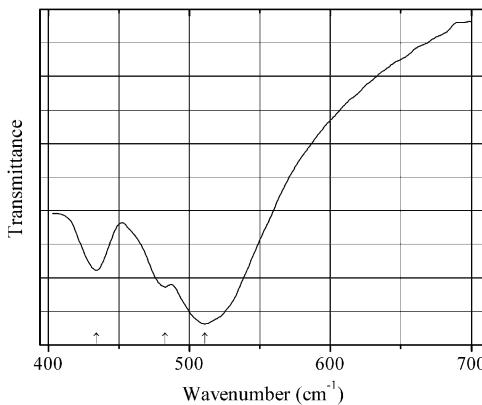
**Source:** Kruger and Heyns (1997).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3190, 3080, 2864w, 1690w, 1417s, 500s.

**Note:** The band at  $1690 \text{ cm}^{-1}$  indicates the presence of  $\text{H}_2\text{O}$ . In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 3146s, 1698, 1412w, 536s, 475w, 377w.

### F78 Barium magnesium fluoride $\text{BaMgF}_4$



**Origin:** Synthetic.

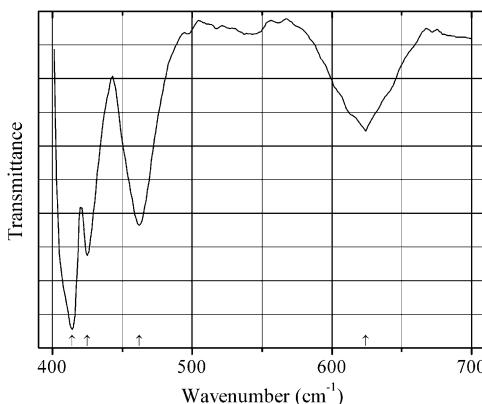
**Description:** Synthesized hydrothermally from  $\text{BaF}_2$  and  $\text{MgF}_2$  in the presence of  $\text{CF}_3\text{COOH}$ , at  $230^\circ\text{C}$  for 24 h. Orthorhombic, space group  $Cmc2_1$ . Characterized by DSC and powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Kim et al. (2010b).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 511s, 483, 434.

### F79 Barium manganese fluoride $\text{BaMnF}_4$



**Origin:** Synthetic.

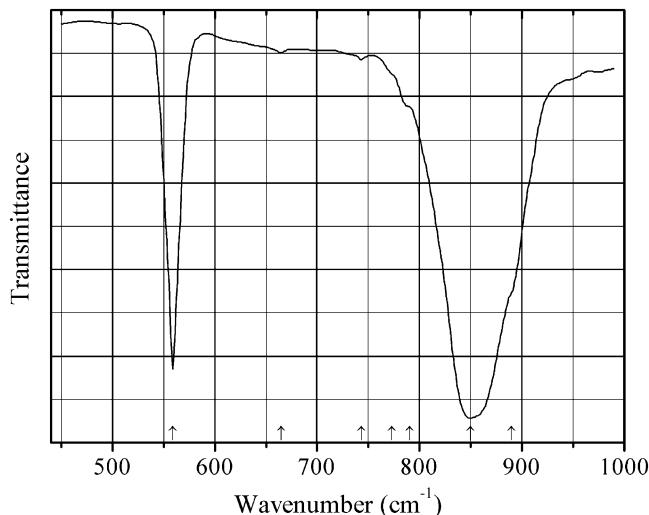
**Description:** Synthesized hydrothermally from  $\text{BaF}_2$  and  $\text{MnF}_2$  in the presence of  $\text{CF}_3\text{COOH}$ , at 230 °C for 24 h. Orthorhombic, space group  $Cmc2_1$ . Characterized by DSC and powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Kim et al. (2010b).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 624, 462, 425, 414s.

#### F80 Cesium hexafluorophosphate $\text{CsPF}_6$



**Origin:** Synthetic.

**Description:** Prepared by crystallization from aqueous solution containing equimolar quantities of  $\text{HPF}_6$  and  $\text{Cs}_2\text{CO}_3$ . Cubic,  $a = 8.218 \text{ \AA}$ . The strongest lines of the powder X-ray diffraction pattern [ $d, \text{ \AA}$  ( $I, \%$ ) ( $hkl$ )] are: 4.113 (100) (200), 2.9051 (29) (220), 2.4787 (29) (311), 2.3726 (8) (222), 1.8381 (9) (420).

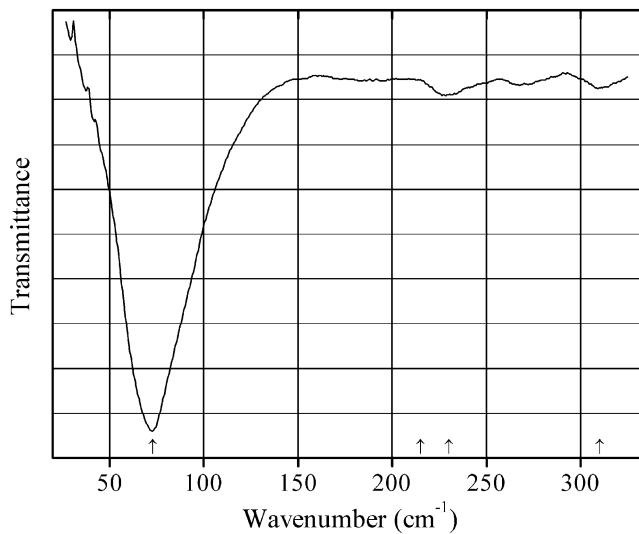
**Kind of sample preparation and/or method of registration of the spectrum:** No data in the cited paper.

**Source:** Heyns et al. (1981).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1410w, (1260w), 890sh, 850s, 790sh, 773sh, 743w, 665w, 559s, 76s.

**Note:** In the cited paper, Raman spectra with different polarization are given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 744, 575–577, 472–475.

**F81 Cesium hexafluorophosphate**  $\text{CsPF}_6$ 

**Origin:** Synthetic.

**Description:** Cubic, space group *Fm3m*,  $a = 8.228(5)$  Å,  $V = 557(1)$  Å<sup>3</sup>,  $Z = 4$ .

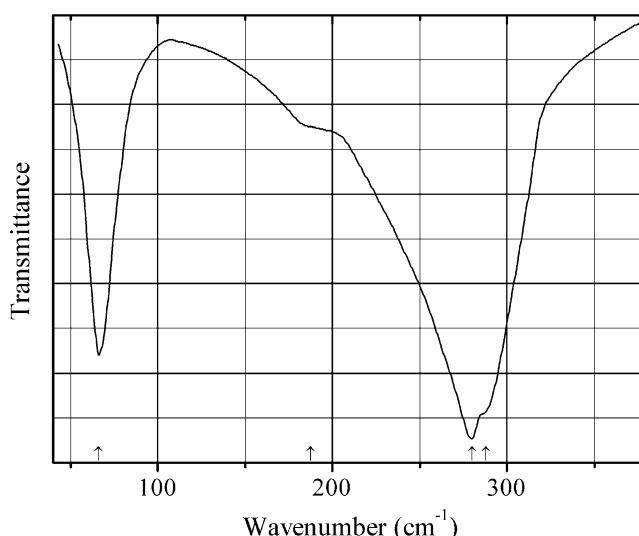
**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

**Source:** English and Heyns (1984).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1405w, 890sh, 846s, 790w, 743w, 559s, 470s, 310w, 230w, 215w, 79.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 744, 578, 476.

**F82 Cesium stibiofluoride**  $\text{CsSbF}_6$ 

**Origin:** Synthetic.

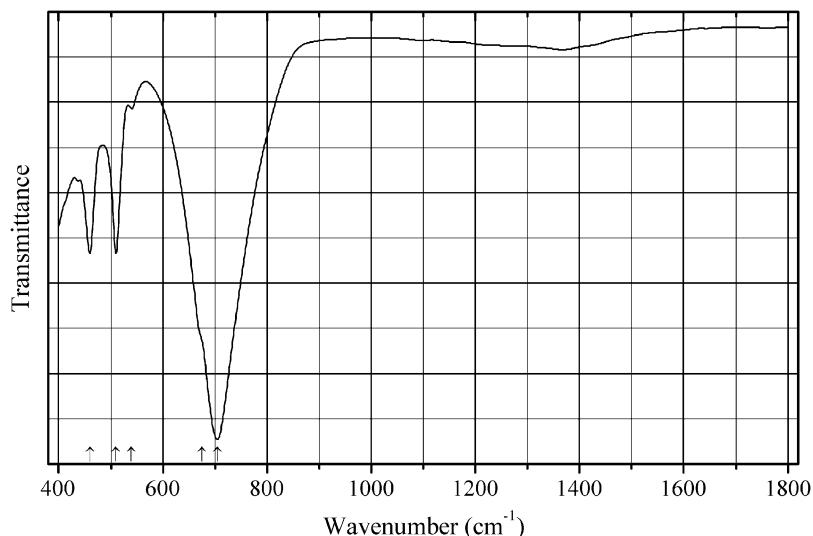
**Description:** Prepared from  $\text{Cs}_2\text{CO}_3$ ,  $\text{Sb}_2\text{O}_5$ , and an excess of hydrofluoric acid. Characterized by powder X-ray diffraction data. Trigonal, space group  $R\text{-}3m$ ,  $a = 7.9037$ ,  $c = 8.2543$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr pellet and Nujol mull. Transmission.

**Source:** De Beer et al. (1980).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1300w, 1260w, 950w, 845w, 668sh, 655s, 635sh, 560w, 450w, 288sh, 280s, 180–195sh, 66s.

### F83 Lithium hexafluorosilicate $\text{Li}_2\text{SiF}_6$



**Origin:** Synthetic.

**Description:** Crystals grown by pressure-induced crystallization at 5.5 GPa and 750 °C. Characterized by powder X-ray diffraction data. The crystal structure is solved. Trigonal, space group  $P\bar{3}21$ ,  $a = 8.219(2)$ ,  $c = 4.5580(9)$  Å,  $V = 266.65(8)$  Å<sup>3</sup>,  $Z = 3$ .  $D_{\text{calc}} = 2.914$  g/cm<sup>3</sup>. Both Li and Si have octahedral coordination.

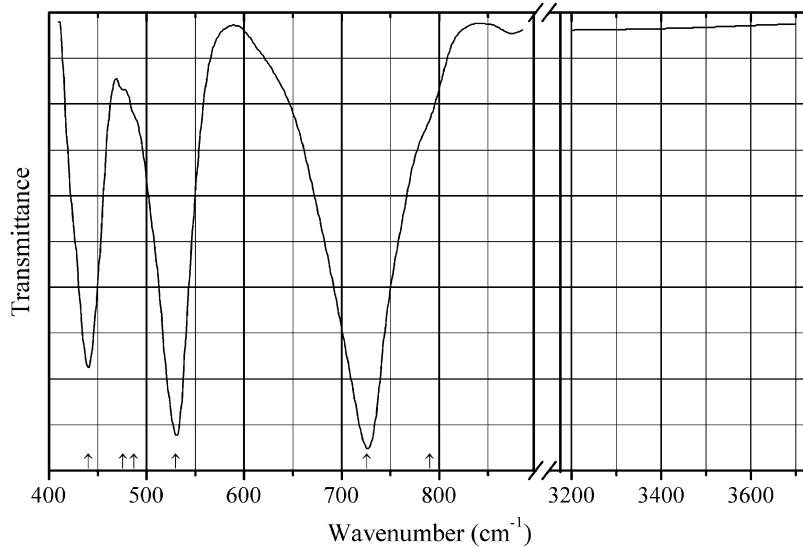
**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of a powdered sample.

**Source:** Hinteregger et al. (2014).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 705s, 675sh, 540w, 510, 460.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, a single-crystal Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1100, 660s, 500, 420.

**F84 Nickel antimonate fluoride  $\text{Ni}_3\text{Sb}_4\text{O}_6\text{F}_6$** 

**Origin:** Synthetic.

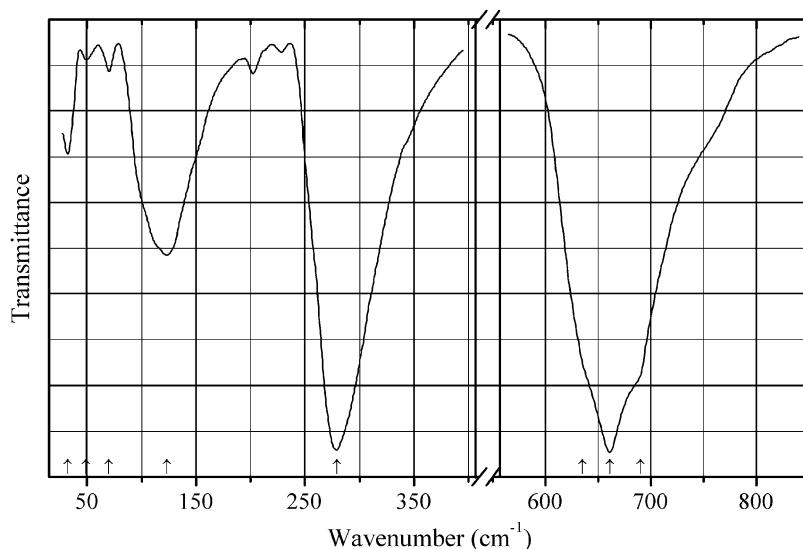
**Description:** Green crystals obtained hydrothermally from  $\text{NiF}_2$  and  $\text{Sb}_2\text{O}_3$  at  $230^\circ\text{C}$  for 4 days. The crystal structure is solved. Cubic, space group  $I-43m$ ,  $a = 8.0778(1)$ ,  $V = 527.08(1)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{calc}} = 5.501$  g/cm $^3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Reflection.

**Source:** Hu et al. (2014).

**Wavenumbers (cm $^{-1}$ ):** 790sh, 726s, 530s, 487sh, 476w, 440s.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**F85 Potassium antimony fluoride  $\text{KSbF}_6$** 

**Origin:** Synthetic.

**Description:** Tetragonal, space group  $P-42m$ ,  $a = 5.16(1)$ ,  $c = 10.07(2)$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

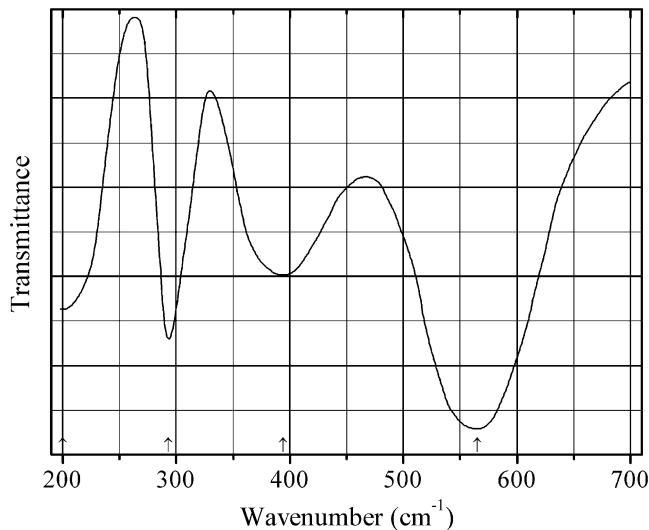
**Source:** Heyns and van den Berg (1995).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 690sh, 661s, 635sh, 279s, 123, 70w, 49w, 32.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 661s, 575, 292s [with the  $z(yy)x$  polarization].

### F86 Potassium manganese(III) fluoride $\text{K}_3\text{MnF}_6$



**Origin:** Synthetic.

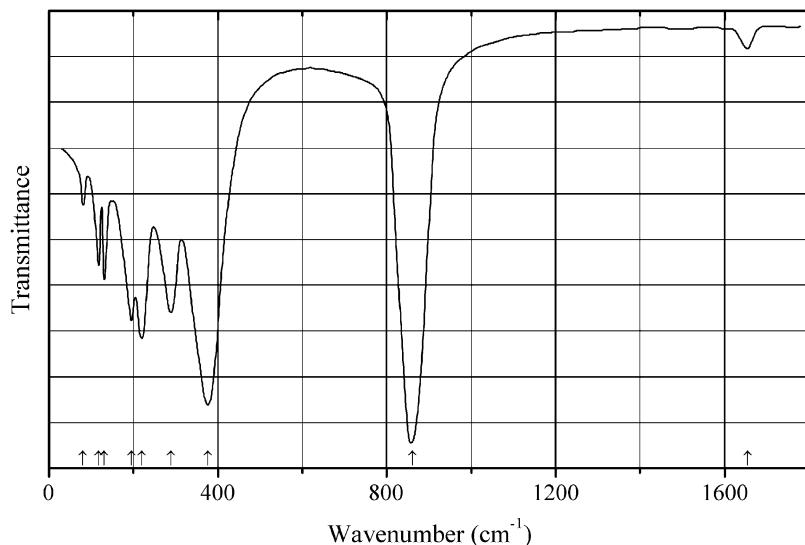
**Description:** The crystal structure contains distorted  $\text{MnF}_6^{3-}$  octahedron.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Wieghardt and Siebert (1971).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 565s, 394, 293, ~200.

### F87 Potassium uranyl fluoride $\text{K}_3(\text{UO}_2)\text{F}_5$



**Origin:** Synthetic.

**Description:** Yellow crystals obtained by heating an aqueous solution containing stoichiometric amounts of uranyl and potassium fluorides to 80 °C with subsequent cooling and adding ethanol.

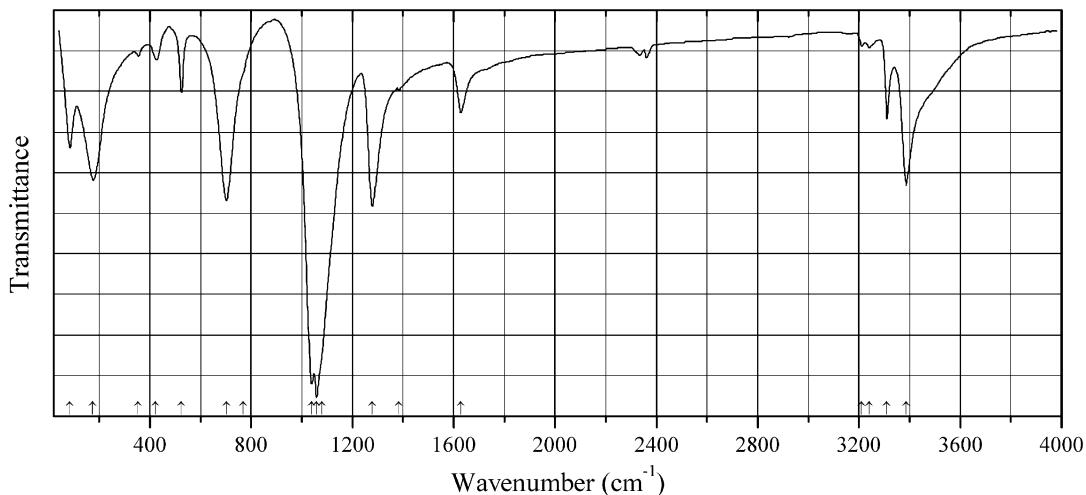
Tetragonal,  $a = 9.160$ ,  $c = 18.167$  Å,  $Z = 8$ . Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull. Transmission.

**Source:** Ohwada et al. (1972).

**Wavenumbers (cm<sup>-1</sup>):** 1655w, 860s, 376s, 289, 220, 195, 131, 118, 81w.

### F88 Tetrammine zinc borofluoride [Zn(NH<sub>3</sub>)<sub>4</sub>](BF<sub>4</sub>)<sub>2</sub>



**Origin:** Synthetic.

**Description:** Orthorhombic, space group *Pnma*,  $a = 10.523$ ,  $b = 7.892$ ,  $c = 13.354$  Å.

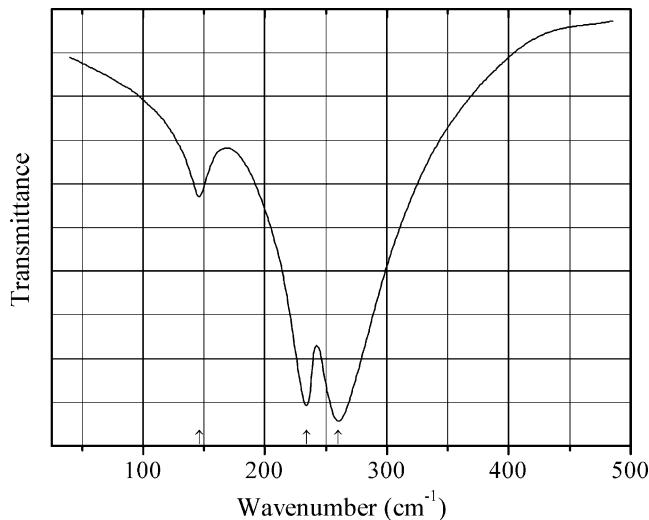
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc and Nujol mull. Absorption.

**Source:** Mikuli et al. (2007).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3385s, 3310, 3240w, 3211w, 1628, 1383sh, 1277s, 1080sh, 1057s, 1039s, 769w, 702s, 523, 423, 354w, 175s, 83.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 3381, 3314s, 3210, 1624, 1085w, 1045sh, 770s, 704w, 525, 436s, 355, 172s.

**F89 Uranyl fluoride  $\text{UO}_2\text{F}_2$** 

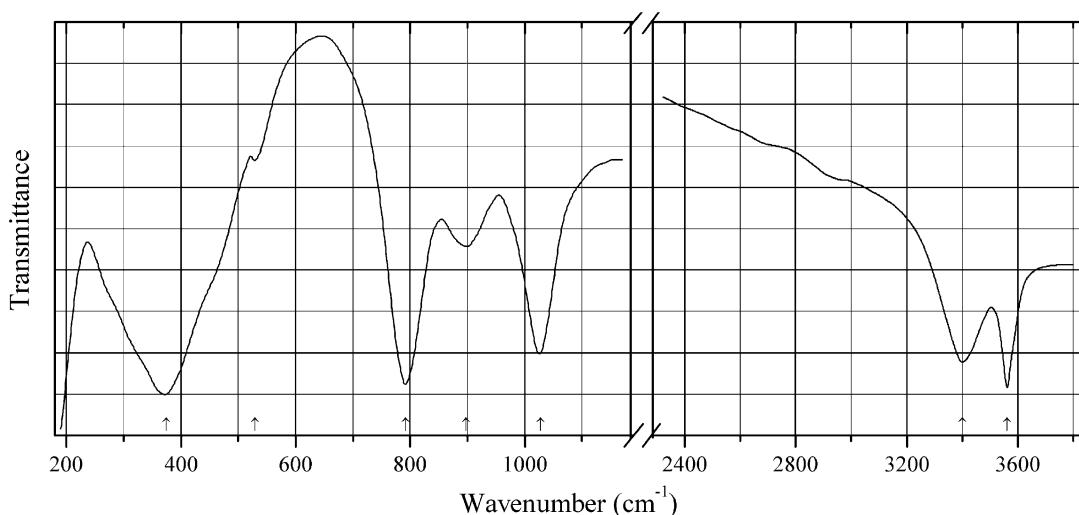
**Origin:** Synthetic.

**Description:** Trigonal, space group  $R-3m$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull. Transmission.

**Source:** Ohwada (1972).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 260s, 234s, 146.

**F90 Zinc hydroxyfluoride  $\text{Zn(OH)F}$** 

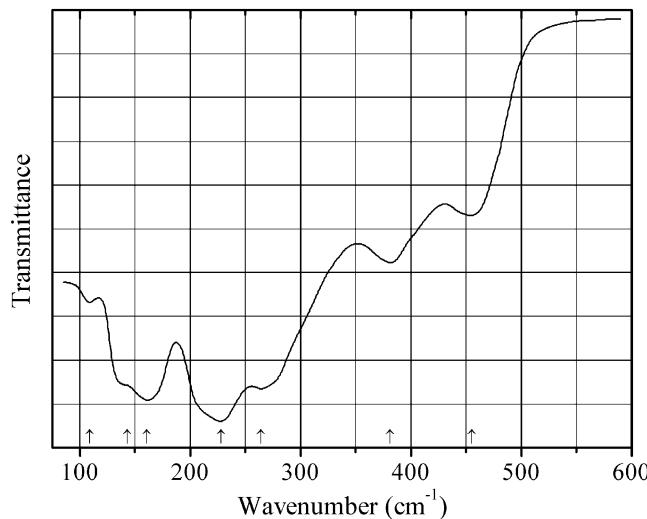
**Origin:** Synthetic.

**Description:** Obtained by boiling an aqueous solution of  $\text{ZnF}_2$ . Orthorhombic, space group  $Pna2_1$ ,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc and Nujol mull. Transmission.

**Source:** Lutz et al. (1993).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3562s, 3401s, 1028s, 898, 792s, 530w, 375s.

**F91 Gananite  $\text{BiF}_3$** 

**Origin:** Synthetic.

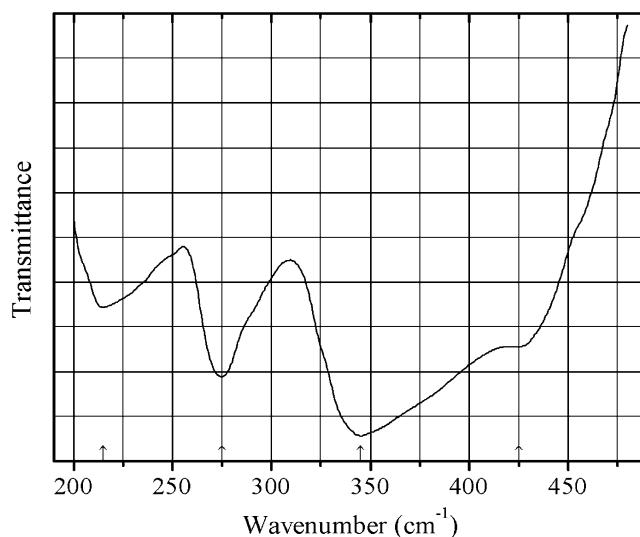
**Description:** Characterized by powder X-ray diffraction data. The crystal structure is solved.

**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull or polyethylene disc.

**Source:** Ignat'eva et al. (2006).

**Wavenumbers (cm⁻¹):** 455w, 381w, 264s, 228s, 161s, 143sh, 109w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**F92 Waimirite-(Yb)  $\text{YbF}_3$** 

**Origin:** Synthetic.

**Description:** Reagent grade commercial product. Orthorhombic.

**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc. Transmission.

**Source:** Taylor et al. (1972).

**Wavenumbers (cm<sup>-1</sup>):** 425, 345s, 275, 215.

### F93 Heklaite

**Origin:** Synthetic.

**Description:** Colorless hexagonal dipyramid. Characterized by powder X-ray diffraction data. Orthorhombic,  $a = 9.3375(5)$ ,  $b = 5.5009(3)$ ,  $c = 9.7912(7)$  Å,  $V = 502.92(4)$  Å<sup>3</sup>,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of powdered mineral.

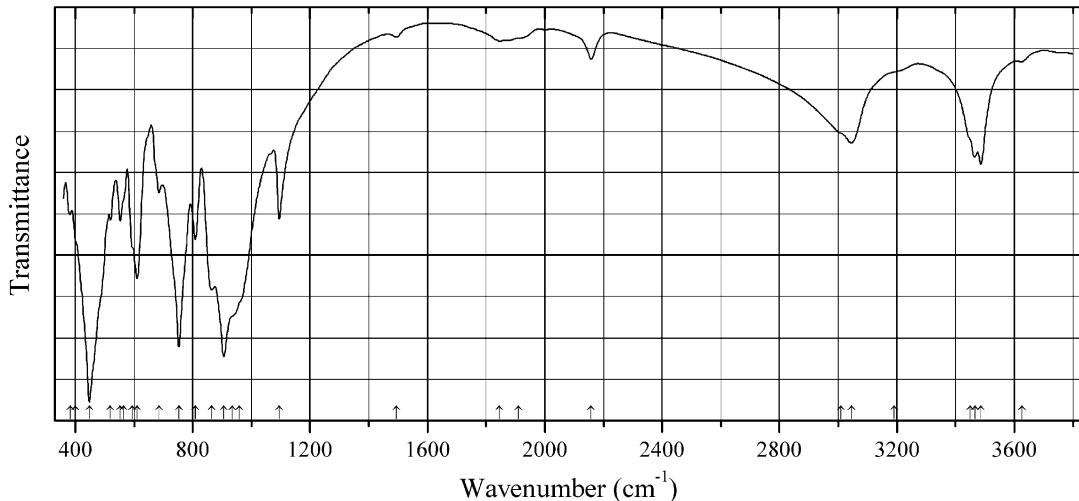
**Source:** RRUFF (2007).

**Wavenumbers (cm<sup>-1</sup>):** 712s, 663w, 479.

**Note:** The wavenumbers were determined by us based on spectral curve analysis.

## 2.7 Silicates

### Sio160 Magnesiochloritoid MgAl<sub>2</sub>O(SiO<sub>4</sub>)(OH)<sub>2</sub>



**Origin:** Allalin glacier, Allalin area, Saas-Almagell, Saas Valley, Zermatt – Saas Fee area, Wallis (Valais), Switzerland (type locality).

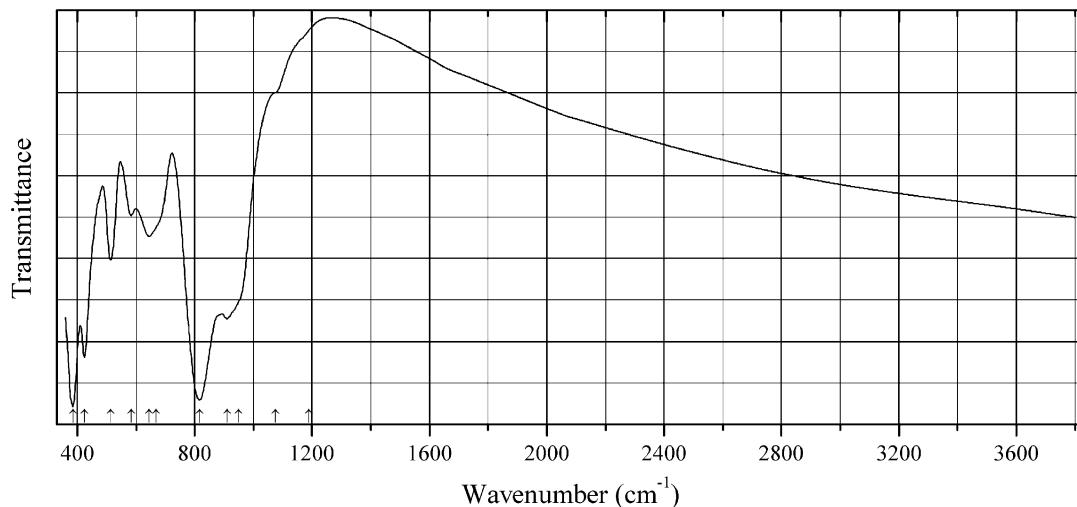
**Description:** Greenish-gray platy grains from the association with chlorite, paragonite, and amphibole. The empirical formula is (electron microprobe):  $(\text{Mg}_{1.22}\text{Fe}^{2+}_{0.77}\text{Mn}_{0.01})(\text{Al}_{3.96}\text{Fe}^{3+}_{0.04})\text{Si}_{2.00}\text{O}_{10}(\text{OH})_4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3627w, 3486, 3467, 3450sh, 3190sh, 3045, 3010sh, 2158, 1910w, 1845, 1495w, 1095, 960sh, 935sh, 906s, 866, 809, 753s, 685, 611, 595sh, 565sh, 553, 520, 448s, 400sh, 383.

**Note:** The spectrum was obtained by N.V. Chukanov.

### Sio161 Morimotoite $\text{Ca}_3(\text{TiFe}^{2+})(\text{SiO}_4)_3$



**Origin:** Odihkincha alkaline massif, Taimyr district, Krasnoyarsk Krai, Siberia, Russia.

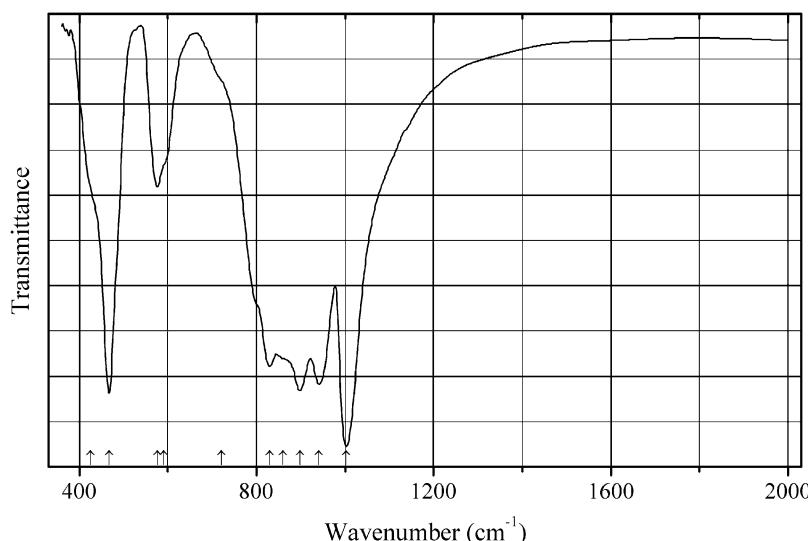
**Description:** Black grains from the association with diopside. Investigated by I.V. Pekov. The empirical formula is (electron microprobe):  $(\text{Ca}_{2.75}\text{Mg}_{0.17}\text{Na}_{0.05}\text{Mn}_{0.03})(\text{Ti}_{0.89}\text{Fe}^{2+}_{0.79}\text{Fe}^{3+}_{0.38}\text{Zr}_{0.02})(\text{Si}_{2.69}\text{Fe}^{3+}_{0.22}\text{Al}_{0.09})\text{O}_{12}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc, Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1190sh, 1075sh, 950sh, 910s, 816s, 670sh, 645, 584, 513, 424s, 385s.

**Note:** The spectrum was obtained by N.V. Chukanov.

## Sio162 Wadalite Ca<sub>6</sub>Al<sub>5</sub>Si<sub>2</sub>O<sub>16</sub>Cl<sub>3</sub>



**Origin:** Bellerberg, near Ettringen, Eifel Mts., Rhineland-Palatinate (Rheinland-Pfalz), Germany.

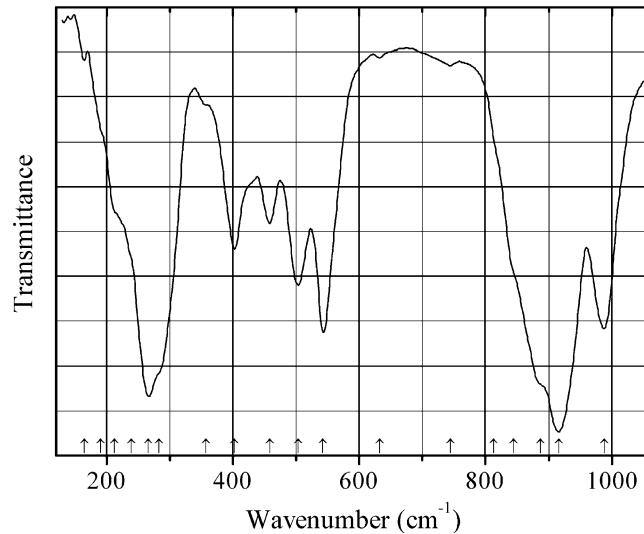
**Description:** Yellow crystals from the association with calcite and gypsum. The empirical formula is (electron microprobe):  $(\text{Ca}_{5.30}\text{Mg}_{0.70})(\text{Al}_{1.62}\text{Fe}_{0.35}\text{Ti}_{0.03})(\text{Si}_{2.04}\text{Al}_{1.96})\text{Cl}_{3.25}\text{O}_r$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 1003s, 941s, 898s, 860sh, 830s, 720sh, 590sh, 576, 467s, 425sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sio163 Lanthanum orthosilicate** La<sub>9.33</sub>(SiO<sub>4</sub>)<sub>6</sub>O<sub>2</sub>



**Origin:** Synthetic.

**Description:** Apatite-type compound.

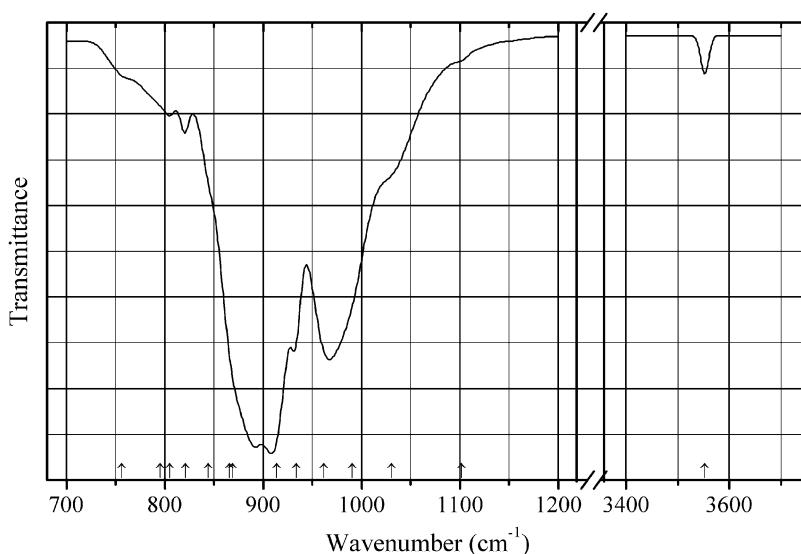
**Kind of sample preparation and/or method of registration of the spectrum:** Absorption. Kind of sample preparation is not indicated.

**Source:** Smirnov et al. (2010).

**Wavenumbers (cm<sup>-1</sup>):** 988s, 916s, 887sh, 844sh, 813sh, 745w, 633w, 543s, 503s, 458, 403, 358sh, 283sh, 266s, 239sh, 213sh, 191sh, 165w.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**Sio164 Fluorche gemite** Ca<sub>7</sub>(SiO<sub>4</sub>)<sub>3</sub>F<sub>2</sub>



**Origin:** Lakargi Mt., Upper Chegem caldera, Kabardino-Balkarian Republic, Northern Caucasus, Russia (type locality).

**Description:** Lens-shaped aggregate. The associated minerals are larnite, edgrewite, wadalite, eltyubyuite, rondorfite, lakargiite, Th-rich kerimasite, as well as their alteration products. Holotype sample. Orthorhombic, space group  $Pbnm$ ,  $a = 5.0620(1)$ ,  $b = 11.3917(2)$ ,  $c = 23.5180(3)$  Å,  $V = 1356.16(4)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 2.91$  g/cm $^3$ . Optically biaxial (−),  $\alpha = 1.610(2)$ ,  $\beta = 1.615(2)$ ,  $\gamma = 1.619(2)$ ,  $2V = 80(8)^\circ$ . The empirical formula is (electron microprobe, OH calculated):  $\text{Ca}_{7.01}\text{Mg}_{0.01}\text{Ti}_{0.01}\text{Si}_{2.98}\text{O}_{12}\text{F}_{1.40}(\text{OH})_{0.60}$ . The experimental powder X-ray diffraction pattern was not obtained.

**Kind of sample preparation and/or method of registration of the spectrum:** Reflection from a polished grain.

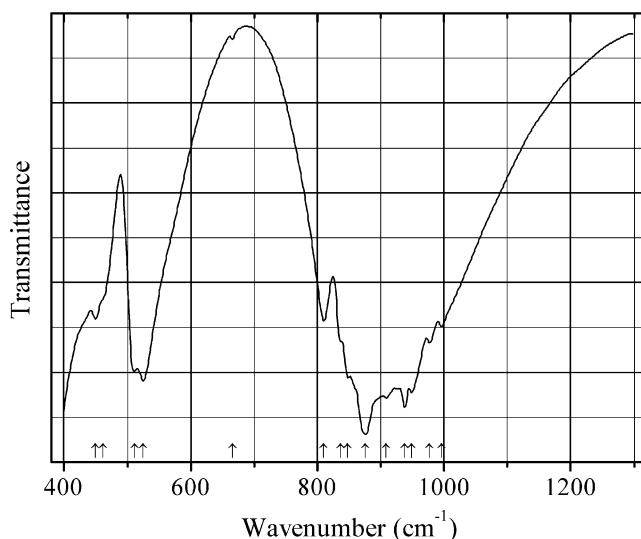
**Source:** Galuskina et al. (2015).

**Wavenumbers (IR, cm $^{-1}$ ):** 3552w, 1102sh, 1031sh, 991sh, 962s, 934, 914s, 889s, 866sh, 844sh, 821w, 805w, 795sh, 756sh.

**Note:** The wavenumbers are indicated only for the maxima of individual bands obtained by Galuskina et al. (2015) as a result of the spectral curve analysis. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 3552, 3548s, 3539, 992s, 843, 817s, 560, 442, 410, 297, 258w.

### Sio165 Hatrurite triclinic polymorph $\text{Ca}_3(\text{SiO}_4)\text{O}$



**Origin:** Synthetic.

**Description:** Prepared by heating a mixture of calcium carbonate and silica gel (with the CaO:SiO<sub>2</sub> molar ratio of 3:1) pressed into a pellet, at 1450 °C. Characterized by powder X-ray diffraction data. Triclinic,  $a = 11.630$ ,  $b = 14.216$ ,  $c = 13.690$  Å,  $\alpha = 105.345^\circ$ ,  $\beta = 94.558^\circ$ ,  $\gamma = 89.845^\circ$ .

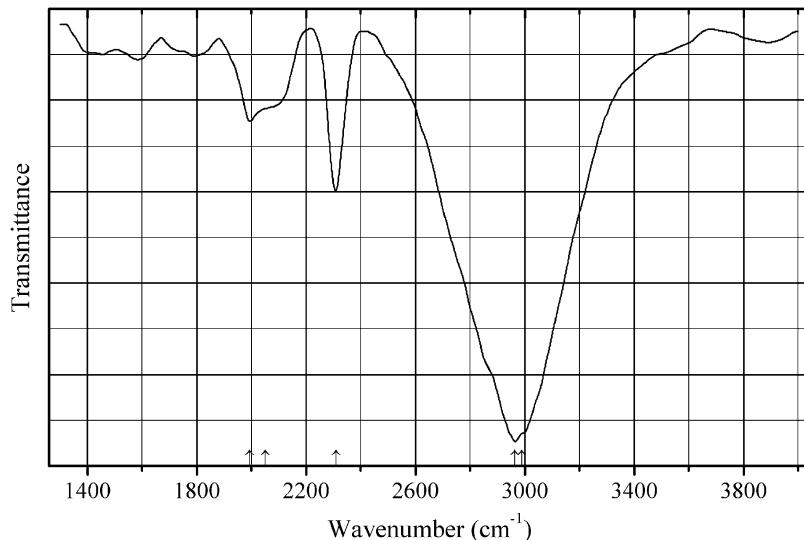
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Del Bosque et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 996, 977, 949, 938s, 909, 875s, 848, 837sh, 810, (666), 525, 511, 462sh, 450.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The band at 666 cm<sup>-1</sup> corresponds to atmospheric CO<sub>2</sub>. In the cited paper, the wavenumber 949 cm<sup>-1</sup> is erroneously indicated as 959 cm<sup>-1</sup>.

### Sio166 Pilawite-(Y) Ca<sub>2</sub>Y<sub>2</sub>Al<sub>4</sub>(SiO<sub>4</sub>)<sub>4</sub>O<sub>2</sub>(OH)<sub>2</sub>



**Origin:** Piława Góra granitic pegmatite, Lower Silesia, Poland (type locality).

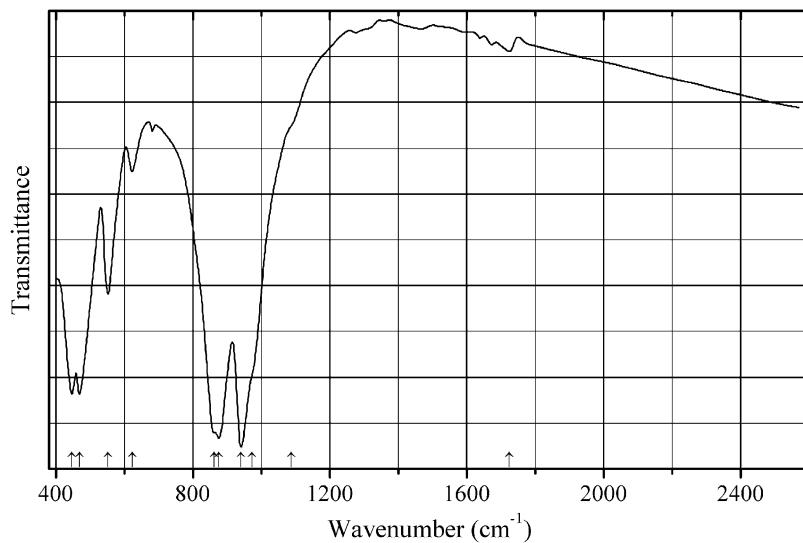
**Description:** White grains from the association with keiviite-(Y), gadolinite-(Y), hingganite-(Y), xenotime-(Y), etc. Holotype sample. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 8.558(3)$  Å,  $b = 7.260(3)$  Å,  $c = 11.182(6)$  Å,  $\beta = 90.61(4)^\circ$ ,  $V = 694.7(4)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 4.007$  g/cm<sup>3</sup>. Optically biaxial (+),  $\alpha = 1.743(5)$ ,  $\beta = 1.754(5)$ ,  $\gamma = 1.779(5)$ ,  $2V = 65(2)^\circ$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 3.044 (100) (022), 2.791 (43) (004), 2.651 (46) (310), 2.583 (54) (-311), 2.485 (62) (-222, 114, 123), 2.408 (45) (-312).

**Kind of sample preparation and/or method of registration of the spectrum:** Absorption. Kind of sample preparation is not indicated.

**Source:** Pieczka et al. (2015).

**Wavenumbers (IR, cm<sup>-1</sup>):** 2990sh, 2965s, 2309, 2050sh, 1995.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The narrow band at 2309 cm<sup>-1</sup> may correspond to CO<sub>2</sub> molecules present in cavities of the heteropolyhedral framework. In the cited paper, a figure of the Raman spectrum is given.

**Sio167 Spessartine Ca-rich** ( $Mn_{1.31}Ca_{1.02}Fe^{2+}_{0.52}Mg_{0.10})(Al_{1.59}Fe^{3+}_{0.46}Ti_{0.06})Si_{2.90}O_{12}$ 

**Origin:** Pit no. 287, Ilmeny Mts., Chelyabinsk region, South Urals, Russia.

**Description:** Brown-red grains from the association with diopside, quartz, and scapolite. Cubic,  $a = 11.736 \text{ \AA}$ . Mössbauer spectroscopy indicates that 46% of iron is trivalent. The strongest lines of the powder X-ray diffraction pattern [ $d, \text{\AA}$  ( $I, \%$ )] are: 2.935 (38), 2.624 (100), 2.396 (26), 1.904 (24), 1.627 (23), 1.569 (33).

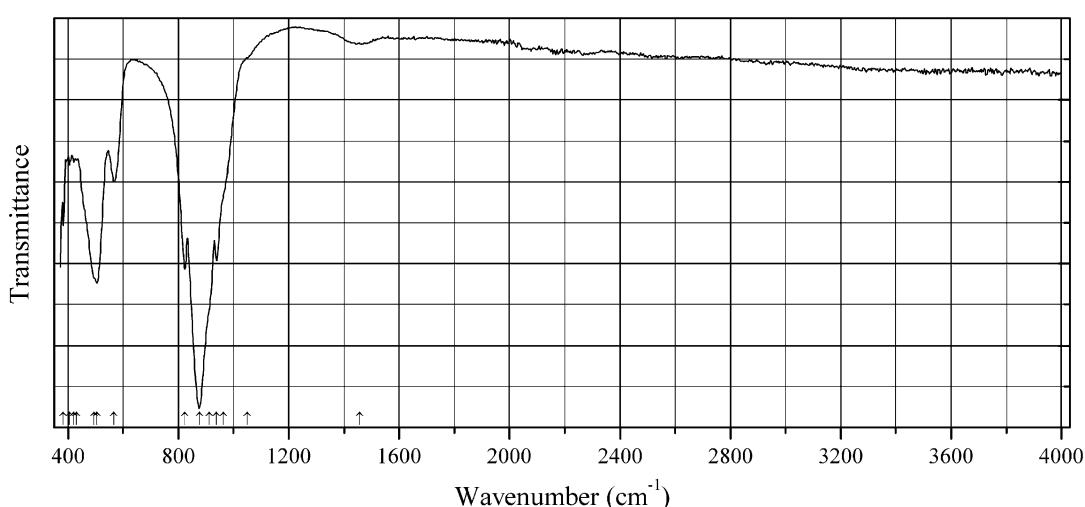
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Korinevsky (2015).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1724w, 1087sh, 972sh, 941s, 876s, 863sh, 623, 553, 469s, 447s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1009, 891s, 834, 623w, 536, 354s, 218, 154.

**Sio168 Kirschsteinite** CaFe<sup>2+</sup>(SiO<sub>4</sub>)

**Origin:** Dolores mine, Pastrana, Mazarrón, Murcia, Spain.

**Description:** Orthorhombic,  $a = 4.8613(3)$ ,  $b = 11.0995(5)$ ,  $c = 6.3989(8)$  Å,  $V = 345.28(4)$  Å<sup>3</sup>.

$D_{\text{meas}} = 2.39(3)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 2.391$  g/cm<sup>3</sup>. The empirical formula is (electron microprobe): (Ca<sub>0.95</sub>Mn<sub>0.02</sub>Mg<sub>0.02</sub>Na<sub>0.01</sub>)(Fe<sup>2+</sup><sub>0.83</sub>Mg<sub>0.16</sub>Fe<sup>3+</sup><sub>0.01</sub>)Si<sub>1.00</sub>O<sub>4</sub>.

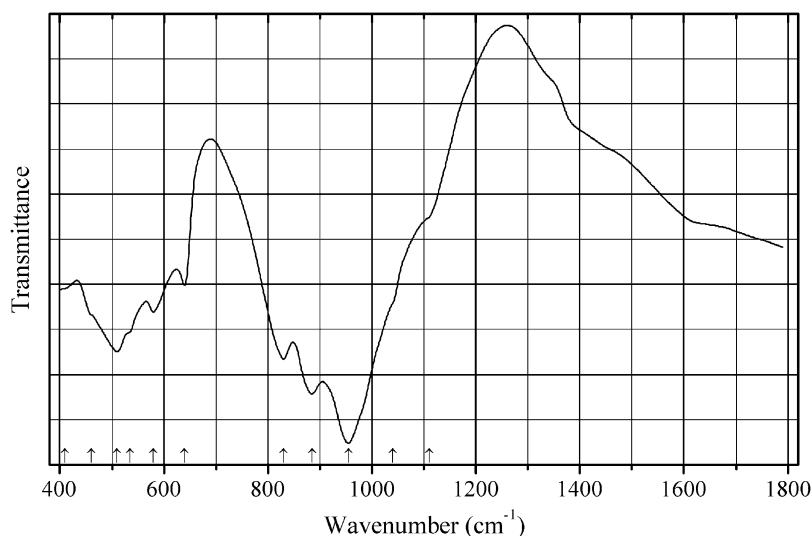
**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of powdered mineral.

**Source:** RRUFF (2007).

**Wavenumbers (cm<sup>-1</sup>):** 1456, 1049, 964sh, 939, 912sh, 876s, 823, 567, 504s, 496sh, 432, 420, 405, 384.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

### Sio169 Laihunite (Fe<sup>3+</sup>,Fe<sup>2+</sup>,□)<sub>2</sub>(SiO<sub>4</sub>)



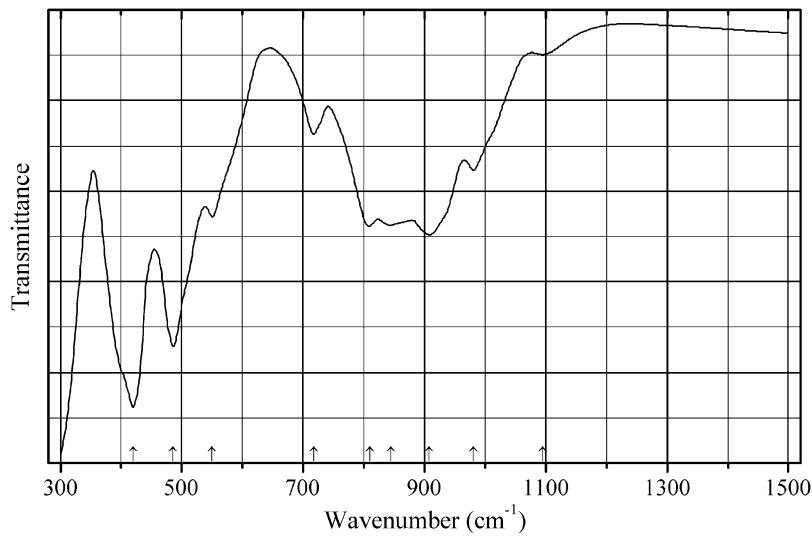
**Origin:** Laihe Fe deposit, Qianshan District, Liaoning Province, China (type locality).

**Description:** Black tabular crystals. Holotype sample. Characterized by Mössbauer spectroscopy and powder X-ray diffraction data. Orthorhombic, space group  $Pb2_1m$ ,  $a = 4.800(5)$ ,  $b = 10.238(5)$ ,  $c = 5.857(5)$  Å.  $D_{\text{meas}} = 3.92$  g/cm<sup>3</sup>. The empirical formula is Fe<sup>3+</sup><sub>1.50</sub>Fe<sup>2+</sup><sub>0.58</sub>Mg<sub>0.03</sub>Si<sub>0.96</sub>O<sub>4</sub>.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission.

**Source:** Laihunite Resh Group (1976).

**Wavenumbers (cm<sup>-1</sup>):** 1110sh, 1040sh, 955s, 885s, 830s, 640, 580, 535sh, 510s, 460sh, 410sh.

**Sio170 Oxybritholite thorium analogue**  $\text{Th}_2\text{Ca}_3(\text{SiO}_4)_3\text{O}$ 

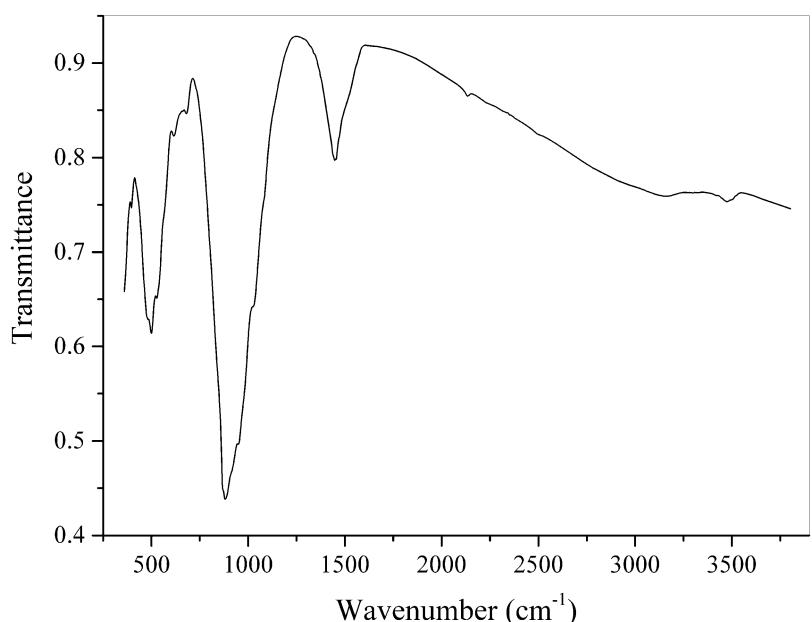
**Origin:** Synthetic.

**Description:** Synthesized by solid-state reaction between thorium nitrate, calcium nitrate, and silicon oxide at 1553 K for 30 h with intermediate grindings every 2 h. The crystal structure is solved. Hexagonal, space group  $P6_3/m$ ,  $a = 9.50172(9)$ ,  $c = 6.98302(8)$  Å,  $V = 545.98(1)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 4.966$  g/cm<sup>3</sup>. The crystal-chemical formula is  $(\text{Ca}_{3.84}\text{Th}_{0.16})(\text{Th}_{3.21}\text{Ca}_{2.79})(\text{SiO}_4)_6\text{O}_2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of a powdered sample.

**Source:** Bulanov et al. (2015).

**Wavenumbers (cm<sup>-1</sup>):** 1095w, 981, 908s, 845, 810, 718, 550, 485s, 420s.

**Sio171 Ulfanderssonite-(Ce)**  $(\text{Ce}_{15}\text{Ca})\text{Mg}_2(\text{SiO}_4)_{10}(\text{SiO}_3\text{OH})(\text{OH},\text{F})_5\text{Cl}_3$ 

**Origin:** Malmkärra Mine, Norberg, Västmanland, Sweden (type locality).

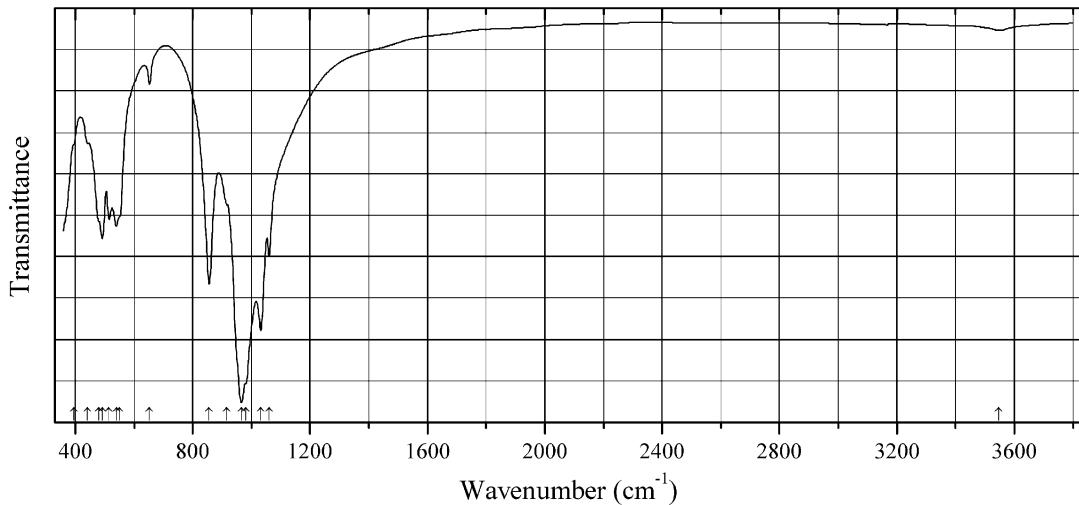
**Description:** Grey grains from the association with cerite-(Ce) and bastnäsite-(Ce). Confirmed by semiquantitative electron microprobe analyses.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 475w, 3160w, 2135w, (1448), 1025, 950, 915sh, 881s, (875sh), 682w, 616w, 565sh, 528, 500, 485sh, 395w.

**Note:** The spectrum was obtained by N.V. Chukanov. The bands at 1448 and 857 cm<sup>-1</sup> correspond to admixed bastnäsite-(Ce).

#### Sid47 Cuspidine Ca<sub>8</sub>(Si<sub>2</sub>O<sub>7</sub>)<sub>2</sub>F<sub>4</sub>



**Origin:** Bellerberg, near Ettringen, Eifel Mts., Rhineland-Palatinate (Rheinland-Pfalz), Germany.

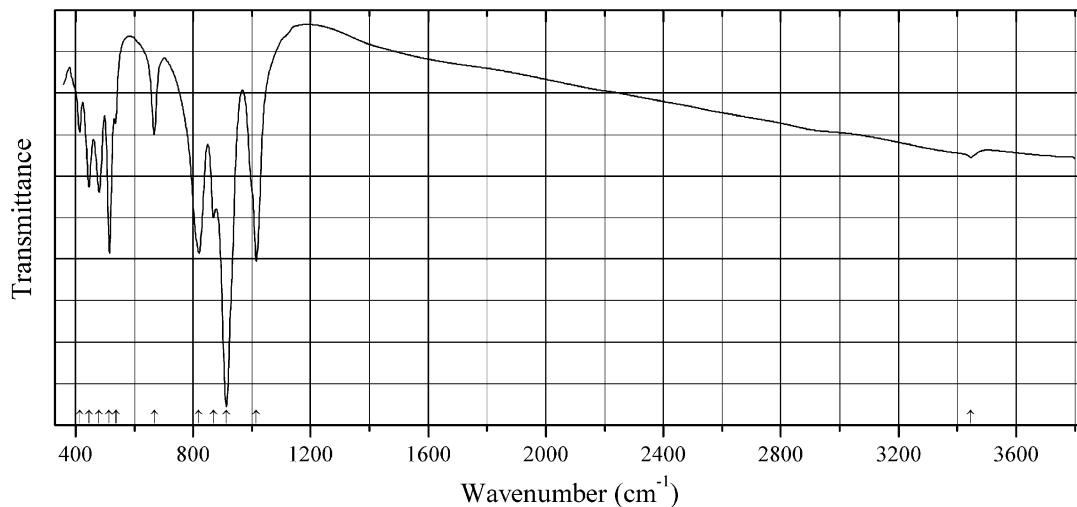
**Description:** Colorless crystals from the association with dorrite, clinopyroxene, spinel, and gypsum. Confirmed by the IR spectrum.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3547w, 1061, 1032s, 980sh, 966s, 915sh, 856s, 653, 550sh, 540, 515, 491, 480sh, 442, 395sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

## **Sid48 Nasonite** $\text{Ca}_4\text{Pb}_6(\text{Si}_2\text{O}_7)_3\text{Cl}_2$



**Origin:** Långban deposit, Bergslagen ore region, Filipstad district, Värmland, Sweden.

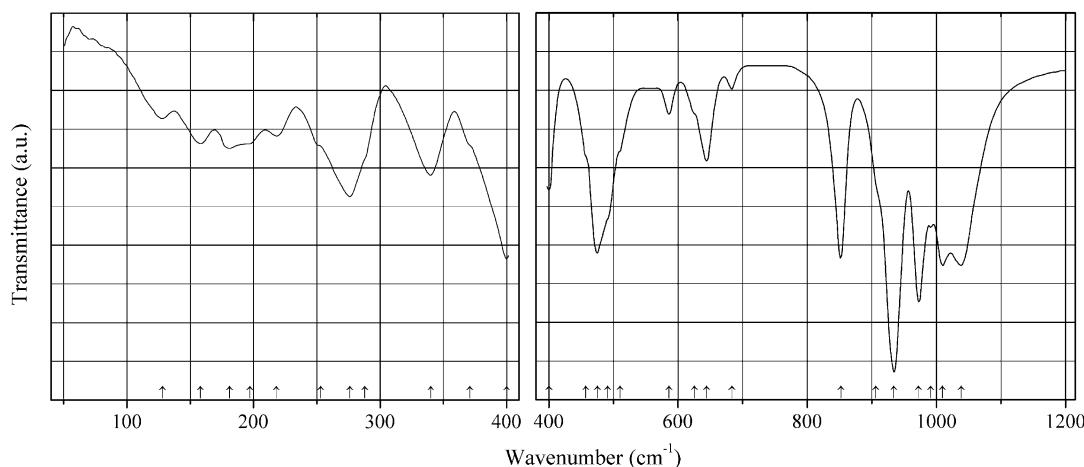
**Description:** Lemon yellow grains from the association with barysilite and jacobsite. The empirical formula is (electron microprobe):  $(\text{Pb}_{5.78}\text{Ca}_{0.22})(\text{Ca}_{3.98}\text{Mn}_x)\text{Si}_{6.00}\text{O}_{21}[\text{Cl}_{1.75}(\text{OH})_{0.25}]$  ( $x \ll 1$ ).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3446w, 1015s, 913s, 869, 820s, 668, 537, 515s, 481, 446, 415.

**Note:** The spectrum was obtained by N.V. Chukanov.

## Sid49 Åkermanite Ca<sub>2</sub>Mg(Si<sub>2</sub>O<sub>7</sub>)



**Origin:** Synthetic.

**Description:** Single crystal grown by Czochralski method. Characterized by X-ray diffraction data. Tetragonal, space group  $P-42_1m$ ,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Absorption. Kind of sample preparation is not indicated.

Source: Hanuza et al. (2012).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1038s, 1009s, 991, 972s, 934s, 906sh, 852s, 683w, 644w, 625sh, 586w, 510sh, 491sh, 475s, 457sh, 400, 371sh, 340w, 288sh, 276w, 253sh, 218w, 197, 181, 158, 128.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 992w, 941w, 910s, 666, 605w, 450w, 318w, 227w, 211w, 107w.

### Sid50 Barysilite $\text{Pb}_8\text{Mn}(\text{Si}_2\text{O}_7)_3$

**Origin:** Långban deposit, Bergslagen ore region, Filipstad district, Värmland, Sweden.

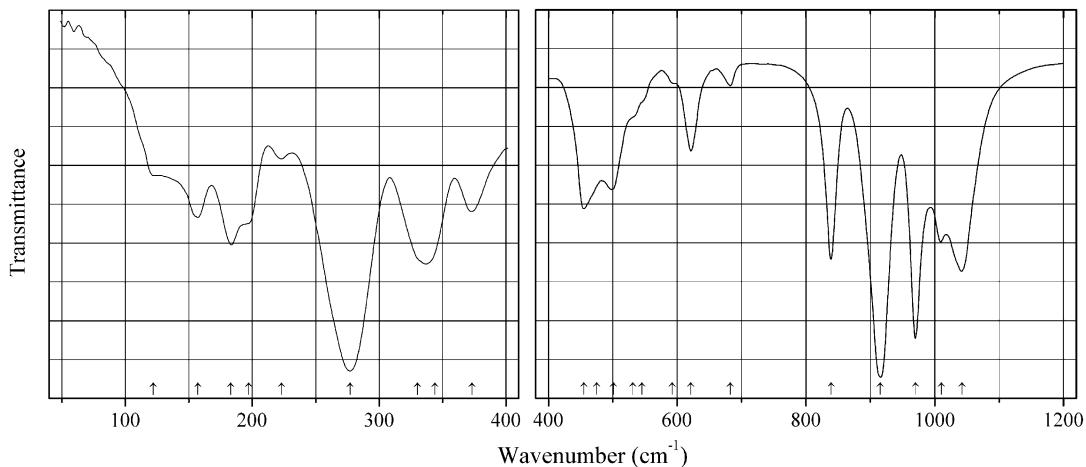
**Description:** The crystal structure is solved. Trigonal, space group  $R\bar{3}c$ ,  $a = 9.821(5)$ ,  $c = 38.38(6)$  Å,  $Z = 6$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Lajzérowicz (1966).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 970sh, 934s, 914s, 892s, 872sh, 832s, (780), 702, 553, 528, 479, 464, 446–444, 423–418, 393, 258.

### Sid51 Hardystonite $\text{Ca}_2\text{Zn}(\text{Si}_2\text{O}_7)$



**Origin:** Synthetic.

**Description:** Single crystal grown by Czochralski method. Characterized by powder X-ray diffraction data. Characterized by X-ray diffraction data. Tetragonal, space group  $P-42_1m$ ,  $Z = 2$ .

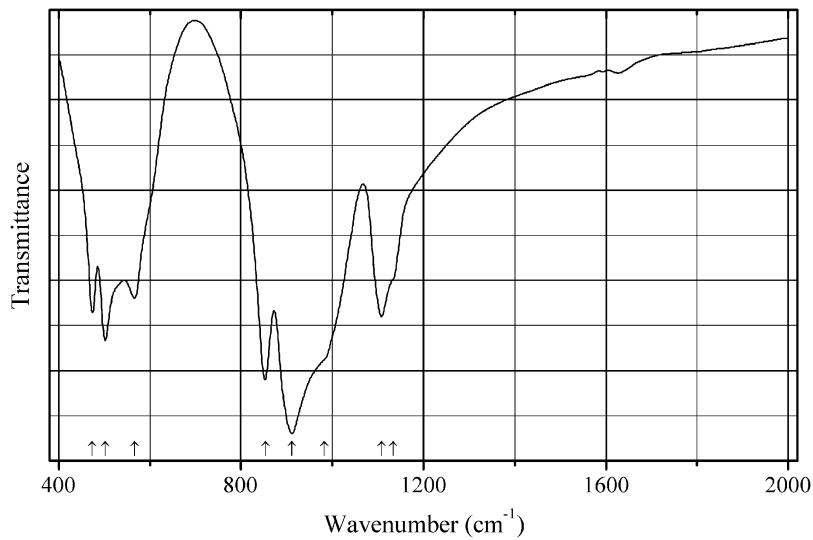
**Kind of sample preparation and/or method of registration of the spectrum:** Absorption. Kind of sample preparation is not indicated.

**Source:** Hanuza et al. (2012).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1042s, 1010, 970s, 915s, 839s, 682w, 621, 592sh, 545sh, 531sh, 501, 475sh, 455, 373w, 344w, 330w, 277, 223w, 197w, 183w, 157w, 122w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1019w, 1004w, 994w, 939w, 908s, 664s, 615w, 551w, 480w, 445w, 315w, 280w, 204w, 147w, 100w.

**Sid52 Keiviite-(Yb)  $\beta\text{-Yb}_2\text{Si}_2\text{O}_7$** 

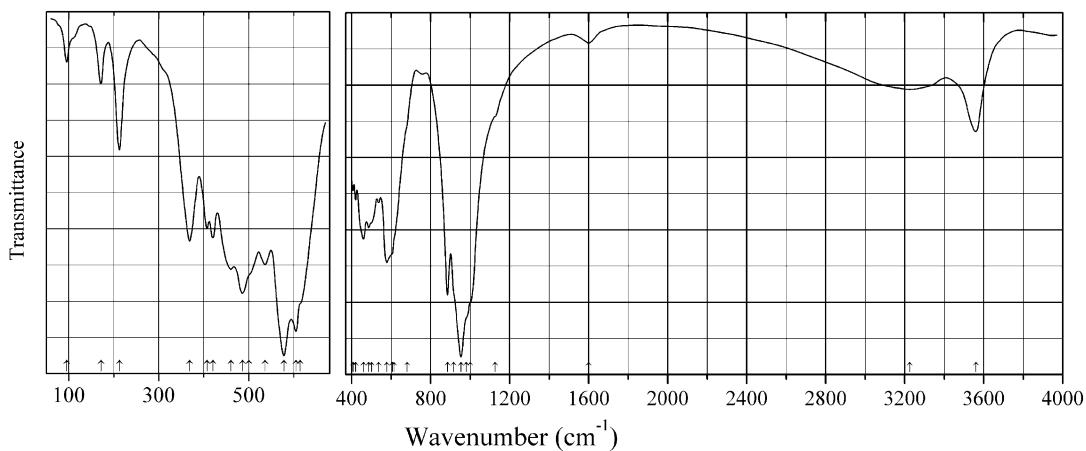
**Origin:** Synthetic.

**Description:** Synthesized from  $\text{Yb}(\text{NO}_3)_3$  and  $\text{Si}(\text{OC}_2\text{H}_5)_4$  by a sol-gel method with subsequent calcination at 1200 °C for 2 h. Characterized by powder X-ray diffraction data. Monoclinic, space group  $C2/m$ ,  $a = 6.80053$ ,  $b = 8.87508$ ,  $c = 4.70740 \text{ \AA}$ ,  $\beta = 101.984$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Zhao et al. (2013a).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1133sh, 1108, 983sh, 912s, 853s, 567, 502, 474.

**Sid53 Lawsonite  $\text{CaAl}_2(\text{Si}_2\text{O}_7)(\text{OH})_2 \cdot \text{H}_2\text{O}$** 

**Origin:** Tiburon Peninsula, California, USA.

**Description:** Equant to tabular crystals. Characterized by electron microprobe analyses and powder X-ray diffraction data. Orthorhombic, space group  $Ccmm$ ,  $a = 8.795 \text{ \AA}$ ,  $b = 5.847 \text{ \AA}$ ,  $c = 13.142 \text{ \AA}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Powder dispersed in KBr disc and in polyethylene substrate. Absorption.

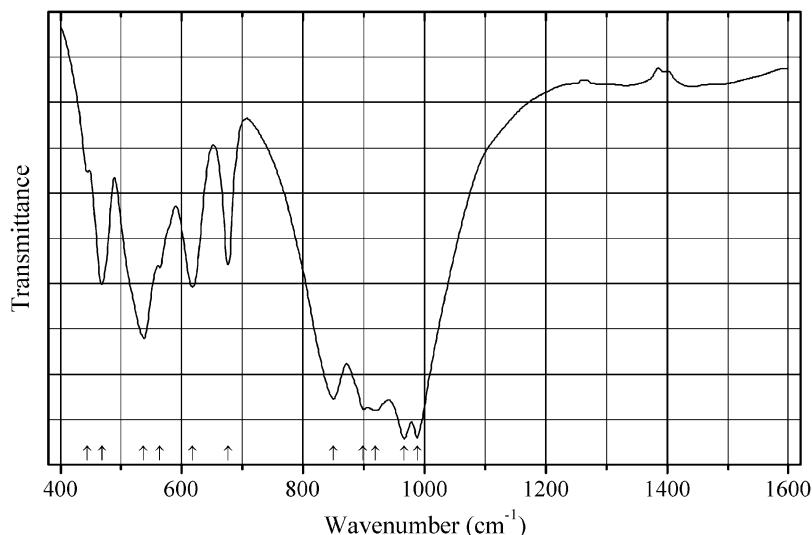
**Source:** Le Cléac'h and Gillet (1990).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3560, 3225, 1600w, 1125sh, 1000sh, 980sh, 953s, 915sh, 885s, 680sh, 614sh, 605sh, 578, 536, 500sh, 486s, 460, 420, 407 (in KBr); 614sh, 605sh, 578s, 536, 500sh, 486, 460, 420, 407, 368, 212, 171w, 95w (in polyethylene).

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 3540, 1578, 1047, 955sh, 935s, 915sh, 810, 694s, 455w, 400w, 372w, 328, 280s.

#### Sid54 Scottyite $\text{BaCu}_2\text{Si}_2\text{O}_7$



**Origin:** Synthetic.

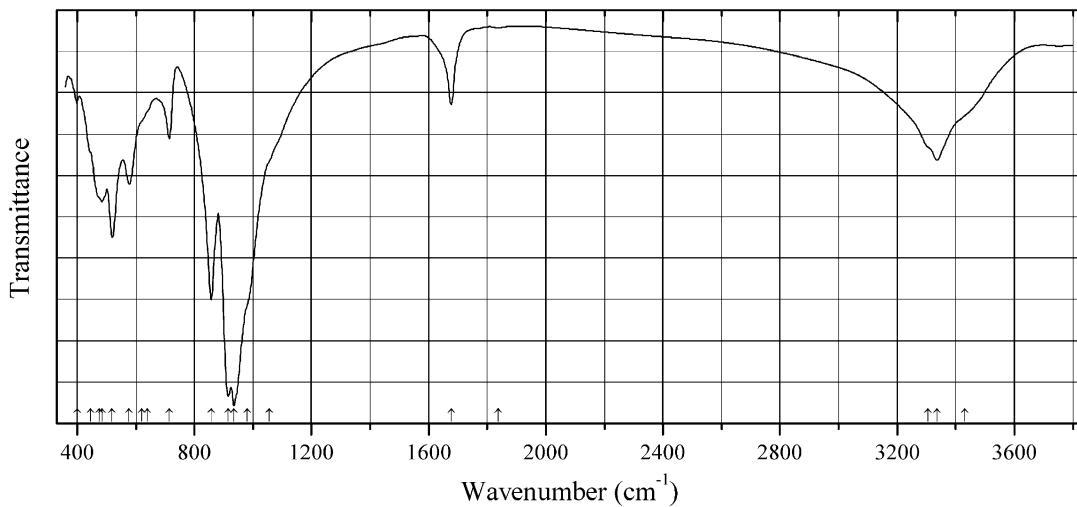
**Description:** Dark blue polycrystalline sample synthesized by a mild hydrothermal method from  $\text{BaCl}_2 \cdot 4\text{H}_2\text{O}$ ,  $\text{Na}_2\text{SiO}_3 \cdot 9\text{H}_2\text{O}$ , and  $\text{CuO}$ . Characterized by energy dispersive spectroscopy and powder X-ray diffraction data. Orthorhombic, space group  $Pnma$ ,  $a = 6.86317(15)$ ,  $b = 13.1773(3)$ ,  $c = 6.86317(15) \text{ \AA}$ ,  $V = 623.68(2) \text{ \AA}^3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Chen et al. (2014b).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 988s, 967s, 919s, 899s, 850s, 676, 617, 564, 537, 468, 444w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Sid57 Junitoite**  $\text{CaZn}_2\text{Si}_2\text{O}_7 \cdot \text{H}_2\text{O}$ 

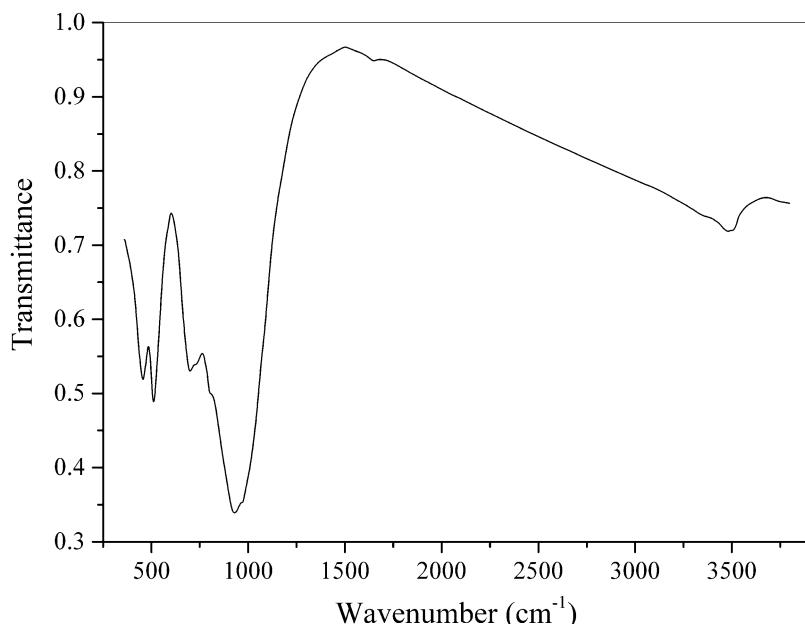
**Origin:** Christmas Mine, Christmas area, Banner District, Dripping Spring Mts, Gila Co., Arizona, USA (type locality).

**Description:** Aggregate of colorless platelets. The empirical formula is (electron microprobe):  $\text{Ca}_{1.05}\text{Zn}_{2.07}\text{Si}_{1.85}\text{Al}_{0.02}\text{Fe}_{0.01}\text{O}_7 \cdot \text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3430sh, 3336, 3305sh, 1838w, 1677, 1055sh, 980sh, 935s, 915s, 857s, 715, 640sh, 620sh, 578, 520, 484, 475sh, 445sh, 399w.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sid58 Rowlandite-like mineral**  $\text{REE}_4\text{FeSi}_4(\text{O},\text{F},\text{OH})_{16} \cdot n\text{H}_2\text{O}$ 

**Origin:** Heftetjern pegmatite, Tørdal, Telemark, Norway.

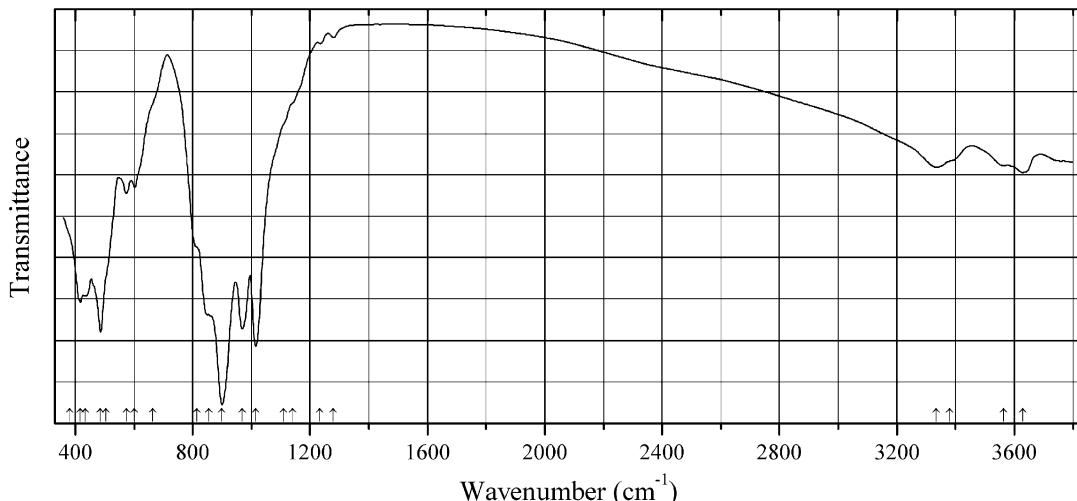
**Description:** Anhedral grains from the association with fluorite. Amorphous, metamict. The empirical formula is (electron microprobe):  $\text{Y}_{2.5}\text{Ln}_{1.6}\text{Fe}_{0.8}\text{Si}_{4.05}\text{O}_{14}(\text{F},\text{OH})_2 \cdot n\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3500sh, 3483, 3380sh, 1649w, 965sh, 931s, 807sh, 765sh, 699, 511, 457.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Siod66 Cyprine**  $\text{Ca}_{19}\text{Cu}^{2+}(\text{Al}_{10}\text{Mg}_2)\text{Si}_{18}\text{O}_{68}(\text{OH})_{10}$



**Origin:** Wessels mine, near Hotazel, Kalahari Manganese Field, North Cape province, South Africa (type locality).

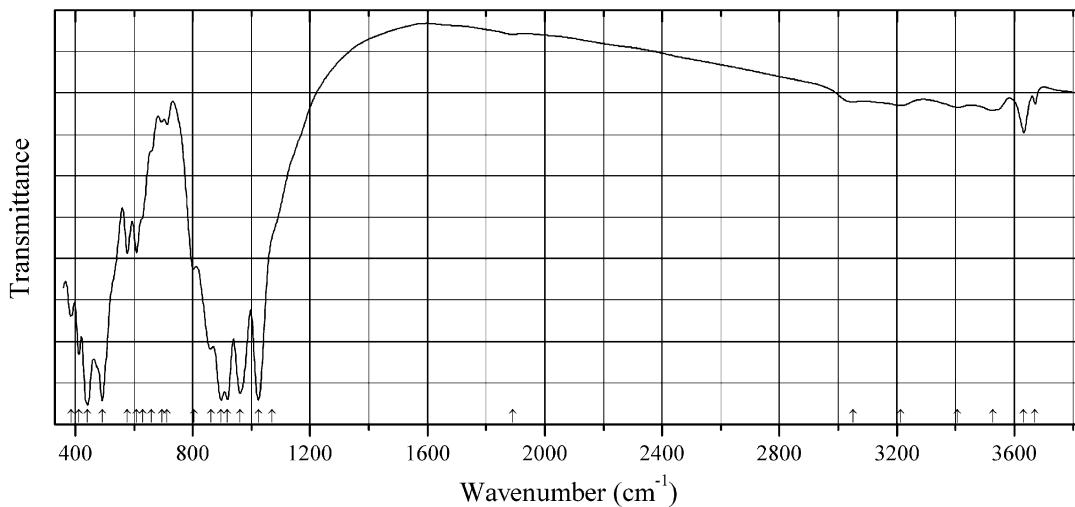
**Description:** Dark red prismatic crystals from the association with calcite, apatite, andradite, henrictierite, and rhodochrosite. Holotype sample. The crystal structure is solved. Tetragonal, space group  $P4/n$ ,  $a = 15.569(1)$ ,  $c = 11.804(1)$  Å,  $V = 2861.6(2)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 2.65$  g/cm<sup>3</sup>. Optically uniaxial (-),  $\omega = 1.744(2)$ ,  $\epsilon = 1.732(2)$ . The empirical formula is (electron microprobe):  $\text{Ca}_{19}(\text{Cu}_{0.91}\text{Mg}_{0.09})_{\Sigma 1.00}(\text{Al}_{8.38}\text{Mg}_{1.64}\text{Mn}^{3+}_{1.87}\text{Fe}^{3+}_{0.29}\text{Cr}_{0.10})_{\Sigma 12.28}\text{Si}_{17.86}\text{O}_{67.86}(\text{OH}_{9.28}\text{O}_{0.72})$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å (I, %) ( $hkl$ )] are: 5.89 (12) (002), 2.950 (47) (004), 2.752 (100) (432), 2.594 (76) (522), 2.459 (35) (620), 1.622 (28) (672).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3630, 3563, 3380sh, 3335, 1280w, 1234w, 1140sh, 1110sh, 1015s, 969s, 900s, 855sh, 815sh, 665sh, 602, 574, 505sh, 486s, 434, 418, (380sh).

**Note:** The weak bands at 1280, 1234, 1140, and 1110 cm<sup>-1</sup> correspond to stretching vibrations of admixed borate groups.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Siod67 Alumovesuvianite**  $\text{Ca}_{19}\text{Al}(\text{Al}_{10}\text{Mg}_2)\text{Si}_{18}\text{O}_{69}(\text{OH})_9$ 

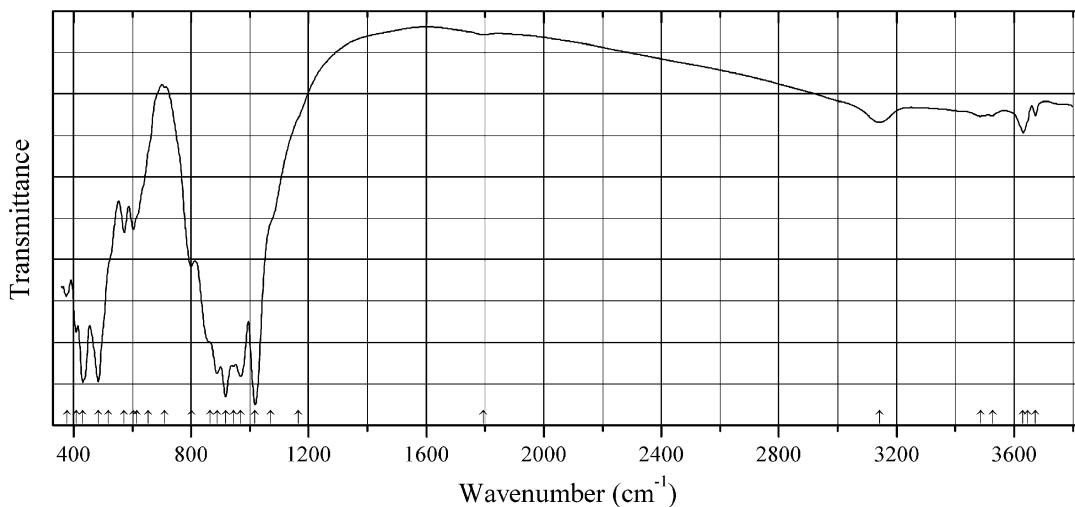
**Origin:** Jeffrey mine, Asbestos, Estrie Region, Québec, Canada (type locality).

**Description:** Pink prismatic tetragonal crystals from the association with diopside and prehnite. Holotype sample. Characterized by powder MAS NMR data. The crystal structure is solved. Tetragonal, space group  $P4/n$ , unit-cell parameters refined from the powder data are  $a = 15.5603(5)$  Å,  $c = 11.8467(4)$  Å,  $V = 2868.3(4)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{meas}} = 3.31(1)$  g/cm $^3$ ,  $D_{\text{calc}} = 3.36$  g/cm $^3$ . Optically uniaxial (−),  $\omega = 1.725(2)$ ,  $\epsilon = 1.722(2)$ . The empirical formula is  $\text{Ca}_{19.00}(\text{Al}_{0.92}\text{Fe}^{3+}_{0.08})\Sigma 1.00(\text{Al}_{9.83}\text{Mg}_{1.80}\text{Mn}^{3+}_{0.25})\Sigma 11.88\text{Si}_{17.98}\text{O}_{69.16}(\text{OH})_{8.44}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 2.96 (22) (004), 2.761 (100) (432), 2.612 (61) (224), 2.593 (25) (600), 1.7658 (20) (831), 1.6672 (20) (734), 1.6247 (21) (912), 1.3443 (22) (880).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm $^{-1}$ ):** 3671w, 3632, 3527, 3407, 3212, 3051, 1890w, 1070sh, 1024s, 962s, 919s, 897s, 863, 804, 713w, 695w, 660sh, 630sh, 609, 577, 491s, 442s, 412, 386.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Siod68 “Ferrovesuvianite”**  $\text{Ca}_{19}\text{Fe}^{2+}(\text{Al,Mg})_{12}\text{Si}_{18}\text{O}_{69}(\text{OH})_9$ 

**Origin:** Valle d'Aosta (Aosta valley), Italy.

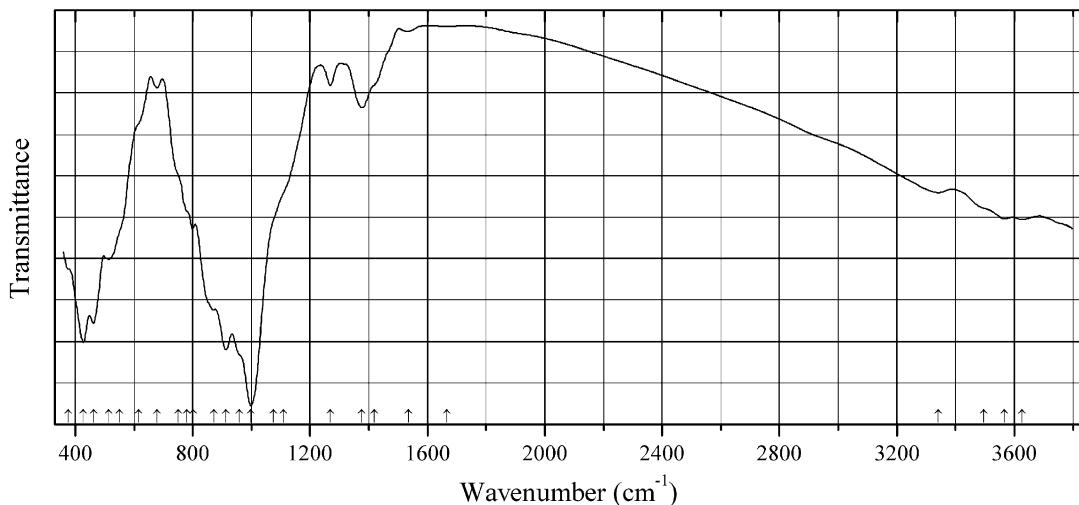
**Description:** Dark brownish-green crystals. The empirical formula is (electron microprobe):  $\text{Ca}_{19.0}(\text{Al}_{9.3}\text{Mg}_{1.9}\text{Fe}_{1.2}\text{Ti}_{0.4}\text{Mn}_{0.1}\text{Cr}_{0.1})\text{Si}_{18}(\text{O},\text{OH})_{78}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3673w, 3645sh, 3630, 3527w, 3487w, 3143, 1795w, 1165sh, 1070sh, 1018s, 969s, 944, 917s, 888s, 865sh, 802, 711w, 655, 615sh, 603, 573, 520sh, 484s, 432s, 409, 379.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Siod69 Wiluite**  $\text{Ca}_{19}(\text{Al,Mg})_{13}(\text{B},\square,\text{Al})_5(\text{SiO}_4)_{10}(\text{Si}_2\text{O}_7)_4(\text{O},\text{OH})_{10}$



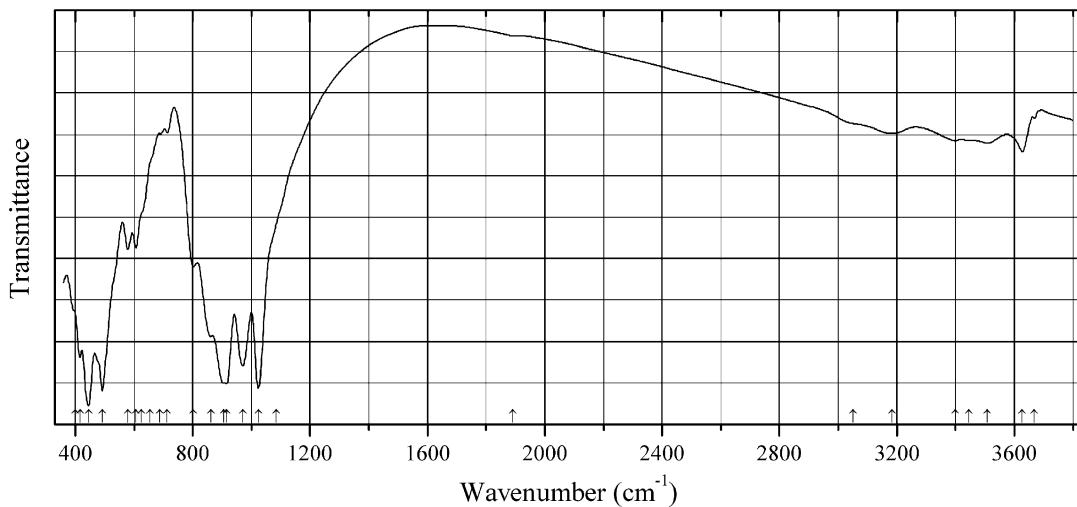
**Origin:** Siki-Yadunskiy fault, Siki River basin, Evenki Autonomous Area, Siberia, Russia.

**Description:** Greenish-gray short-prismatic crystals from the association with grossular. The empirical formula is (electron microprobe):  $(\text{Ca}_{18.78}\text{Na}_{0.17})(\text{Al}_{5.77}\text{Mg}_{5.16}\text{Fe}_{1.37}\text{Ti}_{0.58}\text{Mn}_{0.06}\text{Cr}_{0.06})(\text{B}_x\text{Al}_{1.03}\square_y)\text{Si}_{18}\text{O}_{68}(\text{O},\text{OH})_{10}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3626w, 3566, 3495sh, 3340, 1667w, 1535w, 1420sh, 1376, 1269, 1110sh, 1075sh, 998s, 960sh, 913s, 871, 801, 780sh, 750sh, 679w, 615sh, 550sh, 514, 463, 427s, 377sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Siod70 Magnesiovesuvianite**  $\text{Ca}_{19}\text{Mg}(\text{Al}_{10}\text{Mg}_2)\text{Si}_{18}\text{O}_{68}(\text{OH})_{10}$ 

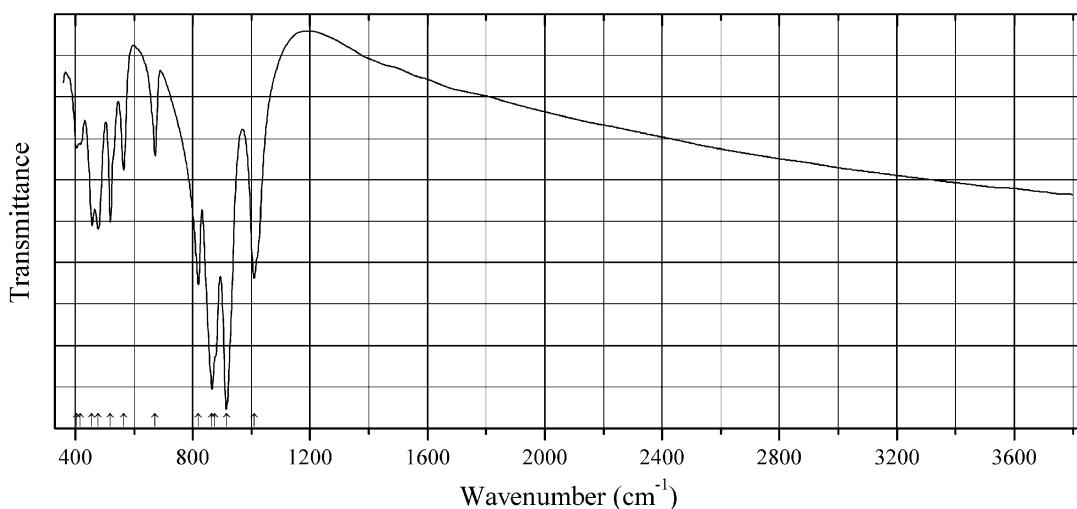
**Origin:** Tuydo combe, near Lojane, Republic of Macedonia (type locality).

**Description:** Light pink acicular tetragonal crystals from the association with calcite, garnet of the grossular-andradite series, and clinochlore. Holotype sample. The crystal structure is solved. Tetragonal, space group  $P4/h$ ,  $a = 15.5026(3)$ ,  $c = 11.7858(5)$  Å,  $V = 2832.4(2)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{meas}} = 3.30(3)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 3.35$  g/cm<sup>3</sup>. Optically uniaxial (-),  $\omega = 1.725(2)$ ,  $\epsilon = 1.721(2)$ . The empirical formula is (electron microprobe):  $(\text{Ca}_{18.99}\text{Na}_{0.01})\Sigma 19.00(\text{Mg}_{0.60}\text{Al}_{0.40})\Sigma 1.00(\text{Al}_{11.05}\text{Mg}_{0.70}\text{Mn}_{0.07}\text{Fe}_{0.02})\Sigma 11.84\text{Si}_{17.84}\text{O}_{68.72}(\text{OH})_9$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 10.96 (23) (110), 3.46 (22) (240), 3.038 (33) (510), 2.740 (100) (432), 2.583 (21) (522), 2.365 (94) (620), 2.192 (19) (710), 1.6165 (25) (672).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3668w, 3627, 3508, (3445), 3398, 3183, 3050sh, 1890w, (1085sh), 1024s, 971s, 915s, 905s, 862, 803, 713w, 689w, 655sh, 625sh, 607, 579, 491s, 445s, 416, 400sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Siod71 Ganolomite**  $\text{Pb}_9\text{Ca}_6(\text{Si}_2\text{O}_7)_4(\text{SiO}_4)\text{O}$ 

**Origin:** Långban deposit, Bergslagen ore region, Filipstad district, Värmland, Sweden (type locality).

**Description:** Colorless anhedral grains from the association with native lead, baryte, calcite, and pyrochroite.

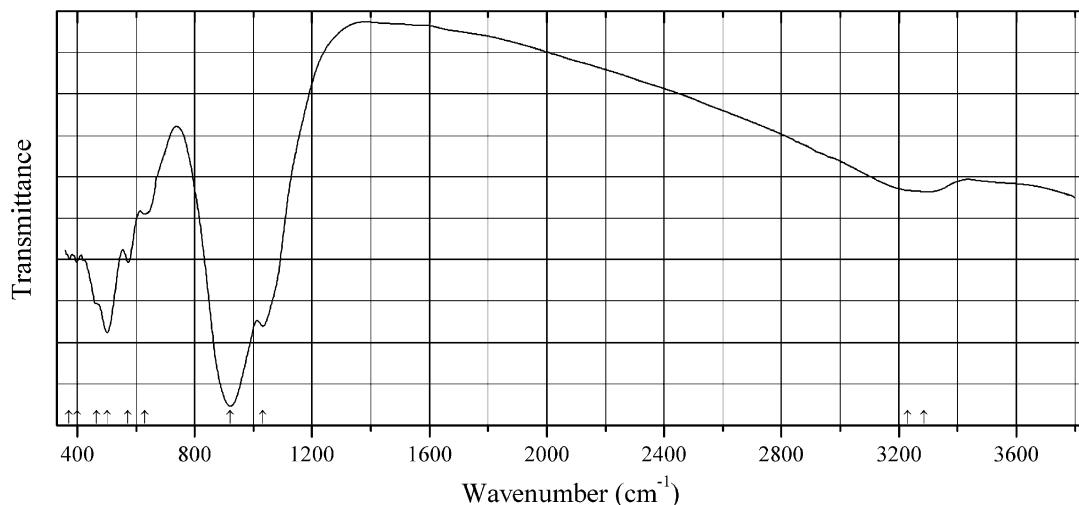
The empirical formula is (electron microprobe):  $(\text{Pb}_{0.58}\text{Ca}_{0.42})\text{Ca}_{5.00}(\text{Mn}_{0.68}\text{Ca}_{0.32})(\text{Si}_2\text{O}_7)_4(\text{SiO}_4)\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1009, 915s, 875sh, 866s, 819, 672, 565, 520, 478, 457, 416, 405.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Siod72 Uedaite-(Ce)**  $Mn^{2+}CeAl_2Fe^{2+}(Si_2O_7)(SiO_4)O(OH)$



**Origin:** Heftetjern amazonite pegmatite, Tørdal, Telemark, Norway.

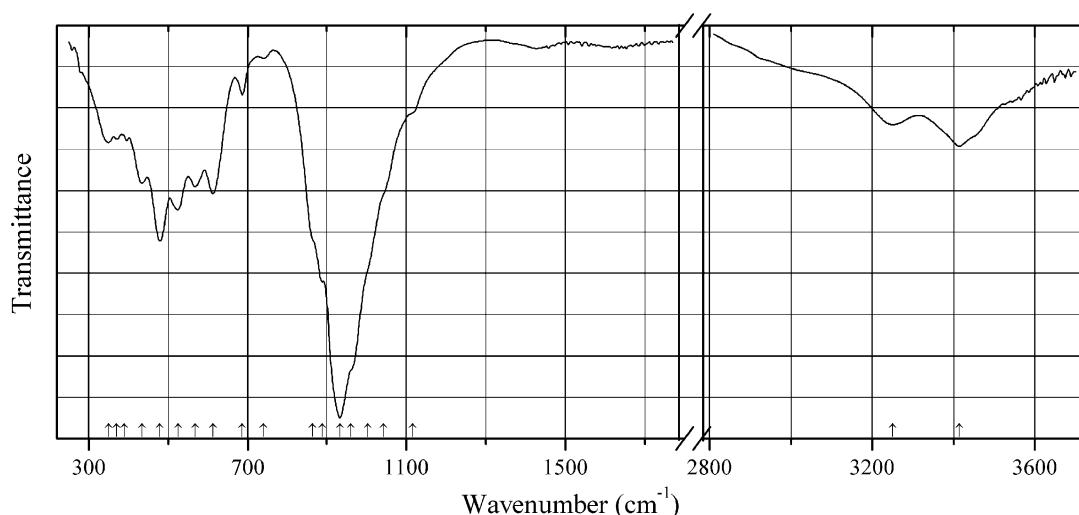
**Description:** Black zone in an allanite-(Ce) crystal. The empirical formula is (electron microprobe):  $(\text{Ce}_{0.59}\text{La}_{0.27}\text{Nd}_{0.12})(\text{Mn}_{0.61}\text{Ca}_{0.39})(\text{Al}_{1.54}\text{Fe}_{1.35}\text{Ti}_{0.04}\text{Mg}_{0.04}\text{Mn}_{0.04})(\text{Si}_{2.94}\text{Al}_{0.06})(\text{O},\text{OH})_{13}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3285, 3230sh, 1033s, 921s, 630, 573, 502s, 465sh, 400, 372.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Siod73 Okhotskite**  $\text{Ca}_2(\text{Mn,Mg})(\text{Mn}^{3+},\text{Al,Fe}^{3+})_2(\text{Si}_2\text{O}_7)(\text{SiO}_4)(\text{OH})_2 \cdot \text{H}_2\text{O}$



**Origin:** South Minusa Intermontane Trough, Siberia, Russia.

**Description:** Main component of the okhotskite-braunite ore. Characterized by powder X-ray diffraction data and electron microprobe analyses. Contains Al-enriched zones corresponding to pumpellyite-(Mn<sup>2+</sup>).

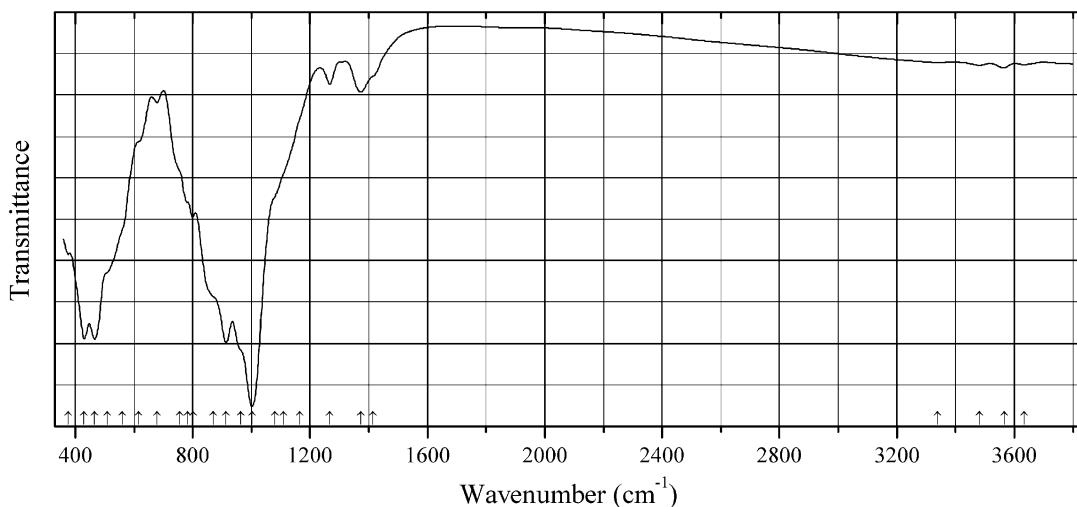
**Kind of sample preparation and/or method of registration of the spectrum:** Absorption. Kind of sample preparation is not indicated.

**Source:** Kassandrov and Mazurov (2009).

**Wavenumbers (cm<sup>-1</sup>):** 3414, 3250, 1115sh, 1042sh, 1002sh, 960sh, 933s, 888s, 864sh, 741, 687, 613, 568, 525, 480s, 435, 390, 371, 350.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**Siod74 Wiluite** Ca<sub>19</sub>(Al,Mg)<sub>13</sub>(B, $\square$ ,Al)<sub>5</sub>(SiO<sub>4</sub>)<sub>10</sub>(Si<sub>2</sub>O<sub>7</sub>)<sub>4</sub>(O,OH)<sub>10</sub>



**Origin:** Wiluy River, Yakutia, Russia (type locality).

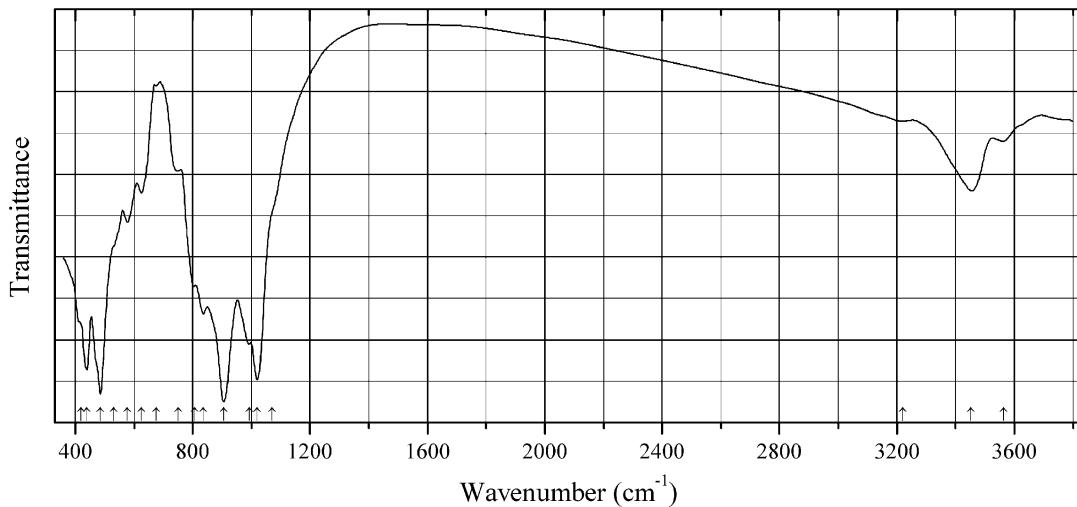
**Description:** Dark green crystal from the association with a chlorite-group mineral, Al-bearing diopside, fluorapatite, goethite, pyrite, grossular, apatite, wollastonite, and perovskite. Characterized by Mössbauer spectroscopy. The crystal structure is solved. Tetragonal, space group  $P4/nnc$ ,  $a = 15.7027(3)$ ,  $c = 11.7008(3)$  Å,  $V = 2885.1(1)$  Å<sup>3</sup>. The crystal-chemical formula is  $x_1^{Y_1}(\text{Ca})_{2.00}^{X_2}(\text{Ca})_{8.00}^{X_3}(\text{Ca})_{8.00}^{X_4}(\text{Ca})_{1.00}^{Y_1}(\text{Mg}_{0.56}\text{Fe}^{2+}_{0.27}\text{Fe}^{3+}_{0.17})_{\Sigma 1.00}^{Y_2}(\text{Al}_{3.90}^{T1+T2}\text{Fe}^{2+}_{0.10})_{\Sigma 4.00}^{Y_3}(\text{Al}_{3.82}\text{Mg}_{3.14}\text{Ti}_{0.63}\text{Fe}^{3+}_{0.21}\text{Fe}^{2+}_{0.16}\text{Mn}_{0.04})_{\Sigma 8.00}^{Z_1}(\text{Si})_{2.00}^{Z_2}(\text{Si})_{8.00}^{Z_3}(\text{Si})_{8.00}(\text{O})_{68.00}^{W}(\text{B}_{3.04}\text{Al}_{0.72}\square_{1.24})_{\Sigma 5.00}^{W}(\text{O}_{8.32}\text{OH}_{0.96})_{\Sigma 9.28}^{W}(\text{O}_{1.52})$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3634w, 3566w, 3481w, 3338w, 1415sh, 1373, 1267, 1165sh, 1110sh, 1080sh, 1002s, 965sh, 914s, 870sh, 803, 782, 755sh, 679w, 615sh, 560sh, 510sh, 466s, 430s, 376.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Siod75 Ferrovesuvianite**  $\text{Ca}_{19}\text{Fe}^{2+}(\text{Al},\text{Fe},\text{Ti})_{12}(\text{SiO}_4)_{10}(\text{Si}_2\text{O}_7)_4(\text{OH},\text{O})_{10}$



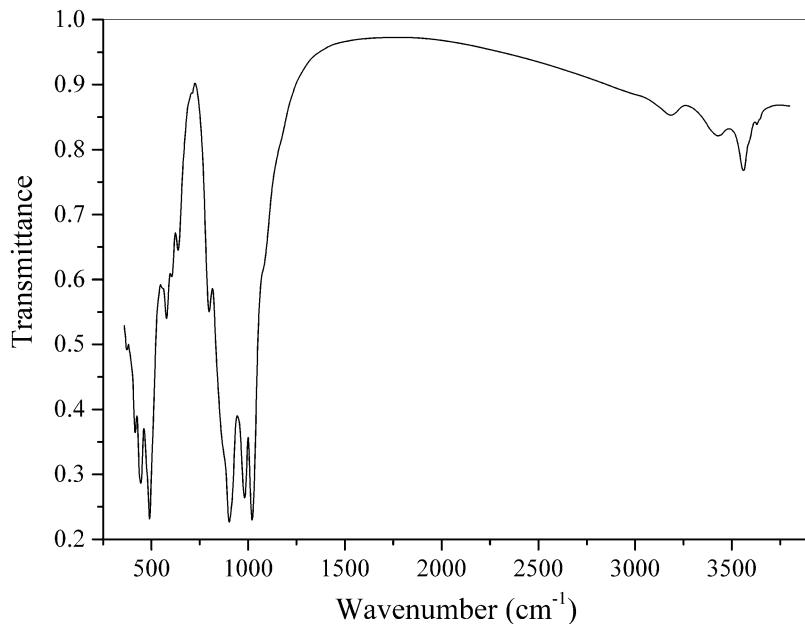
**Origin:** Alchuri, Shigar Valley, Northern Areas, Pakistan.

**Description:** Reddish-brown blocky prismatic crystals from the association with quartz, clinochlore, albite, potassium feldspar, aegirine-augite, andradite, zoisite, calcite, titanite, fluorapatite, and zircon. Characterized by <sup>27</sup>Al NMR and Mössbauer spectroscopy. The crystal structure is solved. Tetragonal, space group  $P4/nmc$ ,  $a = 15.5326(2)$ ,  $c = 11.8040(2)$  Å,  $V = 2847.87(8)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 3.460$  g/cm<sup>3</sup>. Optically uniaxial (-),  $\epsilon = 1.740(4)$ ,  $\omega = 1.749(2)$ . The empirical formula is (electron microprobe):  $(\text{Ca}_{18.11}\text{Na}_{0.885})(\text{Mg}_{0.63}\text{Fe}^{2+}_{0.79}\text{Fe}^{3+}_{1.765}\text{Al}_{7.99}\text{Ti}_{2.21})\text{Si}_{17.62}\text{O}_{69.92}(\text{OH})_{7.37}\text{F}_{1.33}$ . The crystal-chemical formula is  $^{[8-9]}(\text{Ca}_{17.1}\text{Na}_{0.9})^{[8]}\text{Ca}_{1.0}^{[5]}(\text{Fe}^{2+}_{0.44}\text{Fe}^{3+}_{0.34}\text{Mg}_{0.22})^{[6]}(\text{Al}_{3.59}\text{Mg}_{0.41})^{[6]}(\text{Al}_{4.03}\text{Ti}_{2.20}\text{Fe}^{3+}_{1.37}\text{Fe}^{2+}_{0.40})\text{Si}_{18}\text{O}_{68}^{[(\text{OH})_{5.84}\text{O}_{2.83}\text{F}_{1.33}]}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3563w, 3453, 3220w, 1070sh, 1021s, 993s, 906s, 836s, 806, 750, 677w, 626, 578, 530sh, 485s, 439s, 420sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Siod76 Fluorvesuvianite**  $\text{A}_3\text{O}_4\text{H}_2\text{O}_3\text{P}_4\text{O}_3(\text{H})\cdot\text{H}_2\text{O}$ 

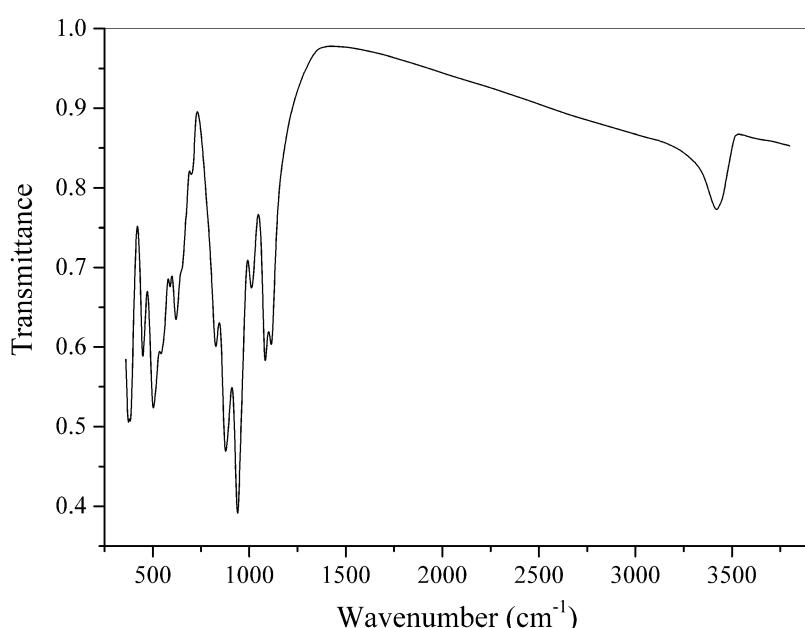
**Origin:** Abandoned Lupikko iron mine, Pitkäranta, Karelia, Russia (type locality).

**Description:** Colorless acicular crystals from the association with sphalerite and clinochlore. Confirmed by the IR spectrum.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3645sh, 3630w, 3560, 3431, 3183w, 1160sh, 1075sh, 1020s, 982s, 903s, 875sh, 799, 710w, 638, 605, 578, 560sh, 491s, 445s, 416, 376.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Siod77 Epidote-(Sr)**  $\text{CaSr}(\text{Al}_2\text{Fe}^{3+})(\text{Si}_2\text{O}_7)(\text{SiO}_4)\text{O(OH)}$ 

**Origin:** N'Chwaning Mine, Kuruman, Kalahari manganese fields, Northern Cape province, South Africa.

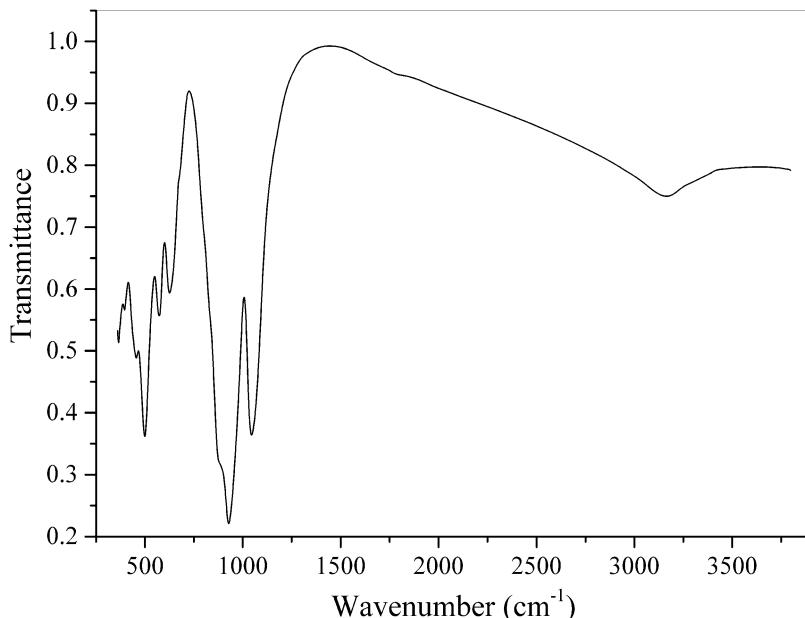
**Description:** Clusters of dark red crystals with thin zones of manganipiemontite-(Sr). The typical composition corresponds to the formula  $\text{Ca}_{1.0}\text{Sr}_{1.0}(\text{Al}_{1.8}\text{Fe}_{0.9}\text{Mn}_{0.3}(\text{Si}_2\text{O}_7)(\text{SiO}_4)\text{O(OH)}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3420, 1114, 1083, 1012, 940s, 878s, 827, 669w, 650sh, 620, 589, 543, 503s, 449, 394s, 376s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Siod78 Ferriakasakaite-(La)**  $\text{CaLaFe}^{3+}\text{AlMn}^{2+}(\text{Si}_2\text{O}_7)(\text{SiO}_4)\text{O(OH)}$



**Origin:** In den Dellen pumice quarry, Niedermendig, Mendig, Laach Lake volcanic complex, Eifel, Rhineland-Palatinate, Germany.

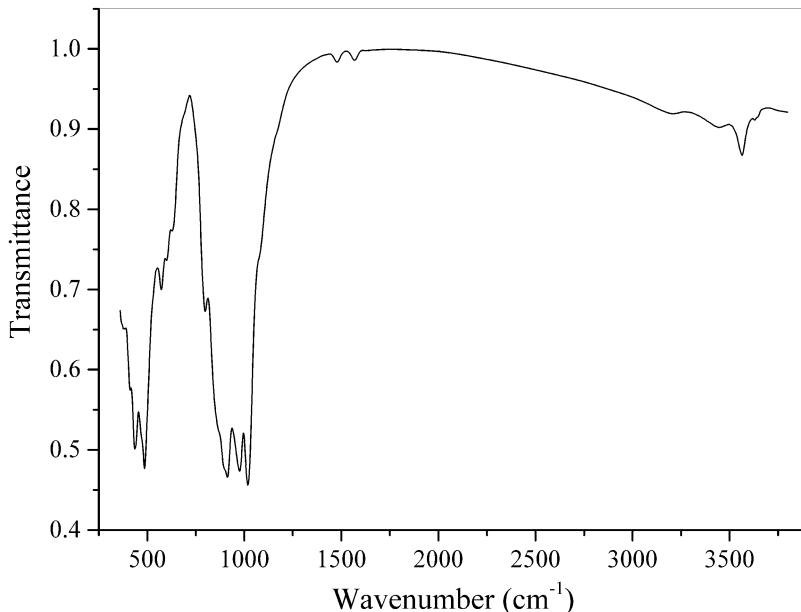
**Description:** Black thick-tabular crystals from sanidinite, from the association with nosean and/or haüyne, Mn-bearing biotite, magnetite, ilmenite-pyrophanite series members, Mn-bearing zirconolite, and secondary jarosite. The crystal structure is solved. Monoclinic, space group  $P2_1/m$ ,  $a = 8.90540$  (13),  $b = 5.75454(7)$ ,  $c = 10.10367(15)$  Å,  $\beta = 114.1030(18)^\circ$ ,  $V = 472.634(11)$  Å<sup>3</sup>. The empirical formula is  $(\text{Ca}_{0.68}\text{Mn}^{2+}_{0.32})_{\Sigma 1.00}(\text{La}_{0.49}\text{Ce}_{0.39}\text{Pr}_{0.02}\text{Nd}_{0.02}\text{Sm}_{0.01}\text{Eu}_{0.01}\text{Gd}_{0.01}\text{Th}_{0.01}\text{Ca}_{0.04})_{\Sigma 1.00}(\text{Fe}^{3+}_{0.52}\text{Fe}^{2+}_{0.04}\text{Al}_{0.34}\text{Ti}^{4+}_{0.10})_{\Sigma 1.00}\text{Al}_{1.00}(\text{Mn}^{2+}_{0.53}\text{Fe}^{2+}_{0.34}\text{Mg}_{0.13})_{\Sigma 1.00}(\text{Si}_{2.98}\text{Al}_{0.02})_{\Sigma 3.00}\text{O}_{12.00}(\text{OH})$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** (3300sh), 3164, 1045s, 928s, 885sh, 675sh, 626, 573, 499s, 455, 394, 366.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Siod79 Vesuvianite**  $\text{Ca}_{19}\text{Fe}^{3+}[\text{Al}_{10}(\text{Fe}^{2+}, \text{Mn}^{2+}, \text{Mg})_2](\text{Si}_2\text{O}_7)_4(\text{SiO}_4)_{10}\text{O(OH)}_9$ ,



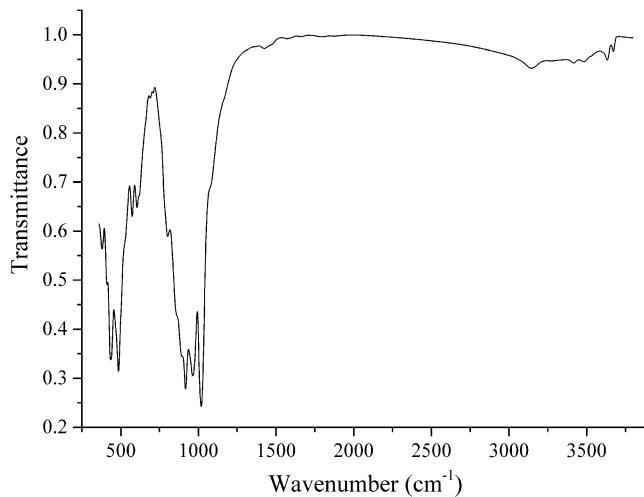
**Origin:** Somma-Vesuvius volcanic complex, Campania region, Italy (type locality).

**Description:** Greenish brown crystals from skarn xenolith. Neotype sample used for vesuvianite formula revision. Characterized by Mössbauer spectroscopy, <sup>27</sup>Al MAS NMR, powder X-ray diffraction and thermal analysis. The crystal structure is solved. Tetragonal, space group *P4/nnc*; *a* = 15.5720(3), *c* = 11.8158(5). The crystal-chemical formula is  $\text{X}^1(\text{Ca})_{2.00} \text{X}^2(\text{Ca})_{8.00} \text{X}^3(\text{Ca})_{8.00} \text{X}^4(\text{Ca}_{0.97}\text{Na}_{0.03})_{1.00} \text{Y}^1(\text{Fe}^{3+}_{0.50}\text{Mg}_{0.28}\text{Fe}^{2+}_{0.22}) \text{Y}^2(\text{Al}_{3.85}\text{Fe}^{2+}_{0.15}) \text{Y}^3(\text{Al}_{5.26}\text{Mg}_{1.83}\text{Fe}^{3+}_{0.54}\text{Fe}^{2+}_{0.26}\text{Mn}_{0.11}) \text{Z}^1(\text{Si})_{2.00} \text{Z}^2(\text{Si})_{8.00} \text{Z}^3(\text{Si})_{8.00} (\text{O})_{68.00} \text{T}^{1+2}(\text{Al}_{0.44}\text{B}_{0.25}\square_{4.31})^W (\text{OH}_{5.65}\text{F}_{2.00}\text{O}_{1.30}\text{Cl}_{0.05})$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3565, 3450w, 3629w, 3210w, 1568w, 1478w, 1170sh, 1075 sh, 1018s, 976s, 914s, 900sh, 870sh, 799, 629, 599, 572, 486s, 436s, 415, 384.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Siod80 Vesuvianite Cr-bearing**  $\text{Ca}_{19}\text{Fe}^{3+}[(\text{Al},\text{Cr})_{10}(\text{Fe}^{2+},\text{Mn}^{2+},\text{Mg})_2](\text{Si}_2\text{O}_7)_4(\text{SiO}_4)_{10}\text{O(OH)}_9$ 

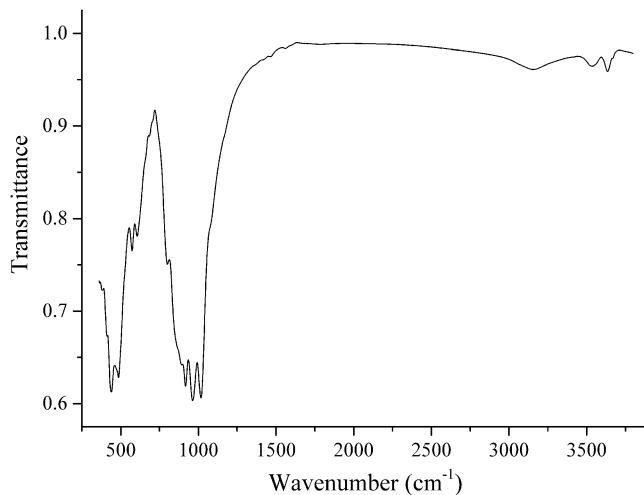
**Origin:** Lekhoilinskoe Cr deposit, Voikaro-Syn'inskiy ultrabasite massif, Polar Urals.

**Description:** Emerald-green crystals on chromite. Investigated by T.L. Panikorovskiy.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3672w, 3633, 3520sh, 3483, 3416, 3146, 1880w, 1796w, 1661w, 1577w, 1465sh, 1424w, 1160sh, 1075sh, 1018s, 964s, 918s, 895sh, 865sh, 803, 710w, 690w, 615sh, 605, 573, 520sh, 485s, 434s, 412, 380.

**Note:** The spectrum was obtained by N.V. Chukanov. The band at 3416 cm<sup>-1</sup> is characteristic for Cr-bearing vesuvianite.

**Siod81 Vesuvianite S-bearing**  $\text{Ca}_{19}\text{Fe}^{3+}[\text{Al}_{10}(\text{Fe}^{2+},\text{Mn}^{2+},\text{Mg})_2](\text{Si}_2\text{O}_7)_4(\text{SiO}_4)_{10}\text{S}_x(\text{OH},\text{O})_{10}$  (?)

**Origin:** Monzoni Mts., Fassa valley, Trento Province, Trentino-Alto Adige (Trentino-Südtirol), Italy.

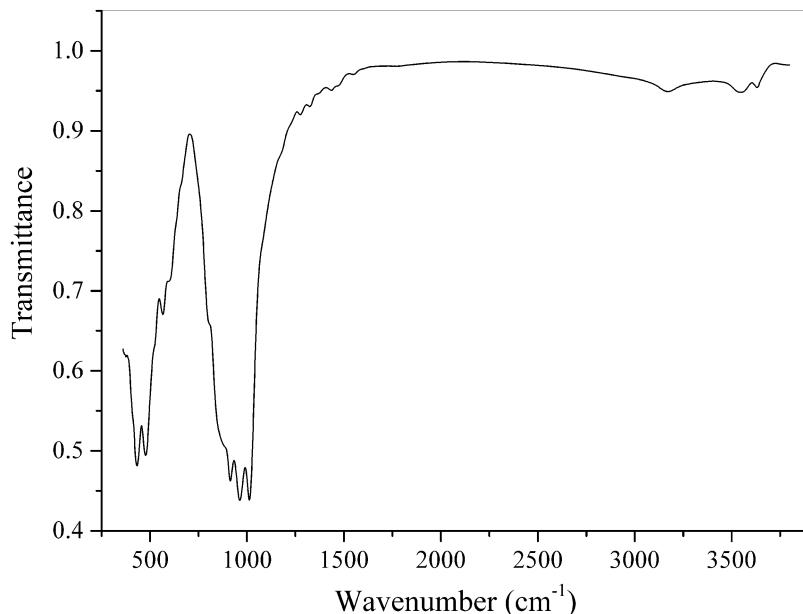
**Description:** Yellow crystal. Investigated by T.L. Panikorovskiy.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3665w, 3634, 3535, 3146, 1588sh, 1560w, 1463w, 1412sh, 1355sh, 1165sh, 1075sh, 1017s, 963s, 918s, 894, 870sh, 803, 705sh, 683w, 606, 573, 485s, 440s, 415, 384.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Siod82 “Hydrovesuvianite”** Ca<sub>19</sub>Fe<sup>3+</sup>[Al<sub>10</sub>(Fe<sup>2+</sup>,Mn<sup>2+</sup>,Mg)<sub>2</sub>](Si<sub>2</sub>O<sub>7</sub>)<sub>4</sub>[SiO<sub>4</sub>,(OH)<sub>4</sub>]<sub>10</sub>O(OH)<sub>9</sub>



**Origin:** Vilyui River Basin (Wilui River Basin), Sakha Republic (Yakutia), Eastern-Siberian Region, Russia.

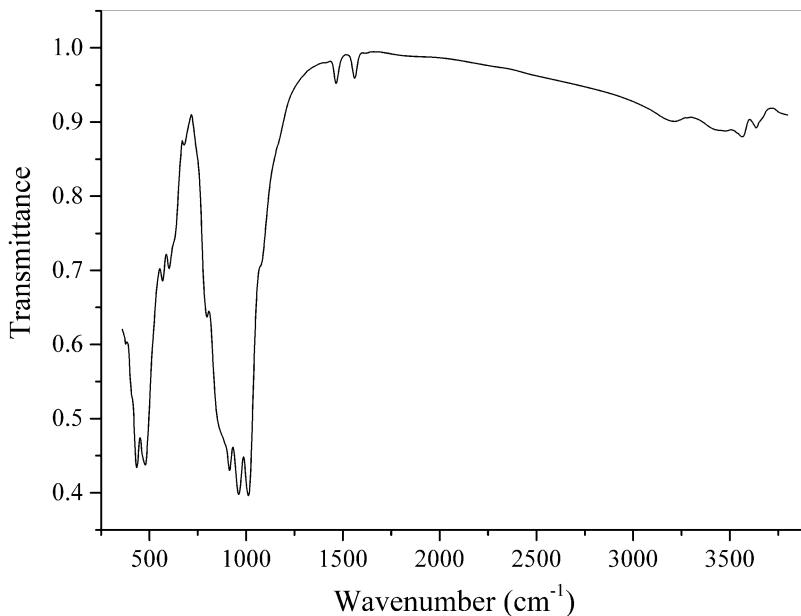
**Description:** Epitaxy on wiluite crystals from the association with grossular. Investigated by T.L. Panikorovskiy.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3631, 3546, 3160, 1547w, 1465sh, 1435w, 1363sh, 1323w, 1275w, 1165sh, 1013s, 963s, 914s, 880sh, 655sh, 595, 566, 520sh, 477s, 433s, 376.

**Note:** The spectrum was obtained by N.V. Chukanov. The band at 3546 cm<sup>-1</sup> may correspond to (OH)<sub>4</sub> tetrahedra.

### Siod83 Vesuvianite B-bearing



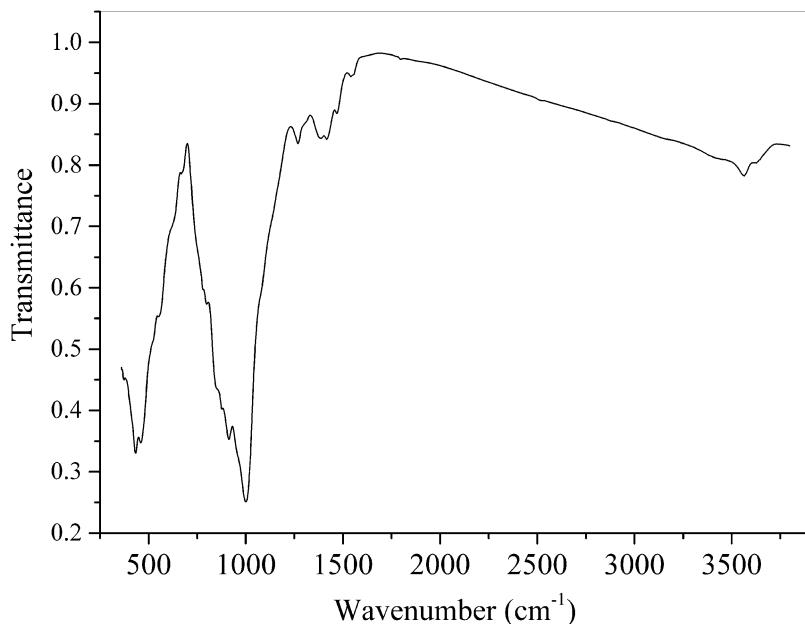
**Origin:** Gulshad, Northern Balkhash Lake Area, Kazakhstan.

**Description:** Investigated by T.L. Panikorovskiy. The crystal structure is solved. The crystal-chemical formula is  $\text{Ca}_{19.00}^{Y1}(\text{Fe}_{0.62}\text{Mg}_{0.38})^{Y2}\text{Al}_{4.00}^{Y3}[(\text{Al},\text{Mg})_{7.34}(\text{Fe},\text{Ti})_{0.66}]^{T1}[\text{B}_{0.45}\text{Al}_{0.80}]_{1.25}^{T2}\text{B}_{0.50}\text{Si}_{18}\text{O}_{68}(\text{OH},\text{O})_{10}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3669sh, 3636, 3563, 3463, 3210, 1562, 1464, 1160sh, 1075sh, 1012s, 962s, 915s, 875sh, 800, 680w, 625sh, 601, 568, 479s, 434s, 415sh, 380.

**Note:** The spectrum was obtained by N.V. Chukanov. The bands at 1562 and 1464 cm<sup>-1</sup> correspond to BO<sub>3</sub> triangles with shortened (as compared to wiluite) B–O bonds.

**Siod84 Vesuvianite B-bearing**

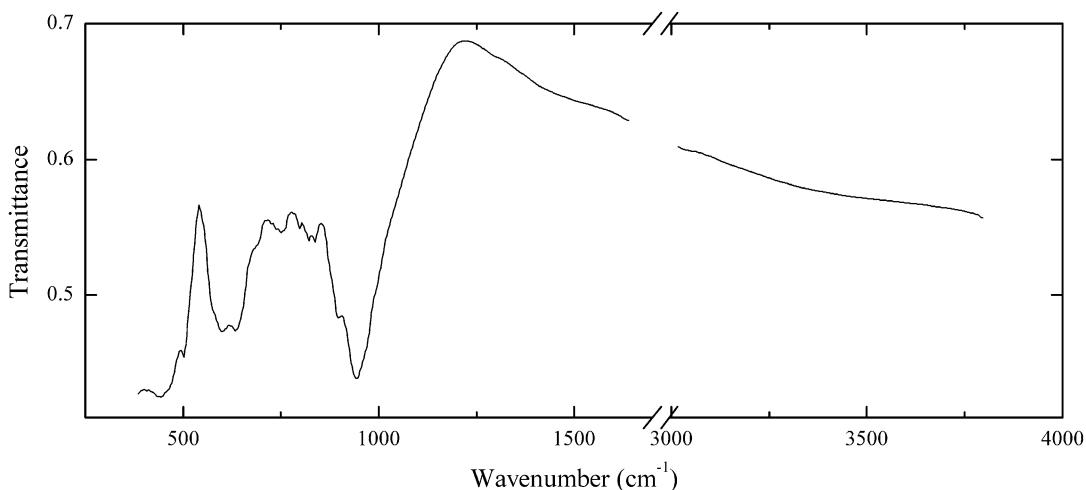
**Origin:** Gulshad, Northern Balkhash Lake Area, Kazakhstan.

**Description:** Investigated by T.L. Panikorovskiy. The crystal structure is solved. The crystal-chemical formula is  $\text{Ca}_{19.00}^{Y_1}(\text{Fe}_{0.87}\text{Mg}_{0.13})^{Y_2}\text{Al}_{4.00}^{Y_3}[(\text{Al},\text{Mg})_{6.45}(\text{Fe},\text{Mn})_{1.55}]^{T_1}\text{B}_{2.06}^{T_2}\text{B}_{1.00}\text{Si}_{18}\text{O}_{68}(\text{OH},\text{O})_{12}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm⁻¹):** 3623w, 3565, 3450sh, 1800w, 1543w, 1469, 1417, 1388, 1300sh, 1269, 1130sh, 1070sh, 1000s, 913s, 882, 855sh, 802, 782, 670w, 620sh, 552, 520sh, 460s, 434s, 376.

**Note:** The spectrum was obtained by N.V. Chukanov. The bands at 1543 and 1469 cm⁻¹ correspond to  $\text{BO}_3$  triangles with shortened (as compared to wiluite) B–O bonds.

**Sic27 Khesinite  $\text{Ca}_4(\text{Mg}_3\text{Fe}^{3+})_9\text{O}_4(\text{Fe}^{3+})_9\text{Si}_3\text{O}_{36}$** 

**Origin:** Burned dump of the Korkinskiy quarry, Chelyabinsk coal basin, Kopeisk, South Urals, Russia.

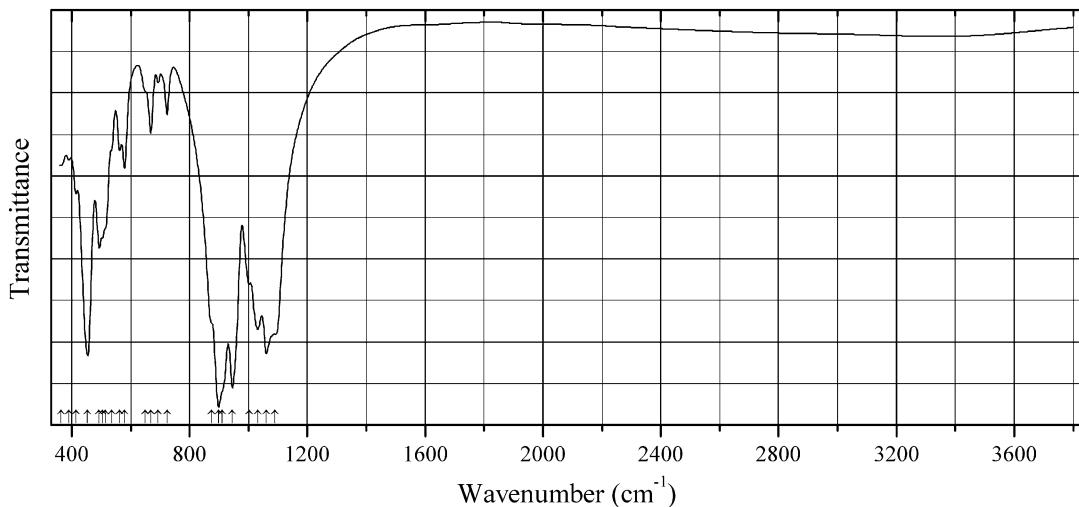
**Description:** Black tabular crystals from the association with melilite, pyroxene, amphibole, wollastonite, anorthite, and calcium ferrites. Technogenetic. Investigated by B.V. Chesnokov. Related to aenigmatite-group minerals. Triclinic,  $a = 10.58(3)$ ,  $b = 10.90(3)$ ,  $c = 9.10(4)$  Å,  $\alpha = 107.08(2)^\circ$ ,  $\beta = 95.02(2)^\circ$ ,  $\gamma = 124.45(2)^\circ$ . The empirical formula is  $\text{Ca}_{1.16}\text{Fe}^{3+}_{4.16}\text{Mg}_{0.32}\text{Ti}_{0.02}\text{Al}_{0.64}\text{Si}_{0.65}\text{O}_{10}$ .  $D_{\text{calc}} = 4.09$  g/cm<sup>3</sup>. The strongest lines of powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %)] are 2.993 (70), 2.721 (80), 2.587 (100), 2.526 (90), 2.473 (40), 2.132 (55), 1.626 (52), 1.517 (70), 1.506 (50).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 953s, 902s, 838, 824, 801, 750, 690sh, 640s, 596s, 500s, 463s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sic105 Fowlerite**  $\text{CaMn}_3\text{Zn}(\text{Si}_5\text{O}_{15})$



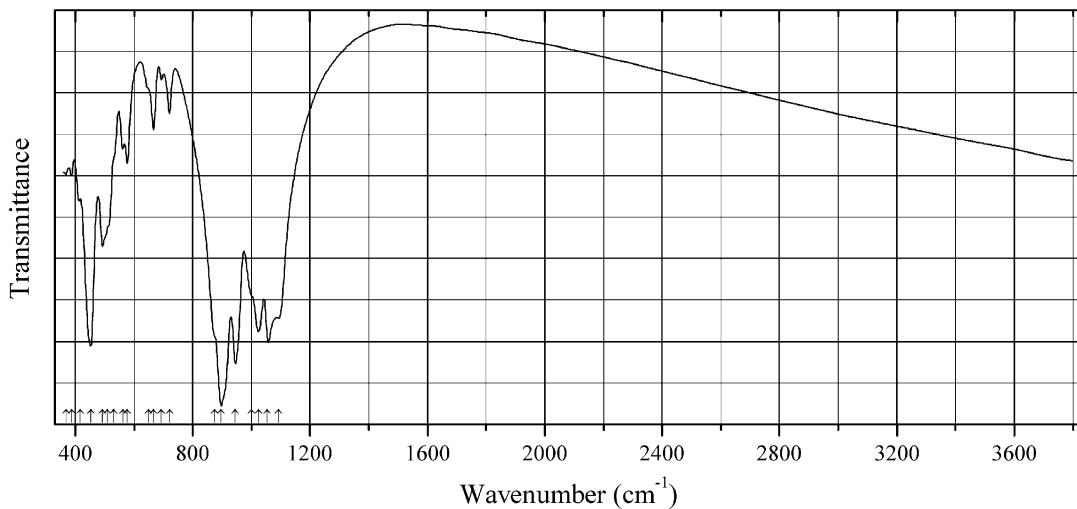
**Origin:** Franklin, Ogdensburg, Sussex Co., New Jersey, USA.

**Description:** Pinkish-brown grains. The empirical formula is  $\text{Ca}_{0.75}\text{Mn}_{3.16}\text{Zn}_{0.56}\text{Fe}_{0.31}\text{Mg}_{0.25}(\text{Si}_5\text{O}_{15})$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 1089s, 1061s, 1032s, 1003, 945s, 910sh, 899s, 875sh, 724, 693w, 669, 650sh, 579, 562, 535sh, 515sh, 505sh, 493, 454s, 415, 390, 365.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sic106 Ferrorhodonite**  $\text{CaMn}_3\text{Fe}(\text{Si}_5\text{O}_{15})$ 

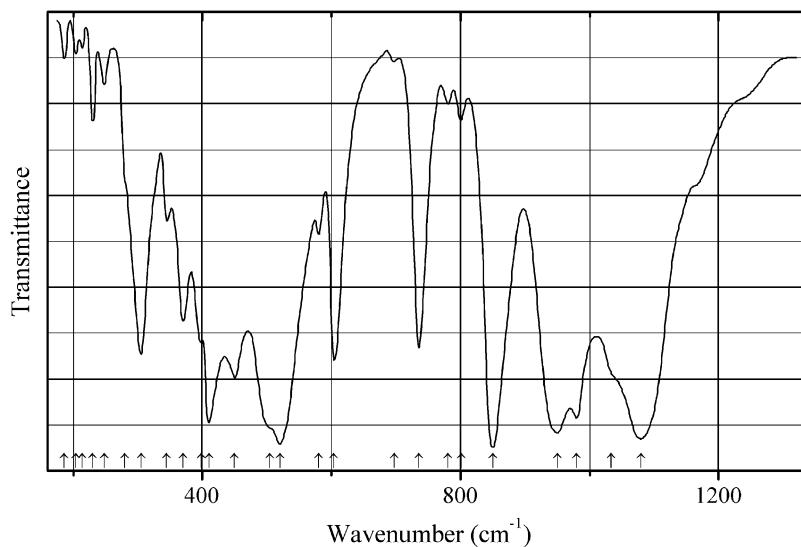
**Origin:** Broken Hill Pb-Zn deposit, Yancowinna Co., New South Wales, Australia (type locality).

**Description:** Brownish red coarse crystalline aggregates in the association with galena, chalcopyrite, spessartine, and quartz. Holotype sample. The crystal structure is solved. Triclinic, space group  $P-1$ ,  $a = 6.6766(5)$ ,  $b = 7.6754(6)$ ,  $c = 11.803(1)$  Å,  $\alpha = 105.501(1)^\circ$ ,  $\beta = 92.275(1)^\circ$ ,  $\gamma = 93.919(1)^\circ$ ,  $V = 580.44(1)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{meas}} = 3.71(2)$  g/cm $^3$ ,  $D_{\text{calc}} = 3.701$  g/cm $^3$ . Optically biaxial (+),  $\alpha = 1.731(4)$ ,  $\beta = 1.736(4)$ ,  $\gamma = 1.745(5)$ ,  $2V = 80(10)^\circ$ . The crystal-chemical formula is  $(\text{Ca}_{0.81}\text{Mn}_{0.19})(\text{Mn}_{2.52}\text{Fe}_{0.48})(\text{Fe}^{2+}_{0.81}\text{Mn}_{0.12}\text{Mg}_{0.04}\text{Zn}_{0.03})(\text{Si}_5\text{O}_{15})$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 3.337 (32) (-1-13), 3.132 (54) (-210), 3.091 (41) (0-23), 2.968 (100) (-2-11), 2.770 (91) (022), 2.223 (34) (-204), 2.173 (30) (-310).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm $^{-1}$ ):** 1092s, 1053s, 1025, 1000sh, 946, 897, 875sh, 721, 694, 667, 650sh, 577, 563sh, 530sh, 510sh, 492, 453s, 416sh, 388, 368.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sic107 Lithium metasilicate**  $\text{Li}_2\text{SiO}_3$ 

**Origin:** Synthetic.

**Description:** Commercial reactant. Orthorhombic, space group  $Cmc2_1$ ,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc.  
Transmission.

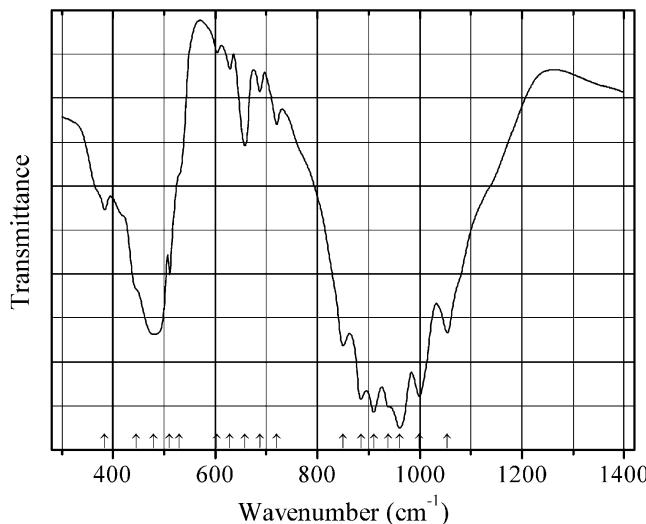
**Source:** Devarajan and Shurvell (1977).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1080s, 1034sh, 980, 950s, 850s, 801w, 781w, 735, 697w, 604, 580w, 520s, 505sh, 450, 410, 398, 370, 345w, 305, 280sh, 248w, 230w, 214w, 204w, 196w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1087, 1034, 1001sh, 983s, 945, 852, 731, 645, 610s, 587sh, 567, 520, 496, 465, 450w, 410, 398sh, 345w, 325w, 291sh, 297, 273w, 258w, 234, 210, 186, 141.

### Sic108 Alamosite polymorph $\text{PbSiO}_3$



**Origin:** Synthetic.

**Description:** Prepared by crystallization at 650 °C from the undercooled melt. Characterized by powder X-ray diffraction data. Hexagonal.

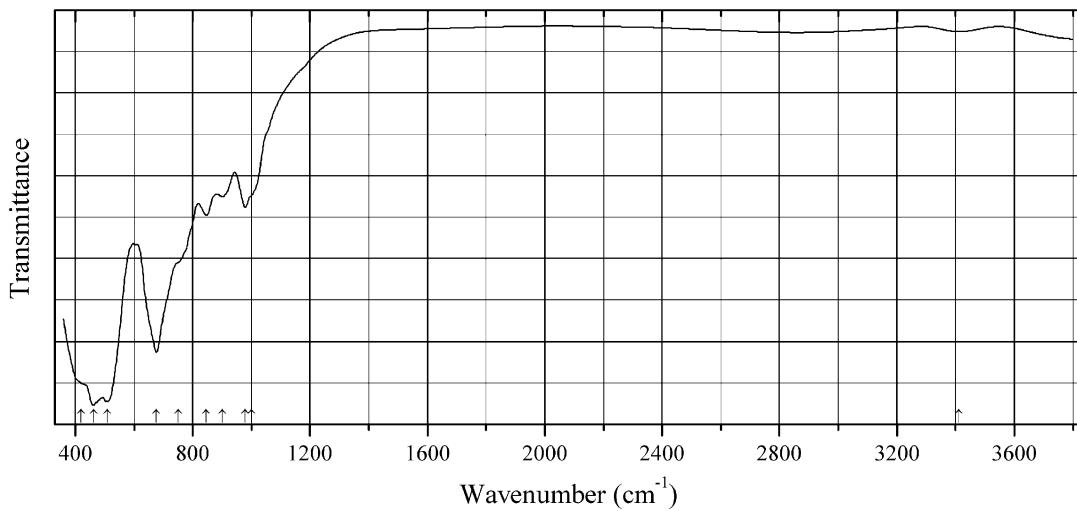
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Furukawa et al. (1979).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1054, 999s, 961s, 938sh, 910s, 885s, 850, 720, 687w, 658, 629w, 604w, 530, 511, 480, 445, 384.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1070, 1012, 936, 915s, 871, 850, 731w, 685w, 669w, 628w, 615w, 545, 513, 503, 484, 438, 406, 358s, 316, 294, 263s, 243, 231, 144, 106, 91, 52.

**Sic109 Dorrite**  $\text{Ca}_4[\text{Mg}_3\text{Fe}^{3+}_9]\text{O}_4[\text{Si}_3\text{Al}_8\text{Fe}^{3+}\text{O}_{36}]$ 

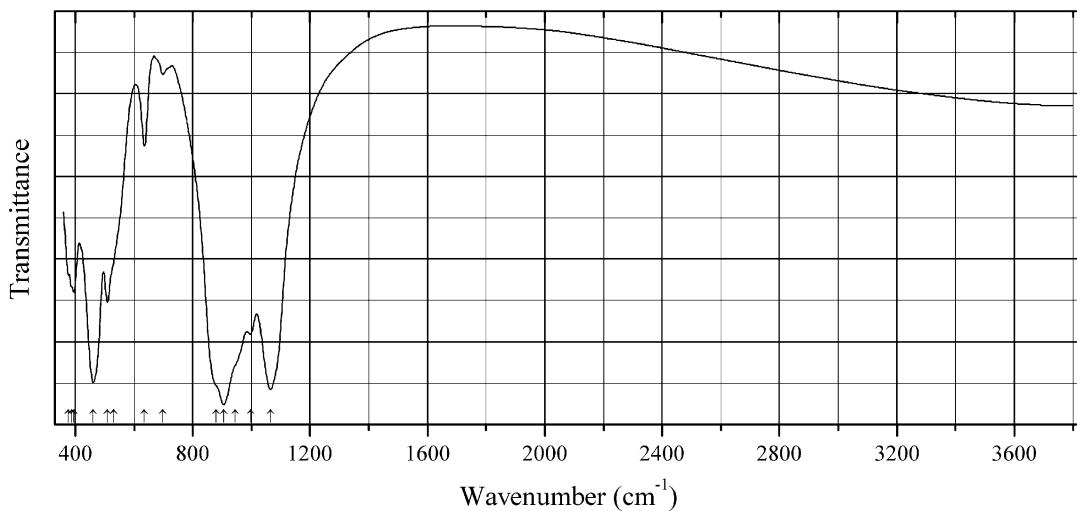
**Origin:** Bellerberg, near Ettringen, Eifel Mts., Rhineland-Palatinate (Rheinland-Pfalz), Germany.

**Description:** Brown equant crystals from the association with cuspidine, clinopyroxene, spinel, and gypsum. The empirical formula is (electron microprobe):  $\text{Ca}_{4.1}(\text{Mg}_{3.6}\text{Mn}_{0.2}\text{Fe}_{7.4}\text{Al}_{0.4}\text{Ti}_{0.3})(\text{Si}_{3.8}\text{Al}_{8.2})\text{O}_{40}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** (3412w), 1000sh, 979, 902, 846, 750sh, 677s, 510s, 463s, 420sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sic110 Aegirine-augite**  $(\text{Ca},\text{Na})(\text{Fe}^{3+},\text{Mg},\text{Fe}^{2+})\text{Si}_2\text{O}_6$ 

**Origin:** Harstigen Mine, Pajsberg, Persberg district, Filipstad, Värmland, Sweden.

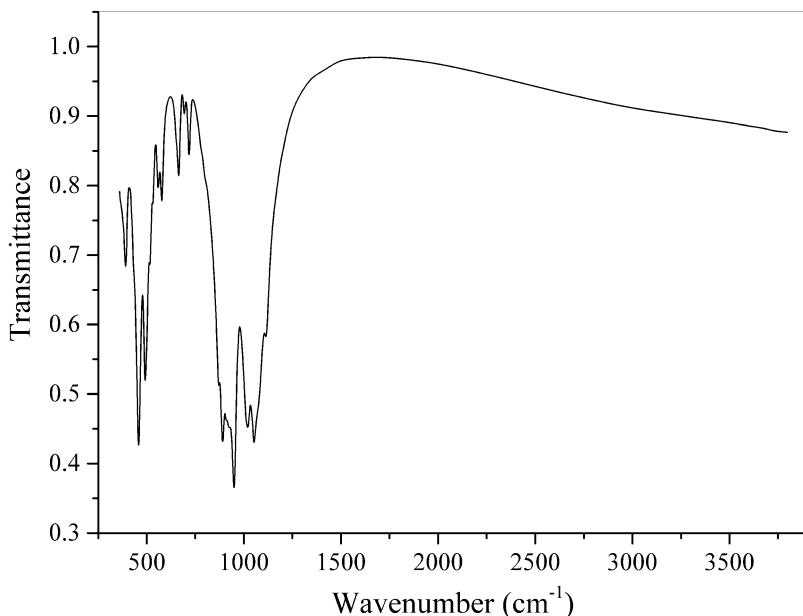
**Description:** Olive-green anhedral grains from the association with julgoldite-(Fe<sup>3+</sup>) and calcite. The empirical formula is (electron microprobe):  $(\text{Ca}_{0.49}\text{Na}_{0.42}\text{Mn}_{0.09})(\text{Fe}_{0.52}\text{Mg}_{0.44}\text{Mn}_{0.04})(\text{Si}_{1.96}\text{Al}_{0.03}\text{Fe}_{0.01}\text{O}_6)$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 1066s, 997s, 945sh, 905s, 880sh, 698w, 636, 530sh, 509, 461s, 395, 387sh, 377sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

### Sic111 Vittingeite Mn<sub>5</sub>(Si<sub>5</sub>O<sub>15</sub>)



**Origin:** Vittinge iron mines, Isokyrö, Western and Inner Finland Region, Finland (type locality).

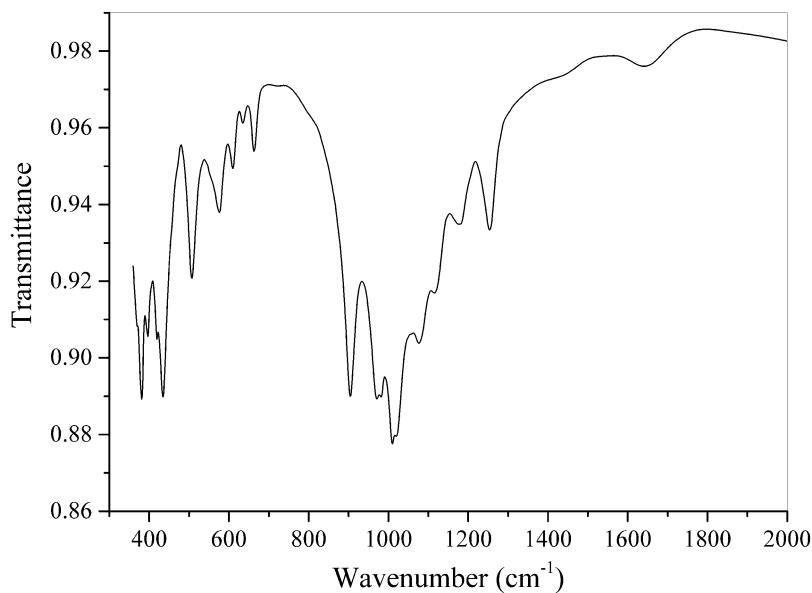
**Description:** Anhedral grains from the association with quartz and pyroxmangite. Holotype sample.

The crystal structure is solved. Triclinic, space group *P*-1,  $a = 6.6980(3)$ ,  $b = 7.6203(3)$ ,  $c = 11.8473(5)$  Å,  $\alpha = 105.663(3)^\circ$ ,  $\beta = 92.400(3)^\circ$ ,  $\gamma = 94.309(3)^\circ$ ,  $V = 579.38(7)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{meas}} = 3.62(2)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 3.737$  g/cm<sup>3</sup>. Optically biaxial (+),(+),  $\alpha = 1.725(4)$ ,  $\beta = 1.733(4)$ ,  $\gamma = 1.745(5)$ ,  $2V = 75(10)^\circ$ . The empirical formula is (electron microprobe):  $\text{Ca}_{0.11}\text{Mn}_{4.71}\text{Fe}_{0.11}\text{Mg}_{0.08}\text{Zn}_{0.01}\text{Si}_{4.99}\text{O}_{15}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 1112, 1053s, 1020s, 950s, 930sh, 915sh, 891s, 824, 718, 693, 664, 578, 559, 515, 492, 458s, 391.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sic112 Haradaite Sr(VO)(Si<sub>2</sub>O<sub>6</sub>)**

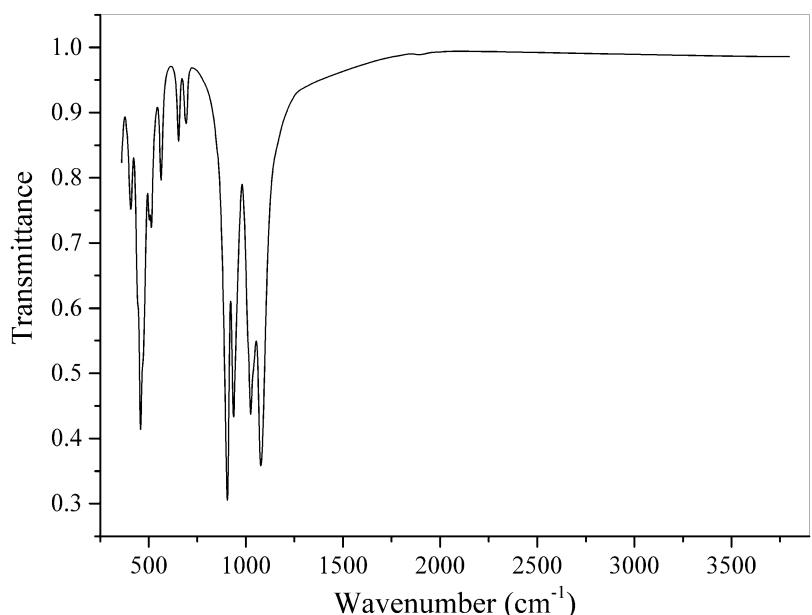
**Origin:** Yamato mine, Amami-Oshima Island, Kagoshima Prefecture, Nansei Archipelago, Kyushu region, Japan (type locality).

**Description:** Bright green grains.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 1254, 1177, 1115, 1076s, 1020s, 1010s, 971s, 904s, 663, 635w, 610, 576, 507, 434s, 394, 380s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sic113 Dalnegorskite Ca<sub>5</sub>Mn(Si<sub>3</sub>O<sub>9</sub>)<sub>2</sub>**

**Origin:** Dalnegorskoe boron deposit, town of Dalnegorsk, Primorskiy Kray, Russian Far East, Russia (type locality).

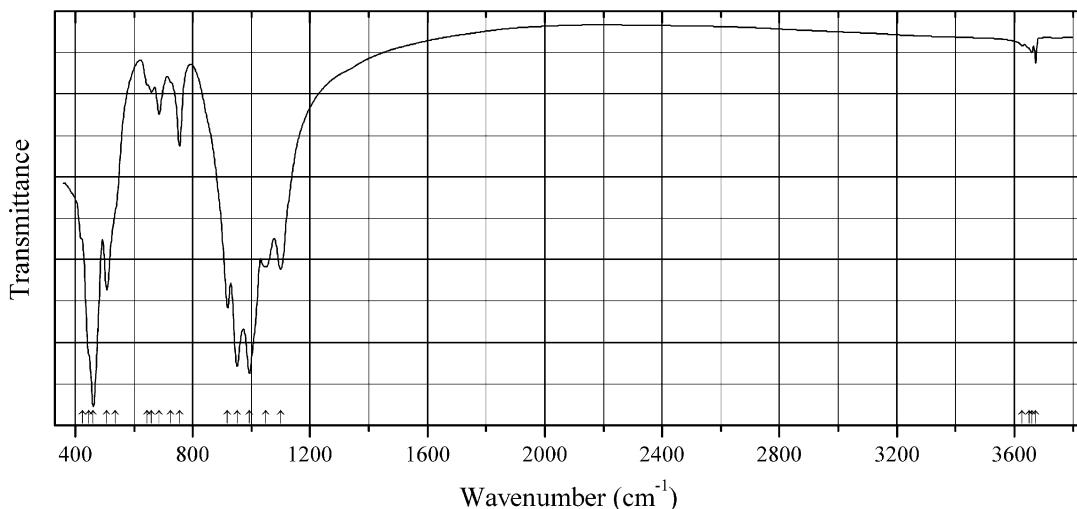
**Description:** Tight aggregate consisting of split thin fiber-like individuals from the association with Mn-bearing hedenbergite and datolite. Holotype sample. Triclinic, Space group:  $P\bar{1}$ ,  $a = 7.2588(11)$ ,  $b = 7.8574(15)$ ,  $c = 7.8765(6)$  Å,  $\alpha = 88.550(15)^\circ$ ,  $\beta = 62.582(15)^\circ$ ,  $\gamma = 76.621(6)^\circ$ ,  $V = 386.23(11)$  Å<sup>3</sup>,  $Z = 1$ .  $D_{\text{meas}} = 3.02(2)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 3.062$  g/cm<sup>3</sup>. Optically biaxial (−),  $\alpha = 1.640(3)$ ,  $\beta = 1.647(3)$ ,  $\gamma = 1.650(3)$ ,  $2V = 75(10)^\circ$ . The empirical formula is (electron microprobe): Ca<sub>5.03</sub>Mn<sub>0.50</sub>Fe<sub>0.36</sub>Mg<sub>0.04</sub>Si<sub>6.03</sub>O<sub>18</sub>. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %)] are: 3.80 (57), 3.48 (57), 3.28 (42), 2.952 (100), 2.951 (66), 1.815 (34), 1.708 (34), 1.703 (34).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 1892w, 1077s, 1025s, 937s, 905s, 693, 653, 563, 513, 505, 470sh, 458s, 445sh, 407.

**Note:** The spectrum was obtained by N.V. Chukanov.

### Sib152 Magnesio-ferri-hornblende



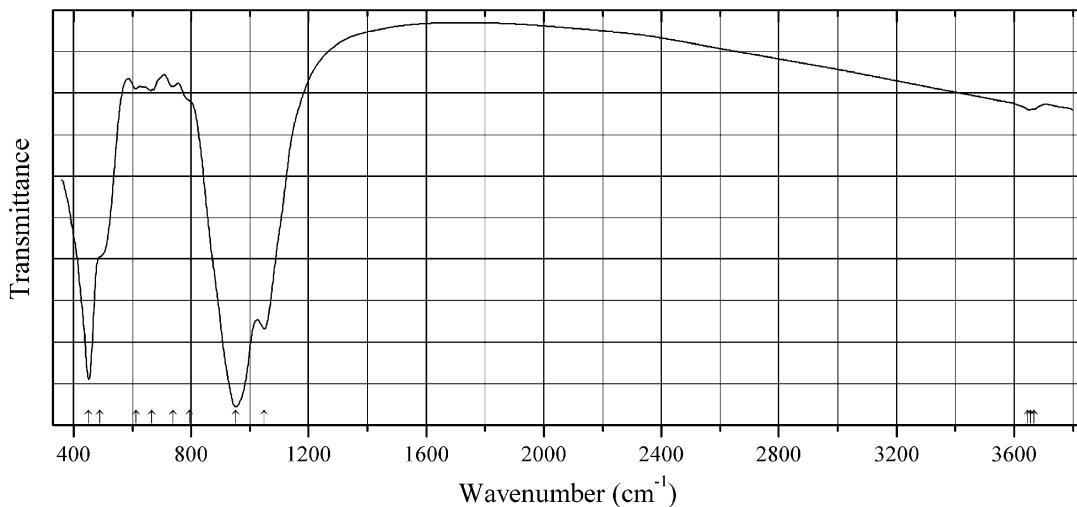
**Origin:** Otamo dolomite quarry, Siikainen, Finland.

**Description:** Dark green grains from the association with plagioclase, dolomite, and calcite. The crystal structure is solved. Monoclinic, space group  $C2/m$ ,  $a = 9.855(1)$ ,  $b = 18.084(1)$ ,  $c = 5.289(1)$  Å,  $\beta = 91.141(6)^\circ$ ,  $V = 104.853(2)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 3.057$  g/cm<sup>3</sup>. The empirical formula is K<sub>0.03</sub>(Ca<sub>1.92</sub>Na<sub>0.07</sub>)[(Mg<sub>4.01</sub>Fe<sup>2+</sup><sub>0.33</sub>Mn<sup>2+</sup><sub>0.03</sub>)(Fe<sup>3+</sup><sub>0.48</sub>Al<sub>0.15</sub>)][(Si<sub>7.43</sub>Al<sub>0.57</sub>O<sub>22</sub>](OH)<sub>2</sub>].

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3673, 3660w, 3650sh, 3627w, 1099s, 1049s, 993s, 951s, 919s, 755, 725sh, 686, 660, 645sh, 535sh, 507s, 461s, 445sh, 425sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sib153 Ferro-ferriferri-katophorite**  $\text{Na}(\text{NaCa})(\text{Fe}^{2+}_4\text{Fe}^{3+}_4)(\text{Si}_7\text{Al})\text{O}_{22}(\text{OH})_2$ 

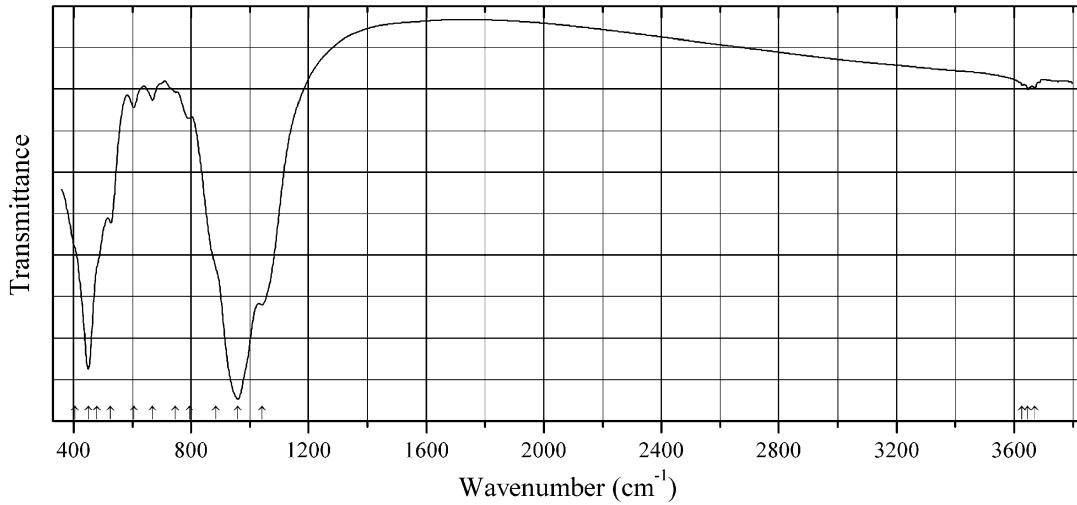
**Origin:** In den Dellen (Ziegłowski) pumice quarry, 1.5 km NE of Mendig, Laacher See volcano, Eifel region, Rhineland-Palatinate (Rheinland-Pfalz), Germany.

**Description:** Black crystals on sanidinite. Characterized by Mössbauer spectrum. The empirical formula is (electron microprobe):  $(\text{Na}_{0.68}\text{K}_{0.32})(\text{Ca}_{1.31}\text{Na}_{0.69})(\text{Mg}_{1.17}\text{Fe}^{2+}_{1.79}\text{Mn}_{0.66}\text{Fe}^{3+}_{1.19}\text{Ti}_{0.19})(\text{Si}_{6.20}\text{Al}_{1.80}\text{O}_{22})(\text{OH})_{1.92}\text{O}_{0.08}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3667w, 3655sh, 3647w, 1050s, 953s, 795sh, 738, 667, 613, 490sh, 452s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sib154 Ferro-pargasite**  $\text{NaCa}_2(\text{Fe}^{2+}_4\text{Al})(\text{Si}_6\text{Al}_2)\text{O}_{22}(\text{OH})_2$ 

**Origin:** Ilmeny (Il'menskie) Mts., South Urals, Russia.

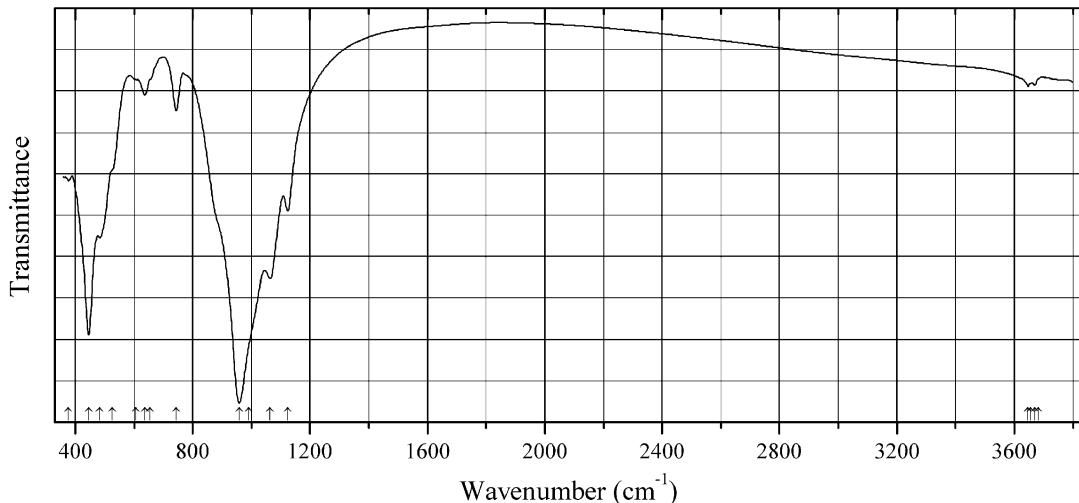
**Description:** Black grains with blue streak from fenite. The empirical formula is (electron microprobe):  $K_{0.4}Na_{1.5}Ca_{1.1}(Fe_{3.2}Mg_{0.8}Mn_{0.3}Al_{0.6}Ti_{0.1})(Si_{6.3}Al_{1.7}O_{22})(OH)_2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3670w, 3647w, 3627w, 1041s, 960s, 885sh, 794, 747w, 669, 605, 526, 480sh, 450s, 405sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sib155 Ferro-ferriniybøite**  $NaNa_2(Fe^{2+}Fe^{3+})_2(Si_7Al)O_{22}(OH)_2$



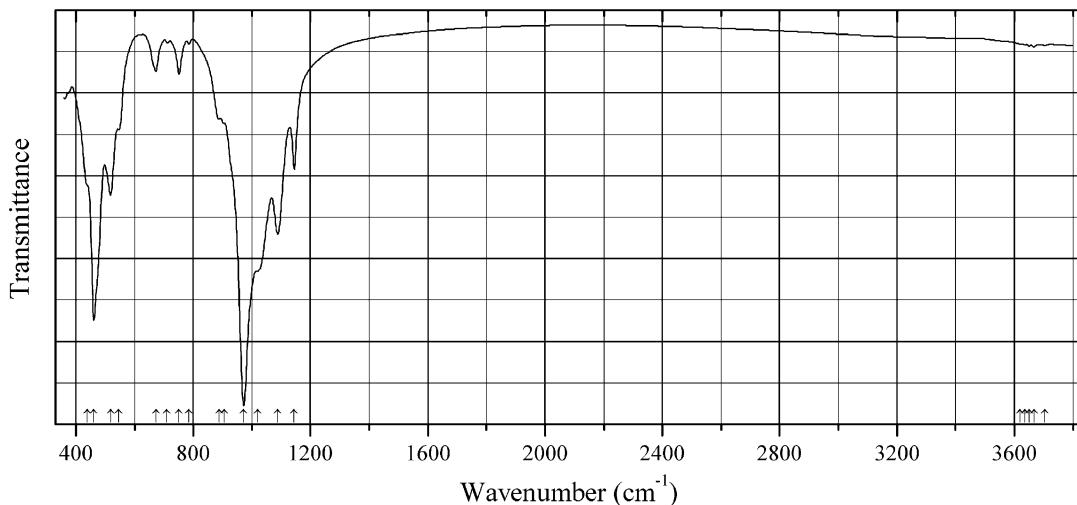
**Origin:** Poudrette quarry, Mont Saint-Hilaire, La Vallée-du-Richelieu RCM, Montérégie (Rouville) Co., Québec, Canada (type locality).

**Description:** Black crystals from the association with a eudialyte-group mineral, an astrophyllite-group mineral, albite, and nepheline. Fragment of the holotype sample kindly granted by A.V. Kasatkin. The crystal structure is solved. Monoclinic, space group  $C2/m$ ,  $a = 9.9190(5)$ ,  $b = 18.0885(8)$ ,  $c = 5.3440(3)$  Å,  $\beta = 103.813(1)$ °,  $V = 931.09(13)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 3.424$  g/cm<sup>3</sup>. The empirical formula is  $(Na_{0.68}K_{0.27})(Na_{1.83}Ca_{0.17})(Mg_{0.06}Fe^{2+}_{3.17}Mn_{0.31}Zn_{0.01}Fe^{3+}_{1.36}Ti_{0.06})(Si_{7.41}Al_{0.59}O_{22})(OH)_{1.58}F_{0.42}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 8.520 (100) (110), 3.162 (55) (310), 2.834 (24) (330), 1.671 (19) (461), 2.732 (10) (151), 2.552 (10) (-202), 2.344 (9) (-351), 3.298 (7) (240), 2.606 (6) (061), 1.446 (6) (-661, 4.10.0).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3683sh, 3670w, 3655w, 3647w, 1124, 1064s, 990sh, 959s, 744, 655sh, 637, 607w, 525sh, 483, 446s, 376.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sib156 Potassic-magnesio-fluoro-arfvedsonite**  $\text{KNa}_2(\text{Mg}_4\text{Fe}^{3+})\text{Si}_8\text{O}_{22}\text{F}_2$ 

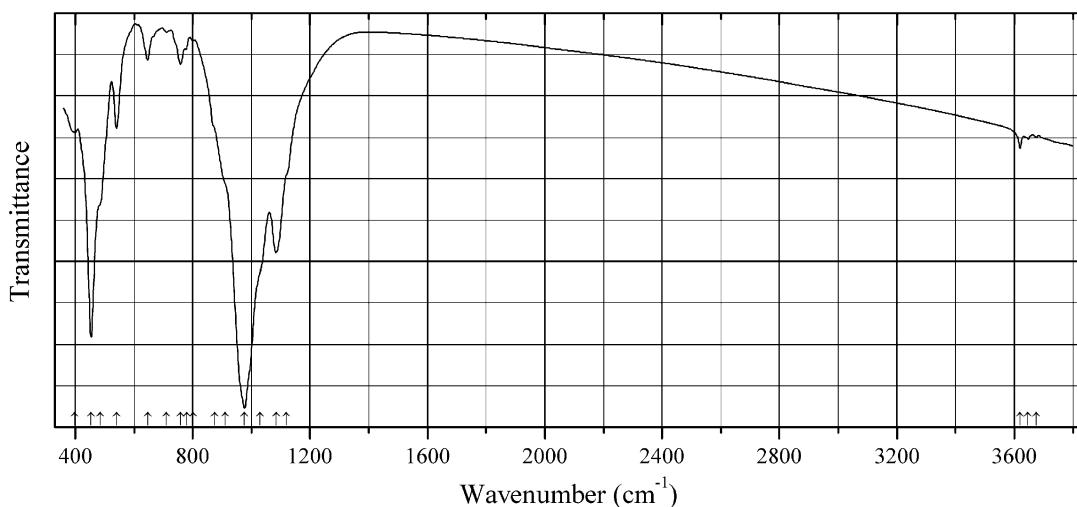
**Origin:** Highway 366 road cut, Val-des-Monts, Québec, Canada (type locality).

**Description:** Fragment of the holotype sample kindly granted by A.V. Kasatkin.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm⁻¹):** 3704w, 3667w, 3651w, (3636w), (3619w), 1144, 1088s, 1020s, 972s, 905sh, 890, 785w, 752, 711w, 673, 546, 518s, 461s, 440sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sib157 Ferro-ferriferro-fluoro-leakeite**  $\text{NaNa}_2(\text{Fe}^{2+}, \text{Fe}^{3+}, \text{Li})\text{Si}_8\text{O}_{22}\text{F}_2$ 

**Origin:** Aryskan REE deposit, Tyva Republic, Russia.

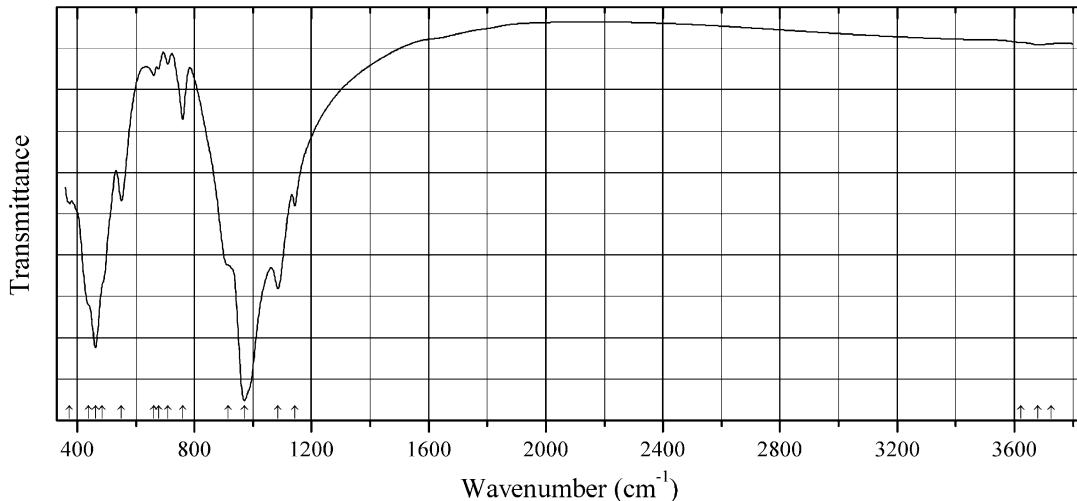
**Description:** Black prismatic crystals from the association with aegirine, polylithionite, quartz, and albite. Investigated by A.V. Kasatkin. The empirical formula is (electron microprobe, Li calculated):  $(\text{Na}_{0.46}\text{K}_{0.32})\text{Na}_{2.00}(\text{Mg}_{0.09}\text{Fe}^{2+}_{1.99}\text{Li}_{0.80}\text{Mn}_{0.10}\text{Zn}_{0.06}\text{Fe}^{3+}_{1.73}\text{Al}_{0.16}\text{Ti}_{0.06})(\text{Si}_{8.00}\text{O}_{22})\text{F}_{1.42}(\text{OH})_{0.58}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3674w, 3646w, 3620w, 1120sh, 1084s, 1030sh, 977s, 910sh, 875sh, (801w), (779w), 758, 710w, 646, 540, 485sh, 454s, 397.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sib160 Ferri-fluoro-leakeite** NaNa<sub>2</sub>(Mg<sub>2</sub>Fe<sup>3+</sup><sub>2</sub>Li)Si<sub>8</sub>O<sub>22</sub>F<sub>2</sub>



**Origin:** Norra Kärr, Gränna, Jönköping, Småland, Sweden.

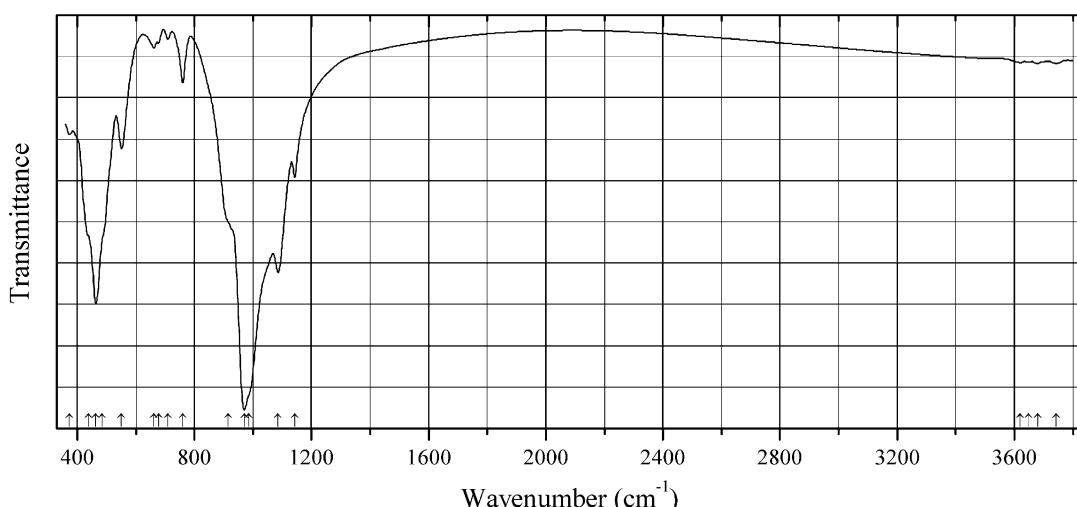
**Description:** Dark green prismatic crystals from the association with aegirine and albite. The empirical formula is (electron microprobe; ICP MS analysis for Li): (Na<sub>0.55</sub>K<sub>0.44</sub>)(Na<sub>1.97</sub>Ca<sub>0.02</sub>Mn<sub>0.01</sub>) (Mg<sub>1.78</sub>Mn<sub>0.09</sub>Zn<sub>0.06</sub>)Li<sub>1.05</sub>(Fe<sub>1.44</sub>Al<sub>0.51</sub>Ti<sub>0.08</sub>)(Si<sub>7.83</sub>Al<sub>0.17</sub>O<sub>22</sub>)F<sub>1.18</sub>(OH)<sub>0.82</sub>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** (3727w), 3681w, 3622w, 1143, 1085s, 971s, 915sh, 760, 710w, 679w, 661, 551, 485sh, 462s, 439sh, 374.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sib161 Ferri-leakeite** NaNa<sub>2</sub>(Mg<sub>2</sub>Fe<sup>3+</sup><sub>2</sub>Li)Si<sub>8</sub>O<sub>22</sub>(OH)<sub>2</sub>



**Origin:** Norra Kärr, Gränna, Jönköping, Småland, Sweden.

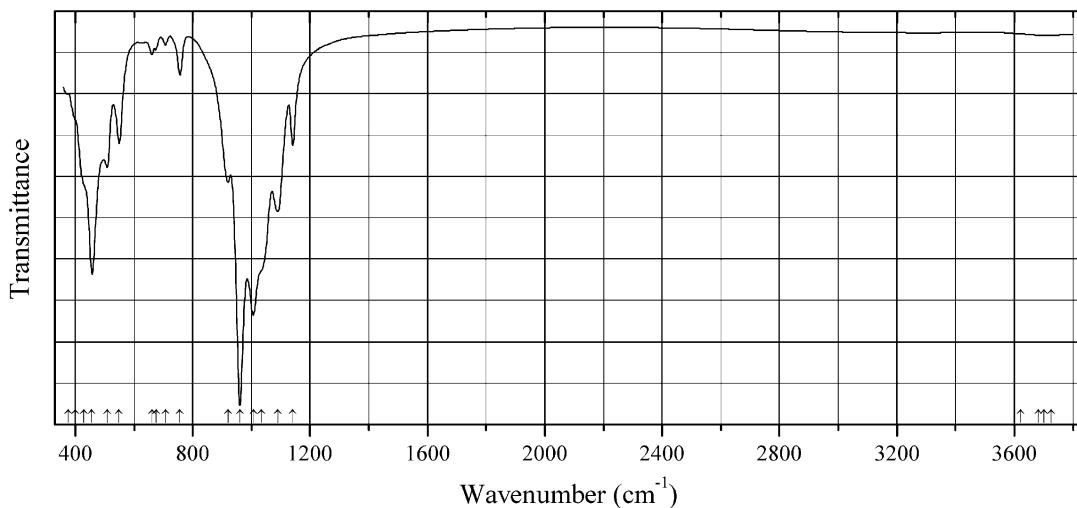
**Description:** Dark green prismatic crystals from the association with aegirine and albite. Characterized by Mössbauer spectroscopy. The empirical formula is (electron microprobe; ICP MS analysis for Li):  $(Na_{0.56}K_{0.44})(Na_{1.90}Mn_{0.08}Ca_{0.02})(Mg_{1.88}Fe^{2+}_{0.10}Mn_{0.02})Li_{1.12}(Fe^{3+}_{1.08}Al_{0.50}Fe^{2+}_{0.24}Ti_{0.06})(Si_{7.97}Al_{0.03}O_{22})(OH)_{1.11}F_{0.89}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** (3742w), 3680w, 3648w, 3620w, 1143, 1086s, 985sh, 971s, 915sh, 761, 710w, 679w, 661, 551, 485sh, 464s, 440sh, 374.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sib162 Potassic-ferri-leakeite**  $KNa_2(Mg_2Fe^{3+}_2Li)Si_8O_{22}(OH)_2$



**Origin:** Kedykverpakhk Mt., Lovozero alkaline complex, Kola peninsula, Murmansk region, Russia.

**Description:** Greenish-gray fibrous aggregate from the association with natrolite and ussingite.

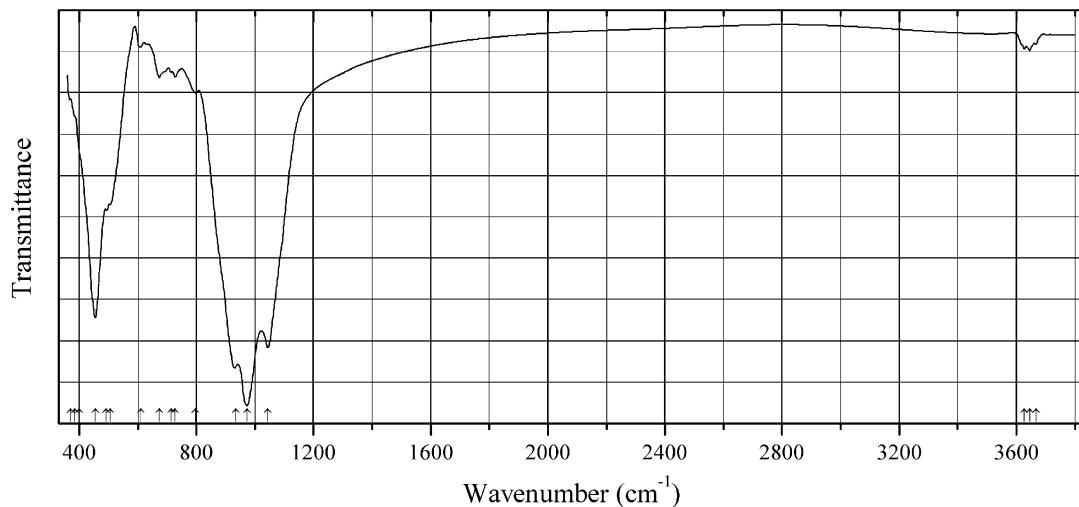
Investigated by I.V. Pekov.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3727w, 3701w, 3683w, 3622w, 1141, 1089s, 1035sh, 1007s, 961s, 920, 757, 707w, 675w, 661, 549, 508, 457s, 430sh, 400sh, 375.

**Note:** Actually, this sample may be the F-dominant analogue of potassic-ferri-leakeite. The spectrum was obtained by N.V. Chukanov.

**Sib163 Potassic-ferro-pargasite**  $KCa_2(Fe^{2+}Al)(Si_6Al_2)O_{22}(OH)_2$



**Origin:** Sal'nye Tundry Mts., Kola Peninsula, Russia.

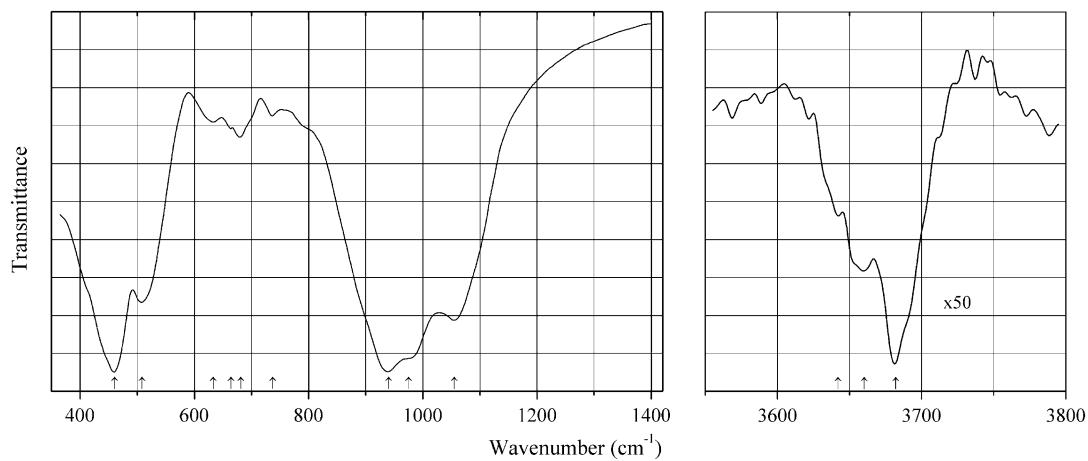
**Description:** Black grains from the association with chlorapatite, almandine, diopside, enstatite, Cl-rich biotite, potassio-chloropargasite, marialite, and plagioclase. The empirical formula is (electron microprobe):  $(K_{0.55}Na_{0.42})(Ca_{1.98}Na_{0.02})(Mg_{1.98}Fe^{2+}_{2.11}Al_{0.65}Ti_{0.26})(Si_{6.03}Al_{1.97}O_{22})(OH)_{1.62}Cl_{0.38}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3667w, 3645w, 3627w, 1044s, 973s, 934s, 798, 727, 715, 674, 611w, 507, 493, 455s, 401sh, 385sh, 370.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sib164 Oxo-magnesio-hastingsite**  $\text{NaCa}_2(\text{Mg}_2\text{Fe}^{3+}_3)(\text{Si}_6\text{Al}_2)\text{O}_{22}\text{O}_2$



**Origin:** Deeti volcanic cone, Gregory rift, northern Tanzania (type locality).

**Description:** Brown megacryst from volcanic tuff. Holotype sample. The crystal structure is solved.

Monoclinic, space group  $C2/m$ ,  $a = 9.8837(3)$ ,  $b = 18.0662(6)$ ,  $c = 5.3107(2)$  Å,  $\beta = 105.278(1)^\circ$ ,  $V = 914.77(5)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{meas}} = 3.19(1)$  g/cm $^3$ . Optically biaxial (−),  $\alpha = 1.706(2)$ ,  $\beta = 1.715(2)$ ,  $\gamma = 1.720(2)$ . The empirical formula is  $(\text{Na}_{0.67}\text{K}_{0.33})(\text{Ca}_{1.87}\text{Mn}_{0.14}\text{Mn}_{0.01})(\text{Mg}_{3.27}\text{Fe}^{3+}_{1.25}\text{Ti}_{0.44}\text{Al}_{0.08})(\text{Si}_{6.20}\text{Al}_{1.80}\text{O}_{22})[\text{O}_{1.40}(\text{OH})_{0.60}]$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 3.383 (62) (131), 2.708 (97) (151), 2.555 (100) (−202), 2.349 (29) (−351), 2.162 (36) (261).

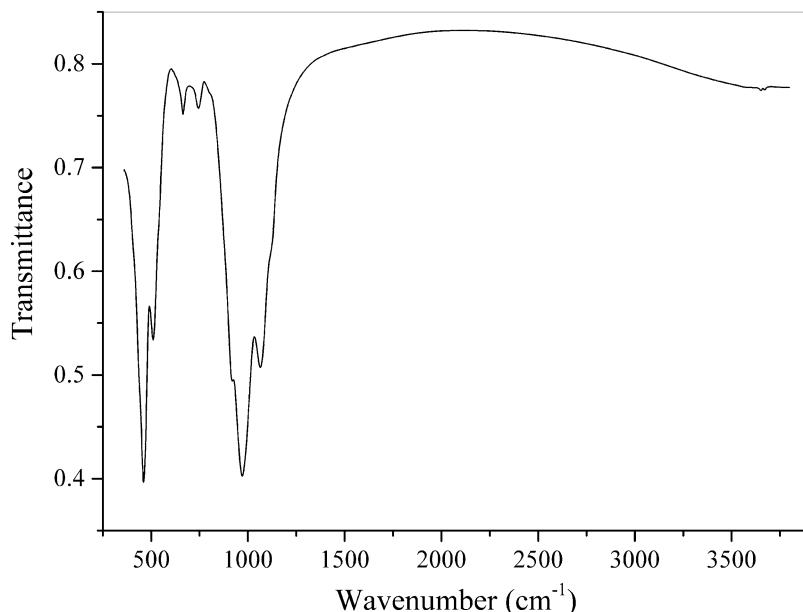
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Zaitsev et al. (2013).

**Wavenumbers (cm $^{-1}$ ):** 3682w, 3660w, 3642w, 1055s, 975sh, 940s, 737w, 681, 664, 633, 508s, 460s.

**Note:** The band positions denoted by Zaitsev et al. (2013) as 3662, 3652, and 3645 cm $^{-1}$  were determined by us at 3682, 3660, and 3642 cm $^{-1}$ , respectively.

### Sib165 Ferri-fluoro-katophorite $\text{Na}(\text{CaNa})(\text{Mg}_4\text{Fe}^{3+})(\text{AlSi}_7\text{O}_{22})\text{F}_2$



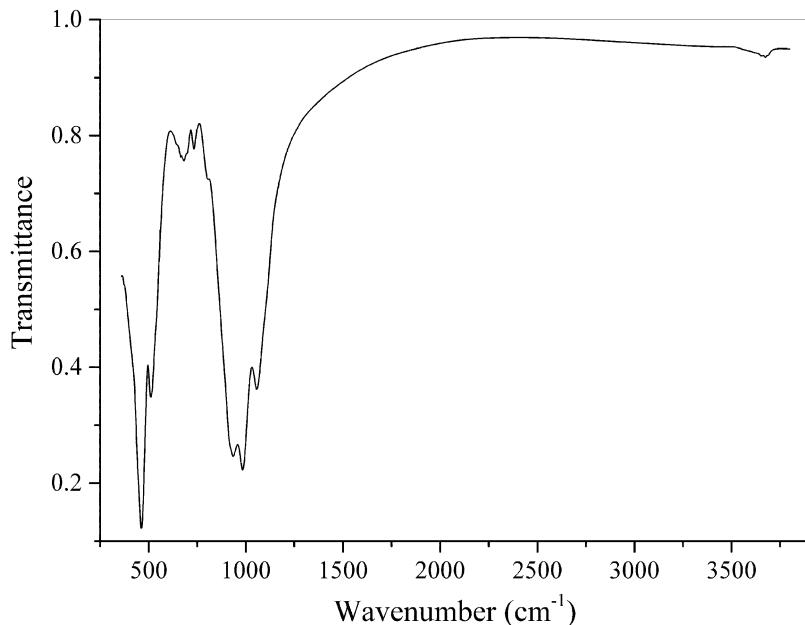
**Origin:** Bear Lake diggings, Monmouth township, Haliburton Co., Ontario, Canada (type locality).

**Description:** Black crystal. Fragment of holotype.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm $^{-1}$ ):** 3671w, 3652w, 1115sh, 1065s, 971s, 922s, 805sh, 745, 664, 510s, 460s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sib166 Fluoro-pargasite**  $\text{NaCa}_2\text{Mg}_4\text{Al}(\text{Al}_2\text{Si}_6\text{O}_{22})(\text{F},\text{OH})_2$ 

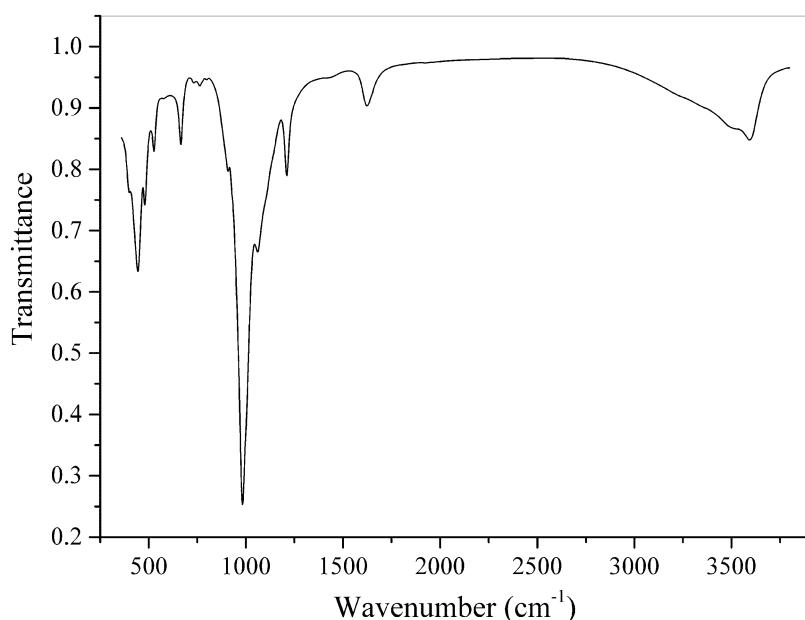
**Origin:** Pargas (Parainen), Southwestern Finland Region, Finland.

**Description:** Dark green crystals from the association with fluorphlogopite and calcite. The empirical formula is (electron microprobe):  $(\text{Na}_{0.7}\text{K}_{0.3})\text{Ca}_{2.0}(\text{Mg}_{3.6}\text{Fe}_{0.7}\text{Al}_{0.6}\text{Ti}_{0.1})(\text{Si}_{6.4}\text{Al}_{1.6}\text{O}_{22})\text{F}_{1.7}(\text{OH})_{0.3}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm⁻¹):** 3688w, 3674w, 3653w, 3630w, 1056s, 984s, 935s, 925sh, 808, 734, 695sh, 681, 667, 650sh, 510s, 462s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sib167 Tobermorite**  $[\text{Ca}_4\text{Si}_6\text{O}_{17} \cdot 2\text{H}_2\text{O}](\text{Ca} \cdot 3\text{H}_2\text{O})$ 

**Origin:** Pervomaiskiy quarry, Crimea, Russia.

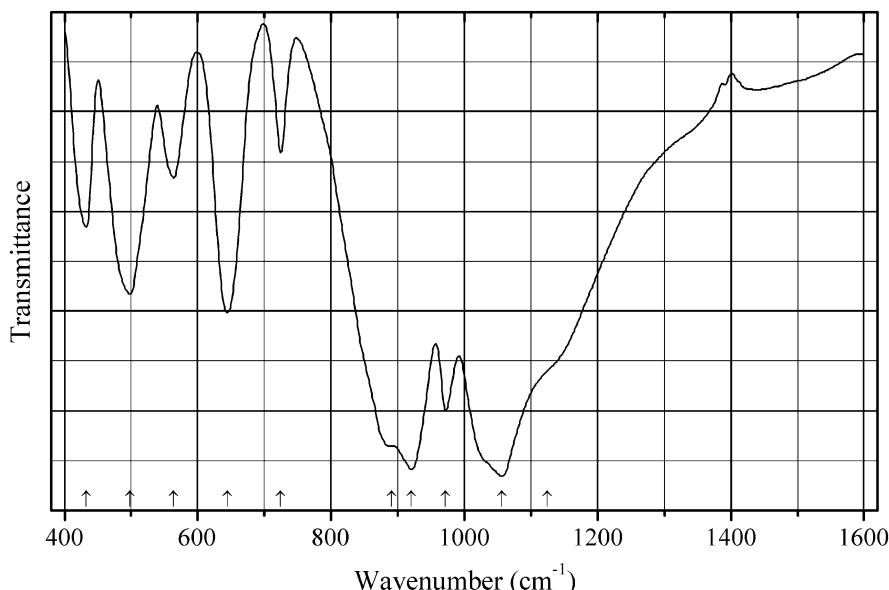
**Description:** White fibrous aggregate from the association with prehnite and laumontite. Investigated by I.S. Lykova. The empirical formula is (electron microprobe):  $\text{Ca}_{4.68}\text{Si}_6\text{O}_{15}(\text{O},\text{OH})_2 \cdot n\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3594, 3525sh, 3355sh, 3240sh, 1624, 1420w, 1211, 1061, 983s, 910, 798w, 764w, 732w, 665, 527, 480, 444s, 402.

**Note:** The spectrum was obtained by N.V. Chukanov.

### Sir199 Colinowensite $\text{BaCuSi}_2\text{O}_6$



**Origin:** Synthetic.

**Description:** Prepared hydrothermally from  $\text{BaCl}_2 \cdot 4\text{H}_2\text{O}$ ,  $\text{Na}_2\text{SiO}_3 \cdot 9\text{H}_2\text{O}$ , and  $\text{CuO}$  at 250 °C for 48 h. Characterized by powder X-ray diffraction data. Tetragonal, space group  $I4_1/acd$ ,  $a = 9.97511(17)$ ,  $c = 22.2887(5)$  Å,  $V = 2217.79(7)$  Å<sup>3</sup>,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Chen et al. (2014b).

**Wavenumbers (cm<sup>-1</sup>):** 1125sh, 1057s, 972, 920s, 891sh, 724, 644, 564, 498, 432.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### Sir200 Gerenite-(Y) $(\text{Ca},\text{Na})_2\text{Y}_3\text{Si}_6\text{O}_{18} \cdot 2\text{H}_2\text{O}$

**Origin:** Strange Lake peralkaline complex, Quebec-Labrador boundary, Canada (type locality).

**Description:** Creamy aggregate. Holotype sample. Triclinic,  $a = 9.245(5)$ ,  $b = 9.684(6)$ ,  $c = 5.510(3)$  Å,  $\alpha = 97.44(6)^\circ$ ,  $\beta = 100.40(6)^\circ$ ,  $\gamma = 116.70(6)^\circ$ .  $D_{\text{calc}} = 3.46$  g/cm<sup>3</sup>. Optically biaxial (−),  $\alpha = 1.602(l)$ ,  $\beta = 1.607(1)$ ,  $\gamma = 1.611(1)$ ,  $2V = 73(3)^\circ$ .

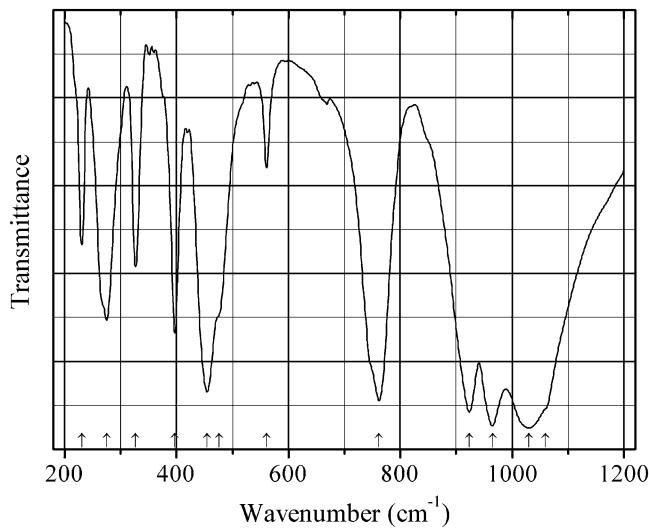
**Kind of sample preparation and/or method of registration of the spectrum:** No data.

**Source:** Jambor et al. (1998).

**Wavenumbers (cm<sup>-1</sup>):** 3480, 1655, 943, 668, 430, 340, 328, 306.

**Note:** Some other bands overlap with strong bands of admixed quartz.

**Sir201 Pabstite BaSnSi<sub>3</sub>O<sub>9</sub>**



**Origin:** Synthetic.

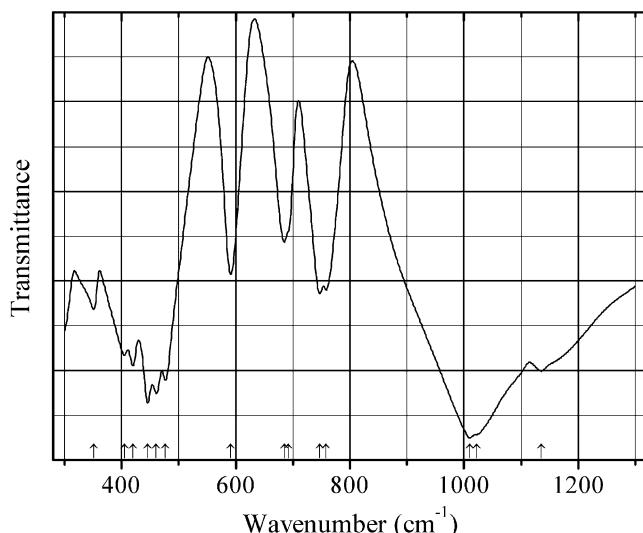
**Description:** Synthesized using a solid-state reaction technique.

**Kind of sample preparation and/or method of registration of the spectrum:** KI disc. Transmission.

**Source:** Choisnet et al. (1975).

**Wavenumbers (cm<sup>-1</sup>):** 1060sh, 1030s, 965s, 923s, 762s, 561, 476sh, 455s, 397, 327, 275, 231.

**Sir202 Wadeite dimorph K<sub>2</sub>ZrSi<sub>3</sub>O<sub>9</sub>**



**Origin:** Synthetic.

**Description:** Synthesized from a glass having wadeite composition by repeatedly crushing and heating at 973–993 K. Characterized by powder X-ray diffraction data. The structure contains four-membered rings of  $\text{SiO}_4$  tetrahedra.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

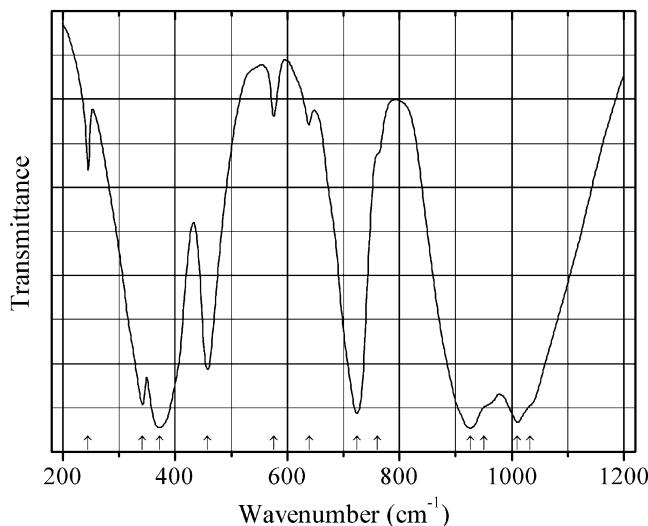
**Source:** Geisinger et al. (1987).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1135, 1022sh, 1010s, 758, 747, 692, 685, 591, 477, 461, 446s, 420, 405, 351.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1154, 1074, 1014w, 800, 744w, 539, 524, 511s, 419s, 400, 339, 311, 304, 215, 179, 149, 111, 90, 67, 52.

### Sir203 Wadeite Rb analogue $\text{Rb}_2\text{TiSi}_3\text{O}_9$



**Origin:** Synthetic.

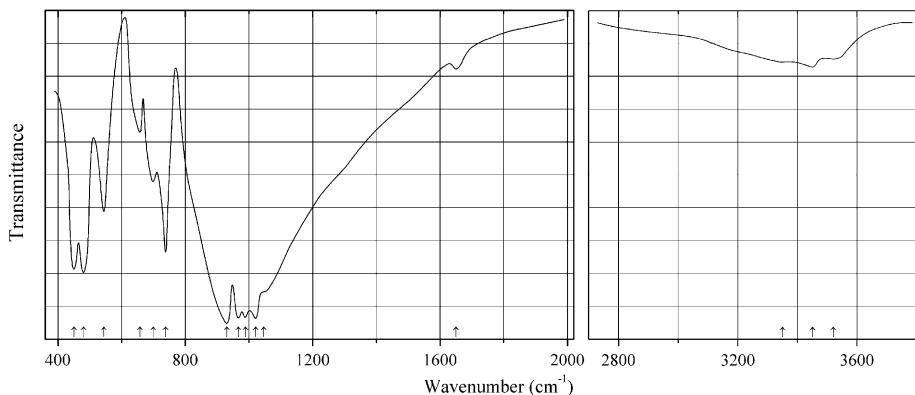
**Description:** Prepared from  $\text{Rb}_2\text{CO}_3$ ,  $\text{TiO}_2$ , and  $\text{SiO}_2$  using a solid-state reaction technique.

**Kind of sample preparation and/or method of registration of the spectrum:** KI disc. Transmission.

**Source:** Choisnet et al. (1975).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1033sh, 1010s, 950sh, 926s, 760sh, 724s, 639w, 576, 458, 372s, 342s, 245.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Sir204 Davinciite**  $\text{Na}_{12}\text{K}_3\text{Ca}_6\text{Fe}^{2+}_3\text{Zr}_3(\text{Si}_{26}\text{O}_{73}\text{OH})\text{Cl}_2$ 

**Origin:** Rasvumchorr Mt., Khibiny alkaline complex, Kola peninsula, Murmansk region, Russia (type locality).

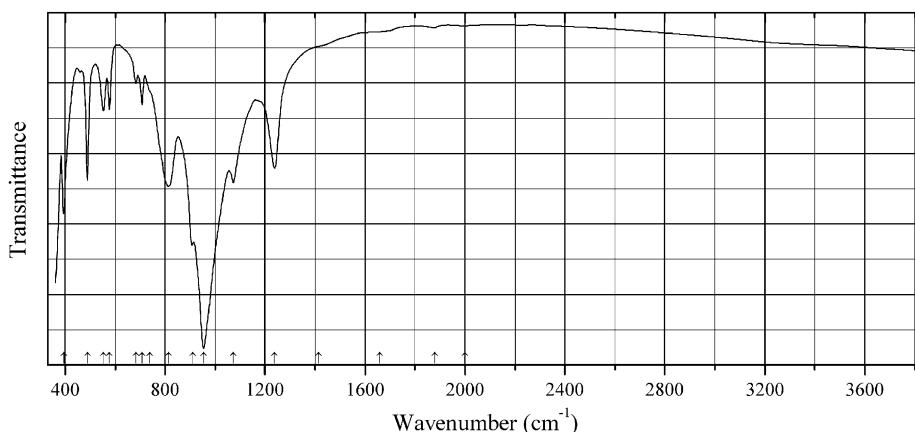
**Description:** Dark lavender grains from the association with nepheline, sodalite, potassium feldspar, delhayelite, aegirine, shcherbakovite, villiaumite, natrite, nacaphite, rasvumite, and djerfisherite. Holotype sample. The crystal structure is solved. Trigonal, space group  $R\bar{3}m$ ,  $a = 14.2956(2)$ ,  $c = 30.0228(5)$  Å,  $V = 5313.6(2)$  Å<sup>3</sup>,  $Z = 3$ .  $D_{\text{meas}} = 2.82(2)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 2.848$  g/cm<sup>3</sup>. Optically uniaxial (+),  $\omega = 1.603(2)$ ,  $\epsilon = 1.605(2)$ . The empirical formula is (electron microprobe, H<sub>2</sub>O calculated):  $(\text{Na}_{11.75}\text{Sr}_{0.29}\text{Ba}_{0.03})(\text{K}_{2.28}\text{Na}_{0.72})\text{Ca}_{5.99}(\text{Fe}_{2.26}\text{Mn}_{0.16})(\text{Zr}_{2.80}\text{Ti}_{0.15}\text{Hf}_{0.03}\text{Nb}_{0.02})(\text{Si}_{1.96}\text{Al}_{0.04})(\text{Si}_3\text{O}_9)_2(\text{Si}_9\text{O}_{27})_2[(\text{OH})_{1.42}\text{O}_{0.58}]\text{Cl}_{1.62}\cdot 0.48\text{H}_2\text{O}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 2.981 (100) (315), 2.860 (96) (404), 4.309 (66) (205), 3.207 (63) (208), 6.415 (54) (104), 3.162 (43) (217).

**Kind of sample preparation and/or method of registration of the spectrum:** No data.

**Source:** Khomyakov et al. (2013).

**Wavenumbers (cm<sup>-1</sup>):** 3520w, 3450w, 3350w, 1650w, 1046sh, 1021s, 989s, 967s, 930s, 738s, 699, 657, 544, 480s, 450s.

**Note:** The band position denoted by Khomyakov et al. (2013) as 3590 cm<sup>-1</sup> was determined by us at 3520 cm<sup>-1</sup>.

**Sir205 Rippite**  $\text{K}_2(\text{Nb},\text{Ti})_2(\text{Si}_4\text{O}_{12})\text{O(O,F)}$ 

**Origin:** Chuktukon carbonatite massif, Chadobets upland, southern Siberian craton, Krasnoyarsky Kray, Russia (type locality).

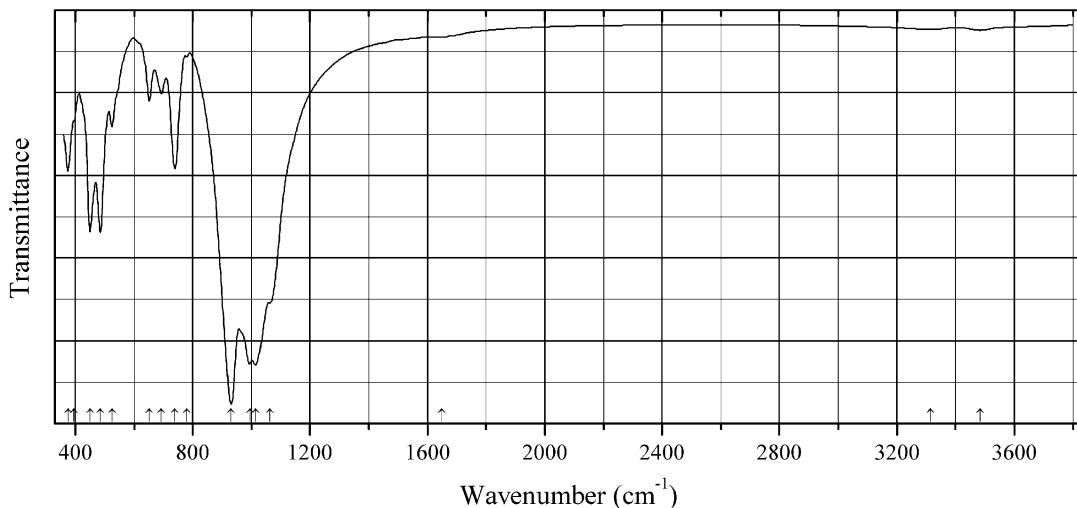
**Description:** Prismatic crystals from the association with pyrochlore-supergroup minerals, quartz, goethite, baryte, monazite-(Ce), K-feldspar, fluorite, fluorapatite, Ca-REE-fluorcarbonates, Nb-rich rutile, olekminskite, aegirine, etc. Holotype sample. The crystal structure is solved. Tetragonal, space group  $P4bm$ ,  $a = 8.7388(2)$  Å,  $c = 8.1277(2)$  Å,  $V = 620.69(2)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{meas}} = 3.17(2)$  g/cm $^3$ ,  $D_{\text{calc}} = 3.198$  g/cm $^3$ . Optically uniaxial (+),  $\omega = 1.738(2)$ ,  $\epsilon = 1.747(2)$ . The empirical formula is (electron microprobe):  $K_{2.00}(Nb_{1.88}Ti_{0.10}Zr_{0.02})(Si_{4.00}O_{12})O(O_{0.88}F_{0.12})$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å (I, %) ( $hkl$ )] are: 6.205 (100) (001), 4.383 (83) (020), 4.082 (90) (002), 3.530 (87) (121), 2.985 (81) (022), 2.822 (70) (122), 2.768 (99) (130).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm $^{-1}$ ):** 1999w, 1878w, 1660w, 1415sh, 1238s, 1073s, 954s, 910s, 813s, 740sh, 707, 683, 577, 552, 489s, 396s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sir206 Dualite**  $Na_{30}(Ca,Na,Ce,Sr)_{12}(Na,Mn,Fe,Ti)_6Zr_3Ti_3MnSi_{51}O_{144}(OH,H_2O,Cl)_9$



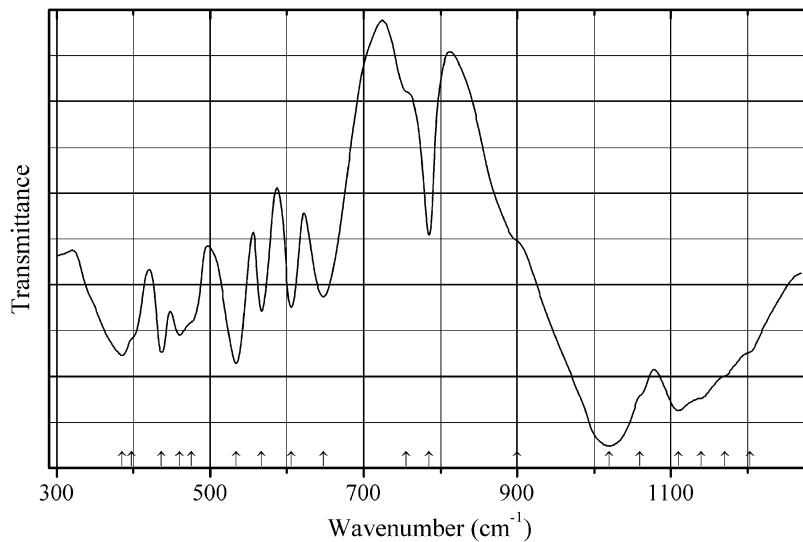
**Origin:** Alluaiv Mt., Lovozerо alkaline complex, Kola peninsula, Murmansk region, Russia (type locality).

**Description:** Yellow anhedral grains from the association with K-Na feldspar, nepheline, sodalite, cancrinite, aegirine, alkaline amphibole, eudialyte, lovozerite, lomonosovite, vuonnemite, lamprophyllite, sphalerite, and villiaumite. Holotype sample. The crystal structure is solved. Trigonal, space group  $R\bar{3}m$ ,  $a = 14.153(9)$  Å,  $c = 60.72(5)$  Å,  $V = 10,533(22)$  Å $^3$ ,  $Z = 3$ .  $D_{\text{meas}} = 2.84$  (3) g/cm $^3$ ,  $D_{\text{calc}} = 2.814$  g/cm $^3$ . Optically uniaxial (+),  $\omega = 1.610(1)$ ,  $\epsilon = 1.613(1)$ . The crystal-chemical formula is  $(Na_{29.79}Ba_{0.1}K_{0.10})_{\Sigma 30}(Ca_{8.55}Na_{1.39}REE_{1.27}Sr_{0.79})(Na_{3.01}Mn_{1.35}Fe^{2+}_{0.87}Ti_{0.77})(Zr_{2.61}Nb_{0.39})(Ti_{2.52}Nb_{0.48})(Mn_{0.82}Si_{0.18})(Si_{50.77}Al_{0.23})O_{144}[(OH)_{6.54}(H_2O)_{1.34}Cl_{0.98}]$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å (I, %) ( $hkl$ )] are: 7.11 (40) (110), 4.31 (50) (0.2.10), 2.964 (100) (1.3.10), 2.839 (90) (048), 2.159 (60) (2.4.10, 0.4.20), 1.770 (60) (2.4.22, 4.0.28, 440), 1362 (50) (5.5.12, 3.0.42).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm $^{-1}$ ):** 3485w, 3314w, 1650w, 1063s, 1015s, 995s, 931s, 780w, 740, 694, 652, 525, 485, 450, 395sh, 375.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sir207 Roedderite Na-free analogue  $K_2Mg_2(Mg_3Si_{12})O_{30}$** 

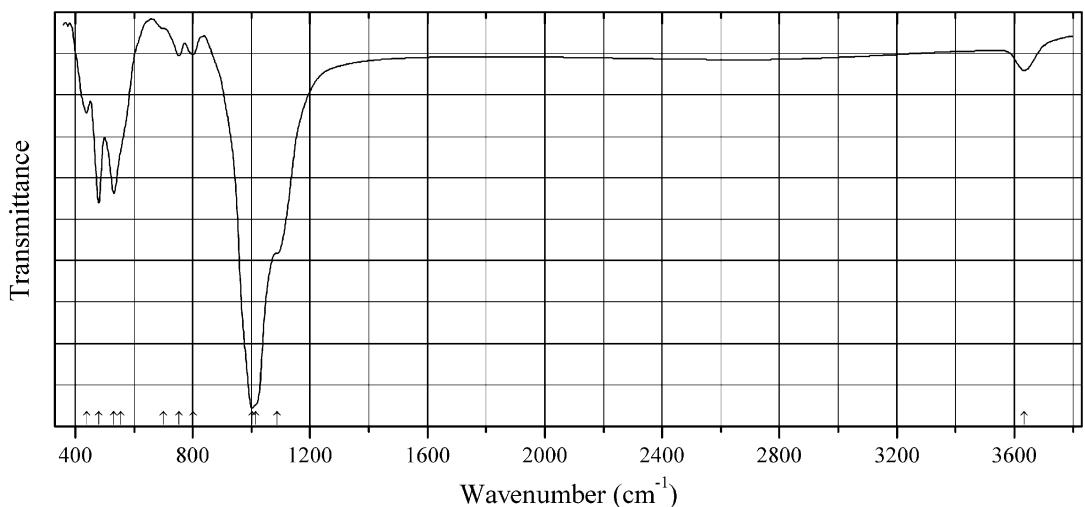
**Origin:** Synthetic.

**Description:** Prepared in a solid-state reaction. The crystal structure is solved. Hexagonal, space group  $P6/mcc$ ,  $a = 10.211$ ,  $c = 14.152 \text{ \AA}$ ,  $V = 1277.8 \text{ \AA}^3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Nguyen et al. (1980).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1203sh, 1170sh, 1140sh, 1110s, 1060sh, 1020s, 900sh, 785, 755sh, 648, 606, 567, 534s, 476sh, 460s, 437s, 398sh, 385s.

**Sil308 Luanshiweiite  $KLiAl_{1.5}(Si_{3.5}Al_{0.5})O_{10}(OH)_2$** 

**Origin:** Ognyovskoe Ta deposit, Ognyovka-Bakennoe pegmatite field, Kalba ridge, Kazakhstan.

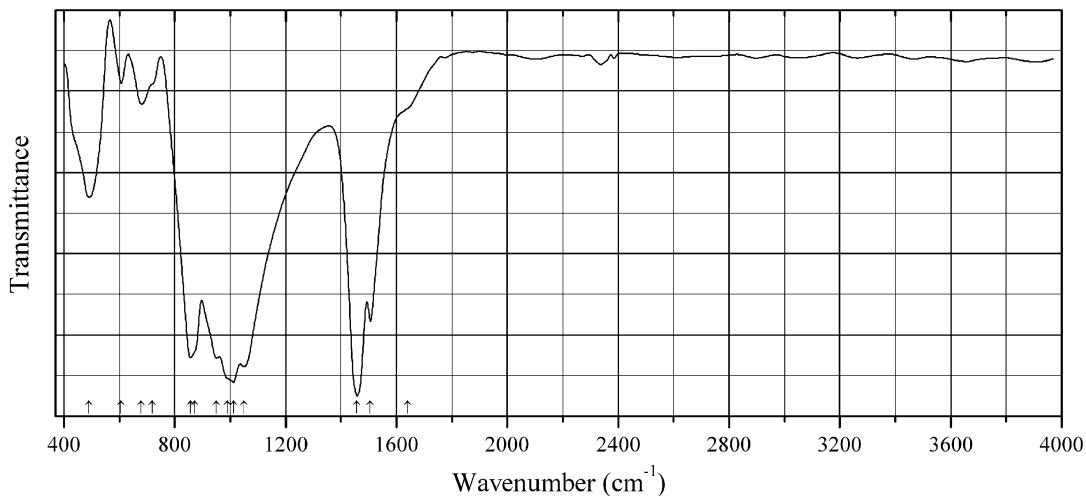
**Description:** Lilac grains from the association with albite, microcline, and quartz. Investigated by A.V. Kasatkin. The empirical formula is  $(K_{0.86}Na_{0.05}Cs_{0.02})(Li_{1.10}Al_{1.51}Mn_{0.09})(Si_{3.26}Al_{0.74}O_{10})(OH)_{1.53}F_{0.47}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3634, 1087s, 1015sh, 1002s, 801, 753, 700sh, 555sh, 531s, 479s, 438.

**Note:** The spectrum was obtained by N.V. Chukanov.

### Sil309 Sodium lithium aluminosilicate $Na_3Li_2(AlSi_2O_8)$ $Na_3Li_2(AlSi_2O_8)$



**Origin:** Synthetic.

**Description:** Synthesized by heating a stoichiometric mixture of  $Li_2CO_3$ ,  $Na_2CO_3$ ,  $Al_2O_3$ , and  $SiO_2$  at 630 °C for 48 h with several intermediate grindings and mixings. Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group  $Cmca$ ,  $a = 14.1045(19)$  Å,  $b = 14.7054(19)$  Å,  $c = 7.0635(9)$  Å,  $V = 1465.1(3)$  Å<sup>3</sup>,  $Z = 8$ .  $D_{\text{calc}} = 2.666$  g/cm<sup>3</sup>. The structure is based on a 2D layer, which is composed of  $[Al_2Si_2O_12]$  rings and  $SiO_4$  tetrahedra.

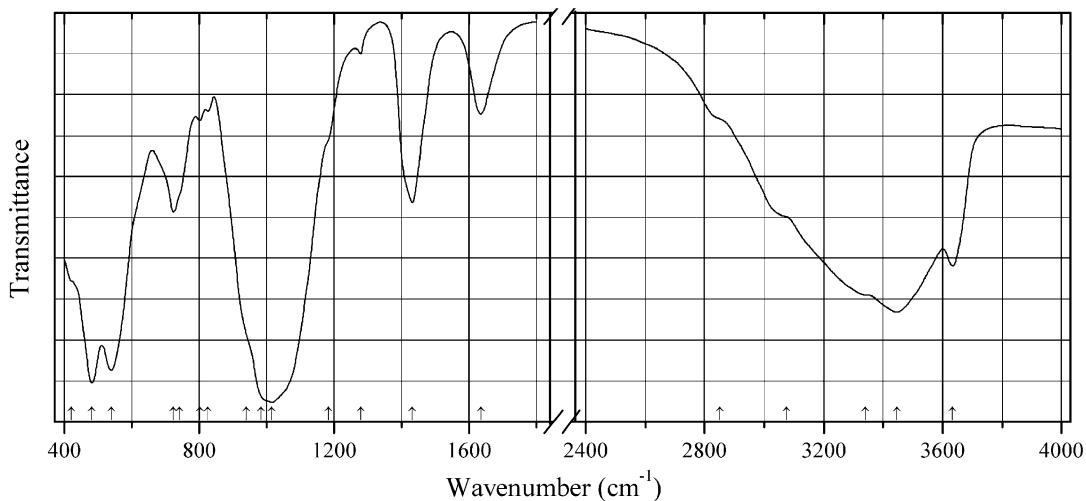
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Han et al. (2013).

**Wavenumbers (cm<sup>-1</sup>):** 1640sh, 1505, 1458s, 1051s, 1012s, 990sh, 951s, 872sh, 858s, 720sh, 680, 607w, 491.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The band at 1458 cm<sup>-1</sup> (erroneously assigned by the authors to the Si–O–Al bridges) indicates that the sample is contaminated by a carbonate.

**Sil310 Tobelite hydrated variety**  $(\text{NH}_4, \text{H}_2\text{O})\text{Al}_2[(\text{Si}, \text{Al})_4\text{O}_{10}](\text{OH})_2 \cdot n\text{H}_2\text{O}$  (?)  
**“Ammonium illite”**



**Origin:** Synthetic.

**Description:** Prepared hydrothermally from metakaolin powder and 25% NH<sub>3</sub> solution at 300 °C for 1 h. Characterized by powder X-ray diffraction data. The basal spacing of the product is 10.74 Å.

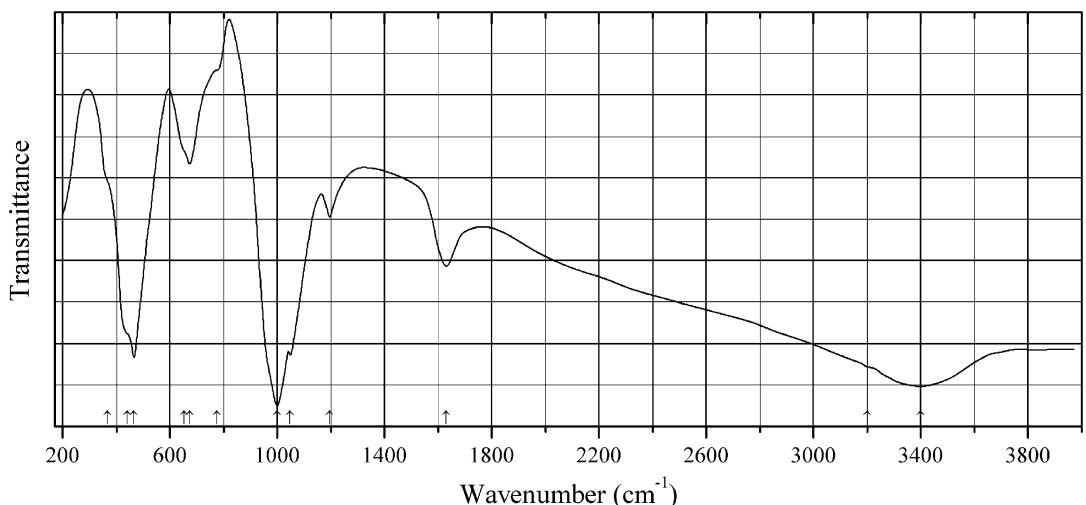
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Wang et al. (2013).

**Wavenumbers (cm<sup>-1</sup>):** 3634, 3446, 3340sh, 3075sh, 2850sh, 1635, 1432, 1278w, 1182sh, 1014s, 982sh, 940sh, 825w, 801w, 741sh, 723, 538s, 481s, 421sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Sil311 Falcondoite** Ni<sub>4</sub>Si<sub>6</sub>O<sub>15</sub>(OH)<sub>2</sub>·6H<sub>2</sub>O



**Origin:** Falcondo Mine, Bonao, La Vega Province, Dominican Republic (type locality).

**Description:** Green sample confirmed by powder X-ray diffraction data.

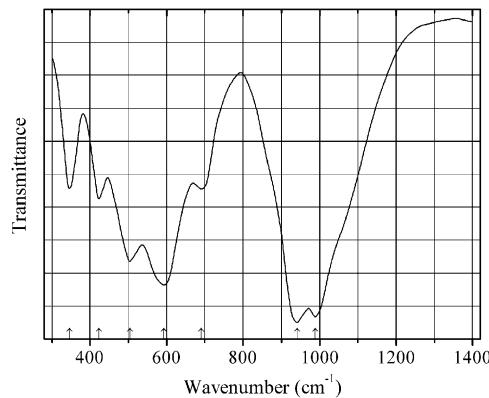
**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull. Transmission.

**Source:** Reddy et al. (1987).

**Wavenumbers (cm<sup>-1</sup>):** 3400, 3200, 1630, 1195, 1048, 1000s, 775sh, 674, 651sh, 465s, 440sh, 365sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### Sil312 Imogolite $\text{Al}_2\text{SiO}_3(\text{OH})_4$



**Origin:** Natural sample; the locality is not indicated.

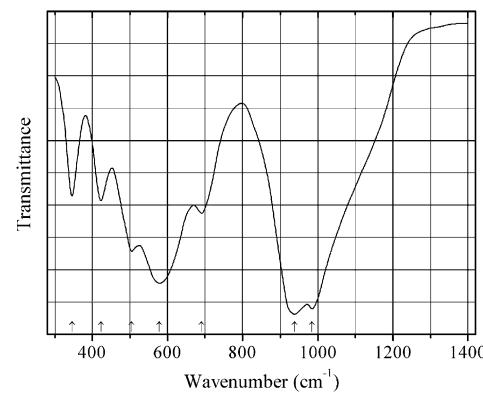
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Farmer et al. (1979).

**Wavenumbers (cm<sup>-1</sup>):** 989s, 941s, 691, 593s, 504, 423, 346.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

### Sil313 Imogolite $\text{Al}_2\text{SiO}_3(\text{OH})_4$



**Origin:** Synthetic.

**Description:** Amorphous product of interaction between hydroxyaluminium and orthosilicic acid in dilute aqueous solutions of pH < 5.

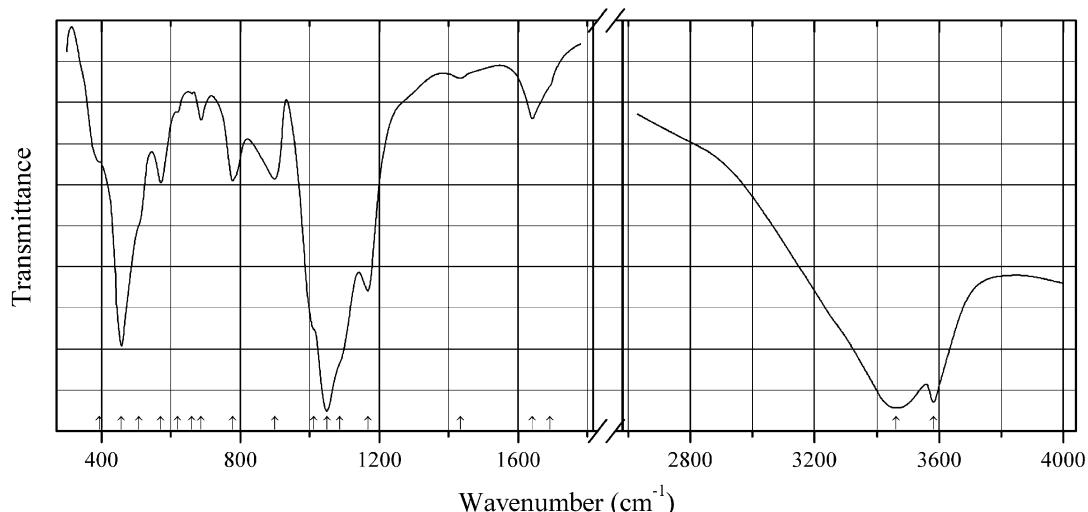
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Farmer et al. (1979).

**Wavenumbers (cm<sup>-1</sup>):** 985s, 938s, 691, 579s, 505, 423, 346.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

## Sil314 Kanemite $\text{HNaSi}_2\text{O}_5 \cdot 3\text{H}_2\text{O}$



**Origin:** Synthetic.

**Description:** Synthesized according to known methods. Characterized by powder X-ray diffraction data.

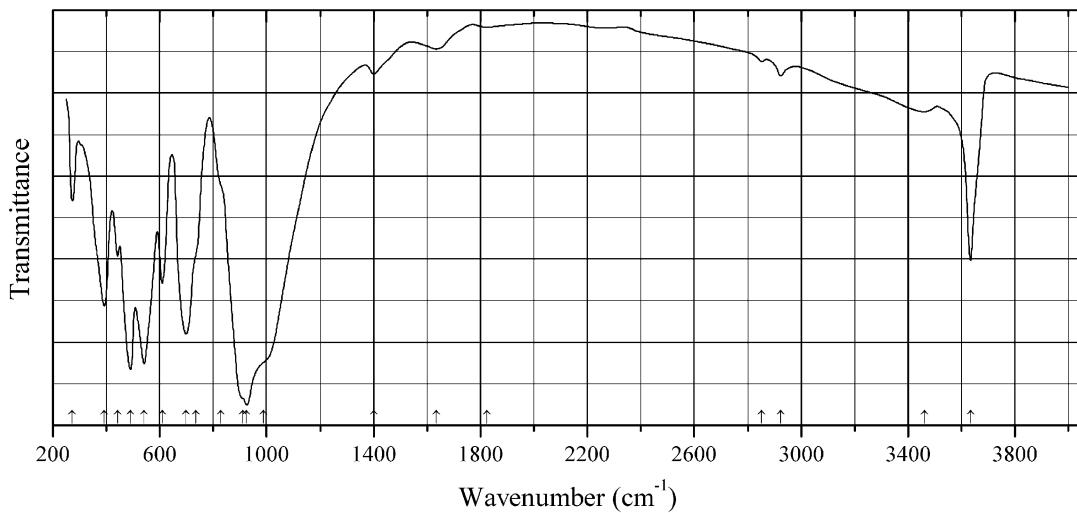
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission

Source: Huang et al. (1998)

**Wavenumbers (IR, cm<sup>-1</sup>)**: 3582, 3463s, 1692sh, 1642, 1433, 1167s, 1087sh, 1049s, 1012sh, 899, 777, 687w, 661w, 619sh, 571, 508sh, 457s, 393sh

Note: In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 3150w, 1060s, 1015s, 788w, 699w, 646w, 503w, 489w, 465s, 419, 372, 285, 261, 237, 185w, 173w, 154w, 137w, 129, 122, 107w, 100w

**Sil315 Margarite**  $\text{CaAl}_2\text{Si}_2\text{Al}_2\text{O}_{10}(\text{OH})_2$ 

**Origin:** Enontekiö, northern Finland.

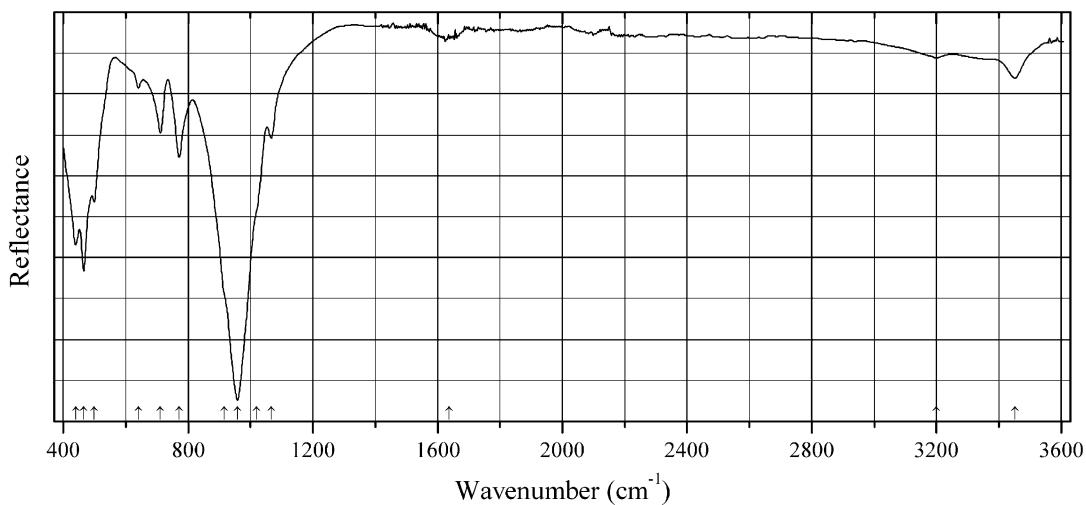
**Description:** A Li- and Be-poor variety.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Lahti and Saikkinen (1985).

**Wavenumbers (cm<sup>-1</sup>):** 3634, 3461w, 1825w, 1634w, 1400w, 987sh, 925s, 910sh, 828sh, 734sh, 698s, 609, 541s, 490s, 442, 392, 273.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. Weak bands in the range from 2800 to 3000 cm<sup>-1</sup> correspond to the admixture of an organic substance.

**Sil316 Plumbophyllite**  $\text{Pb}_2\text{Si}_4\text{O}_{10}\cdot\text{H}_2\text{O}$ 

**Origin:** Blue Bell claims, near Baker, San Bernardino Co., California, USA (type locality).

**Description:** Pale blue prismatic crystals from the association with cerussite, chrysocolla, fluorite, goethite, gypsum, mimetite, opal, plumbotsumite, quartz, sepiolite, and wulfenite. Holotype sample. The crystal structure is solved. Orthorhombic, space group  $Pbcn$ ,  $a = 13.2083(4)$ ,  $b = 9.7832(3)$ ,  $c = 8.6545(2)$  Å,  $V = 1118.33(5)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{meas}} = 3.96(5)$  g/cm $^3$ ,  $D_{\text{calc}} = 3.940$  g/cm $^3$ . Optically biaxial (+),  $\alpha = 1.674(2)$ ,  $\beta = 1.684(2)$ ,  $\gamma = 1.708(2)$ ,  $2V = 66(2)^\circ$ . The empirical formula is  $\text{Pb}_{1.79}\text{Cu}_{0.02}\text{Si}_{4.00}\text{O}_{9.62}(\text{OH})_{0.38} \cdot 1.02\text{H}_2\text{O}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 7.88 (97) (110), 6.63 (35) (200), 4.90 (38) (020), 3.623 (100) (202), 3.166 (45) (130), 2.938 (57) (312, 411, 222), 2.555 (51) (132, 213), 2.243 (50) (521, 332).

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of powdered mineral.

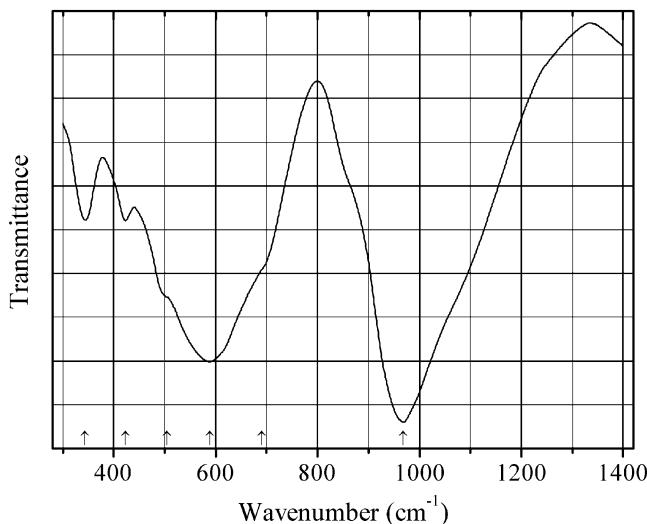
**Source:** Kampf et al. (2009b).

**Wavenumbers (IR, cm $^{-1}$ ):** 3452, 3200w, 1636w, 1067, 1019sh, 958s, 915sh, 771, 711, 640w, 499, 465s, 439s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 3561, 3468, 3338, 3209, 1062, 1024s, 980, 923s, 641, 506, 480, 347, 329, 251, 209, 146, 94s.

### Sil317 Protoimogolite



**Origin:** Synthetic.

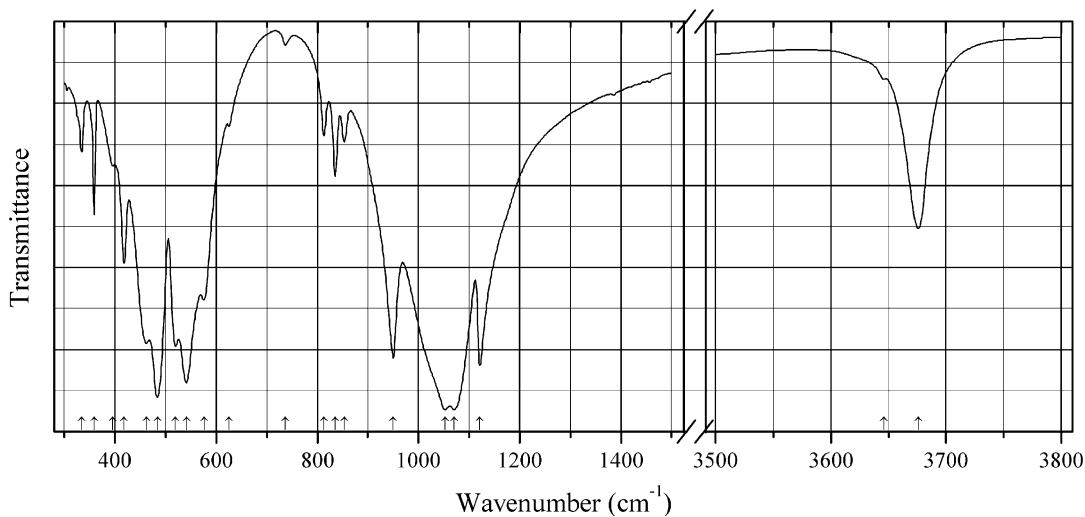
**Description:** Amorphous product of interaction between hydroxyaluminium species and orthosilicic acid in dilute aqueous solutions of pH < 5 at 20 °C.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Farmer et al. (1979).

**Wavenumbers (cm $^{-1}$ ):** 968s, 691sh, 588s, 504sh, 423, 344.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**Sil318 Pyrophyllite**  $\text{Al}_2\text{Si}_4\text{O}_{10}(\text{OH})_2$ 

**Origin:** Nakamuraguchi, Yano-Shokozan area, Hiroshima Prefecture, Japan.

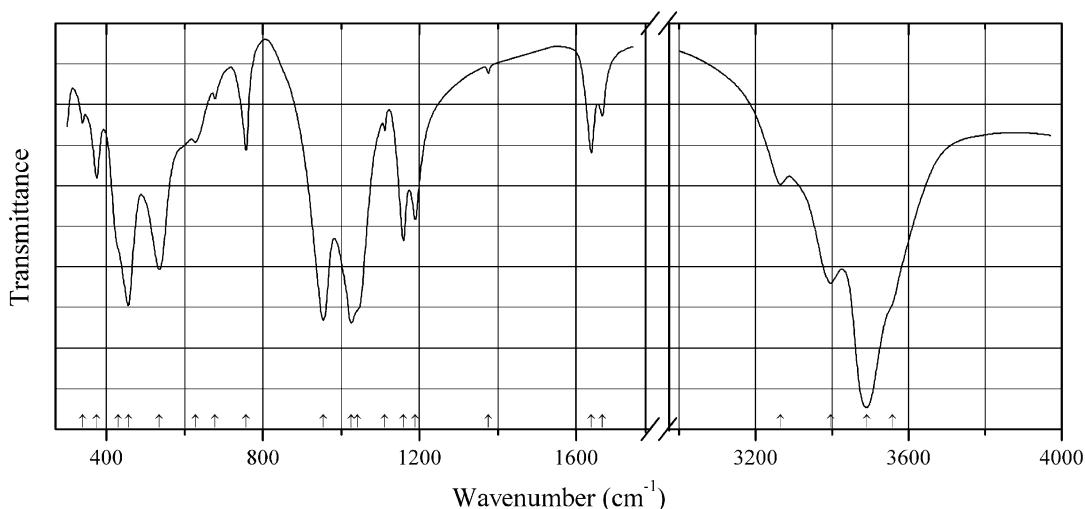
**Description:** Fine-grained aggregate. Characterized by powder X-ray diffraction data and electron microprobe analyses. Triclinic,  $a = 5.16(1)$ ,  $b = 8.96(1)$ ,  $c = 9.37(2)$  Å,  $\alpha = 90.8(2)^\circ$ ,  $\beta = 101.0(2)^\circ$ ,  $\gamma = 89.8(2)^\circ$ . The empirical formula is close to that of the end-member.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Wiewióra and Hida (1996).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3676, 3646, 1121s, 1070s, 1052s, 950s, 853, 835, 813, 737w, 625w, 576, 541s, 520, 484s, 462, 418, 396w, 359, 334w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Sil319 Silinaite**  $\text{NaLiSi}_2\text{O}_5 \cdot 2\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Characterized by powder X-ray diffraction data. Monoclinic, space group  $A2/n$ ,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

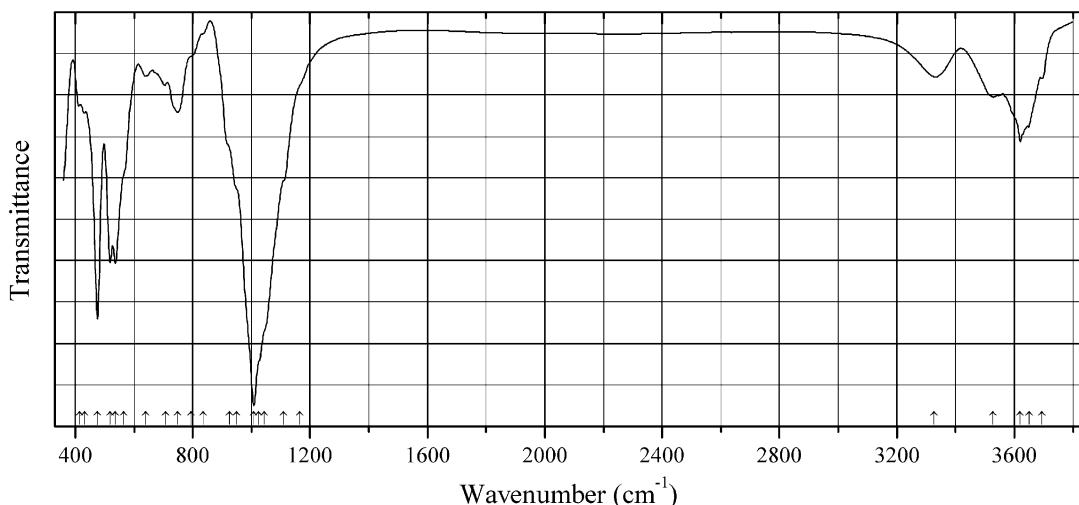
**Source:** Huang et al. (1999a).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3558sh, 3490s, 3396, 3265, 1667, 1639, 1376w, 1189, 1159, 1111, 1042sh, 1026s, 955s, 757, 677w, 627, 535, 456s, 430sh, 375, 339w.

**Note:** The weak band at  $1376 \text{ cm}^{-1}$  corresponds to the admixture of a nitrate in KBr. The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 3472, 3389, 3259, 1652, 1068s, 1000w, 956, 773w, 734w, 635, 609s, 501, 490w, 466, 423, 408, 371, 342, 327, 279, 259, 250, 227, 196, 163, 148, 126, 107.

### Sil320 Cookeite $(\text{Al},\text{Li})_3\text{Al}_2(\text{Si},\text{Al})_4\text{O}_{10}(\text{OH})_8$



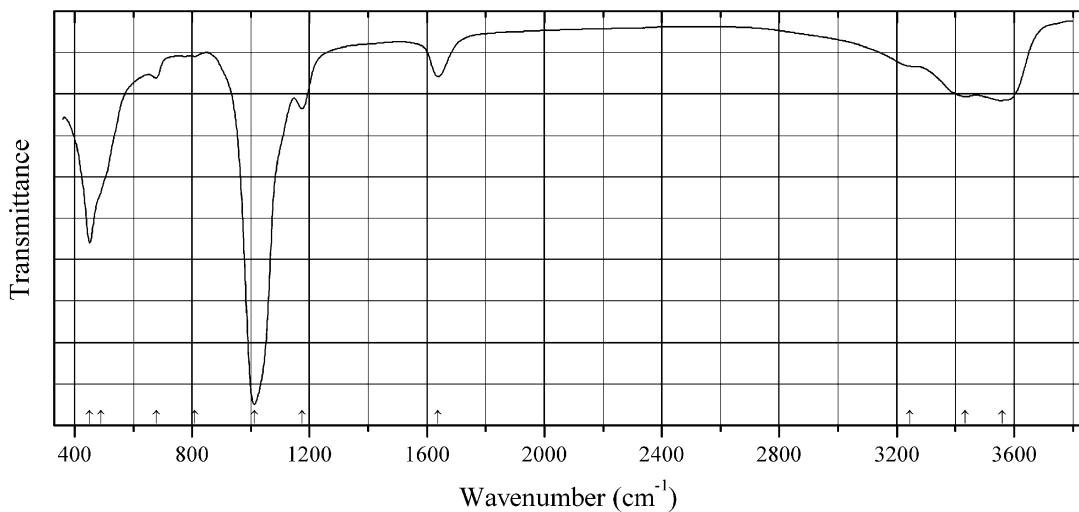
**Origin:** Nagol'nyi Kryazh, Lugansk region, Ukraine (type locality).

**Description:** White scales with pearly lustre from the association with quartz. Investigated by A.V. Kasatkin and Y.V. Bychkova. The empirical formula is  $\text{Li}_{0.92}\text{Al}_{3.97}(\text{Si}_{3.29}\text{Al}_{0.71}\text{O}_{10})(\text{OH},\text{O})_8$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3694, 3650, 3620, 3528, 3327, 1165sh, 1110sh, 1045sh, 1025sh, 1008s, 950sh, 925sh, 835sh, 795sh, 749, 707w, 639w, 565sh, 536s, 518s, 475s, 432w, 415w.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sil321 Windhoekite Na-bearing variety**  $(\text{Ca},\text{Na})_2\text{Fe}^{3+}_{3+x}[\text{Si},\text{Al}]_8\text{O}_{20}](\text{OH})_4 \cdot n\text{H}_2\text{O}$ 


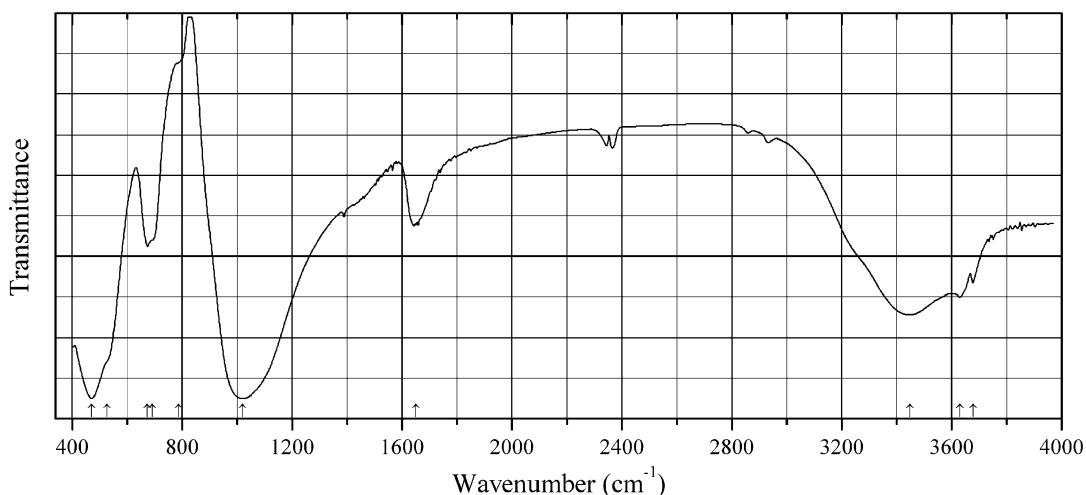
**Origin:** Ariskop Quarry, Aris, near Windhoek, Windhoek district, Khomas Region, Namibia (type locality).

**Description:** Clusters of brown acicular crystals from the association with fluorapofillite, aegirine, and microcline. The crystal structure is solved. Monoclinic, space group  $C2/m$ ,  $a = 14.0626(3)$ ,  $b = 17.9007(8)$ ,  $c = 5.2527(2)$  Å,  $\beta = 104.4(6)^\circ$ ,  $V = 1280.3(2)$  Å<sup>3</sup>,  $Z = 2$ . A specific feature of Na-rich windhoekite is the presence of the fivefold coordination  $M(4)$ -site occupied by Ca and Na in the atomic ratio 1:1, which is attached to a ribbon consisting of Fe<sup>3+</sup>- and Ca-centered octahedra and sandwiched between two opposing tetrahedral ribbons. The empirical formula is (electron microprobe):  $\text{K}_{0.08}\text{Na}_{0.42}\text{Ca}_{1.15}\text{Fe}^{3+}_{3.52}\text{Mn}_{0.41}\text{Cr}_{0.04}\text{Ti}_{10.10}(\text{Si}_{7.44}\text{Al}_{0.56})\text{O}_{20}(\text{OH})_x \cdot n\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3558, 3434, 3245w, 1636, 1175, 1012s, 810w, 678w, 490sh, 452s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sil322 Stevensite**  $(\text{Ca},\text{Na})_x\text{Mg}_{3-y}\text{Si}_4\text{O}_{10}(\text{OH})_2$ 


**Origin:** Ghassoul locality, Atlas Mts., Morocco.

**Description:** Characterized by powder X-ray diffraction data, thermal and chemical analyses. Basal spacing value is equal to 13.5 Å. Weight loss on ignition at 1000 °C is 7.19%.

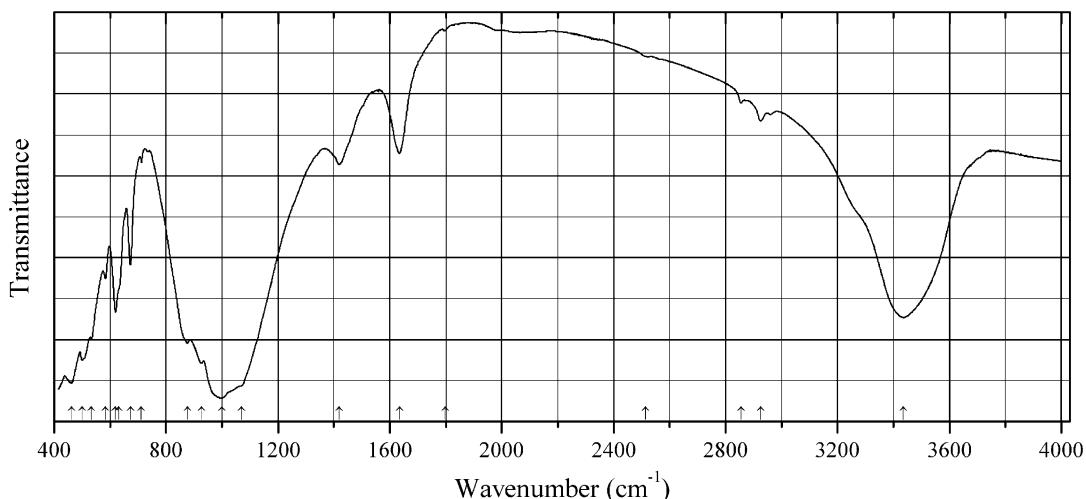
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Benhammou et al. (2011).

**Wavenumbers (cm<sup>-1</sup>):** 3678, 3630, 3447, 1650, 1022s, 787sh, 692sh, 675, 527sh, 471s.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. Weak bands in the ranges from 2800 to 3000 cm<sup>-1</sup> and from 2300 to 2400 cm<sup>-1</sup> correspond to the admixture of an organic substance and to atmospheric CO<sub>2</sub>, respectively.

### Sil323 Sudoite Mg<sub>2</sub>Al<sub>3</sub>(Si<sub>3</sub>Al)O<sub>10</sub>(OH)<sub>8</sub>



**Origin:** Kamikita, Aomori prefecture, Japan.

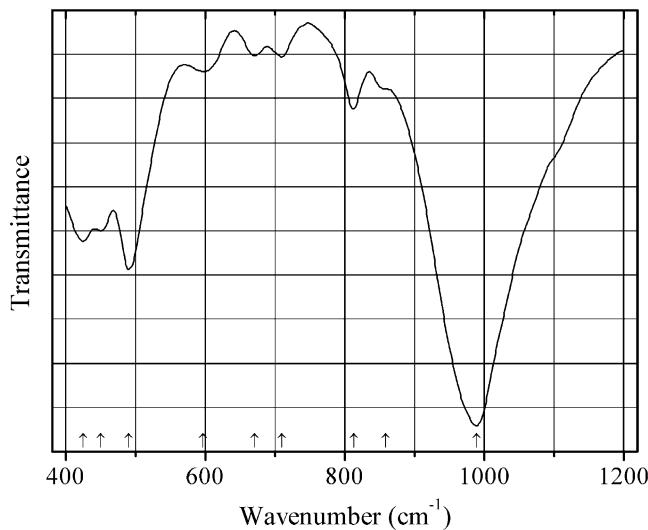
**Description:** The empirical formula is (K<sub>0.01</sub>Na<sub>0.115</sub>Ca<sub>0.005</sub>Mg<sub>1.385</sub>Fe<sup>3+</sup><sub>0.035</sub>Al<sub>3.29</sub>)(Si<sub>3.125</sub>Al<sub>0.875</sub>)O<sub>10</sub>(OH)<sub>8</sub>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Shirozu and Ishida (1982).

**Wavenumbers (cm<sup>-1</sup>):** 3610, 3530, 3340w, 1049sh, 993s, 940sh, 918sh, 835w, 700, 557, 527, 472s, 455s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Sil324 “Tetraferrinontronite”**  $\text{Na}_{0.75}\text{Fe}_2(\text{Si}_{3.25}\text{Fe}_{0.75}\text{O}_{10})(\text{OH})_2$ 

**Origin:** Synthetic.

**Description:** Synthesized hydrothermally. Characterized by powder X-ray diffraction data;  $b \approx 9.25 \text{ \AA}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Petit et al. (2015).

**Wavenumbers (cm⁻¹):** 989, 859sh, 813, 710, 671, 597, 490, 450, 425.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. In the cited paper, the following wavenumbers are given: 3562, 993s, 851sh, 812, 710w, 669w, 598w, 490s, 449, 420.

**Note:** The compound is described as a smectite, but compositional and PXRD data correspond to a dioctahedral mica.

**Sil325 Yangzhumingite**  $\text{KMg}_{2.5}\text{Si}_4\text{O}_{10}\text{F}_2$ 

**Origin:** A lamproitic dyke at the Kvaløya Island, North Norway.

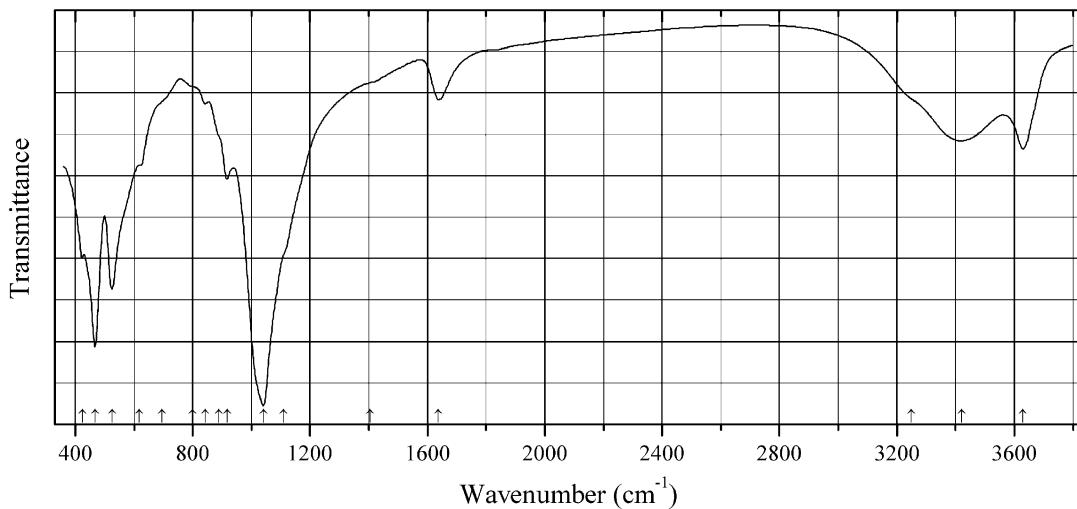
**Description:** Grains from the association with low-Al phlogopite, apatite, Fe-bearing potassium feldspar, quartz, and alkali amphibole. The crystal structure is solved. Monoclinic, space group  $C2/m$ ,  $a = 5.2677(3)$ ,  $b = 9.1208(5)$ ,  $c = 10.1652(6) \text{ \AA}$ ,  $\beta = 100.010(4)^\circ$ . The empirical formula is  $(\text{K}_{0.98}\text{Na}_{0.03})(\text{Mg}_{2.35}\text{Fe}_{0.23}\text{Cr}_{0.01}\text{Ti}_{0.02}\text{Ni}_{0.01}\square_{0.38})(\text{Si}_{3.66}\text{Al}_{0.34}\text{O}_{10})\text{F}_{1.16}(\text{OH})_{0.84}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Micro-FTIR measurement on a crystal mounted on glass capillary.

**Source:** Schingaro et al. (2014).

**Wavenumbers (cm⁻¹):** 3605w, 3586, 3550, 3537, 1638w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Sil326 Montmorillonite**  $(\text{Na,Ca})_{0.3}(\text{Al,Mg})_2(\text{Si}_4\text{O}_{10})(\text{OH})_2 \cdot n\text{H}_2\text{O}$ 

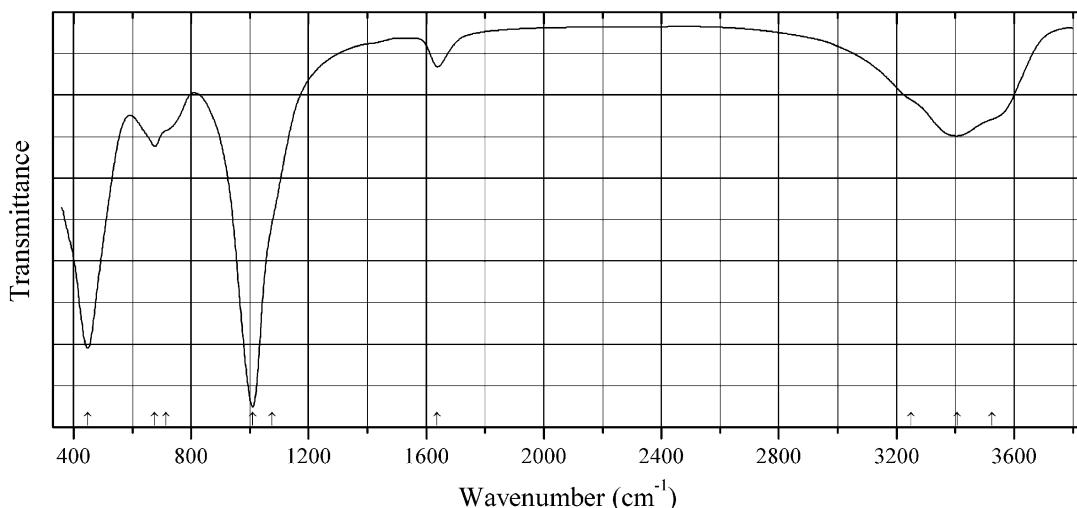
**Origin:** Voudia bentonite quarry, Milos Island, Greece.

**Description:** Gray nodule from the association with natroalunite. The empirical formula is (electron microprobe):  $(\text{Ca}_{0.12}\text{K}_{0.06}\text{Na}_{0.04})(\text{Al}_{1.40}\text{Mg}_{0.35}\text{Fe}_{0.20}\text{Ti}_{0.04}\text{Cr}_{0.01})(\text{Si}_{3.83}\text{Al}_{0.17}\text{O}_{10}) \cdot n\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3630, 3420, 3250sh, 1638, 1405sh, 1110sh, 1041s, 917, 890sh, 842w, 800sh, 695sh, 619, 525s, 467s, 424.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sil328 Hydrobiotite**  $\text{K}(\text{Mg,Fe}^{2+})_6(\text{Si,Al})_8\text{O}_{20}(\text{OH})_4 \cdot n\text{H}_2\text{O}$ 

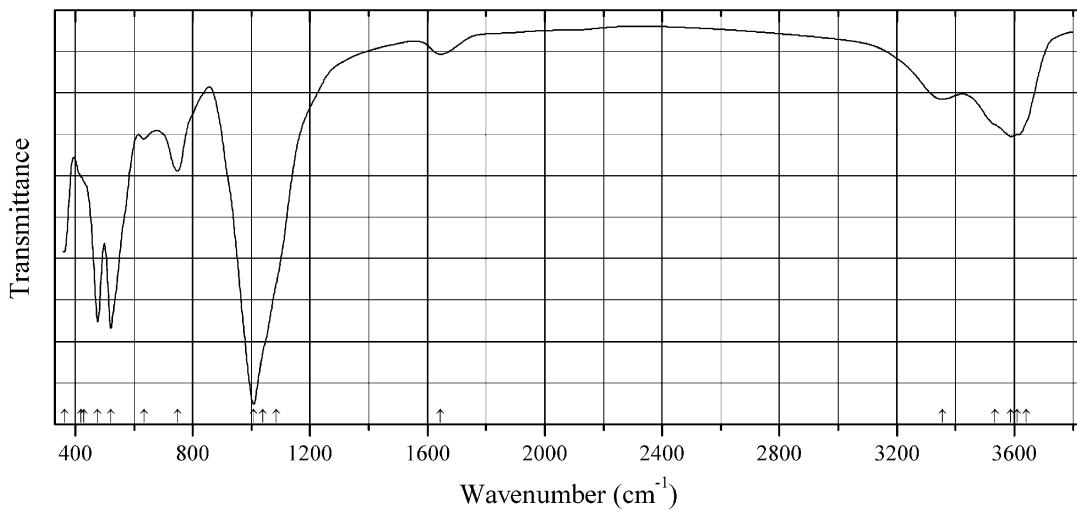
**Origin:** Tsigrado perlite quarry, Milos Island, Greece.

**Description:** Dark brown platy crystals from perlite. The empirical formula is (electron microprobe):  $(\text{K}_{0.35}\text{Na}_{0.10}\text{Ca}_{0.04})(\text{Mg}_{1.67}\text{Fe}_{1.08}\text{Ti}_{0.23}\text{Mn}_{0.02})(\text{Si}_{2.76}\text{Al}_{1.21}\text{Fe}_{0.03}\text{O}_{10})(\text{OH})_2 \cdot n\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3525sh, 3406, 3250sh, 1638, 1075sh, 1010s, 715sh, 677, 448s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sil329 Cookeite**  $(\text{Al},\text{Li})_3\text{Al}_2(\text{Si},\text{Al})_4\text{O}_{10}(\text{OH})_8$ 

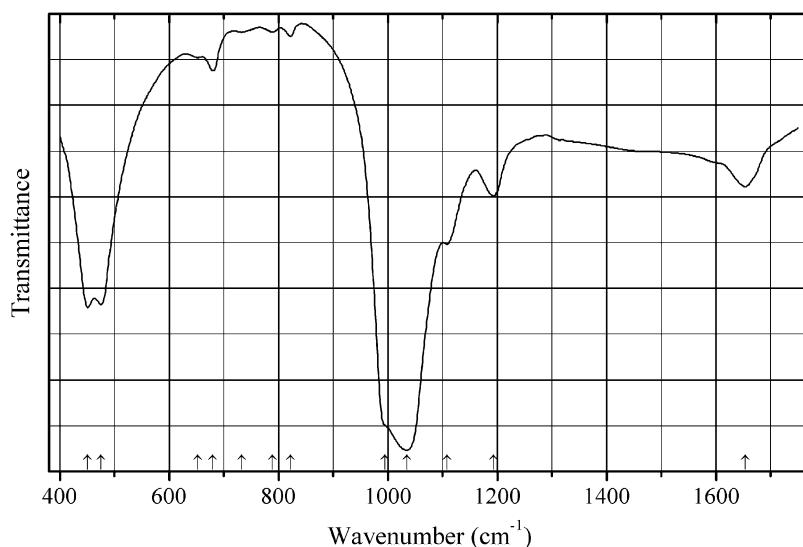
**Origin:** Coronel Murta, Minas Gerais, Brazil.

**Description:** Yellow split platelets from the association with F-rich muscovite and elbaite. A hydrated sample. The empirical formula is  $(\text{Li}_{1.07}\text{Al}_{3.82}\text{Fe}_{0.11})(\text{Si}_{3.14}\text{Al}_{0.86}\text{O}_{10})(\text{OH})_{7.8}\text{F}_{0.2}\cdot\text{nH}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3640sh, 3610sh, 3588, 3535sh, 3355, 1644w, 1085sh, 1040sh, 1008s, 749, 635w, 521s, 476s, 430sh, 420sh, (363).

**Note:** The spectrum was obtained by N.V. Chukanov.

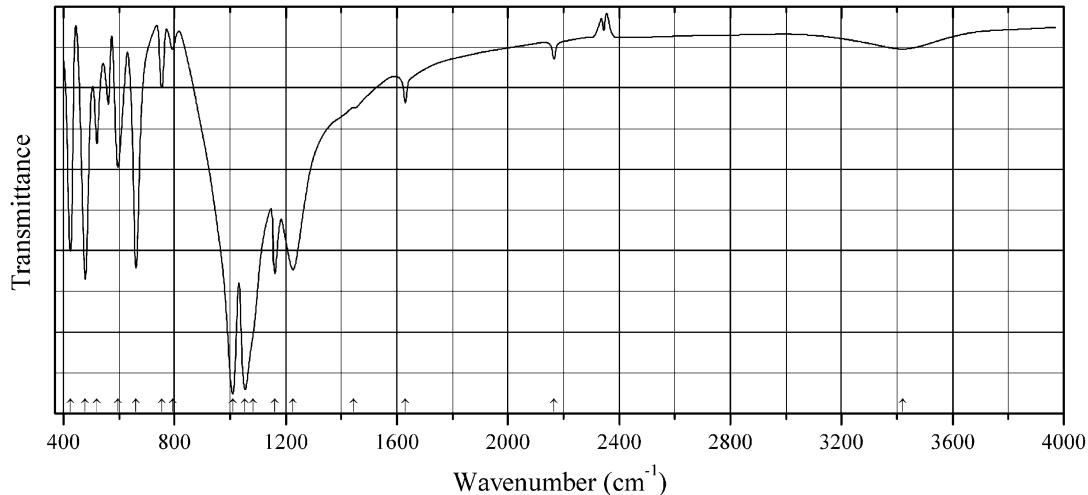
**Sil330 Ferrisepiolite**  $(\text{Fe}^{3+},\text{Fe}^{2+},\text{Mg})_4[(\text{Si},\text{Fe}^{3+})_6\text{O}_{15}](\text{O},\text{OH})_2\cdot 6\text{H}_2\text{O}$ 

**Origin:** Flora (Selsurt) Mt., Lovozero alkaline complex, Kola Peninsula, Murmansk region, Russia.

**Description:** Beige fibrous aggregate from the association with yofortierite and narsarsukite. Characterized by semiquantitative electron microprobe analyses. Confirmed by the IR spectrum.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.  
**Wavenumbers (cm<sup>-1</sup>):** 1653, 1193, 1108, 1034s, 995sh, 822w, 789w, 732w, 680, 652, 475s, 451s.  
**Note:** The spectrum was obtained by N.V. Chukanov.

## Sil331 Wesselsite $\text{SrCuSi}_4\text{O}_{10}$



**Origin:** Synthetic.

**Description:** Synthesized via sol-gel method and calcined at 900 °C. Characterized by powder X-ray diffraction data and EDS analyses. Tetragonal,  $a = 7.366$ ,  $c = 15.574$  Å.

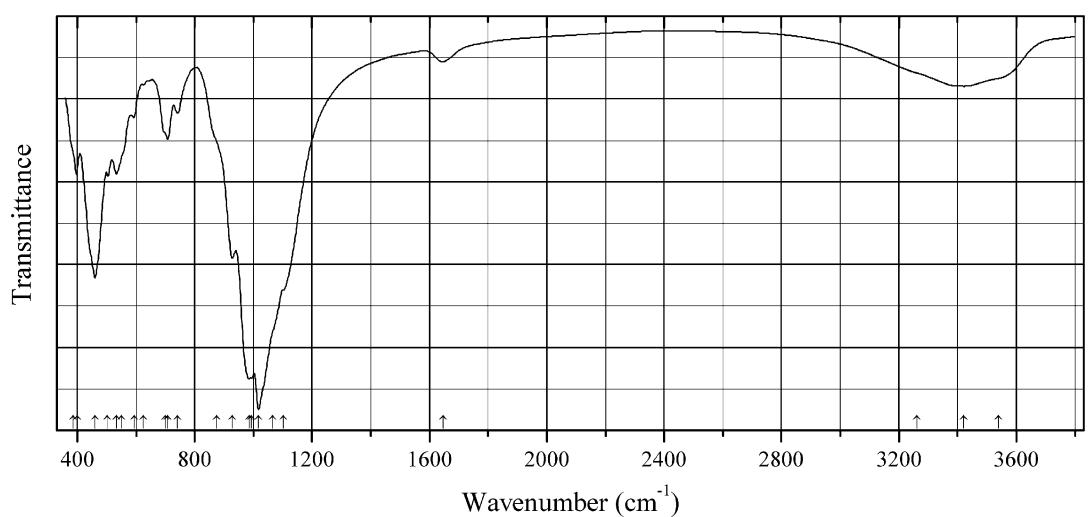
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

Source: Zhang et al. (2016b).

**Wavenumbers (cm<sup>-1</sup>):** 1226s, 1161s, 1082sh, 1054s, 1009s, 793w, 753, 661s, 596, 562, 521, 479s, 425s

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. Bands above  $1400\text{ cm}^{-1}$  are due to impurities.

**Sil332 Hydronaujakasite**  $\text{Na}_2(\text{H}_2\text{O}, \text{H}_3\text{O})_4\text{Fe}[\text{Al}]_4\text{Si}_8\text{O}_{22}(\text{OH}, \text{O})_4$



**Origin:** Toperssuatsiait bay, southern part of the Ilímaussaq alkaline complex, Narsaq, Kujalleq, South Greenland (type locality).

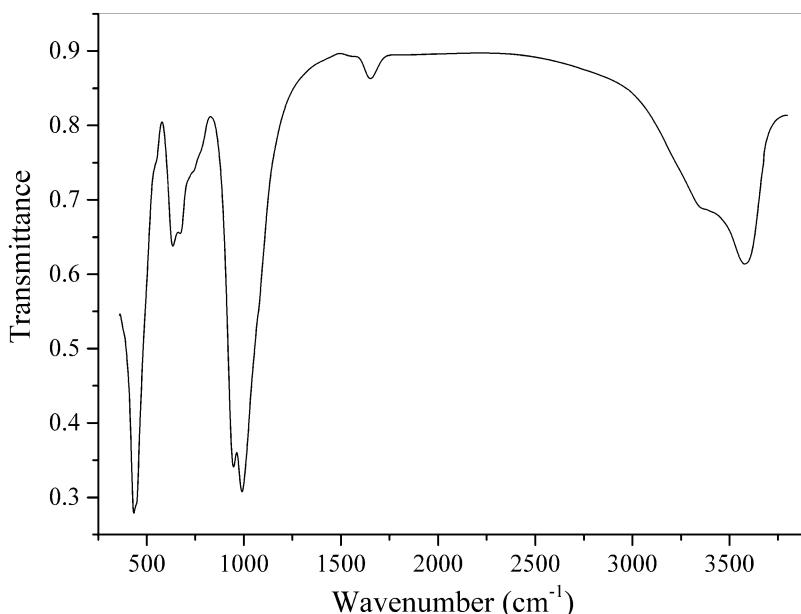
**Description:** Peripheral zones (replacement rims) up to 1 mm thick of naujakasite crystals. The crystal structure is solved. Monoclinic, space group  $C2/m$ ,  $a = 14.983(8)$ ,  $b = 7.998(4)$ ,  $c = 10.403(6)$  Å,  $\beta = 113.874(8)^\circ$ ,  $V = 1140.0(11)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{meas}} = 2.66(1)$  g/cm $^3$ ,  $D_{\text{calc}} = 2.673$  g/cm $^3$ . Optically biaxial (+),  $\alpha = 1.525(2)$ ,  $\beta = 1.530(2)$ ,  $\gamma = 1.545$ . The empirical formula is  $\text{H}_{10.78}\text{Na}_{1.83}\text{Ca}_{0.09}\text{Fe}^{2+}_{0.90}\text{Mn}_{0.20}\text{Al}_{3.95}\text{Si}_{8.05}\text{O}_{29.52}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm $^{-1}$ ):** 3540sh, 3420, 3260sh, 1646w, 1103s, 1065sh, 1018s, 994s, 985s, 928s, 875sh, 742, 708, 700sh, 625w, 593, 550sh, 533, 502, 460s, 399, 385sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

Sil333 “Hydrochamosite-1M”  $(\text{Fe},\text{Al},\text{Mg})_6(\text{Si},\text{Al})_4\text{O}_{10}(\text{OH})_8 \cdot n\text{H}_2\text{O}$



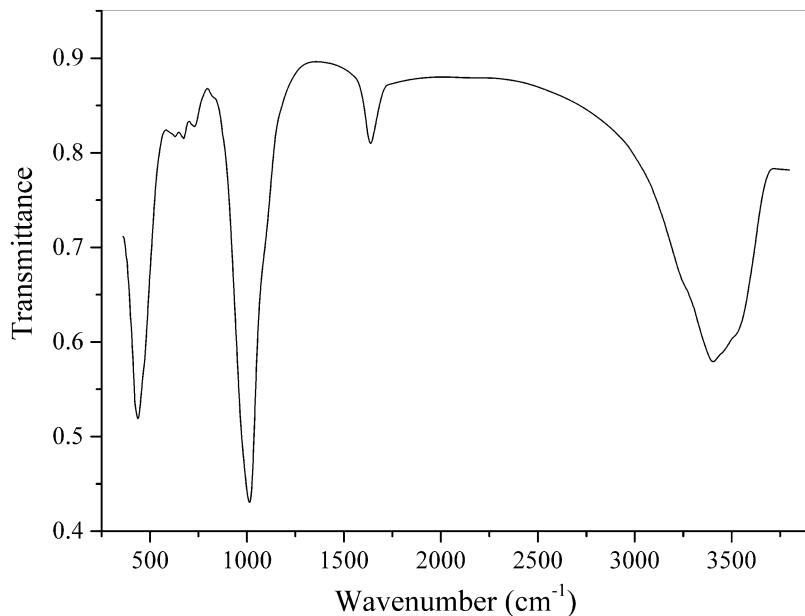
**Origin:** Karagach ridge, Karadag Mts., Crimea Peninsula, Russia.

**Description:** Olive-green, powdery. Investigated by A.V. Kasatkin. The observed lines of the powder X-ray diffraction pattern [ $d$ , Å] are: 14.50s, 7.18s, 4.80w, 4.61, 3.57, 2.85, 2.65, 2.49s, 2.09s, 1.55w, 1.52, 1.47w, 1.42w, 1.34w, 1.30, 1.23w, 1.18w.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm $^{-1}$ ):** 3579s, 3380sh, 1652, 1075sh, 991s, 947s, 770sh, 730sh, 671, 634, 545sh, 445sh, 433s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sil334 “Ferrisaponite”**  $\text{Ca}_x(\text{Fe}^{3+},\text{Mg})_{3-y}[(\text{Si},\text{Al})_4\text{O}_{10}](\text{O},\text{OH})_2 \cdot n\text{H}_2\text{O}$ 


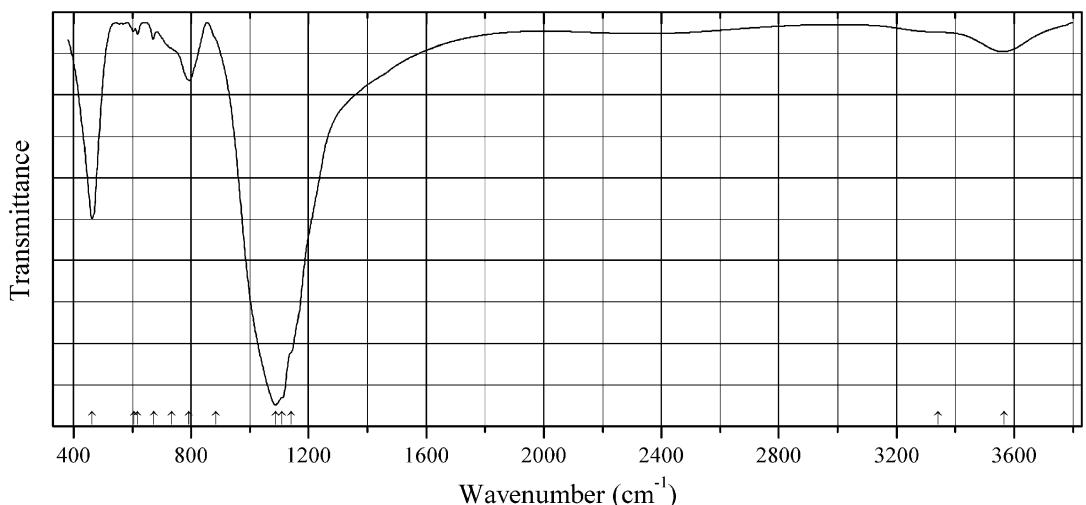
**Origin:** Pervomaiskiy quarry, Crimea Peninsula, Russia.

**Description:** Brownish-black grains with submetallic lustre. A product of ferrosaponite oxidation. The empirical formula is (electron microprobe):  $\text{Ca}_{0.32}\text{Na}_{0.10}(\text{Fe}_{1.7}\text{Mg}_{1.1})(\text{Si}_{3.2}\text{Al}_{0.8}\text{O}_{10})(\text{O},\text{OH})_2 \cdot n\text{H}_2\text{O}$ . The observed lines of the powder X-ray diffraction pattern [ $d$ , Å] are: 14.82w, 4.58s, 2.64s, 2.58, 2.42, 2.30, 1.54s.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3510sh, 3440sh, 3406, 3250sh, 1635, (1420), 1090sh, 1014s, 830sh, 727, 673, 628, 437s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sif148 Glass**  $(\text{K},\text{Cs})\text{AlSi}_{5-6}\text{O}_x$ 


**Origin:** Arsenatnaya fumarole, Second scoria cone of the Northern Breakthrough of the Great Tolbachik Fissure Eruption, Tolbachik volcano, Kamchatka peninsula, Russia.

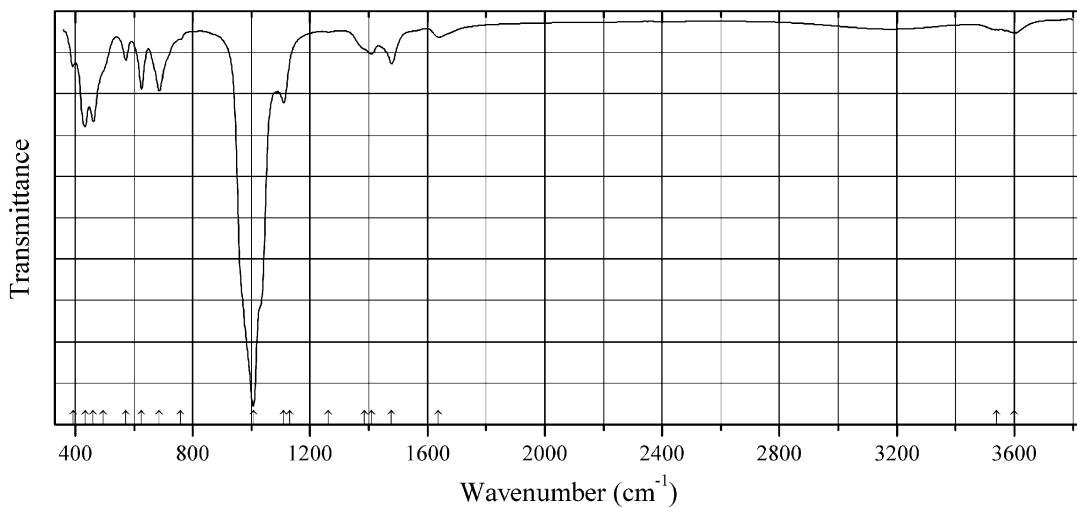
**Description:** Greenish with conchoidal fracture. Investigated by I.V. Pekov. Characterized by qualitative electron microprobe analyses.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3565, (3340w), 1140sh, 1110sh, 1087s, 885sh, 793, 735sh, 673, 619w, 606w, 463s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sif149 Hydroxycancrinite (?)**  $\text{Na}_{8-x}(\text{Si}_6\text{Al}_6\text{O}_{24})(\text{CO}_3)_{<1}\cdot n\text{H}_2\text{O}$   
Cancrinite  $\text{CO}_3$ -deficient



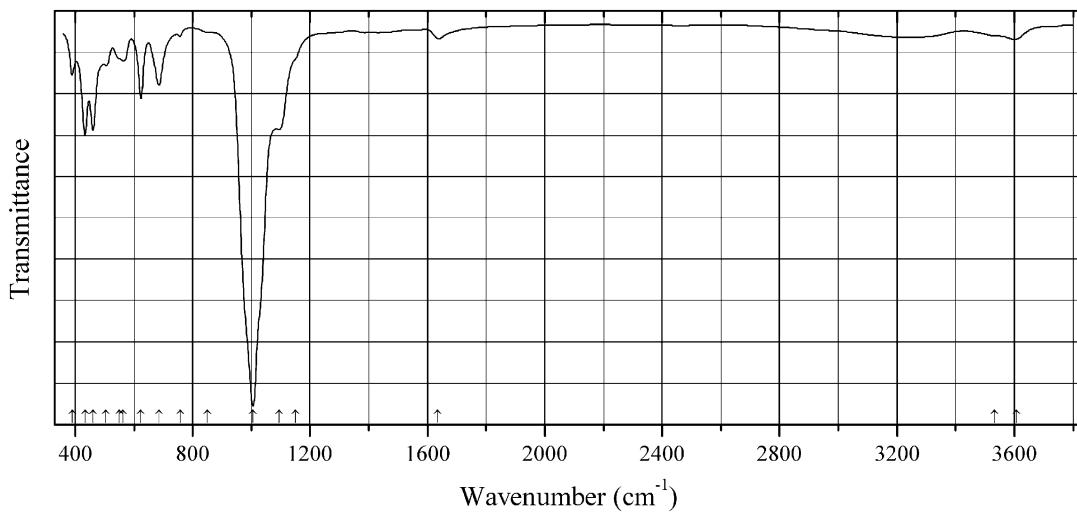
**Origin:** Synthetic.

**Description:** Synthesized hydrothermally at 200 °C from a charge containing 0.7 g of kaolinite, 0.425 g of  $\text{Na}_2\text{CO}_3$ , and 17 ml of 0.8 M NaOH solution during 22 h, see Chukanov et al. (2012a). Characterized by powder X-ray diffraction and semiquantitative electron microprobe analyses. Hexagonal,  $a = 12.703(1)$ ,  $c = 5.181(1)$  Å,  $V = 723.9(3)$  Å<sup>3</sup>. The empirical formula is  $\text{Na}_{6.7}(\text{Si}_{6.1}\text{Al}_{5.9}\text{O}_{24})(\text{CO}_3)_x\cdot n\text{H}_2\text{O}$  ( $x \approx 0.45$ ).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3600, 3540w, 1636, 1477, 1409w, 1385sh, 1262w, 1110, 1130sh, 1007s, 758w, 686, 626, 572, 495sh, 461s, 433s, 394.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sif150 Depmeierite**  $\text{Na}_8[\text{Al}_6\text{Si}_6\text{O}_{24}](\text{PO}_4,\text{CO}_3)_{1-x}\cdot 3\text{H}_2\text{O}$  ( $x < 0.5$ )

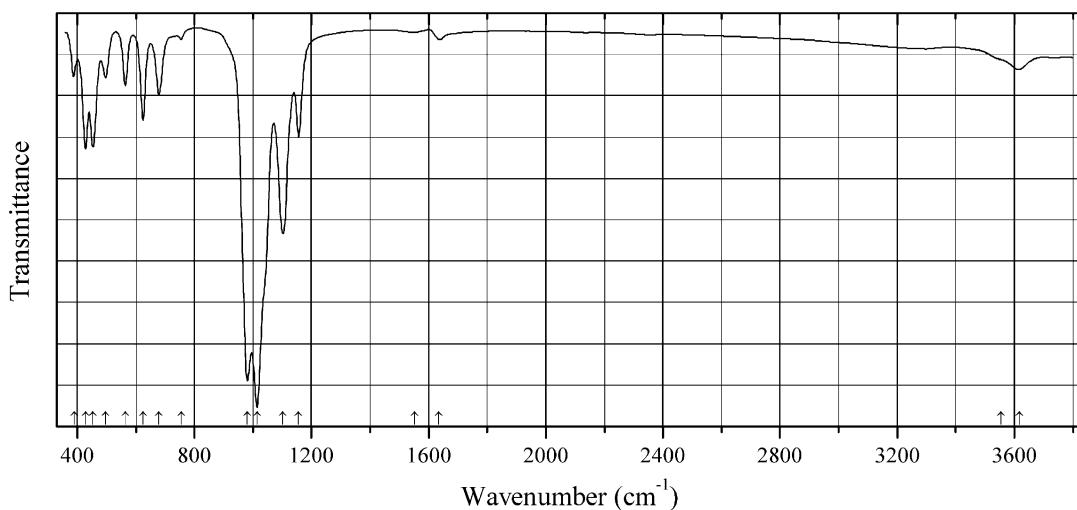
**Origin:** Synthetic.

**Description:** Synthesized hydrothermally at 200 °C from a charge containing 0.7 g of kaolinite, 1.7 g of  $\text{Na}_3\text{PO}_4$ , and 17 ml of 0.8 M NaOH solution during 10 h, see Chukanov et al. (2012a). Characterized by powder X-ray diffraction and electron microprobe analyses. Hexagonal,  $a = 12.703(4)$ ,  $c = 5.166$  (2) Å,  $V = 722.0(5)$  Å<sup>3</sup>. The empirical formula is  $\text{H}_x\text{Na}_{7.15}(\text{Si}_{6.22}\text{Al}_{5.78}\text{O}_{24})(\text{PO}_4)_{0.59}\cdot n\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3607, 3533w, 1635, 1150sh, 1095, 1006s, 850w, 758w, 685, 624, 562, 550sh, 505, 460s, 433s, 391.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sif151 Vishnevite potassium analogue**  $\text{K}_2\text{Na}_6[\text{Al}_6\text{Si}_6\text{O}_{24}](\text{SO}_4)\cdot n\text{H}_2\text{O}$ 

**Origin:** Synthetic.

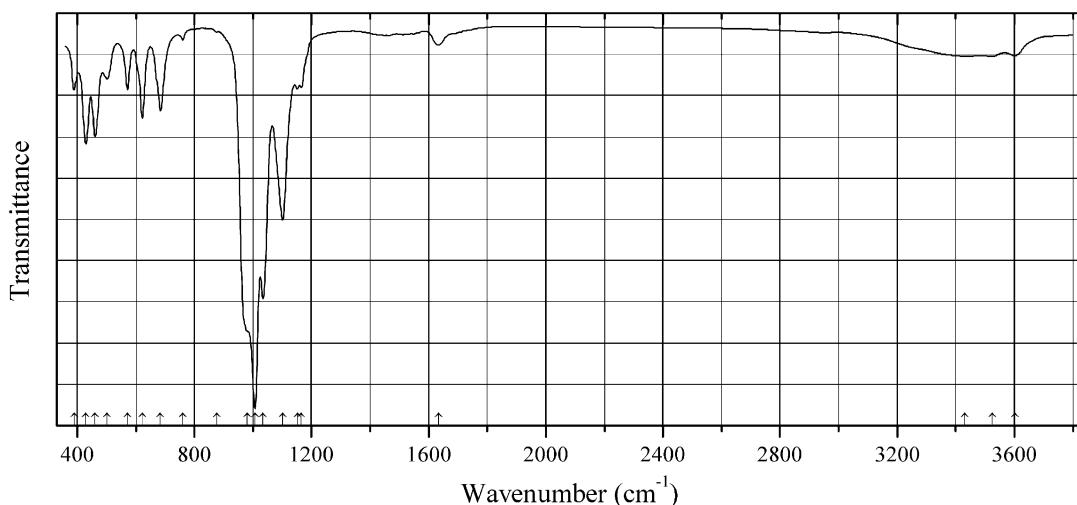
**Description:** Synthesized hydrothermally at 200 °C from a charge containing 0.7 g of kaolinite, 1.7 g of K<sub>2</sub>SO<sub>4</sub>, and 17 ml of 0.8 M NaOH solution during 10 h, *see* Chukanov et al. (2012a). Characterized by powder X-ray diffraction and electron microprobe analyses. Hexagonal,  $a = 12.800(1)$ ,  $c = 5.246(1)$  Å,  $V = 744.3(2)$  Å<sup>3</sup>. The empirical formula is K<sub>2.02</sub>Na<sub>6.17</sub>(Si<sub>6.01</sub>Al<sub>5.99</sub>O<sub>24</sub>)(SO<sub>4</sub>)<sub>0.94</sub>(OH)<sub>x</sub>·nH<sub>2</sub>O.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3617, 3555sh, 1635, (1552w), 1156, 1103s, 1014s, 981s, 756w, 679, 625, 564, 497, 454s, 429s, 391.

**Note:** The spectrum was obtained by N.V. Chukanov.

### Sif152 Vishnevite Na<sub>8</sub>(Si<sub>6</sub>Al<sub>6</sub>O<sub>24</sub>)(SO<sub>4</sub>)·2H<sub>2</sub>O



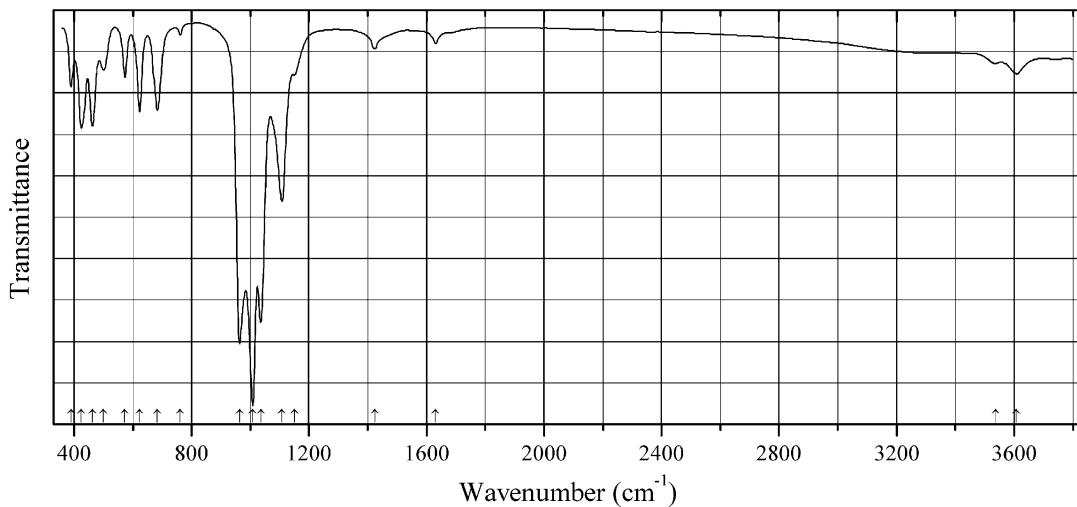
**Origin:** Synthetic.

**Description:** Synthesized hydrothermally at 200 °C from a charge containing 0.7 g of kaolinite, 1.7 g of Na<sub>2</sub>SO<sub>4</sub>, and 17 ml of 0.8 M NaOH solution during 10 h, *see* Chukanov et al. (2012a). Characterized by powder X-ray diffraction and electron microprobe analyses. Hexagonal,  $a = 12.689(1)$ ,  $c = 5.180(1)$  Å,  $V = 722.2(2)$  Å<sup>3</sup>. The empirical formula is Na<sub>8.03</sub>(Si<sub>6.01</sub>Al<sub>5.99</sub>O<sub>24</sub>)(SO<sub>4</sub>)<sub>0.96</sub>(CO<sub>3</sub>,OH)<sub>x</sub>·nH<sub>2</sub>O.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3603, 3526w, 3430, 1635, 1164, 1152, 1101s, 1035s, 1007s, 980sh, 876w, 762w, 684, 622, 572, 503, 461, 430, 391.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sif153 Vishnevite CO<sub>3</sub>-bearing** Na<sub>8</sub>(Si<sub>6</sub>Al<sub>6</sub>O<sub>24</sub>)(SO<sub>4</sub>,CO<sub>3</sub>)·2H<sub>2</sub>O

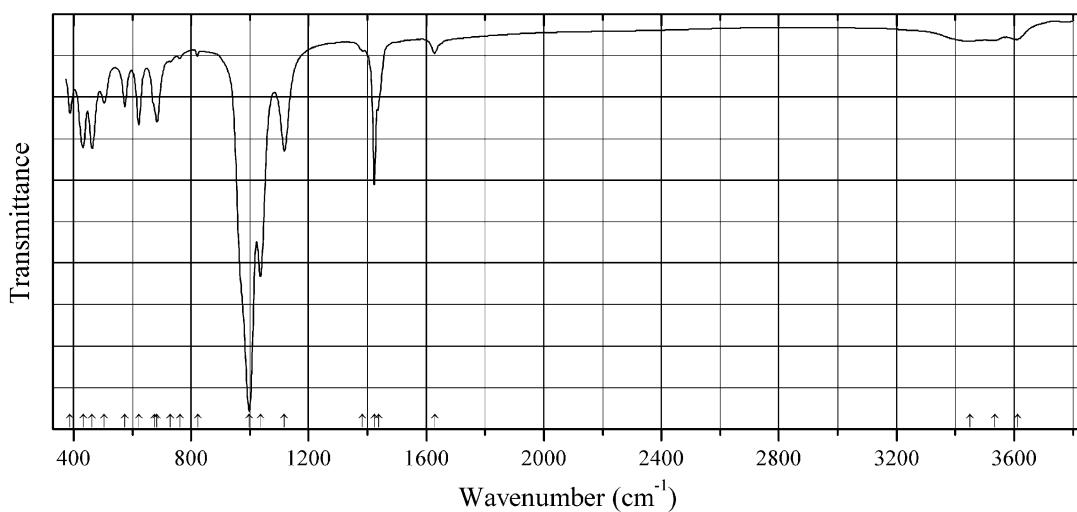
**Origin:** Synthetic.

**Description:** Synthesized hydrothermally at 200 °C from a charge containing 0.7 g of kaolinite, 0.43 g of Na<sub>2</sub>CO<sub>3</sub>, 0.43 g of Na<sub>3</sub>PO<sub>4</sub>, 0.43 g of Na<sub>3</sub>SO<sub>4</sub>, 0.43 g of Na<sub>2</sub>C<sub>2</sub>O<sub>4</sub>, and 17 ml of 0.8 M NaOH solution during 67 h, see Chukanov et al. (2012a). Characterized by powder X-ray diffraction and electron microprobe analyses. Hexagonal,  $a = 12.674(1)$ ,  $c = 5.1667(2)$  Å,  $V = 718.7(4)$  Å<sup>3</sup>. The empirical formula is Na<sub>7.52</sub>(Si<sub>6.18</sub>Al<sub>5.82</sub>O<sub>24</sub>)(SO<sub>4</sub>)<sub>0.62</sub>(CO<sub>3</sub>)<sub>0.19</sub>(PO<sub>4</sub>)<sub>0.03</sub>· $n$ H<sub>2</sub>O.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3608, 3536w, 1631w, 1425w, 1151, 1107s, 1036s, 1008s, 963s, 762w, 684, 623, 573, 500, 463s, 425s, 391.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sif154 Cancrinite NO<sub>3</sub>-analogue** Na<sub>8</sub>(Si<sub>6</sub>Al<sub>6</sub>O<sub>24</sub>)(NO<sub>3</sub>,CO<sub>3</sub>)<sub>2-x</sub>·3H<sub>2</sub>O

**Origin:** Synthetic.

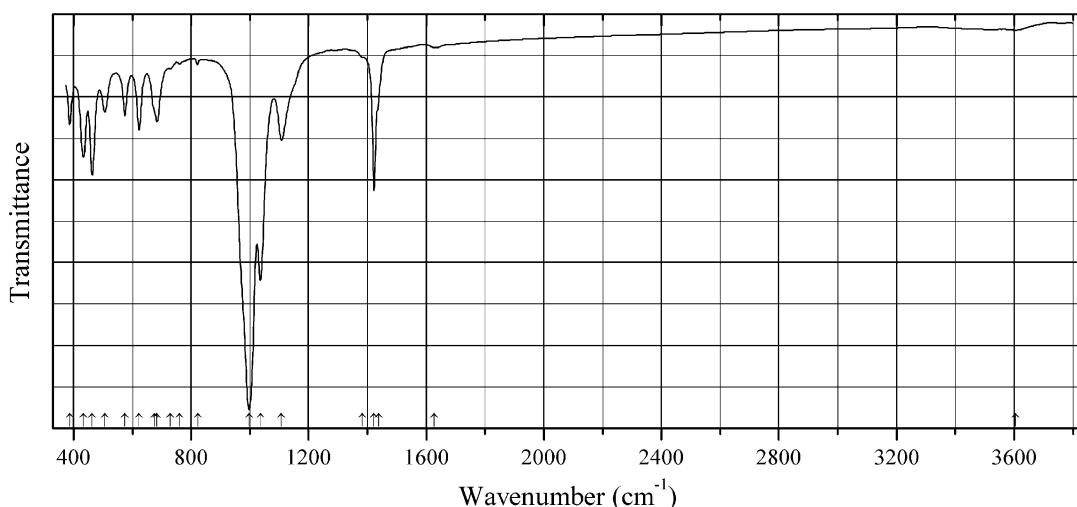
**Description:** Synthesized hydrothermally at 160 °C from a charge containing 1 g of kaolinite, 4 g of NaNO<sub>3</sub>, and 45 ml of 8 M NaOH solution during 120 h (see Chukanov et al. 2011, 2012a). Characterized by powder X-ray diffraction and electron microprobe analyses and gas chromatography of annealing products. The crystal structure is solved. Hexagonal, space group *P*6<sub>3</sub>, *a* = 12.6743(2), *c* = 5.18289(13) Å, *V* = 721.02(2) Å<sup>3</sup>. The empirical formula is Na<sub>7.8</sub>(Si<sub>6.05</sub>Al<sub>5.95</sub>O<sub>24</sub>)(NO<sub>3</sub>)<sub>1.32</sub>(CO<sub>3</sub>)<sub>0.27</sub>·3.3H<sub>2</sub>O.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3611, 3535, 3449, 1629, 1438sh, 1423s, 1384w, 1117, 1036s, 998s, 823w, 763w, 730w, 684, 675sh, 622, 575, 504, 464s, 433s, 389.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sif155 Cancrinit NO<sub>3</sub>-analogue low-hydrous** Na<sub>8</sub>(Si<sub>6</sub>Al<sub>6</sub>O<sub>24</sub>)(NO<sub>3</sub>,CO<sub>3</sub>)<sub>2-x</sub>·H<sub>2</sub>O



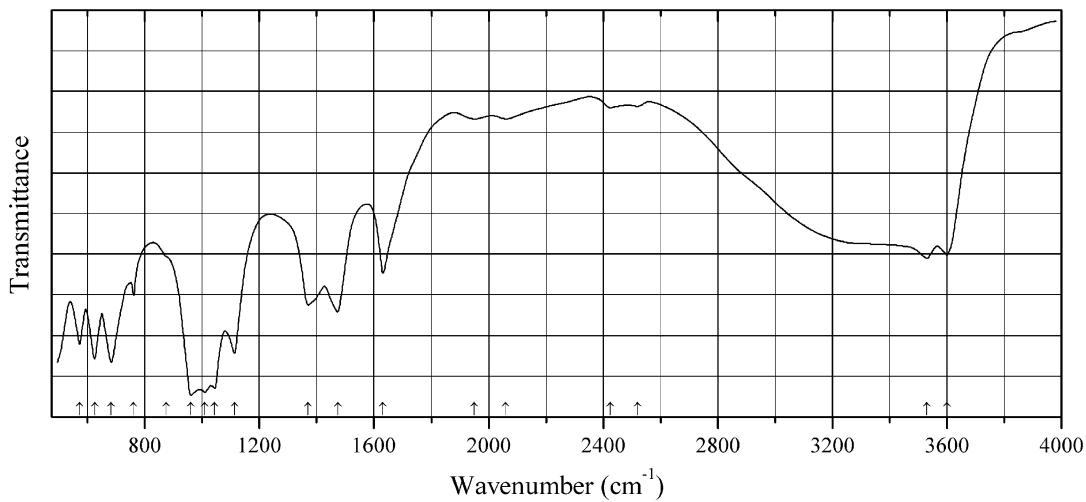
**Origin:** Synthetic.

**Description:** Product of partial dehydration of the NO<sub>3</sub>-analogue of cancrinitite Sif154 at 300 °C (see Chukanov et al. 2011, 2012a). The empirical formula is Na<sub>7.8</sub>(Si<sub>6.05</sub>Al<sub>5.95</sub>O<sub>24</sub>)(NO<sub>3</sub>)<sub>1.32</sub>(CO<sub>3</sub>)<sub>0.27</sub>·*n*H<sub>2</sub>O (*n* ≈ 1).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3604w, 1628w, 1438sh, 1422s, 1384w, 1108, 1036s, 997s, 823w, 762w, 730w, 684, 675sh, 624, 575, 507, 464s, 434s, 387.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sif156 Cancrinite Ca-free analogue**  $\text{Na}_8[\text{Al}_6\text{Si}_6\text{O}_{24}](\text{CO}_3)\cdot 4\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Synthesized hydrothermally from kaolinite, NaOH, and  $\text{NaHCO}_3$  at 473 K for 48 h.

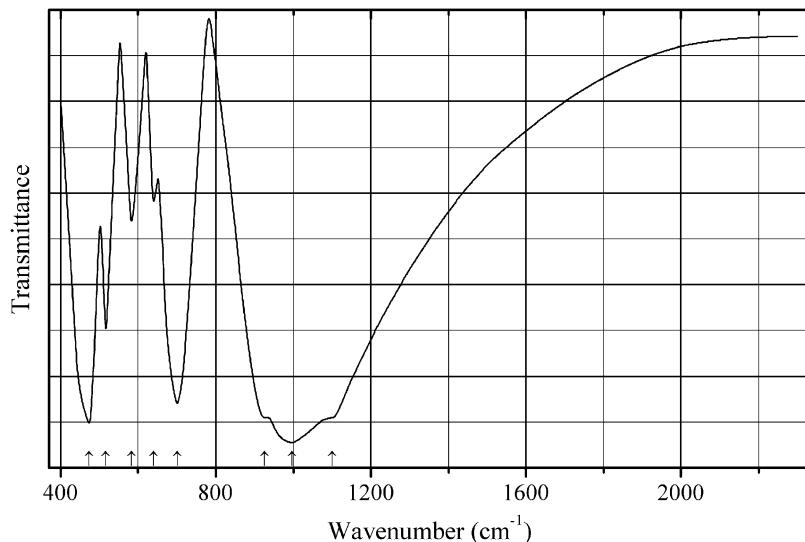
Characterized by thermal data and powder X-ray diffraction. Hexagonal, space group  $P6_3$ ,  $a = 12.663(2)$ ,  $c = 5.1738(9)$  Å. The empirical formula is  $\text{Na}_{8.28}[\text{Al}_{5.93}\text{Si}_{6.07}\text{O}_{24}] (\text{CO}_3)_{0.93}(\text{OH})_{0.49}\cdot 3.64\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Kurdakova et al. (2014).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3601s, 3530s, 2520w, 2425w, 2060w, 1950w, 1630, 1474, 1370, 1114, 1044s, 1010s, 960s, 875sh, 761w, 683, 625, 573.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Sif157 Carnegieite (high)**  $\text{Na}(\text{AlSiO}_4)$ 

**Origin:** Synthetic phase polymorphous with nepheline.

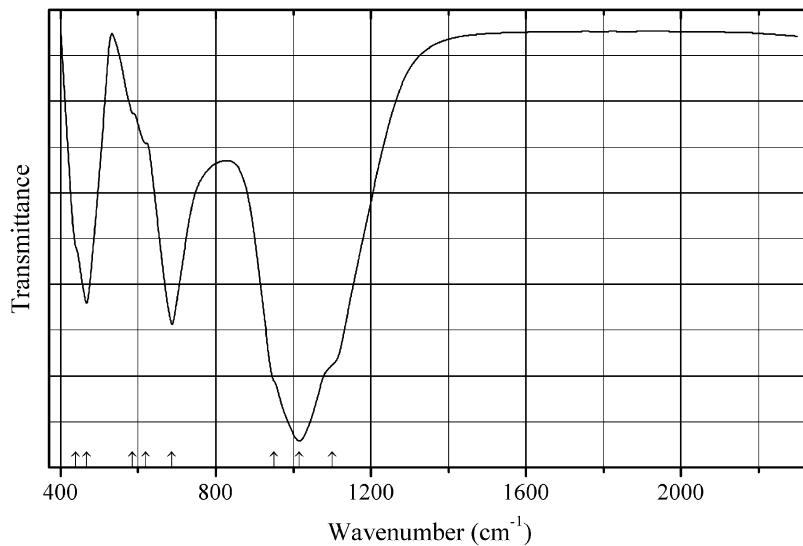
**Description:** Prepared from hydrated alumina gel, NaOH, and highly reactive aerosol silica at 800° with subsequent annealing at 1300 °C. Characterized by powder X-ray diffraction data. Cubic, space group  $P2_13$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Nayak and Kutty (1998).

**Wavenumbers (cm<sup>-1</sup>):** 1100sh, 996s, 925sh, 700s, 640, 583, 517, 474s.

### Sif158 Carnegieite (low) Na(AlSiO<sub>4</sub>)



**Origin:** Synthetic phase polymorphous with nepheline.

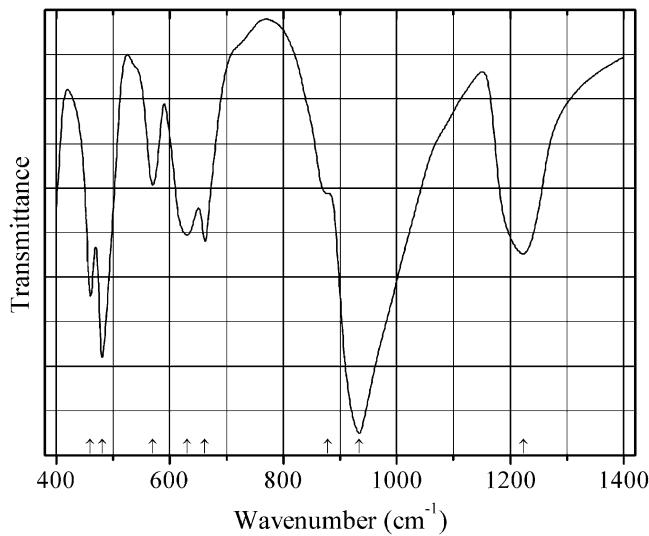
**Description:** Prepared from hydrated alumina gel, NaOH, and highly reactive aerosol silica at 800°.

Characterized by powder X-ray diffraction data. Orthorombic, space group  $Pb2_1a$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Nayak and Kutty (1998).

**Wavenumbers (cm<sup>-1</sup>):** 1100sh, 1016s, 950sh, 687, 620sh, 586sh, 468, 439sh.

**Sif159 Hexacelsian** Ba(Al<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>)

**Origin:** Synthetic.

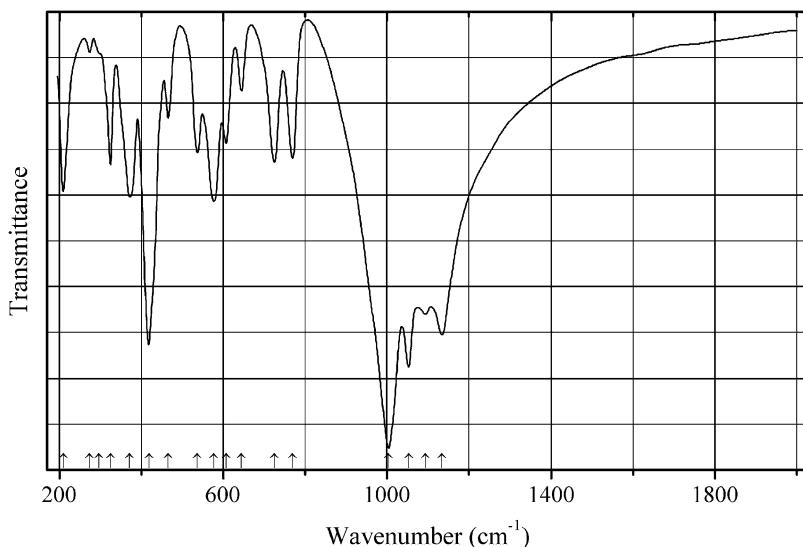
**Description:** Prepared by heating Ba-exchanged synthetic zeolite 4A ( $\text{Na}_{12}\text{Al}_{12}\text{Si}_{12}\text{O}_{48} \cdot 27\text{H}_2\text{O}$ ) up to 1300 °C at a rate of 10 °C/min. Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Aronne et al. (2002).

**Wavenumbers (cm<sup>-1</sup>):** 1223s, 934s, 878sh, 662, 630, 570, 481s, 460s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. For the IR spectra of hexacelsian and its polymorphs see also Dondur et al. (2005) and Colomban et al. (2000).

**Sif160 Rubicline** Rb(AlSi<sub>3</sub>O<sub>8</sub>)

**Origin:** Synthetic.

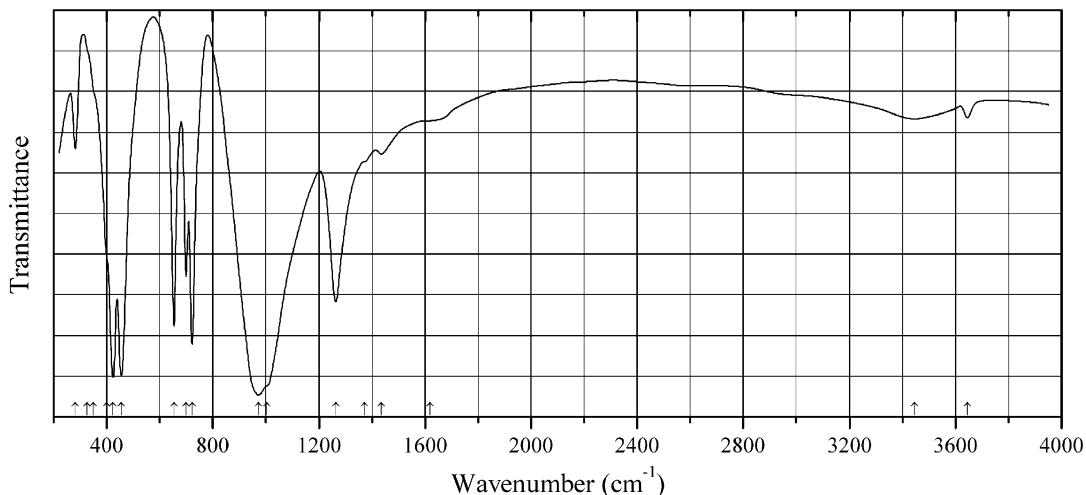
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Roy (1987).

**Wavenumbers (cm<sup>-1</sup>):** 1134s, 1093s, 1053s, 1004s, 770, 725, 645, 607, 578, 537, 465, 419s, 372, 325, 297sh, 274w, 210.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### Sif161 Sodalite nitrite analogue Na<sub>8</sub>[AlSiO<sub>4</sub>]<sub>6</sub>(NO<sub>2</sub>)<sub>2</sub>·nH<sub>2</sub>O



**Origin:** Synthetic.

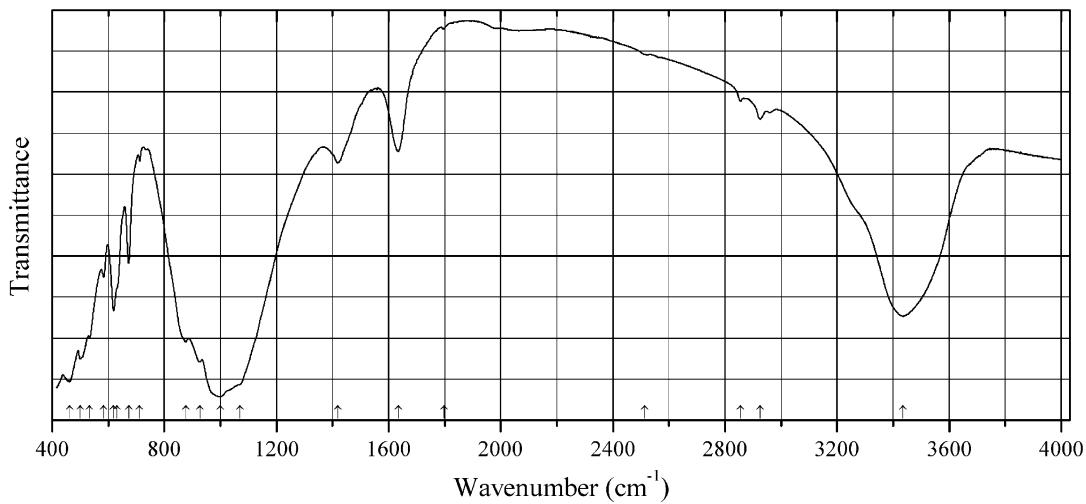
**Description:** Prepared hydrothermally from kaolinite, in the presence of NaNO<sub>2</sub>. Characterized by powder X-ray diffraction data. Cubic,  $a = 8.931(1)$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Buhl (1991).

**Wavenumbers (cm<sup>-1</sup>):** 3645w, 3445w, 1620sh, 1435, 1372sh, 1264, 1005sh, 972s, 722s, 699, 654s, 455s, 424s, 400sh, 350sh, 326sh, 282.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. The bands at 1264 and 1372 cm<sup>-1</sup> correspond to stretching vibrations of NO<sub>2</sub><sup>-</sup> and NO<sub>3</sub><sup>-</sup>, respectively. The band at 1435 cm<sup>-1</sup> indicates the presence of CO<sub>3</sub><sup>2-</sup>.

**Sif162 Sulphydrylbystrite**  $\text{Na}_5\text{K}_2\text{Ca}[\text{Al}_6\text{Si}_6\text{O}_{24}](\text{S}_5)^{2-}(\text{SH})^-$ 


**Origin:** Malobystrinskoye lazurite deposit, Malaya Bystraya River basin, Lake Baikal area, Eastern Siberian Region, Russia (type locality).

**Description:** Anhedral grains from the association with lazurite, calcite, diopside, phlogopite, and pyrite.

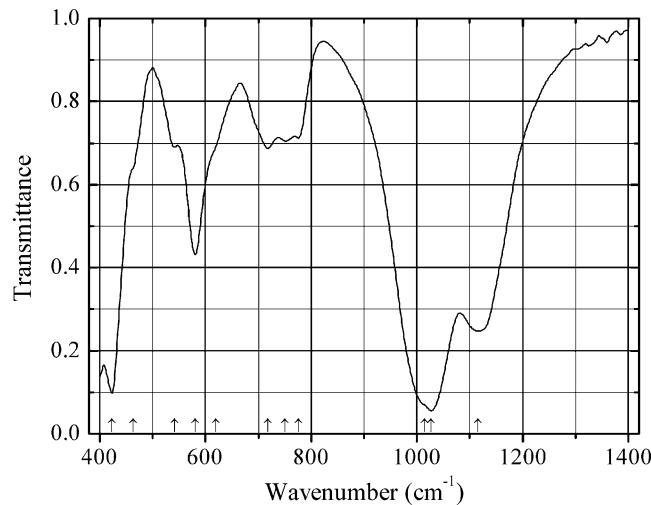
Holotype sample. The crystal structure is solved. Hexagonal, space group  $P31c$ ,  $a = 12.9567(6)$ ,  $c = 10.7711(5)$  Å,  $V = 1566.0(1)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{meas}} = 2.391(1)$  g/cm $^3$ ,  $D_{\text{calc}} = 2.368$  g/cm $^3$ . Optically uniaxial (+),  $\omega = 1.661(2)$ ,  $\epsilon = 1.584(2)$ . The empirical formula is  $\text{Na}_{5.17}\text{K}_{1.87}\text{Ca}_{0.99}(\text{Al}_{6.01}\text{Si}_{5.99}\text{O}_{24})(\text{S}_5)^{2-} \cdot 0.86(\text{SH})_{0.86}\text{Cl}_{0.07}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 4.857 (48) (102), 3.948 (38) (211), 3.739 (94) (300), 3.331 (100) (212), 2.715 (32) (401), 2.692 (56) (004).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Sapozhnikov et al. (2016).

**Wavenumbers (cm $^{-1}$ ):** 3436, 2926, 2855, 2514, 1798, 1634, 1071, 1000, 926, 876, 712, 673, 631sh, 619, 583, 534, 501, 462.

**Note:** The bands at 3436 and 1634  $\text{cm}^{-1}$  correspond to H $_2$ O molecules that are not indicated in the chemical formula of sulphydrylbystrite. Weak bands in the range from 2800 to 3000  $\text{cm}^{-1}$  correspond to the admixture of an organic substance. The assignment of the very weak band at 2514  $\text{cm}^{-1}$  to S–H-stretching vibrations made by the authors is ambiguous and questionable.

**Sif163 Thallium feldspar  $TlAlSi_3O_8$** 

**Origin:** Synthetic.

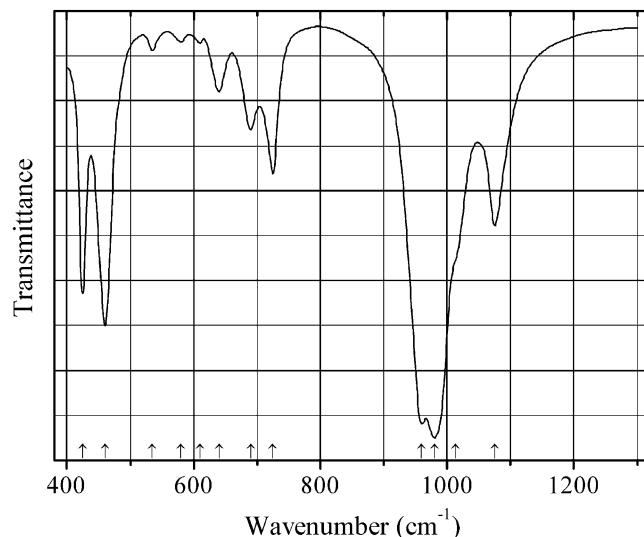
**Description:** Synthesized from a powdered sample of natural low albite and  $TlNO_3$  in a 1:1 weight ratio under hydrothermal conditions, at 550 °C for 5 days. The crystal structure is solved. Monoclinic, space group  $C2/m$ ,  $a = 8.882(3)$ ,  $b = 13.048(2)$ ,  $c = 7.202(2)$  Å,  $\beta = 116.88(1)^\circ$ ,  $V = 744.5(4)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 3.958$  g/cm<sup>3</sup>. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 3.94 (64) (200, 111), 3.63 (70) (13-1), 3.62 (80) (22-1), 3.45 (92) (11-2), 3.372 (100) (220), 3.197 (54) (002), 2.992 (78) (131).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Kyono and Kimata (2001).

**Wavenumbers (cm<sup>-1</sup>):** 1116s, 1027s, 1014sh, 776, 751, 718, 620sh, 581, 542, 463sh, 423s.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**Sif164 Thallium sodalite  $Tl_6(Al_6Si_6O_{24})$** 

**Origin:** Synthetic.

**Description:** Obtained in the ion-exchange reaction between hydroxysodalite  $\text{Na}_8(\text{Al}_6\text{Si}_6\text{O}_{24})(\text{OH})_2 \cdot 2\text{H}_2\text{O}$  and 1 M aqueous solution of  $\text{TINO}_3$  at 100 °C. The product was dried at 425 °C for 5 h under a vacuum of  $10^{-5}$  Torr. Characterized by powder X-ray diffraction data. The structure was refined by Rietveld analysis. Cubic,  $a = 8.9653(1)$  Å.

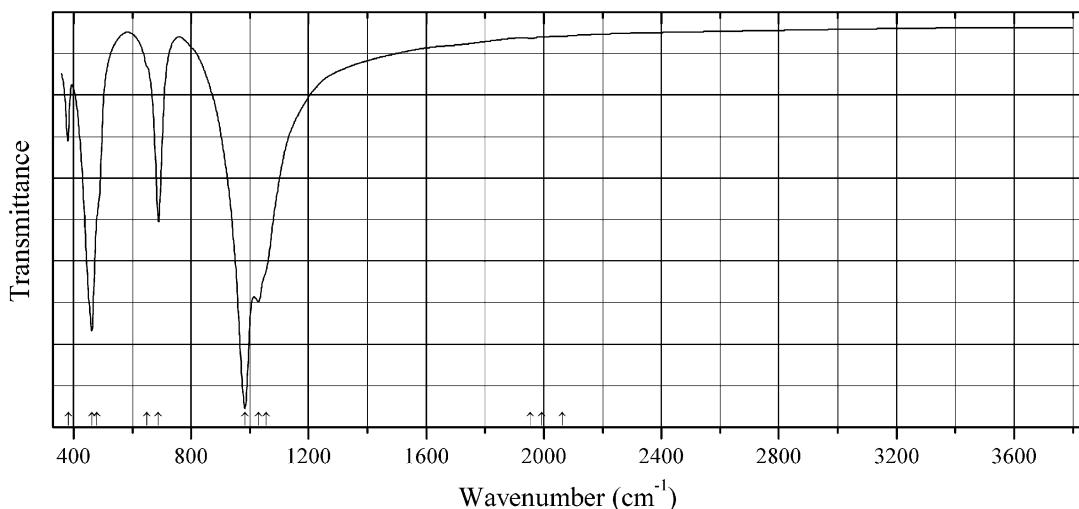
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Lattuner et al. (1999).

**Wavenumbers (cm<sup>-1</sup>):** 1075, 1013sh, 980s, 960s, 725, 690, 640, 610w, 580w, 535w, 460s, 425s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### Sif165 Kalsilite $\text{KAlSiO}_4$



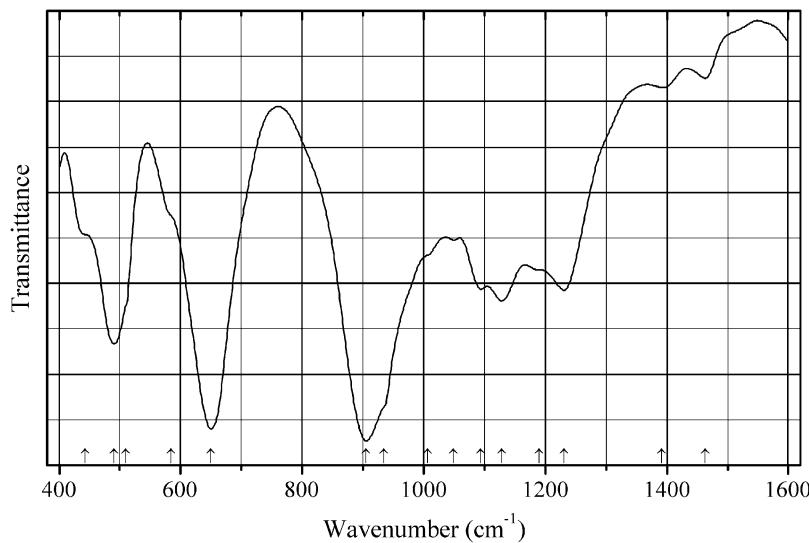
**Origin:** Koashva Mt., Khibiny alkaline complex, Kola peninsula, Murnansk region, Russia.

**Description:** Crystals from the association with carbobystrite. Investigated by I.V. Pekov. Characterized by powder and single-crystal X-ray diffraction data, as well as electron microprobe analyses. Hexagonal, space group  $P6_3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 2063w, 1992w, 1953w, 1055sh, 1030s, 983s, 689s, 650sh, 480sh, 462s, 383.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sif166 Dmisteinbergite**  $\text{Ca}(\text{Al}_2\text{Si}_2\text{O}_8)$ 

**Origin:** Burned dump of the Chelyabinsk coal basin, Kopeisk, South Urals, Russia (type locality).

**Description:** Hexagonal platelets from the association with anorthite, svyatoslavite, troilite, and cohenite. The empirical formula is (electron microprobe):  $\text{Ca}_{1.00}\text{Al}_{2.01}\text{Si}_{2.03}\text{O}_{8.07}$ .

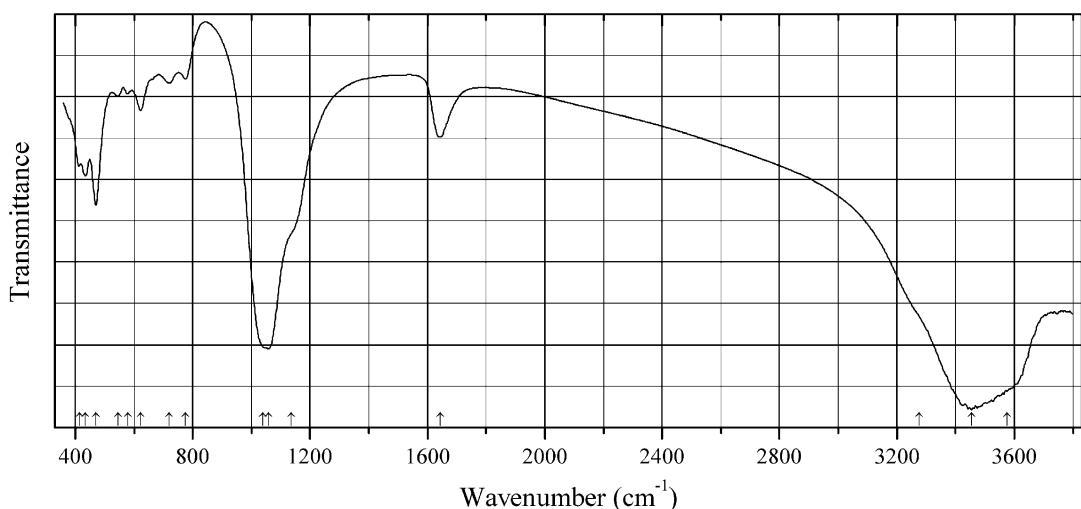
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Simakin et al. (2010).

**Wavenumbers (IR, cm<sup>-1</sup>):** (1463), (1392), 1231, 1190sh, 1128, 1094, 1049, 1007sh, 935sh, 905s, 650s, 584sh, 510sh, 490s, 443sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. Weak bands in the range 1300–1500 cm<sup>-1</sup> correspond to the admixture of a carbonate. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 903s, 809, 651, 485s, 432s.

**Sif\_Z127 Erionite-K**  $\text{K}_{10}[\text{Si}_{26}\text{Al}_{10}\text{O}_{72}] \cdot 30\text{H}_2\text{O}$ 

**Origin:** Karadag Mts., Crimea Peninsula, Russia.

**Description:** Light green crystals of erionite-K with zones of erionite-Na. Investigated by A.V. Kasatkin.

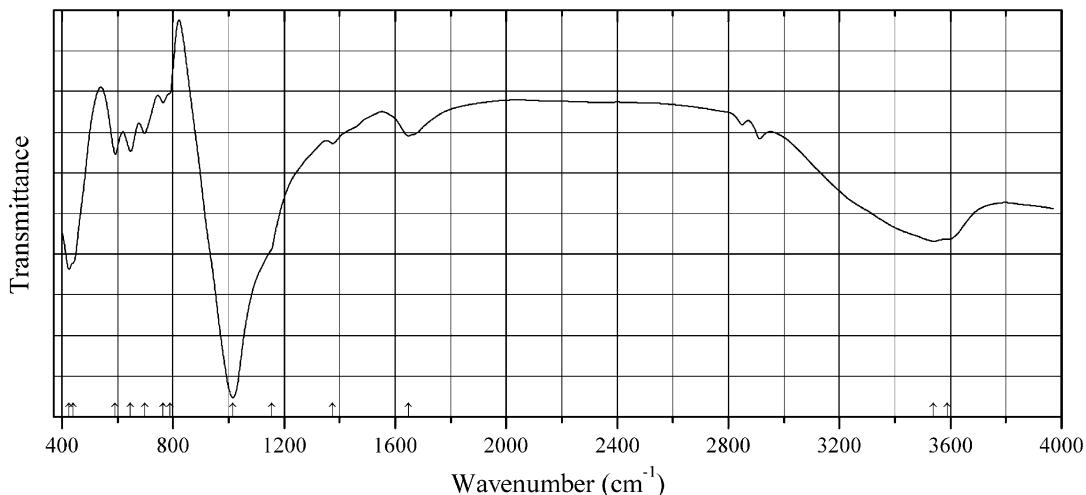
The empirical formula is (electron microprobe):  $K_{1.82}Ca_{1.78}Na_{1.70}Mg_{0.57}(Si_{27.42}Al_{8.27}Fe_{0.30}O_{72}) \cdot nH_2O$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3575sh, 3455s, 3275sh, 1645, 1135sh, 1058s, 1040sh, 775, 720, 623, 579, 545, 470s, 435, 415.

**Note:** The spectrum was obtained by N.V. Chukanov.

### Sif\_Z128 Merlinite $K_5Ca_2(Si_{23}Al_9)O_{64} \cdot 24H_2O$



**Origin:** Fosso Attici, Sacrofano, Italy.

**Description:** Yellowish prismatic crystals from the association with phillipsite. The crystal structure is solved. Orthorhombic, space group  $Immm$ ,  $a = 14.066(5)$ ,  $b = 14.111(5)$ ,  $c = 9.943(3)$  Å (at 100 K).  $D_{\text{calc}} = 2.177$  g/cm<sup>3</sup>. The empirical formula is  $(K_{5.69}Na_{0.37})(Ca_{1.93}Ba_{0.40}Mg_{0.01})(Si_{21.38}Al_{10.55}Fe^{3+}_{0.02})O_{64} \cdot 19.6H_2O$ .

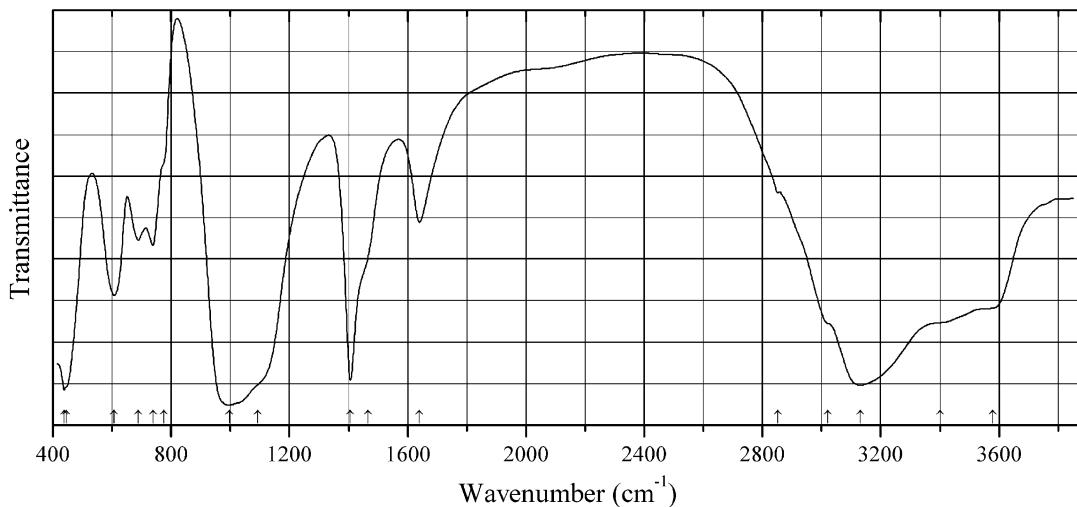
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Gatta et al. (2015a).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3589sh, 3539, 1649, 1375, 1156sh, 1015s, 789sh, 764, 698, 647, 592, 440sh, 425s.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 3470, 1637, (with a 473.1 nm laser); 1087, 496, 422, 320, 125 (with a 632.8 nm laser).

**Sif\_Z129 Phillipsite-NH<sub>4</sub>**  $(\text{NH}_4, \text{Na})_9(\text{Al}_9\text{Si}_{27}\text{O}_{72}) \cdot 24\text{H}_2\text{O}$ 

**Origin:** Artificial.

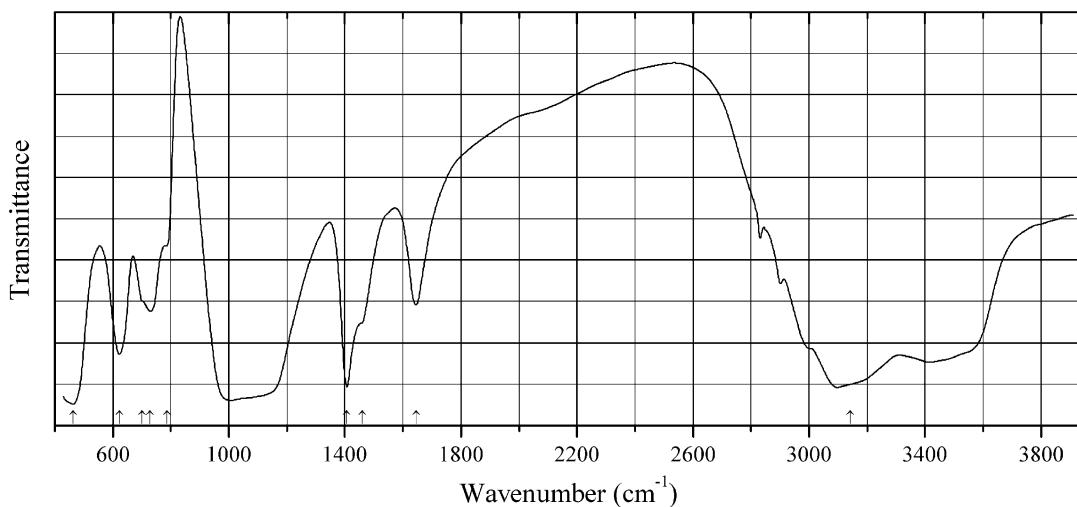
**Description:** NH<sub>4</sub><sup>+</sup>-exchanged Si-poor phillipsite from Vallerano, Rome, Italy. The crystal structure is solved. Monoclinic,  $a = 10.0507(5)$ ,  $b = 14.2016(8)$ ,  $c = 8.7281(8)$  Å,  $\beta = 125.123(5)^\circ$ ,  $V = 1019.0(9)$  Å<sup>3</sup>,  $Z = 4$ . The empirical formula is  $(\text{NH}_4)_{11.41}\text{Na}_{1.36}(\text{Al}_{13.36}\text{Si}_{22.64}\text{O}_{72.45}) \cdot 20.6\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Gualtieri (2000).

**Wavenumbers (cm<sup>-1</sup>):** 3580, 3402sh, 3131s, 3022sh, 1640, 1465sh, 1406s, 1092sh, 996s, 775sh, 739, 689, 607, 446sh, 438s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Sif\_Z130 Phillipsite-NH<sub>4</sub>**  $(\text{NH}_4, \text{Na})_9(\text{Al}_9\text{Si}_{27}\text{O}_{72}) \cdot 24\text{H}_2\text{O}$ 

**Origin:** Artificial.

**Description:**  $\text{NH}_4^+$ -exchanged phillipsite from Perrier, Puy du Dôme, France. The crystal structure is solved. Monoclinic,  $a = 10.0122(8)$ ,  $b = 14.1943(12)$ ,  $c = 8.7284(17)$  Å,  $\beta = 125.024(11)^\circ$ ,  $V = 1015.81(2)$  Å<sup>3</sup>,  $Z = 4$ . The empirical formula is  $(\text{NH}_4)_{9.89}\text{Na}_{0.45}(\text{Al}_{9.92}\text{Si}_{26.08}\text{O}_{71.96}) \cdot 18.2\text{H}_2\text{O}$ .

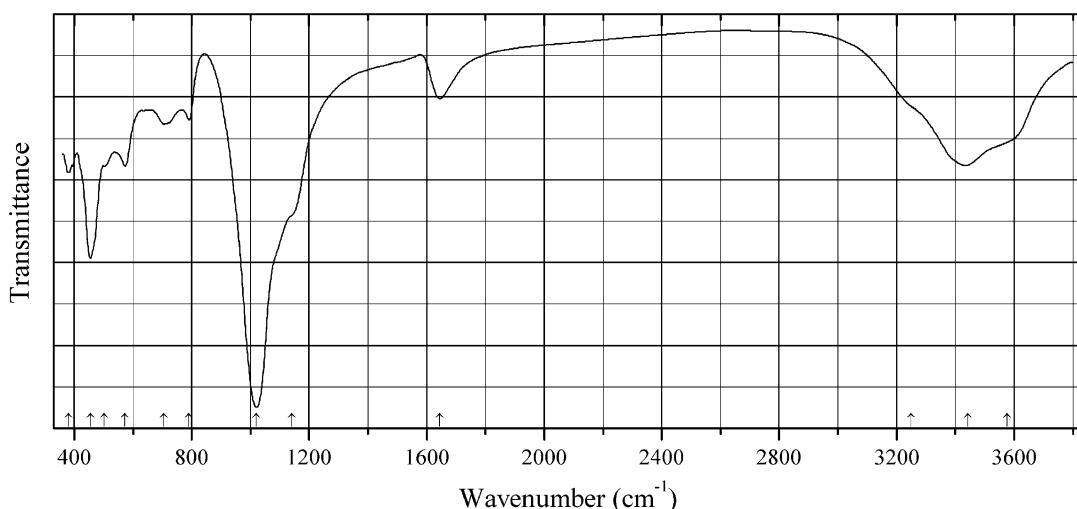
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Gualtieri (2000).

**Wavenumbers (cm<sup>-1</sup>):** 3400–3600 (broad), 3141s, 1645, 1460sh, 1407s, 980–1180 (broad), 786sh, 729, 700, 622, 463s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### Sif\_Z131 Faujasite-Ca (Ca,Na,Mg)<sub>2</sub>(Si,Al)<sub>12</sub>O<sub>24</sub>·15H<sub>2</sub>O



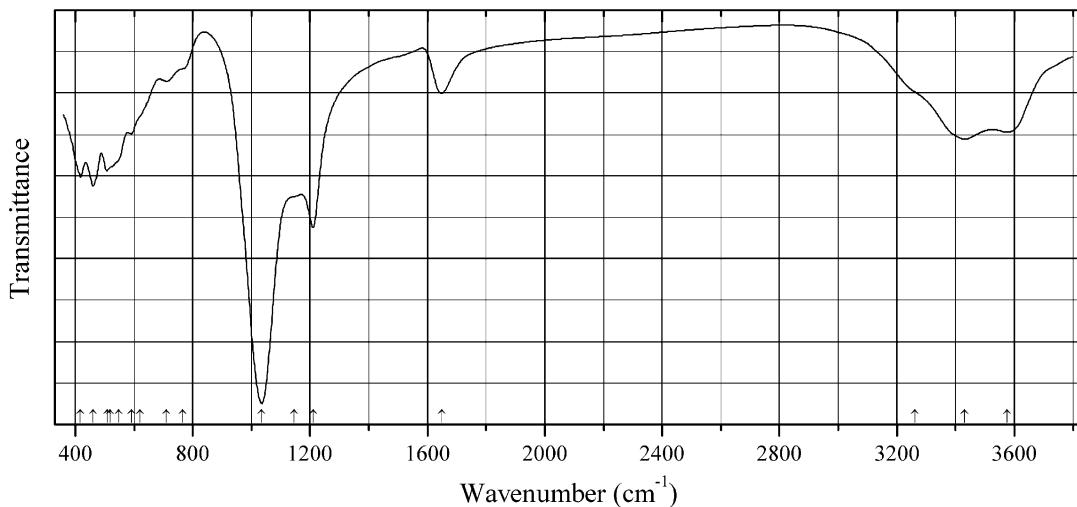
**Origin:** Quarry No. 1, Limberg, Sasbach, Germany.

**Description:** Colorless octahedral crystals from cavities in basalt. The empirical formula is (electron microprobe):  $(\text{Ca}_{11.5}\text{Mg}_{10.5}\text{Na}_7)(\text{Si}_{141}\text{Al}_{51}\text{O}_{384}) \cdot n\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3575sh, 3442, 3250sh, 1645, 1140sh, 1021s, 791, 706, 573, 503, 456s, 381.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sif\_Z132 Tschernichite**  $\text{CaAl}_2\text{Si}_6\text{O}_{16}\cdot8\text{H}_2\text{O}$ 

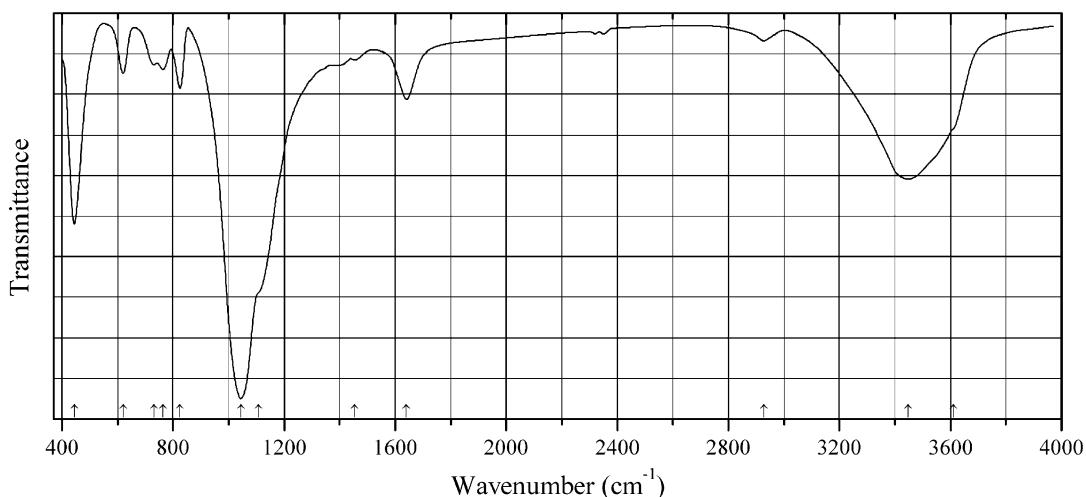
**Origin:** Markaz, Lis-Kas-Kő, Hungary.

**Description:** Colorless crystals. Identified by morphological features and qualitative electron microprobe analyses. Confirmed by the IR spectrum.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3577, 3430, 3260sh, 1648, 1210s, 1145, 1035s, 765sh, 711, 620sh, 591, 549sh, 520sh, 508, 460s, 418.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sif\_Z133 Mazzite-Na**  $\text{Na}_8(\text{Si}_{28}\text{Al}_8)\text{O}_{72}\cdot30\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Prepared hydrothermally in the reaction between magadiite, sodium aluminate, and NaOH in the presence of glycerol, at 120 °C with subsequent crystallization for several days under autogenous pressure. Characterized by powder X-ray diffraction data.

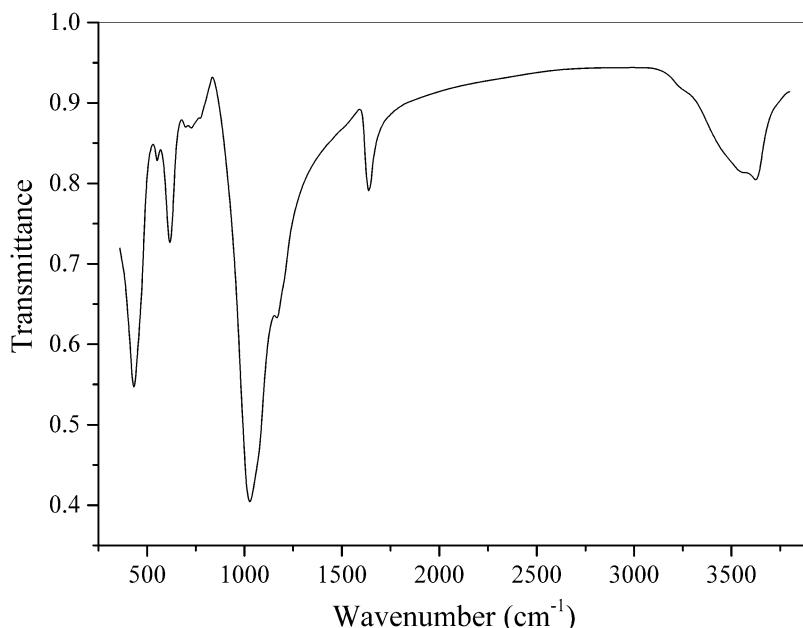
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Cui et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 3610sh, 3447s, 2927w, 1641, 1454w, 1107sh, 1046s, 825, 764, 731, 620, 445s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### Sif\_Z134 Martinandresite Ba<sub>2</sub>(Al<sub>4</sub>Si<sub>12</sub>O<sub>32</sub>)·10H<sub>2</sub>O



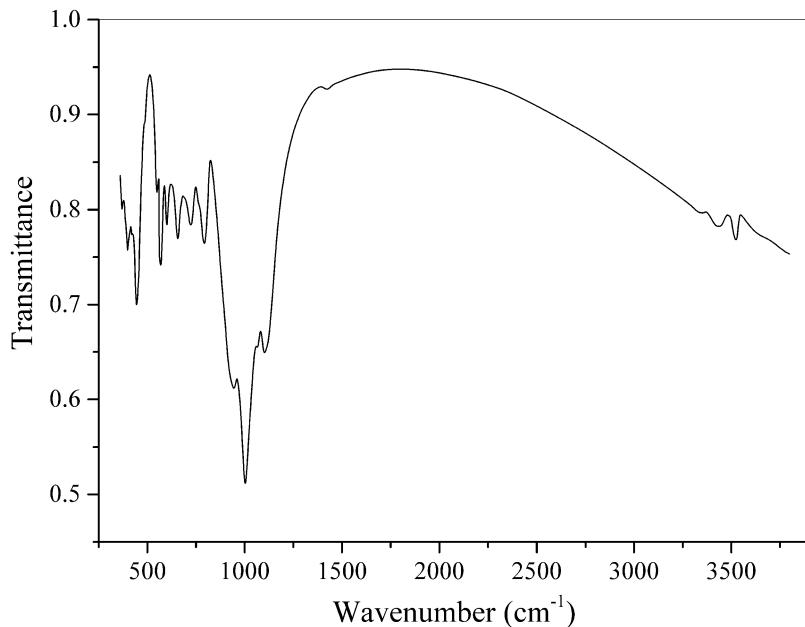
**Origin:** Wasenalp, near the Isenwegg peak, Ganter valley, Simplon region, Switzerland (type locality).

**Description:** Tan-colored blocky crystal from the association with armenite, quartz, dickite, and chlorite. Holotype sample. The crystal structure is solved. Orthorhombic, space group *Pmmn*,  $a = 9.4640(5)$ ,  $b = 14.2288(6)$ ,  $c = 6.9940(4)$  Å,  $V = 941.82(8)$  Å<sup>3</sup>,  $Z = 1$ .  $D_{\text{meas}} = 2.482(5)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 2.495$  g/cm<sup>3</sup>. Optically biaxial (−),  $\alpha = 1.500(2)$ ,  $\beta = 1.512(2)$ ,  $\gamma = 1.515(2)$ ,  $2V = 55$  (10)°. The empirical formula is  $\text{Na}_{0.17}\text{K}_{0.04}\text{Ba}_{2.00}(\text{Al}_{4.19}\text{Si}_{11.81}\text{O}_{32})\text{H}_{19.85}\text{O}_{9.93}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 6.98 (74) (001), 6.26 (83) (011), 5.61 (100) (101), 3.933 (60) (220, 031), 3.191 (50) (112), 3.170 (62) (041), 3.005 (79) (231, 141).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3625, 3570sh, 3260sh, 1638, 1167, 1028s, 774w, 728w, 700w, 616, 551, 432s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sif\_Z135 Rongibbsite**  $\text{Pb}_2(\text{Si}_4\text{Al})\text{O}_{11}(\text{OH})$ 

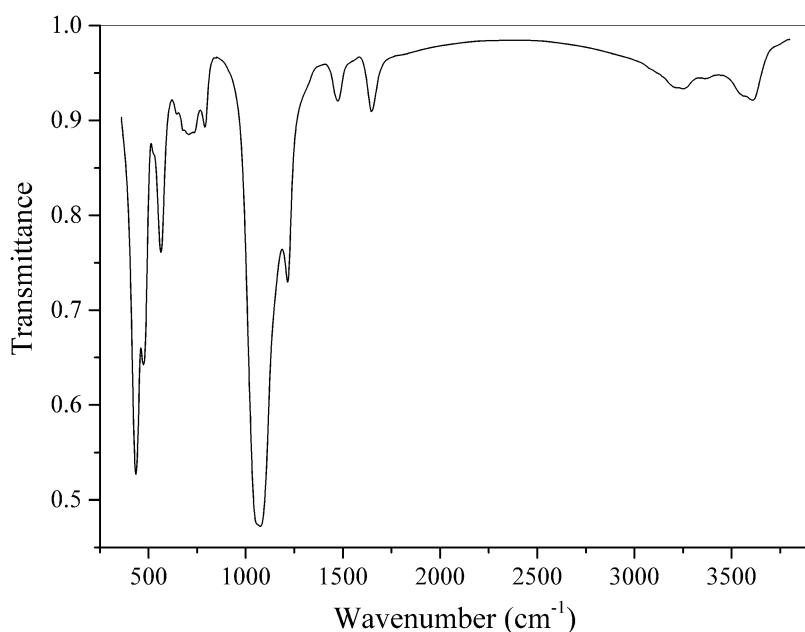
**Origin:** Big Horn Mts, Maricopa Co., Arizona, USA (type locality).

**Description:** Colorless prismatic crystals. The empirical formula is (electron microprobe):  $\text{Pb}_{2.0}\text{Si}_{3.75}\text{Al}_{1.1}\text{Mg}_{0.05}(\text{O},\text{OH})_{12}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm⁻¹):** 3524, 3436, (3347), (1425w), 1103s, 1065s, 1004s, 946s, 794, 724, 656, 600, 569, 549, 485sh, 444s, 425sh, 400, 373.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Sif\_Z136 Ferrierite-NH<sub>4</sub>**  $(\text{NH}_4,\text{Mg}_{0.5})_5(\text{Al}_5\text{Si}_{31}\text{O}_{72}) \cdot 22\text{H}_2\text{O}$ 

**Origin:** Libous lignite quarry, near Chomutov, Ústí Region, Bohemia, Czech Republic (type locality).

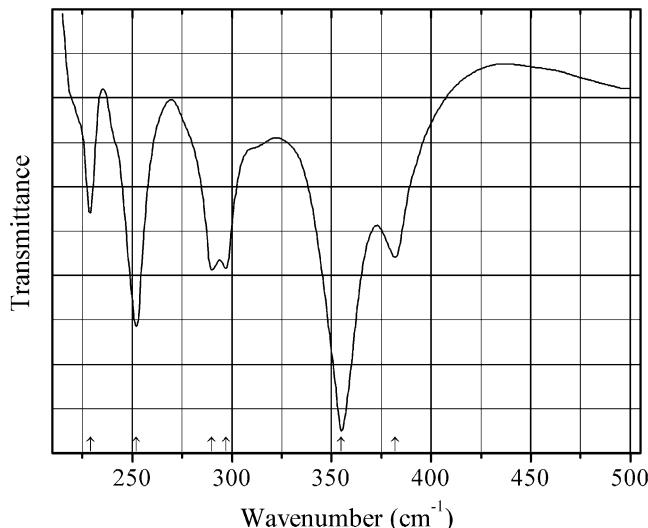
**Description:** Radiated aggregates consisting of fibrous crystals from the association with siderite, opal, kaolinite, goethite, and organic matter. Holotype sample. Orthorhombic, space group *Immm*,  $a = 19.10(1)$ ,  $b = 14.15(1)$ ,  $c = 7.489(3)$  Å,  $V = 2024(3)$  Å $^3$ ,  $Z = 1$ .  $D_{\text{calc}} = 2.154$  g/cm $^3$ . Optically biaxial (+),  $\alpha = 1.518(2)$ ,  $\beta = 1.520(2)$ ,  $\gamma = 1.522(2)$ . The empirical formula is  $\text{H}_{0.35}[(\text{NH}_4)_{2.74}\text{Mg}_{1.07}\text{Na}_{0.21}](\text{Al}_{5.44}\text{Si}_{30.56}\text{O}_{72}) \cdot 21.55\text{H}_2\text{O}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 6.95 (28) (101), 6.60 (19) (011), 3.988 (61) (321, 031, 420), 3.784 (19) (330), 3.547 (73) (112, 040), 3.482 (100) (202), 3.143 (37) (141, 312).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm $^{-1}$ ):** 3610, 3565sh, 3360w, 3250, 3220sh, 1646, 1474, 1216s, 1076s, 1060sh, 791, 730, 707, 681, 647w, 564s, 530sh, 474s, 435s.

**Note:** The spectrum was obtained by N.V. Chukanov.

### Si49 Chromium disilicide CrSi<sub>2</sub>



**Origin:** Synthetic.

**Description:** Thin film prepared by laser ablation of a cast stoichiometric CrSi target under vacuum.

The temperature of the substrate was 773 K. Hexagonal, space group *P<sub>6</sub>222*. Characterized by powder X-ray diffraction data.

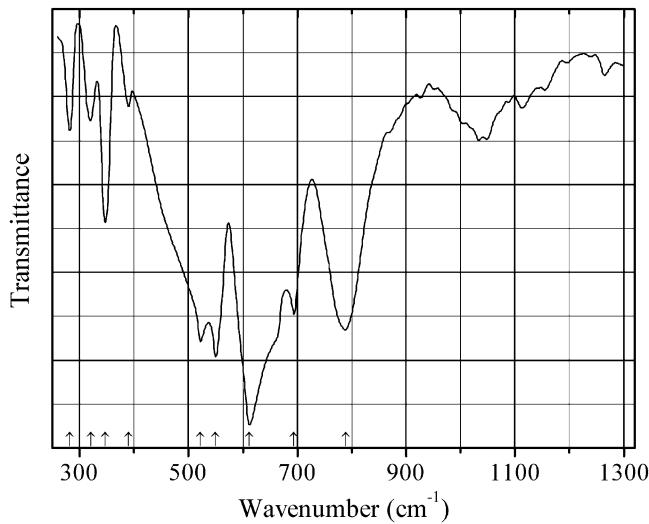
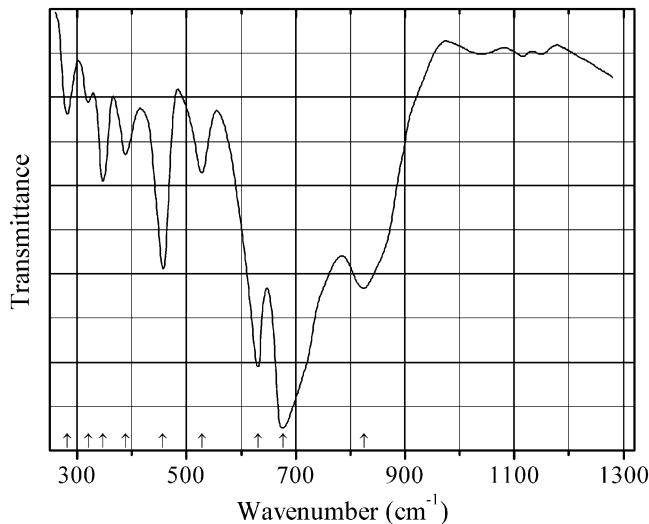
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission of a polycrystalline film.

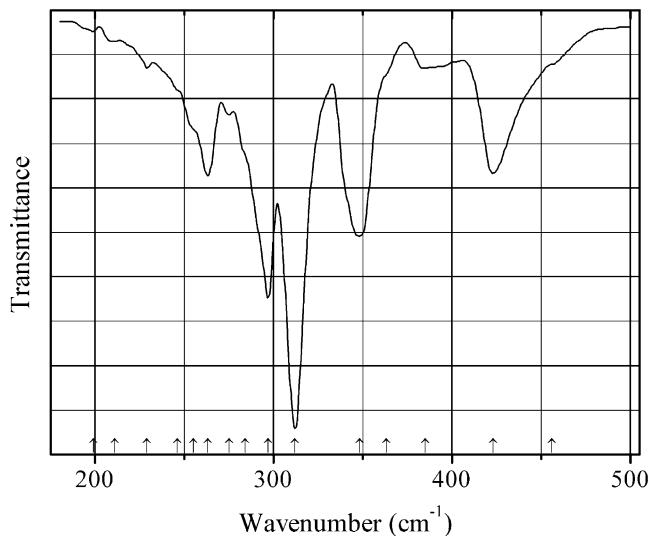
**Source:** Chaix-Pluchery and Lucaleau (1998).

**Wavenumbers (IR, cm $^{-1}$ ):** 382, 355s, 297, 290, 252s, 229.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, single crystal, polarization  $Y(XX)\text{-}Y + eY(XZ)\text{-}Y$ , cm $^{-1}$ ):** 412s, 397, 354, 305s, 300sh, 290w.

**Si50 Bridgmanite  $MgSiO_3$** **Magnesium silicon oxide perovskite-type****Origin:** Synthetic.**Description:** Obtained from the  $MgSiO_3$  glass in a laser heated diamond anvil cell at 500 kbar.**Kind of sample preparation and/or method of registration of the spectrum:** CsI or KBr disc. Absorption.**Source:** Madon and Price (1989).**Wavenumbers ( $\text{cm}^{-1}$ ):** 789s, 694, 612s, 550s, 522s, 390w, 347, 320, 282.**Si51 Akimotoite  $MgSiO_3$** **Origin:** Synthetic.**Description:** Synthesized from  $MgSiO_3$  glass in a laser heated diamond anvil cell at 500 kbar.**Kind of sample preparation and/or method of registration of the spectrum:** KBr or CsI disc. Absorption.**Source:** Madon and Price (1989).**Wavenumbers ( $\text{cm}^{-1}$ ):** 825s, 677s, 631s, 528, 457, 388, 347, 320w, 282.

**Si52 Luobusaite  $\beta\text{-FeSi}_2$** 

**Origin:** Synthetic.

**Kind of sample preparation and/or method of registration of the spectrum:** Thin film on single crystal Si substrate. Absorption.

**Source:** Fenske et al. (1996).

**Wavenumbers (cm<sup>-1</sup>):** 456sh, 423, 385w, 363sh, 348s, 312s, 297s, 284sh, 275w, 263, 255sh, 246sh, 229w, 211sh, 199w.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**Si53 Mendeleevite-(Nd)  $\text{Cs}_6[(\text{Nd},\text{REE})_{23}\text{Ca}_7](\text{Si}_{70}\text{O}_{175})(\text{OH},\text{F})_{19}\cdot16\text{H}_2\text{O}$** 

**Origin:** Dara-i Pioz glacier, Dara-i Pioz alkaline massif, Tien Shan Mts., Tajikistan (type locality).

**Description:** Anhedral grains from the association with pectolite grains, quartz, aegirine, fluorite, etc. Holotype sample. Cubic, space group *Pm-3*,  $a = 21.9106(4)$  Å,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Agakhanov et al. (2016a).

**Wavenumbers (cm<sup>-1</sup>):** 3408, 1612, 1011s, 980s, 695sh, 547sh.

**Si54 Bridgmanite trigonal polymorph  $\text{MgSiO}_3$** 

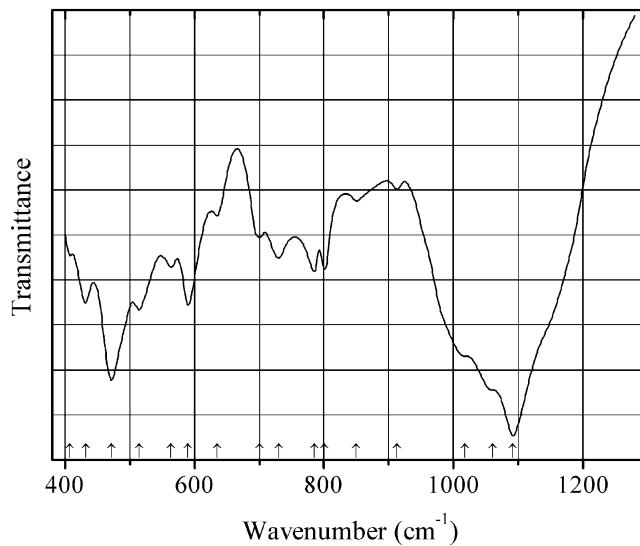
**Origin:** Synthetic.

**Description:** Isostructural with ilmenite. Single crystal.

**Kind of sample preparation and/or method of registration of the spectrum:** Unpolarized reflection.

**Source:** Hofmeister and Ito (1992).

**Wavenumbers (cm<sup>-1</sup>):** 951, 665, 619, 536w, 448, 377.

**Si55 Sapphirine**  $Mg_4(Mg_3Al_9)O_4[Si_3Al_9O_{36}]$ 

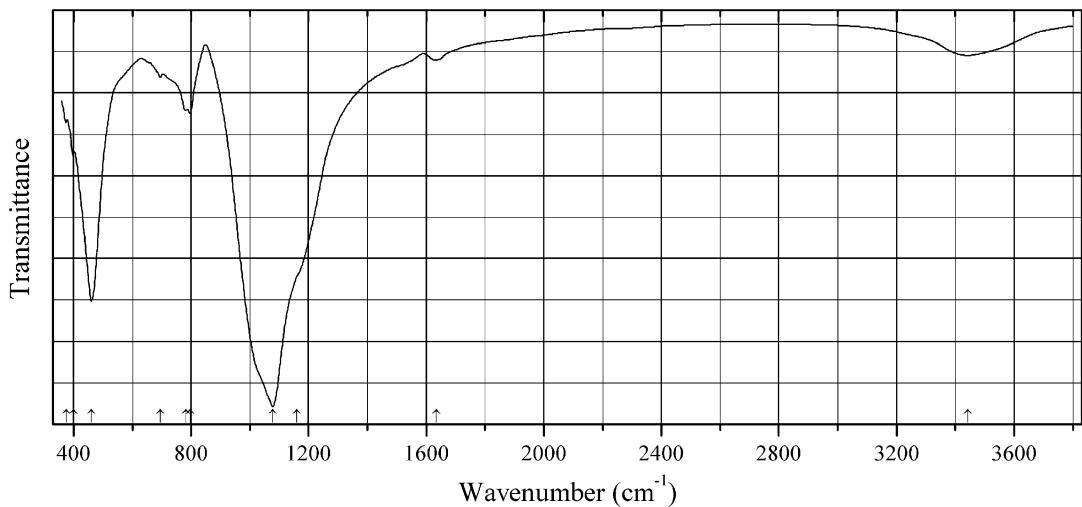
**Origin:** Betroka, Anosy Region, Tuléar (Toliara) province, Madagascar.

**Description:** Metacrystal from metamorphic schist.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Povarennykh (1970).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1092s, 1060sh, 1018sh, 913w, 850w, 801, 785, 730, 700, 635w, 590, 564, 515, 472s, 432, 408w.

**Sia24 Pearlite**  $(Na,K)_x(Si_{1-x}Al_xO_2)\cdot nH_2O$  ( $x \ll 1$ )

**Origin:** Tsigrado quarry, Milos Island, Greece.

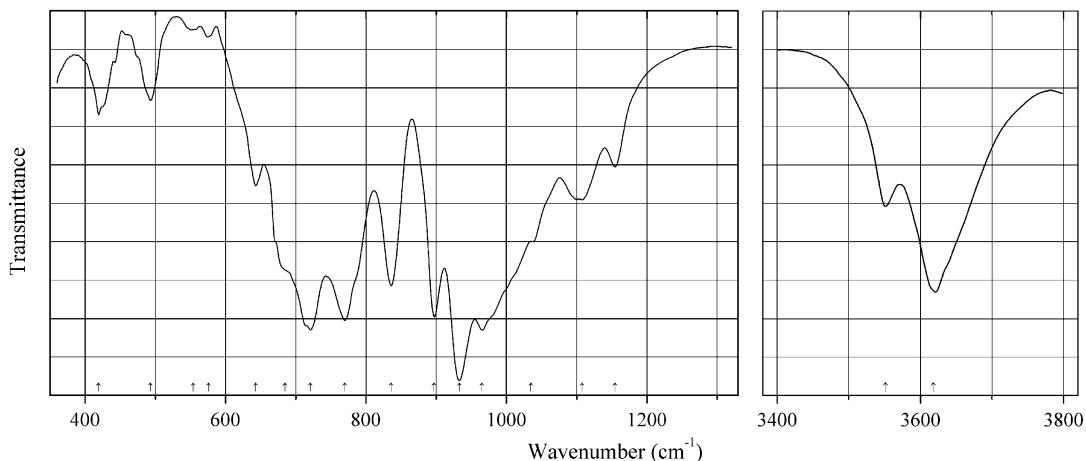
**Description:** Light gray, semitransparent, massive, from the association with hydrobiotite. The sample contains quartz inclusions.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3442, 1634w, 1160sh, 1078s, 796, 783, 695w, 461s, 400, 375.

**Note:** The spectrum was obtained by N.V. Chukanov.

**BeSi74 Sphaerobertrandite Be<sub>3</sub>SiO<sub>4</sub>(OH)<sub>2</sub>**



**Origin:** Sagåsen, Tvedalen, Larvik, S. Norway.

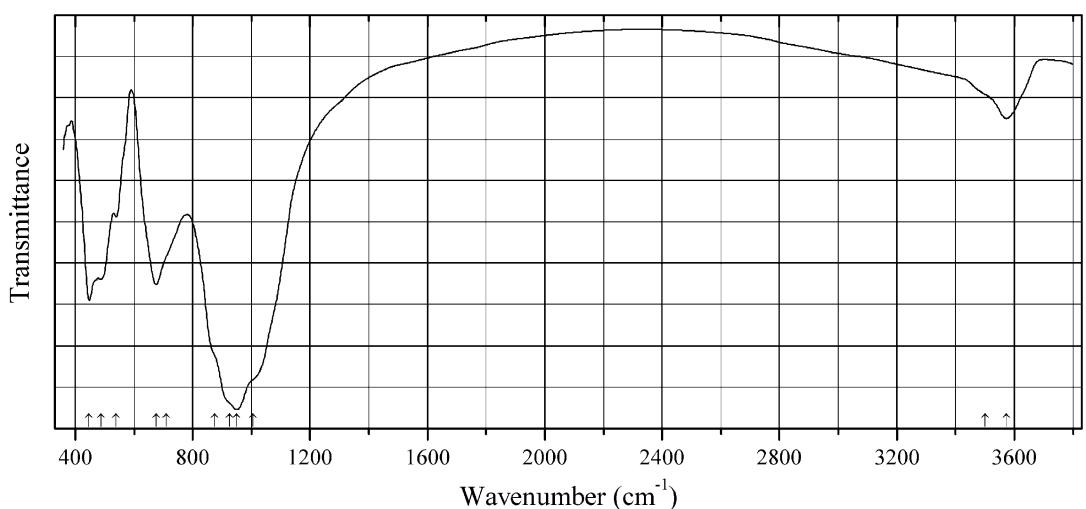
**Description:** Yellow spherulites from the association with diaspore. Identified by the IR spectrum.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3618s, 3551s, 1155, 1108, 1035sh, 965s, 933s, 897s, 836s, 770s, 721s, 685sh, 643, 576w, 554w, 493, 419.

**Note:** The spectrum was obtained by N.V. Chukanov.

**BeSi75 Hydroxylgugiaite (Ca<sub>3</sub>□)(Si<sub>3.5</sub>Be<sub>2.5</sub>)O<sub>11</sub>(OH)<sub>3</sub>**



**Origin:** Larvik plutonic complex, Porsgrunn, Telemark, Norway (type locality).

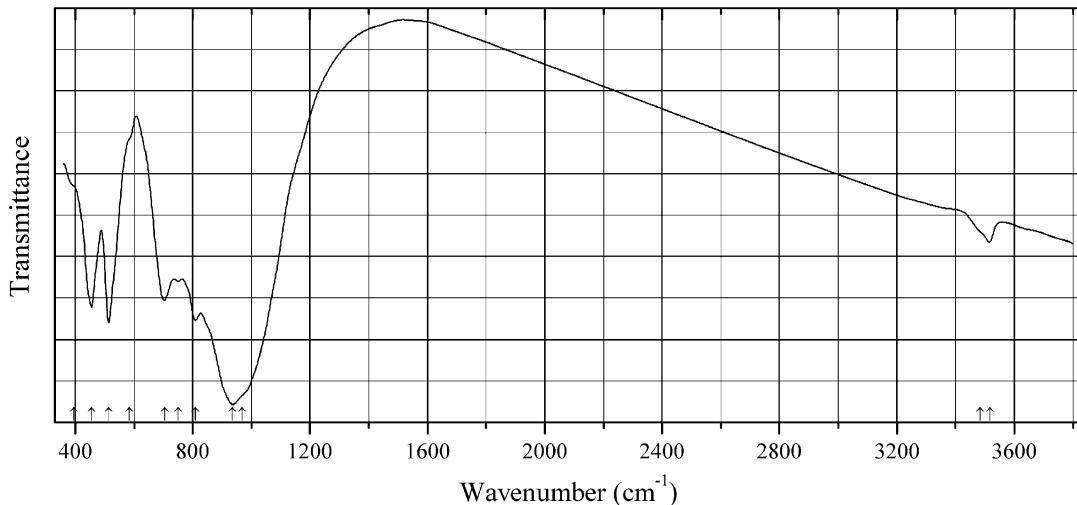
**Description:** Pale grey crystals from the association with chlorite and calcite. Holotype sample. The crystal structure is solved. Tetragonal, space group  $P-42_1/m$ ,  $a = 7.4151(2)$ ,  $c = 4.9652(1)$  Å,  $V = 272.9(1)$  Å $^3$ ,  $Z = 12$ . Optically uniaxial (+),  $\omega = 1.622(2)$ ,  $e = 1.632(2)$ . The empirical formula is  $(\text{Ca}_{2.76}\text{Na}_{0.31}\text{Mn}_{0.05}\text{Fe}_{0.01})(\text{Si}_{3.45}\text{Be}_{2.53}\text{Al}_{0.07})\text{O}_{11}[(\text{OH})_{2.57}\text{F}_{0.43}]$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm $^{-1}$ ):** 3574, 3500sh, 1105sh, 950s, 925sh, 875sh, 710sh, 676, 539, 487, 447.

**Note:** The spectrum was obtained by N.V. Chukanov.

### BeSi76 “Hydroxylgadolinite-(Y)” $(\text{Y},\text{Ca})_2(\text{Fe},\square)\text{Be}_2\text{Si}_2\text{O}_8(\text{OH},\text{O})_2$



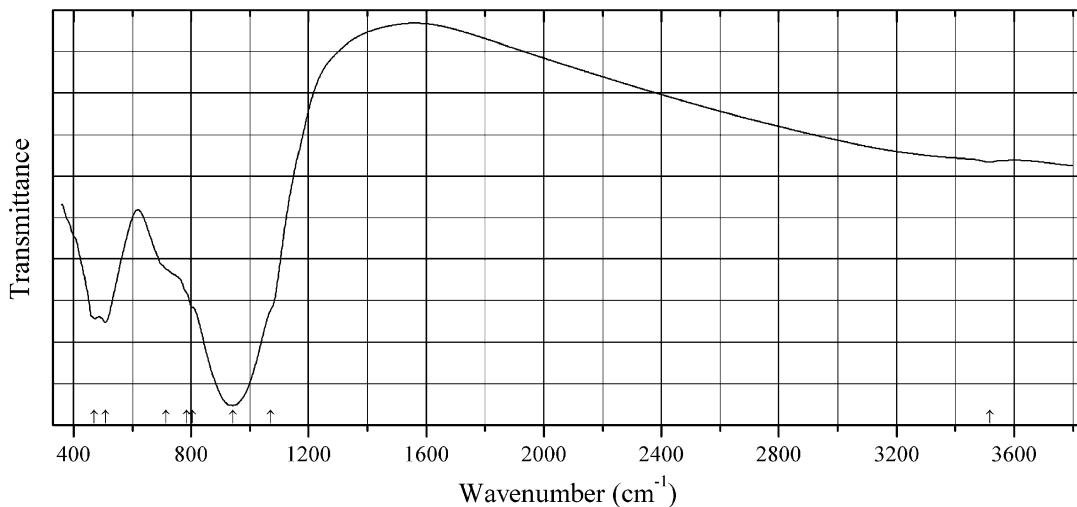
**Origin:** Heftetjern granitic pegmatite, Southern Norway.

**Description:** Bottle-green grains and short-prismatic crystals from the association with feldspar, quartz, and intermediate members of the gadolinite-(Y)-hingganite-(Y) solid-solution series. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 4.7514(10)$ ,  $b = 7.5719(16)$ ,  $c = 9.9414(2)$  Å,  $\beta = 90.015(4)^\circ$ ,  $V = 357.663(3)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{calc}} = 3.967$  g/cm $^3$ . Optically biaxial (+),  $\alpha = 1.760(4)$ ,  $\beta = 1.770(4)$ ,  $\gamma = 1.785(4)$ ,  $2V = 80(10)^\circ$ . The empirical formula is  $(\text{Y}_{1.285}\text{Ca}_{0.55}\text{Ce}_{0.07}\text{La}_{0.04}\text{Nd}_{0.01})\text{Fe}^{2+}_{0.57}\text{Be}_{2.02}\text{Si}_{1.995}\text{O}_{8.48}(\text{OH})_{1.52}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 4.761 (48) (100), 3.554 (30) (021), 3.452 (30) (10-2, 102), 3.138 (81) (11-2, 112), 2.972 (39) (120), 2.849 (100) (12-1, 121), 2.570 (59) (11-3, 113, 12-2), and 2.215 (27) (211, 12-3, 123).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm $^{-1}$ ):** 3517, 3485sh, 970sh, 936s, 809, 752, 704, 585sh, 514, 455, 395sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**BeSi77 Gadolinite-(Y)  $\text{Y}_2\text{Fe}^{2+}\text{Be}_2\text{Si}_2\text{O}_{10}$** 

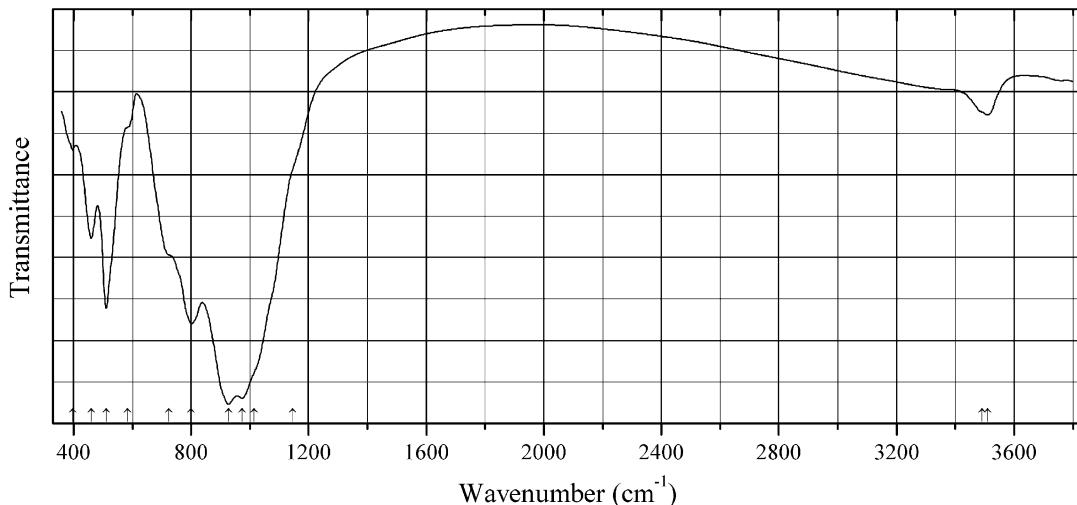
**Origin:** Row Lake, Keivy Mts., Kola Peninsula, Russia.

**Description:** Black grains from pegmatite. X-ray amorphous, metamict. Confirmed by semiquantitative electron microprobe analysis.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm⁻¹):** 3518w, 1070sh, 942s, 805sh, 785sh, 715sh, 508, 470.

**Note:** The spectrum was obtained by N.V. Chukanov.

**BeSi78 Hingganite-(Y)  $\text{Y}_2\text{□Be}_2\text{Si}_2\text{O}_8(\text{OH})_2$** 

**Origin:** Heftetjern pegmatite, Tørdal, Telemark, Norway.

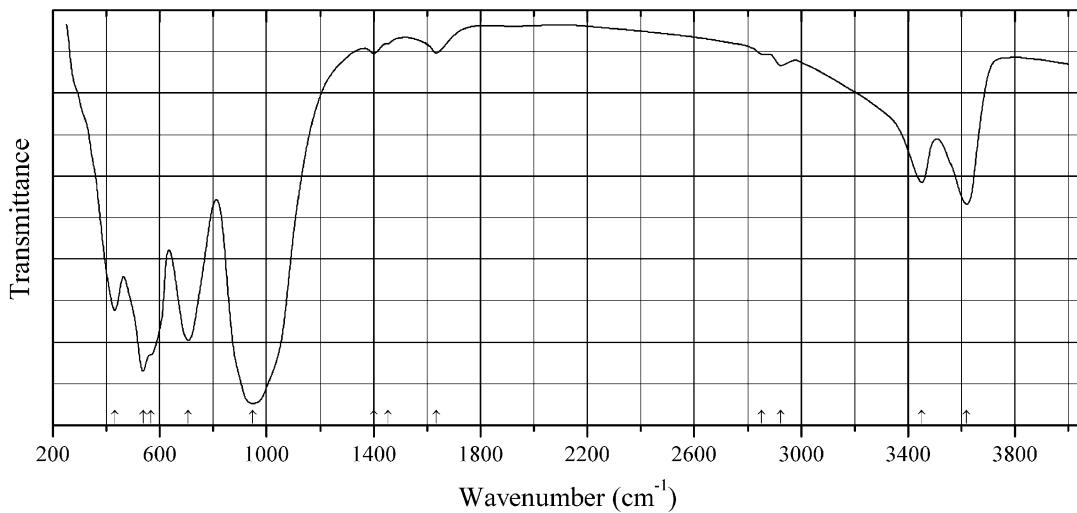
**Description:** Olive-green crystals from the association with REE-bearing epidote. A Ca- and Fe-rich variety.

The empirical formula is (electron microprobe):  $\sim(\text{Y}_{1.1}\text{Ca}_{0.8}\text{Ln}_{0.1})(\text{Fe}_{0.35}\text{Al}_{0.05})\text{Be}_2\text{Si}_2\text{O}_{8.05}(\text{OH})_{1.95}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm⁻¹):** 3510, 3490sh, 1145sh, 1015sh, 973s, 927s, 800, 725sh, 585sh, 511, 460, 398w.

**Note:** The spectrum was obtained by N.V. Chukanov.

**BeSi79 Bityite**  $\text{CaLiAl}_2(\text{Si}_2\text{BeAl})\text{O}_{10}(\text{OH})_2$ 

**Origin:** Maantienvarsni pegmatite, Eräjärvi area, Orivesi, southern Finland.

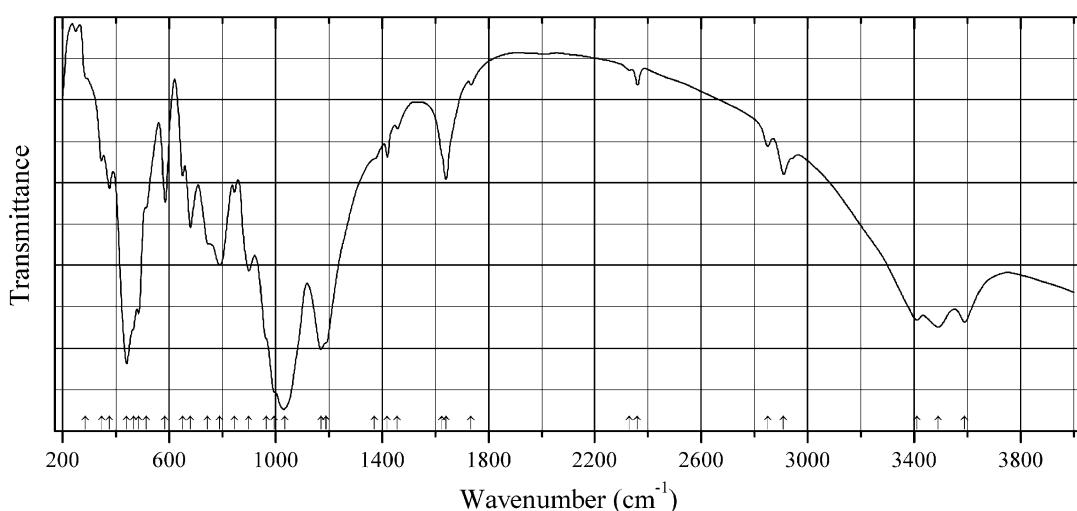
**Description:** Fine-scaled white to yellowish mass with a pearly lustre from the association with beryl, bertrandite, fluorite, and fluorapatite. Characterized by powder X-ray diffraction data. Monoclinic, space group  $C2/c$  or  $Cc$ ,  $a = 4.99$ ,  $b = 8.68$ ,  $c = 19.04 \text{ \AA}$ ,  $\beta = 95.17^\circ$ ,  $V = 821.33 \text{ \AA}^3$ .  $D_{\text{meas}} = 3.05 \text{ g/cm}^3$ ,  $D_{\text{calc}} = 3.12 \text{ g/cm}^3$ . Optically biaxial (-),  $\alpha = 1.650$ ,  $\beta = 1.658$ ,  $\gamma = 1.660$ ,  $2V = 52.9^\circ$ . The empirical formula is (wet chemical analysis,  $Z = 2$ ):  $(\text{Ca}_{1.93}\text{K}_{0.03}\text{Na}_{0.02})(\text{Li}_{1.19}\text{Al}_{3.68}\text{Mg}_{0.35}\text{Fe}_{0.13})(\text{Si}_{4.26}\text{Be}_{2.21}\text{Al}_{1.53})\text{O}_{19.30}(\text{OH})_{4.54}\text{F}_{0.16}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Lahti and Saikonen (1985).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3620, 3451, (2924), (2853sh), 1634w, 1453sh, 1400w, 949s, 707s, 568sh, 537s, 431.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**BeSi80 Chiavennite**  $\text{CaMn}^{2+}(\text{BeOH})_2\text{Si}_5\text{O}_{13} \cdot 2\text{H}_2\text{O}$ 

**Origin:** Chiavenna, Valchiavenna, Sondrio Province, Lombardy, Italy (type locality).

**Description:** Euhedral orange grains and crusts from the association with beryl and bavenite. Holotype sample. Orthorhombic, space group  $P2_1ab$ ,  $a = 8.729(5)$ ,  $b = 31.326(11)$ ,  $c = 4.903(2)$  Å,  $Z = 4$ .  $D_{\text{meas}} = 2.64(1)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 2.657$  g/cm<sup>3</sup>. Optically biaxial (−),  $\alpha = 1.581(1)$ ,  $\gamma = 1.600(1)$ ,  $2V = 70(5)^\circ$ . The empirical formula is  $(\text{Ca}_{0.97}\text{Na}_{0.05})\text{Mn}_{0.97}(\text{Be}_{1.98}\text{Al}_{0.03})(\text{Si}_{4.65}\text{Al}_{0.35})\text{O}_{12.63}(\text{OH})_{2.37} \cdot 2.16\text{H}_2\text{O}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 15.7 (100) (020), 4.15 (30) (041), 3.93 (30) (080), 3.82 (30) (240), 3.28 (75) (201), 2.903 (100) (251, 181), 1.944 (30) (3.12.0).

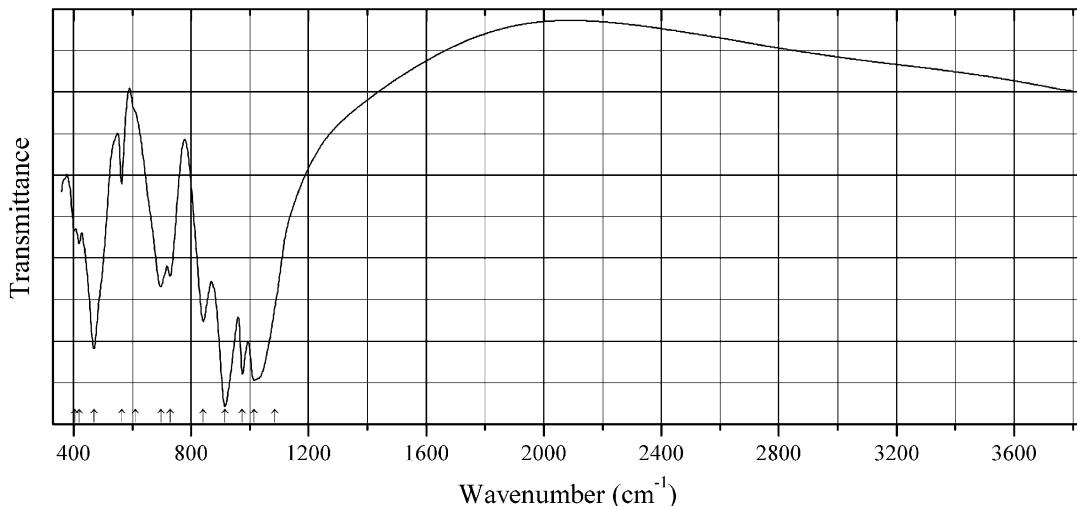
**Kind of sample preparation and/or method of registration of the spectrum:** Absorption. Kind of sample preparation is not indicated.

**Source:** Bondi et al. (1983).

**Wavenumbers (cm<sup>−1</sup>):** 3590, 3490, 3410, (2910), (2850), (2360), (2330), 1735, 1640, 1625sh, 1458, 1420, 1372sh, 1190sh, 1170, 1035, 995sh, 965sh, 900, 845, 790, 745sh, 680, 650, 585, 515sh, 485, 465sh, 440, 375, 345, 285sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. Weak bands in the ranges from 2300 to 2400 cm<sup>−1</sup> and from 2800 to 3000 cm<sup>−1</sup> correspond to atmospheric CO<sub>2</sub> and the admixture of an organic substance.

### BeSi81 Gugiaite $\text{Ca}_2\text{BeSi}_2\text{O}_7$



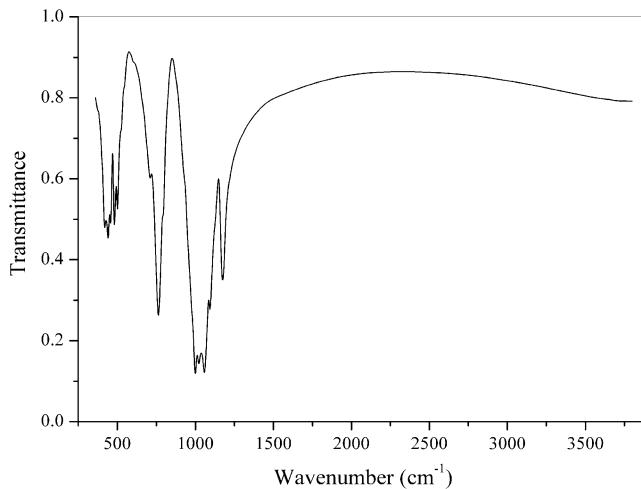
**Origin:** Dugdu alkaline massif, Tuva Republic, Eastern Siberia, Russia.

**Description:** Rosette-like aggregates of white semitransparent crystals from the association with meliphyanite. Confirmed by the IR spectrum.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>−1</sup>):** 1025sh, 1015s, 975s, 915s, 841, 729, 697, 610sh, 564, 470, 419, 404.

**Note:** The spectrum was obtained by N.V. Chukanov.

**BeSi82 Leifite**  $\text{NaNa}_6\text{Be}_2\text{Al}_3\text{Si}_{15}\text{O}_{39}\text{F}_2$ 

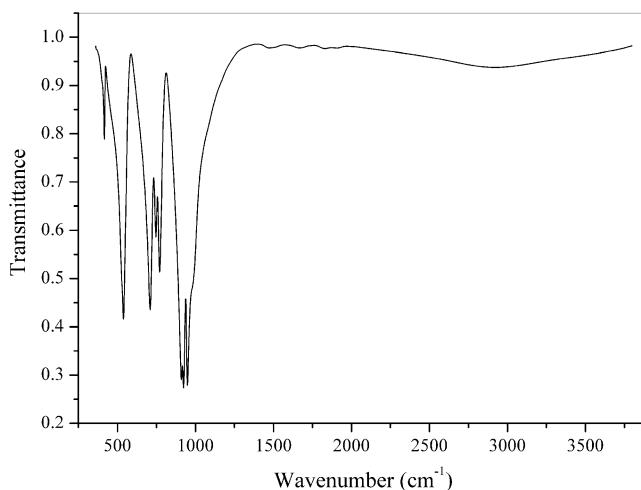
**Origin:** Poudrette (Demix) quarry, Mont Saint-Hilaire, Rouville RCM (Rouville Co.), Montérégie, Québec, Canada.

**Description:** White radiated aggregate of prismatic crystals. Investigated by A.V. Voloshin. Confirmed by the IR spectrum.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 1175s, 1094s, 1058s, 1023s, 1000s, 935sh, 795sh, 764s, 712, 610sh, 545sh, 515sh, 502, 481, 457, 440s, 419.

**Note:** The spectrum was obtained by N.V. Chukanov.

**BeSi83 Danalite**  $\text{Fe}^{2+} \text{Fe}^{2+}_4\text{Be}_3(\text{SiO}_4)_3\text{S}$ 

**Origin:** Lupikko deposit, near Pitkäranta, Ladoga lake, Karelia, Russia.

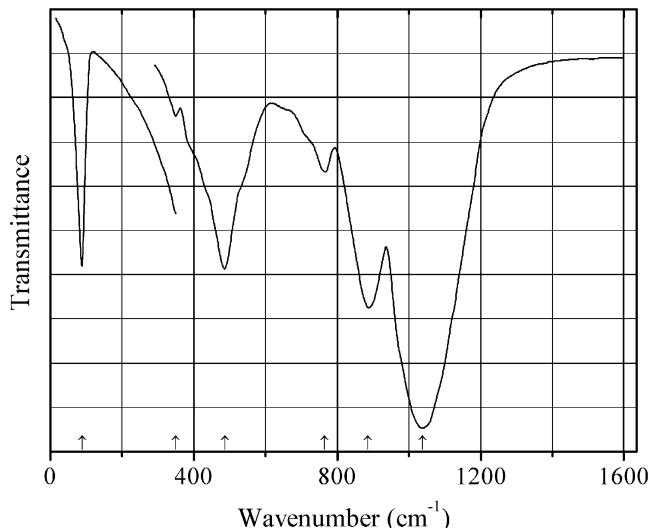
**Description:** Dark red grain in skarn, in the association with clinochlore, calcite, and fluorite. The empirical formula is (electron microprobe):  $\text{H}_x\text{Fe}_{2.6}\text{Mn}_{0.8}\text{Zn}_{0.6}\text{Be}_3\text{Si}_3\text{O}_{12}\text{S}_{0.9}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 2922 (broad), 1907w, 1830w, 1667w, 1473w, 975sh, 948s, 924s, 910s, 771, 747, 710, 538, 416.

**Note:** The spectrum was obtained by N.V. Chukanov. The broad band at  $2922\text{ cm}^{-1}$  indicates the presence of OH groups forming strong hydrogen bonds.

**BSi99 Cesium borosilicate pollucite-type  $\text{CsBSi}_2\text{O}_6$**



**Origin:** Synthetic.

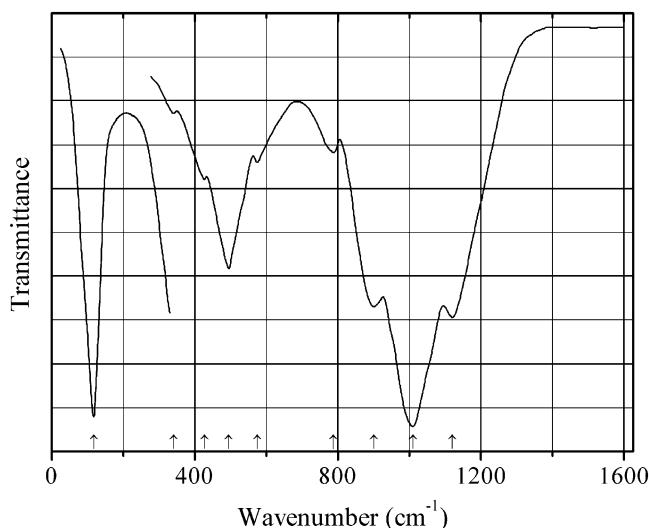
**Description:** Synthesized from the stoichiometric mixture of  $\text{Cs}_2\text{CO}_3$ ,  $\text{H}_3\text{BO}_3$ , and  $\text{SiO}_2$  by a conventional solid-state reaction technique at  $800\text{ }^\circ\text{C}$ . Structurally related to pollucite.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

**Source:** Rulmont and Tarte (1987).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1037s, 886, 765w, 487, 350w, 88.

**BSi100 Potassium borosilicate pollucite-type  $\text{K(BSi}_2\text{O}_6$ )**



**Origin:** Synthetic.

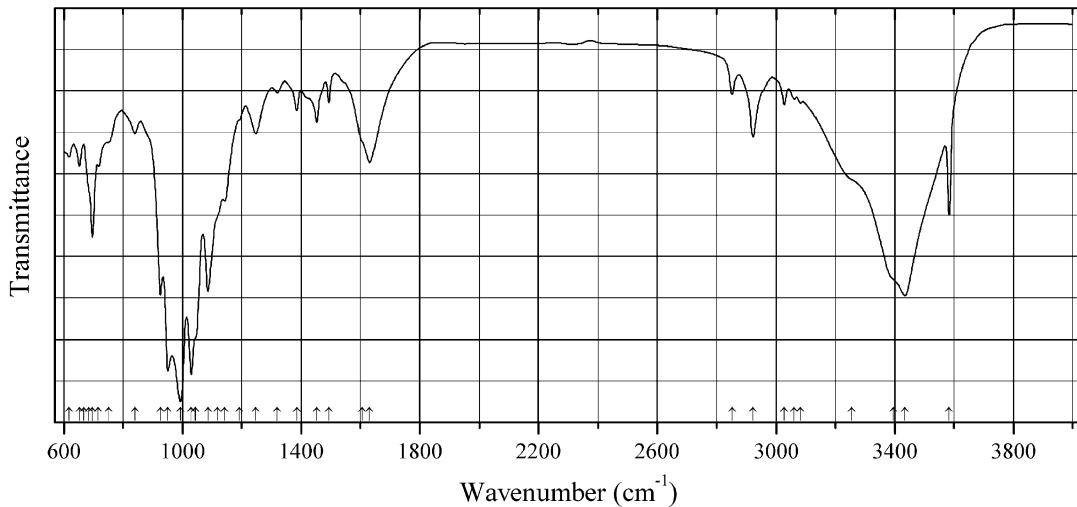
**Description:** Obtained by heating the stoichiometric mixture of  $K_2CO_3$ ,  $H_3BO_3$ , and  $SiO_2$  to 800 °C. Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

**Source:** Rulmont and Tarte (1987).

**Wavenumbers (cm<sup>-1</sup>):** 1120s, 1010s, 900s, 788w, 575w, 495, 427, 340w, 117s.

### BSi101 Nolzeite $NaMn_2(Si_3BO_9)(OH)_2 \cdot 2H_2O$



**Origin:** Poudrette quarry, La Vallée-du-Richelieu, Montérégie (formerly Rouville County), Québec, Canada (type locality).

**Description:** Pale green acicular crystals from the association with aegirine, nepheline, sodalite, eudialyte-group minerals, analcime, natron, pyrrhotite, catapleiite, and steedeite. Holotype sample. The crystal structure is solved. Boron has fourfold coordination. Triclinic, space group  $P-1$ ,  $a = 6.894(1)$ ,  $b = 7.632(2)$ ,  $c = 11.017(2)$  Å,  $\alpha = 108.39(3)$ °,  $\beta = 99.03(3)$ °,  $\gamma = 103.05(3)$ °,  $V = 519.27$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 2.79$  g/cm<sup>3</sup>. Optically biaxial,  $n_{\text{min}} = 1.616(2)$ ,  $n_{\text{max}} = 1.636(2)$ . The empirical formula is  $Na_{1.04}(Mn_{1.69}Fe_{0.24}Ca_{0.02})(Si_{2.96}S_{0.04})(B_{0.70}Si_{0.30})O_9(OH)_2 \cdot 2H_2O$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å (I, %) ( $hkl$ )] are: 10.113 (100) (00-1), 6.911 (16) (0-10), 3.593 (13) (0-13), 3.026 (15) (0-23), 2.808 (50) (211, 2-20), 2.675 (12) (0-1-3).

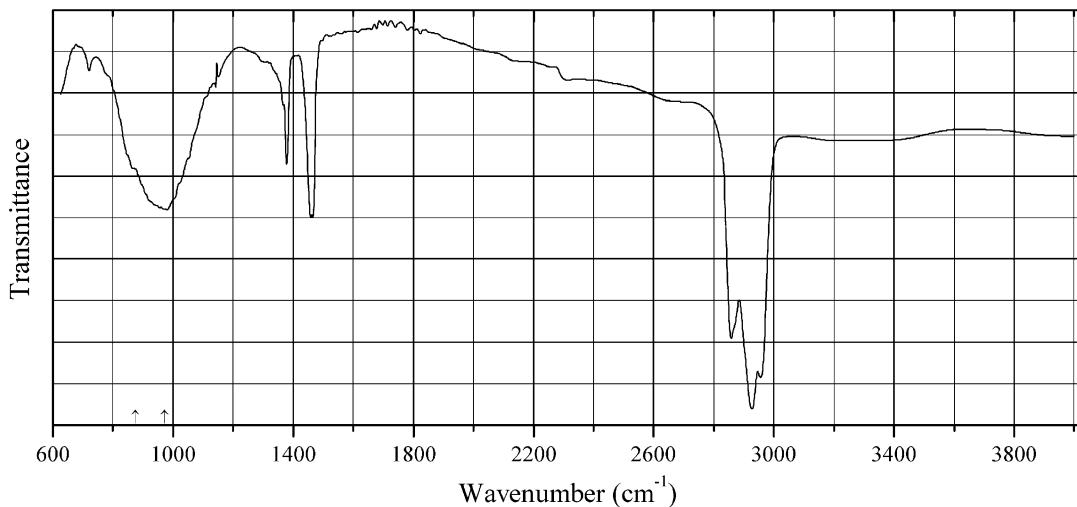
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Haring and McDonald (2016).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3583, 3434s, 3395sh, 3254sh, 3083w, 3062w, 3028w, 2922, 2852w, 1631, 1607sh, 1493w, 1453w, 1385w, 1320w, 1247, 1192sh, 1143s, 1117sh, 1086s, 1044sh, 1030, 993s, 951, 926, 840, 752sh, 717, 697, 685sh, 653w, 618w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. Weak bands in the range from 2800 to 3100 cm<sup>-1</sup> may correspond to the admixture of an organic substance. Weak bands in the range from 1240 to 1500 cm<sup>-1</sup> may correspond to the admixture of an organic substance and/or (partly) carbonate groups. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 3548, 3399, 1588, 1290, 1009, 842, 626, 553, 390, 341, 268, 223, 167.

**BSi102 Proshchenkoite-(Y)  $(Y,REE,Ca,Na,Mn)_{15}Fe^{2+}Ca(P,Si)Si_6B_3(O,F)_{48}$** 

**Origin:** Tommot REE-Nb deposit, Yakutia, Russia (type locality).

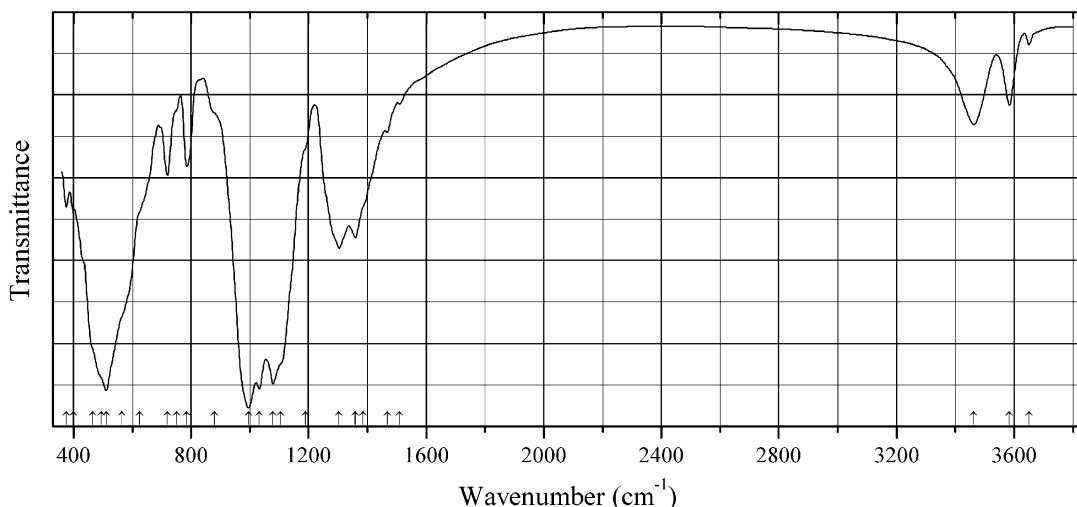
**Description:** Reddish-brown grains. Trigonal, space group  $R\bar{3}m$ ,  $a = 10.7527(7)$ ,  $c = 27.4002(18)$  Å,  $V = 2743.6(6)$  Å<sup>3</sup>,  $Z = 3$ . Uniaxial (-),  $\omega = 1.734(2)$ ,  $e = 1.728(2)$ . The empirical formula is  $(Y_{3.70}REE_{7.54}Ca_{1.55}Na_{1.16}Mn_{0.77}Th_{0.10}Pb_{0.01})(Fe^{2+}_{0.83}Mn_{0.15}Ti_{0.02})Ca_{1.00}(P_{0.70}Si_{0.26}As_{0.04})Si_{6.05}B_{3.20}(O_{34.55}F_{13.45})$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 4.441 (36) (202), 3.144 (77) (214), 3.028 (45) (009), 2.968 (100) (027), 1.782 (32) (330), 1.713 (32) (1.2.14).

**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull. Transmission.

**Source:** Kristiansen (2016); for the sample description see Raade et al. (2008).

**Wavenumbers (cm<sup>-1</sup>):** 972s, 871sh.

**Note:** Strong bands above 1200 cm<sup>-1</sup> correspond to Nujol.

**BSi103 Darrellhenryite  $Na(LiAl_2)Al_6(BO_3)_3Si_6O_{18}(OH)_3O$** 

**Origin:** Nová Ves, Český Krumlov, South Bohemia Region, Czech Republic (type locality).

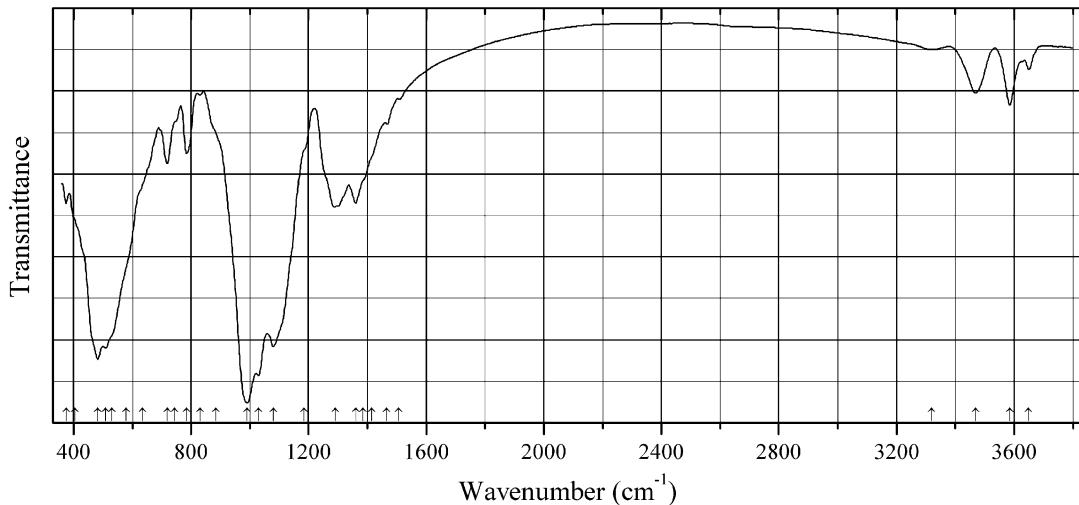
**Description:** Pink grains. Fragments of the cotype sample. Characterized by electron microprobe analyses.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3650w, 3584, 3463, 1509w, 1467w, 1385sh, 1359, 1304, 1190sh, 1105sh, 1079s, 1032s, 996s, 880sh, 786, 750sh, 720, 625sh, 565sh, 511s, 495sh, 465sh, 400w, 376w.

**Note:** The spectrum was obtained by N.V. Chukanov.

**BSi104 Darrellhenryite** Na(LiAl<sub>2</sub>)Al<sub>6</sub>(BO<sub>3</sub>)<sub>3</sub>Si<sub>6</sub>O<sub>18</sub>(OH)<sub>3</sub>O



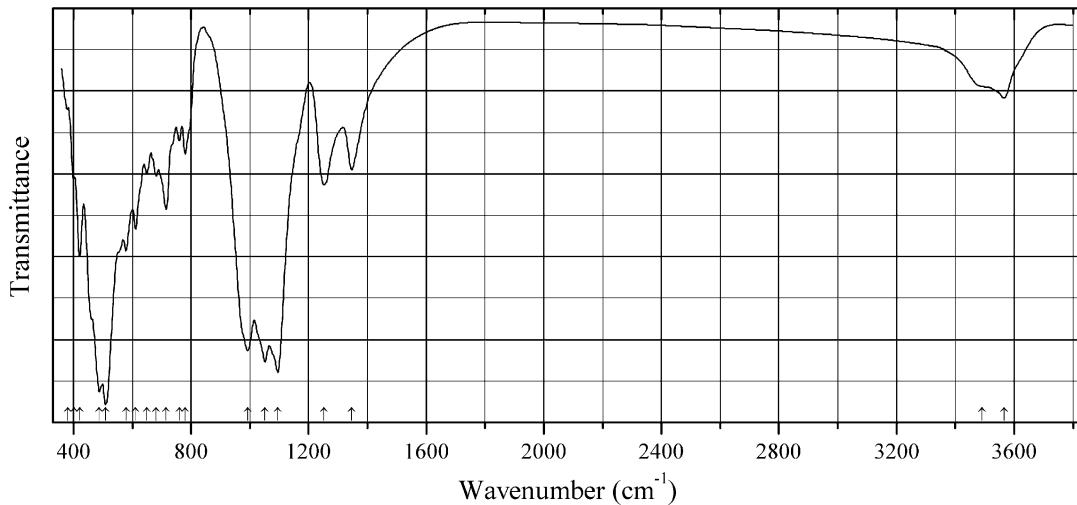
**Origin:** Aleksandrovskoe Ta deposit, Irkutsk region, Siberia, Russia.

**Description:** Colorless grains from pegmatite. Investigated by A.V. Kasatkin. The empirical formula is (electron microprobe, Li calculated): Na<sub>0.59</sub>LiAl<sub>7.98</sub>Ti<sub>0.02</sub>(BO<sub>3</sub>)<sub>3</sub>(Si<sub>6</sub>O<sub>18</sub>)(OH)<sub>3</sub>(O,OH).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3649w, 3585, 3469, 3320w, 1507w, 1465w, 1415sh, 1385sh, 1360, 1280, 1185sh, 1080s, 1029s, 990s, 885sh, 830w, 785, 745sh, 719, 635sh, 580sh, 530sh, 510s, 483s, 405sh, 375.

**Note:** The spectrum was obtained by N.V. Chukanov.

**BSi105 Fluor-drawite**  $\text{NaMg}_3\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3\text{F}$ 

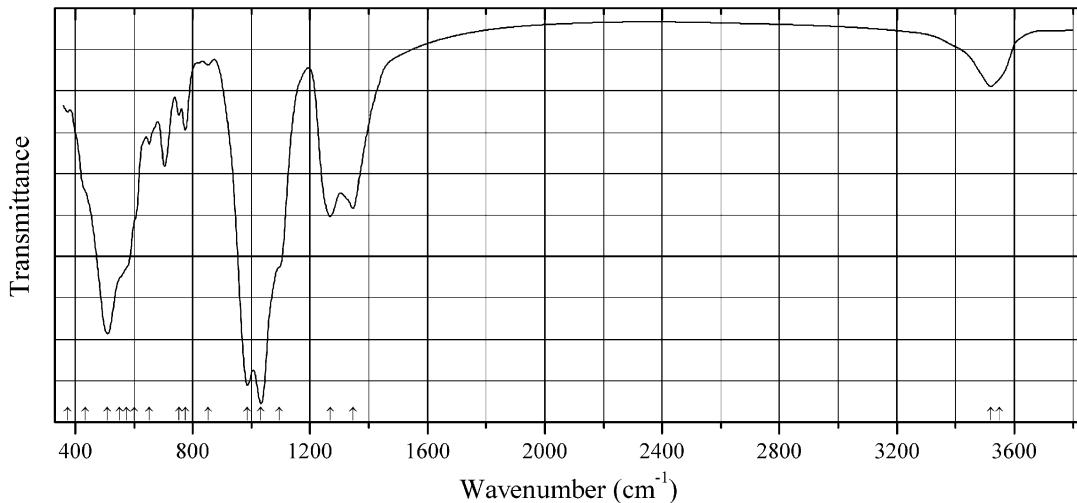
**Origin:** Crabtree Emerald mine, Mitchell Co., North Carolina, USA (type locality).

**Description:** Olive-green grains from the association with quartz. The empirical formula is (electron microprobe):  $(\text{Na}_{0.78}\text{Ca}_{0.05})(\text{Mg}_{1.75}\text{Fe}_{1.14}\text{Mn}_{0.11})(\text{Al}_{5.78}\text{Fe}_{0.17}\text{Ti}_{0.05})(\text{Si}_{5.91}\text{Al}_{0.09})(\text{BO}_3)_3(\text{OH})_3\text{F}_{0.68}(\text{O}, \text{OH})_{0.32}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3566, 3490sh, 1347, 1253, 1095s, 1052s, 992s, 780, 760, 715, 681, 649, 611, 579, 508s, 488s, 421, 402w, 381w.

**Note:** The spectrum was obtained by N.V. Chukanov.

**BSi106 Luinaite-(OH)**  $\text{NaFe}^{2+}_3\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3(\text{OH})$ 

**Origin:** Cleavland Tin mine, Luina, Waratah, Tasmania, Australia (type locality).

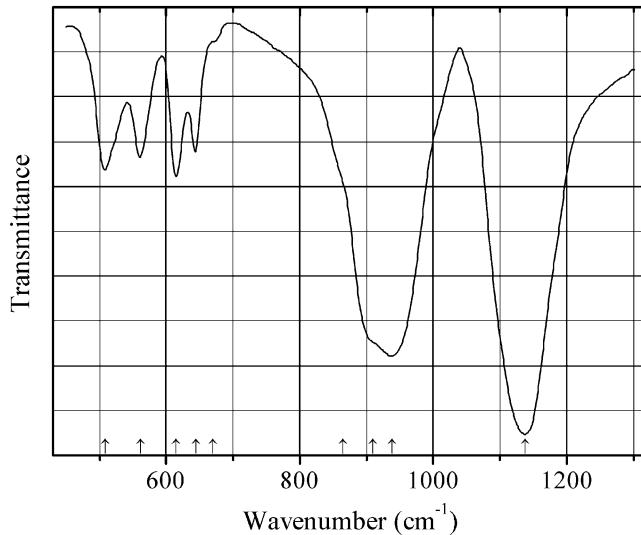
**Description:** Aggregate of light green acicular crystals.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3550sh, 3521, 1346, 1268, 1093sh, 1033s, 986s, 854w, 775, 753, 704, 652, 600sh, 575sh, 550sh, 509s, 435sh, 374w.

**Note:** The spectrum was obtained by N.V. Chukanov.

### SSi14 Chlorellstadite $\text{Ca}_{10}[(\text{SiO}_4)_3(\text{SO}_4)_3]\text{Cl}_2$



**Origin:** Synthetic.

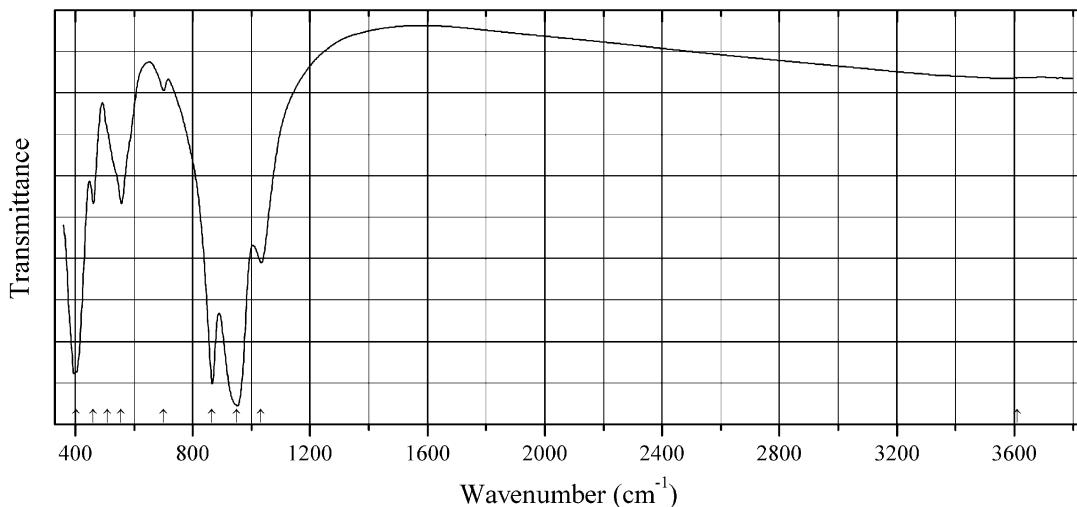
**Description:** Synthesized by heating of an appropriate mixture of CaO, CaSO<sub>4</sub>, SiO<sub>2</sub>, CaCl<sub>2</sub>, and CaF<sub>2</sub> first at 900 °C for 5 h and then at 950 °C for 9 h with intermediate grinding. Characterized by powder X-ray diffraction data. The crystal structure is solved. Hexagonal, space group  $P6_3/m$ ,  $a = 9.6239(3)$ ,  $c = 6.87749(3)$  Å,  $V = 551.64(2)$  Å<sup>3</sup>. The formula is  $\text{Ca}_{10}(\text{SiO}_4)_3(\text{SO}_4)_3\text{Cl}_{1.6}\text{F}_{0.4}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Fang et al. (2011).

**Wavenumbers (cm<sup>-1</sup>):** 1138s, 938s, 910sh, 865sh, 670sh, 644, 615, 561, 508.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, the wavenumber 670 cm<sup>-1</sup> is erroneously indicated as 660 cm<sup>-1</sup>.

**TiSi318 Fluorbarytolamprophyllite**  $(\text{Ba},\text{Sr})_2[(\text{Na},\text{Fe}^{2+})_3(\text{Ti},\text{Mg})\text{F}_2][\text{Ti}_2(\text{Si}_2\text{O}_7)_2\text{O}_2]$ 

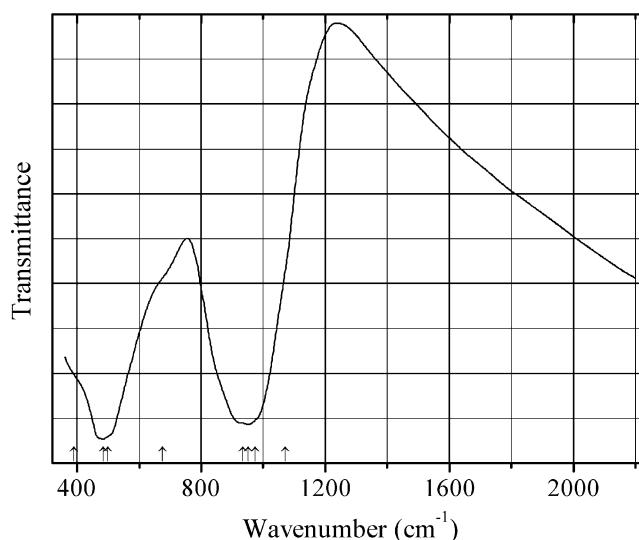
**Origin:** Niva alkaline intrusion, Kola Alkaline Province, Murmansk Region, Russia (type locality).

**Description:** Brown prismatic crystals from the association with orthoclase, titanian aegirine-augite, arfvedsonite, aenigmatite, lamprophyllite, fluorlamprophyllite, barytolamprophyllite, shcherbakovite, and natrolite. Holotype sample. The crystal structure is solved. Monoclinic, space group:  $C2/m$ ,  $a = 19.538(1)$ ,  $b = 7.092(1)$ ,  $c = 5.391(2)$  Å,  $\beta = 96.704(8)^\circ$ ,  $V = 741.8(3)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 3.662$  g/cm<sup>3</sup>. Optically biaxial (+),  $\alpha = 1.738(3)$ ,  $\beta = 1.745(4)$ ,  $\gamma = 1.777(4)$ ,  $2V = 55(5)^\circ$ . The empirical formula is  $(\text{Ba}_{0.865}\text{Sr}_{0.44}\text{K}_{0.46}\text{Na}_{0.26})(\text{Na}_{2.38}\text{Ca}_{0.09}\text{Fe}_{0.47}\text{Mn}_{0.06})(\text{Ti}_{2.79}\text{Mg}_{0.09}\text{Fe}_{0.035}\text{Nb}_{0.06}\text{Zr}_{0.015}\text{Ta}_{0.01})(\text{Si}_{3.99}\text{Al}_{0.01})\text{O}_{16}[\text{F}_{1.04}\text{O}_{0.72}(\text{OH})_{0.24}]$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 9.692 (40) (200), 3.726 (59) (-311), 3.414 (67) (311, 510, 401), 3.230 (96) (600), 3.013 (53) (-5-11), 2.780 (100) (221).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** (3610w), 1031, 950s, 866s, 701w, 556, 510sh, 461, 402s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**TiSi319 Polyakovite-(Ce)**  $(\text{Ce},\text{Ca})_4\text{MgCr}_2(\text{Ti},\text{Nb})_2\text{Si}_4\text{O}_{22}$ 

**Origin:** Pit No. 97, Ilmen (Il'menskie) Mts, Chelyabinsk region, Southern Urals, Russia (type locality).

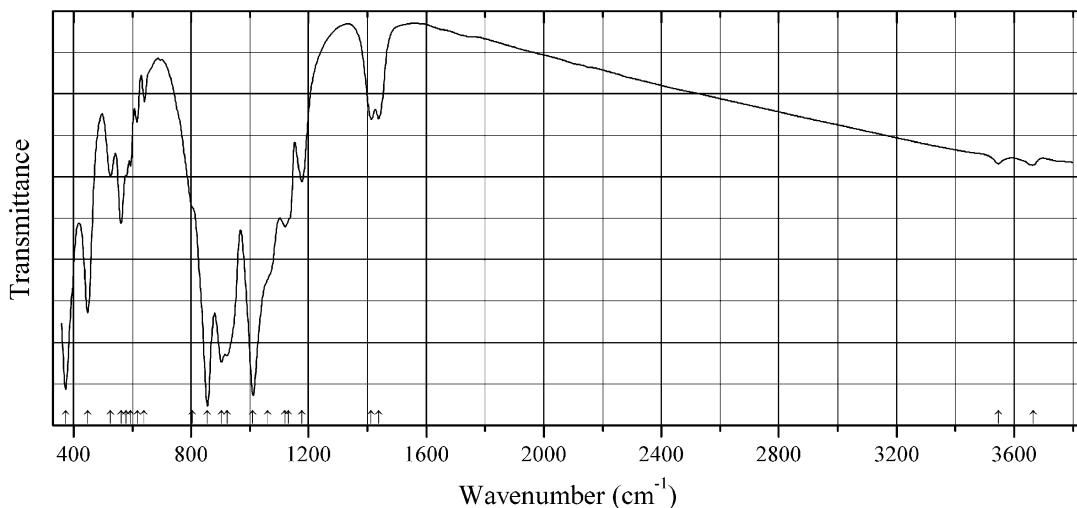
**Description:** Black grain from the association with calcite, dolomite, fluororichterite, phlogopite, forsterite, monazite-(Ce), clinohumite, chromite, and davidite-(Ce). X-ray amorphous, metamict. The empirical formula is (electron microprobe):  $(\text{Ce}_{1.8}\text{La}_{1.2}\text{Nd}_{0.4}\text{Pr}_{0.2}\text{Ca}_{0.3}\text{Th}_{1.15})(\text{Cr}_{1.3}\text{Fe}_{0.8}\text{Mg}_{0.7}\text{Ti}_{1.6}\text{Nb}_{0.4}\text{Si}_4\text{O}_{22})$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 1070sh, 975sh, 952s, 935sh, 675sh, 500sh, 483s, 390sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**TiSi320 Yoshimuraite**  $\text{Ba}_2\text{Mn}^{2+}_2\text{Ti}(\text{Si}_2\text{O}_7)(\text{PO}_4)\text{O}(\text{OH})$



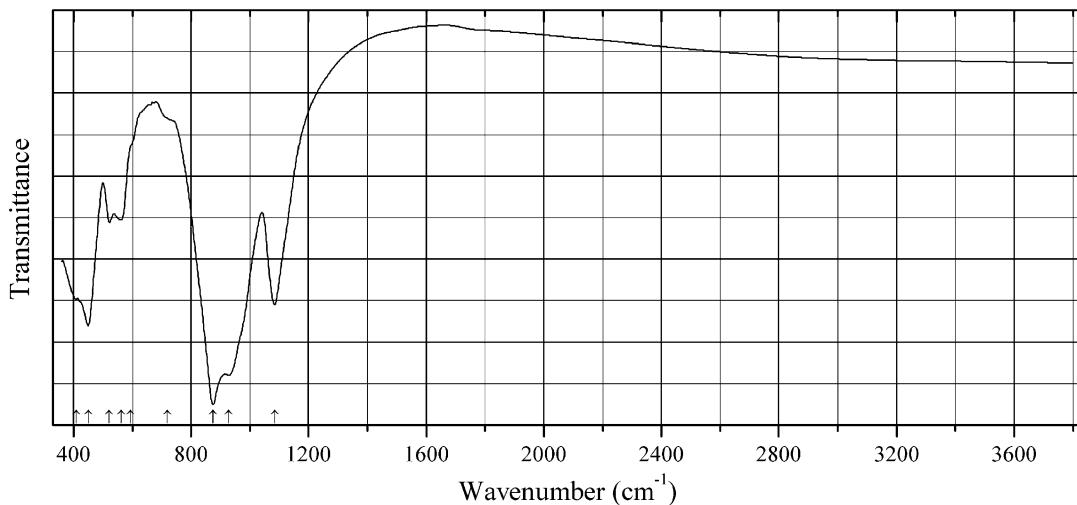
**Origin:** Tanohata mine, Tanohata-mura, Shimohei-gun, Iwate Prefecture, Tohoku Region, Honshu Island, Japan.

**Description:** Brown platelets. The empirical formula is (electron microprobe):  $(\text{Ba}_{3.6}\text{Sr}_{0.3}\text{Na}_{0.1})(\text{Mn}_{3.5}\text{Fe}_{0.3}\text{Mg}_{0.1})(\text{Ti}_{1.8}\text{Fe}_{0.2})(\text{Si}_2\text{O}_7)_{2.05}[(\text{PO}_4)_{1.1}(\text{SO}_4)_{0.7}(\text{CO}_3)_x]\text{O}_2(\text{OH})_{1.1}\text{F}_{0.9}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3665w, 3546w, 1438, 1413, 1177, 1130sh, 1120, 1060sh, 1011s, 922s, 904s, 856s, 805sh, 641w, 617w, 594, 580sh, 562, 526, 448, 374s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**TiSi321 Lavenite Fe-analogue**  $(\text{Na,Ca})_2(\text{Fe,Mn})(\text{Zr,Ti,Nb})(\text{Si}_2\text{O}_7)(\text{O,F})_2$ 

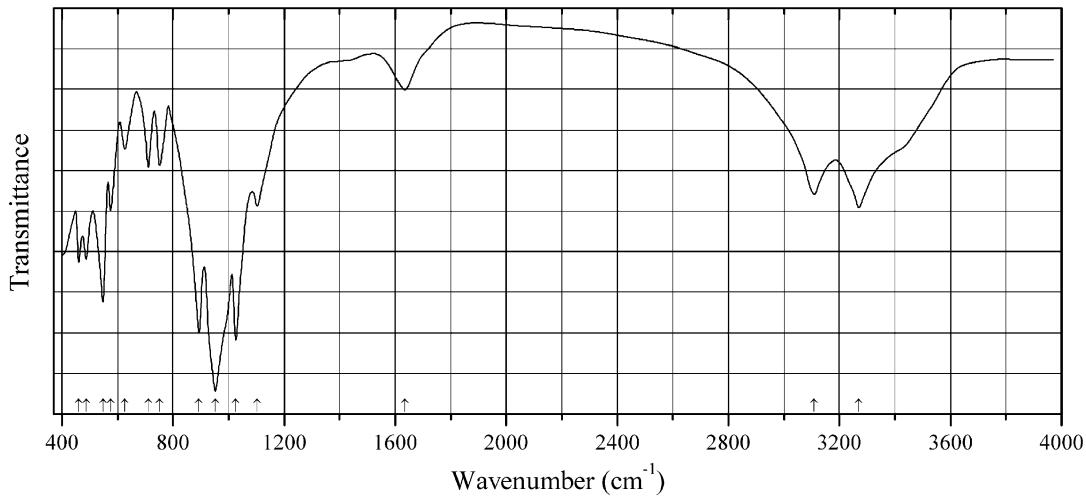
**Origin:** Ankisuai valley, Suoluav Mt., southeastern part of Lovozero alkaline complex, Kola peninsula, Murnansk region, Russia.

**Description:** Brown crystals from the association with seidozerite, aegirine and K-feldspar. The empirical formula is (electron microprobe):  $(\text{Na}_{1.66}\text{Ca}_{0.34})(\text{Fe}_{0.27}\text{Mn}_{0.24}\text{Ti}_{0.24}\text{Ca}_{0.18}\text{Al}_{0.05})(\text{Zr}_{0.84}\text{Nb}_{0.15}\text{Ti}_{0.01})(\text{Si}_{1.99}\text{Al}_{0.01})\text{O}_7(\text{OH,F})_2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1084s, 928s, 875s, 720sh, 595sh, 562, 522, 450s, 411.

**Note:** The spectrum was obtained by N.V. Chukanov.

**TiSi322 Potassium titanium silicate**  $\text{K}_2\text{TiSi}_3\text{O}_9 \cdot \text{H}_2\text{O}$   $\text{K}_2\text{TiSi}_3\text{O}_9 \cdot \text{H}_2\text{O}$ 

**Origin:** Synthetic.

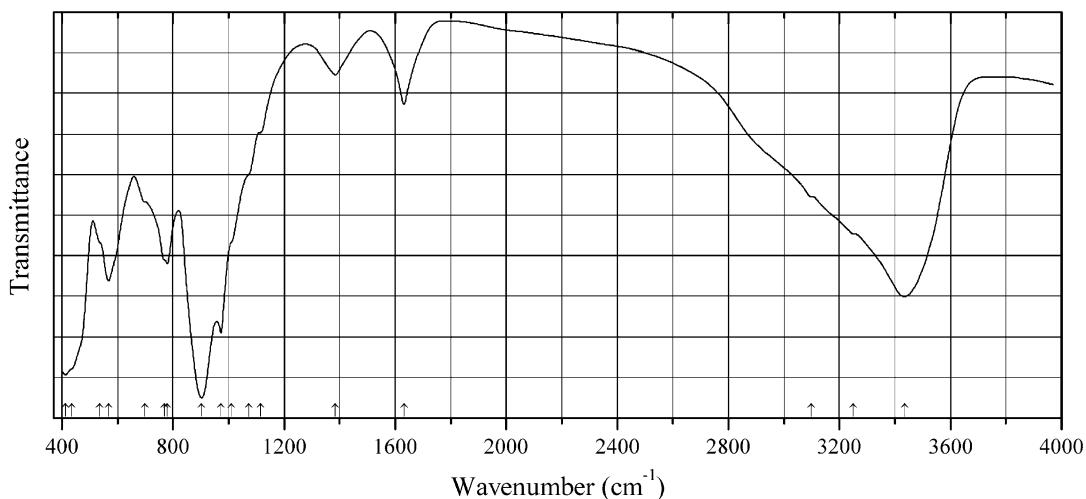
**Description:** Prepared hydrothermally from a solution containing  $\text{TiCl}_4$ ,  $\text{H}_2\text{O}_2$ ,  $\text{SiO}_2$ ,  $\text{KOH}$ , and  $\text{NaOH}$ , at  $180^\circ\text{C}$  for 7 days. Characterized by powder X-ray diffraction data and elemental analysis. The crystal structure is solved. Orthorhombic, space group  $P2_12_12_1$ ,  $a = 9.9081(4)$ ,  $b = 12.9445(5)$ ,  $c = 7.1384(3)$  Å,  $V = 915.5$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 2.701$  g/cm $^3$ . The microporous structure is based on a heteropolyhedral framework containing  $\text{Si}_3\text{O}_9$  chains.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Bortun et al. (2000).

**Wavenumbers (cm $^{-1}$ ):** 3270, 3110, 1635, 1103, 1026s, 952s, 893s, 752, 711, 626w, 575, 547, 487, 461.

### TiSi323 Sodium titanium silicate $\text{Na}_2\text{TiSi}_2\text{O}_7 \cdot 2\text{H}_2\text{O}$ $\text{Na}_2\text{TiSi}_2\text{O}_7 \cdot 2\text{H}_2\text{O}$



**Origin:** Synthetic.

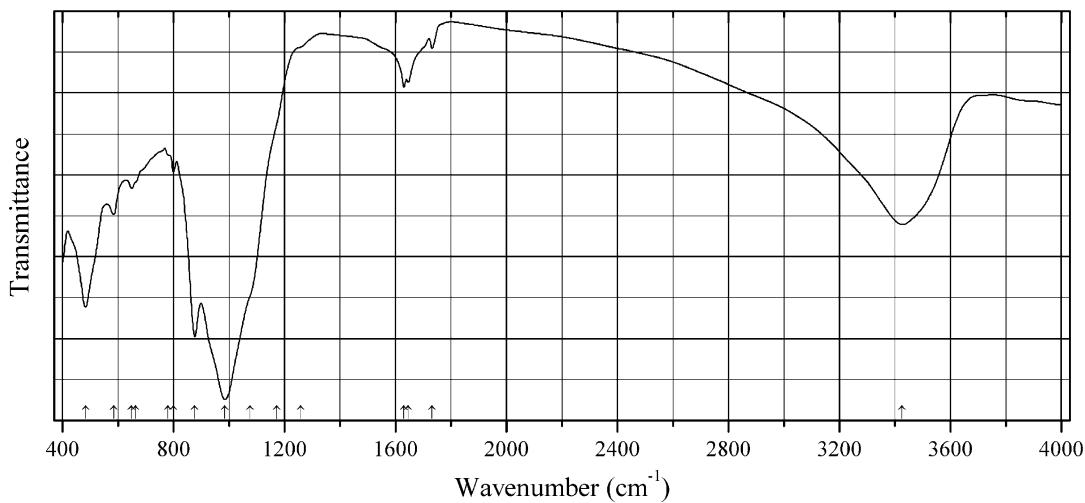
**Description:** White powder. A compound with layered structure synthesized hydrothermally from  $\text{TiCl}_4$ , silicic acid,  $\text{NaOH}$ , and  $\text{H}_2\text{O}_2$  at  $200^\circ\text{C}$  for 7 days. Characterized by powder X-ray diffraction, TG analysis, MAS  $^{29}\text{Si}$ , and  $^{23}\text{Na}$  NMR. The strongest reflection is observed at 14.97 Å.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Clearfield et al. (1997).

**Wavenumbers (cm $^{-1}$ ):** 3436s, (3250), (3100), 1632, 1385w, 1115sh, 1073sh, 1011sh, 973s, 902s, 779, 768sh, 698sh, 568, 536sh, 435sh, 412s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**TiSi324 Batievaite-(Y)  $\text{Y}_2\text{Ca}_2\text{Ti}(\text{Si}_2\text{O}_7)_2(\text{OH})_2 \cdot 4\text{H}_2\text{O}$** 


**Origin:** Sakharjok alkaline massif, Kola Peninsula, Russia (type locality).

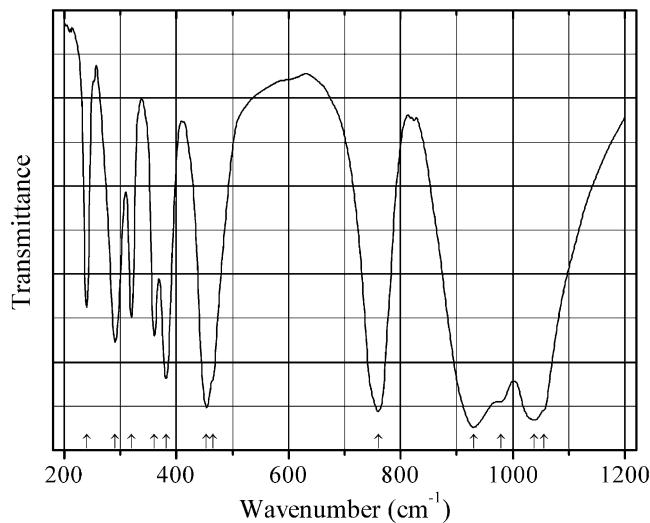
**Description:** Brownish euhedral crystals from the association with hainite, nepheline, albite, calcite, and zeolite-group minerals. Holotype sample. The crystal structure is solved. Triclinic, space group  $P-1$ ,  $a = 9.4024(8)$ ,  $b = 5.5623(5)$ ,  $c = 7.3784(6)$  Å,  $\alpha = 89.919(2)^\circ$ ,  $\beta = 101.408(2)^\circ$ ,  $\gamma = 96.621(2)^\circ$ ,  $V = 375.65(6)$  Å<sup>3</sup>,  $Z = 1$ .  $D_{\text{meas}} = 3.45(5)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 3.357$  g/cm<sup>3</sup>. Optically biaxial (+),  $\alpha = 1.745(5)$ ,  $\beta = 1.745(7)$ ,  $\gamma = 1.752(5)$ ,  $2V = 60(5)^\circ$ . The empirical formula is (electron microprobe; grouping of the components is based on structural data):  $(\text{Y}_{0.81}\text{Ca}_{0.65}\text{Ln}_{0.23}\text{Mn}_{0.15}\text{Zr}_{0.12}\text{Fe}_{0.04})[(\text{H}_2\text{O})_{0.75}\text{Ca}_{0.70}\square_{0.55}]\text{Ca}_{2.00}[\square_{0.61}\text{Na}_{0.25}(\text{H}_2\text{O})_{0.14}](\text{Ti}_{0.76}\text{Nb}_{0.15}\text{Zr}_{0.09})[\text{Si}_{3.91}\text{Al}_{0.09}\text{O}_{14}]$ [(OH)<sub>1.56</sub>F<sub>0.44</sub>][(H<sub>2</sub>O)<sub>1.27</sub>F<sub>0.73</sub>]. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 9.145 (17) (100), 7.238 (36) (00-1), 4.350 (23) (0-1-1), 4.042 (16) (11-1), 3.745 (13) (2-10), 3.061 (30) (300), 2.991 (100) (11-2), 2.819 (16) (3-10).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Lyalina et al. (2016).

**Wavenumbers (cm<sup>-1</sup>):** 3426, 1732w, 1646, 1630, 1258sh, 1172sh, 1077sh, 985s, 877, 800w, 780sh, 664sh, 649, 584, 493s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The band at 1732 cm<sup>-1</sup> indicates possible presence of H<sub>3</sub>O<sup>+</sup> or H<sub>5</sub>O<sub>2</sub><sup>+</sup> groups.

**TiSi325 Bazirite** BaZr(Si<sub>3</sub>O<sub>9</sub>)

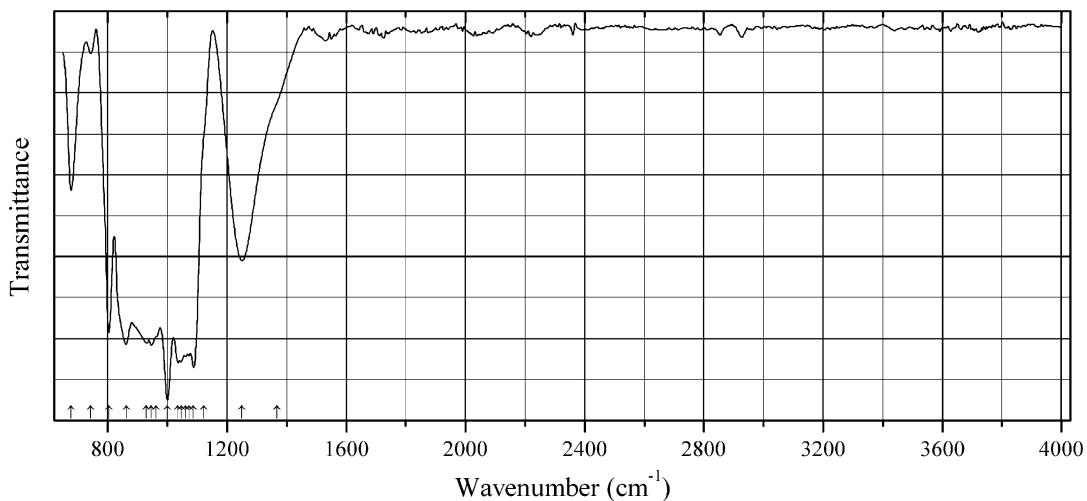
**Origin:** Synthetic.

**Description:** Synthesized using solid-state reaction techniques from the stoichiometric mixture of BaCO<sub>3</sub>, ZrO<sub>2</sub>, and SiO<sub>2</sub>.

**Kind of sample preparation and/or method of registration of the spectrum:** KI disc. Transmission.

**Source:** Choisnet et al. (1975).

**Wavenumbers (cm<sup>-1</sup>):** 1055sh, 1038s, 979sh, 930s, 760s, 465sh, 454s, 382, 361, 320, 291, 240.

**TiSi326 Fogoite-(Y)** Na<sub>3</sub>Ca<sub>2</sub>Y<sub>2</sub>Ti(Si<sub>2</sub>O<sub>7</sub>)<sub>2</sub>OF<sub>3</sub>

**Origin:** Lagoa do Fogo, the São Miguel Island, the Azores, Portugal (type locality).

**Description:** Colorless long-prismatic crystals from the association with sanidine, astrophyllite, fluornatropyrochlore, ferrokentbrooksite, quartz, and ferro-katophorite. Holotype sample. The crystal structure is solved. Triclinic, space group  $P\bar{1}$ ,  $a = 9.575(6)$ ,  $b = 5.685(4)$ ,  $c = 7.279(5)$  Å,  $\alpha = 89.985(6)^\circ$ ,  $\beta = 100.933(4)^\circ$ ,  $\gamma = 101.300(5)^\circ$ ,  $V = 381.2(7)$  Å $^3$ ,  $Z = 1$ .  $D_{\text{calc}} = 3.523$  g/cm $^3$ . Optically biaxial (+),  $\alpha = 1.686(2)$ ,  $\beta = 1.690(2)$ ,  $\gamma = 1.702(5)$ ,  $2V = 57(1)^\circ$ . The empirical formula is (electron microprobe):  $(\text{Na}_{2.74}\text{Mn}_{0.15})\text{Ca}_2(\text{Y}_{1.21}\text{Ln}_{0.35}\text{Mn}_{0.16}\text{Zr}_{0.11}\text{Nb}_{0.09}\text{Fe}_{0.07}\text{Ca}_{0.01})(\text{Ti}_{0.76}\text{Nb}_{0.23}\text{Ta}_{0.01})(\text{Si}_{4.03}\text{O}_{14})\text{O}_{1.12}\text{F}_{2.88}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 2.954 (100) (-1-12, -310), 3.069 (42) (300, 0-12), 2.486 (24) (310, 2-12), 3.960 (23) (-1-11, -210), 2.626 (21) (-220), 1.820 (20) (-104).

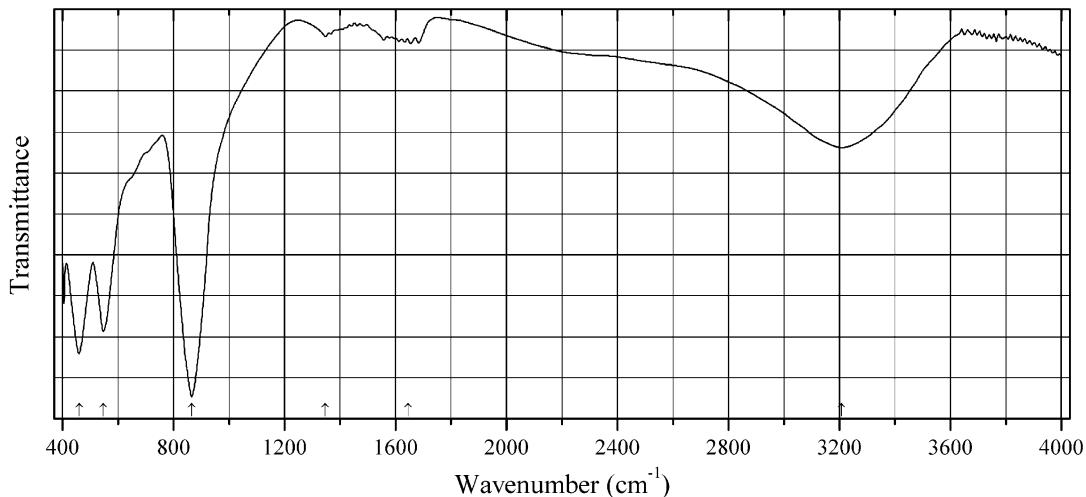
**Kind of sample preparation and/or method of registration of the spectrum:** Absorption of a crystal fragment using an IR microscope. A procedure of baseline correction was applied.

**Source:** Câmara et al. (2016b).

**Wavenumbers (cm $^{-1}$ ):** 1367sh, 1250, 1122sh, 1088s, 1072s, 1061s, 1046s, 1036s, 1000s, 963sh, 946s, 930s, 862s, 803, 743w, 677.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### TiSi327 Ivanyukite-Cs $\text{Cs}_3\text{HTi}_4\text{O}_4(\text{SiO}_4)_3 \cdot 4\text{H}_2\text{O}$



**Origin:** Synthetic.

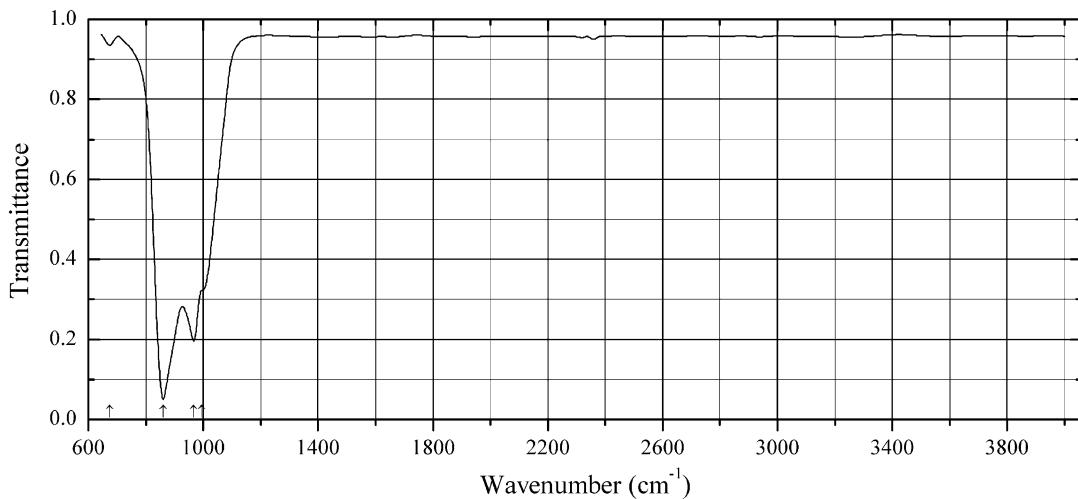
**Description:** Prepared using a gel technique at 200 °C for 48 h. Characterized by TG and powder X-ray diffraction data. Cubic, space group  $P\bar{4}3m$ ,  $a = 7.7644(3)$ ,  $Z = 1$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Behrens et al. (1996).

**Wavenumbers (cm $^{-1}$ ):** 3208, 1645w, (1347w), 866s, 546s, 460s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**TiSi328 Schüllerite-type mineral**  $\text{Ba}_2\text{Na}_2\text{Mg}_2\text{Ti}_2(\text{Si}_2\text{O}_7)_2\text{O}_2\text{F}_2$ 

**Origin:** Eifel volcanic region, Germany.

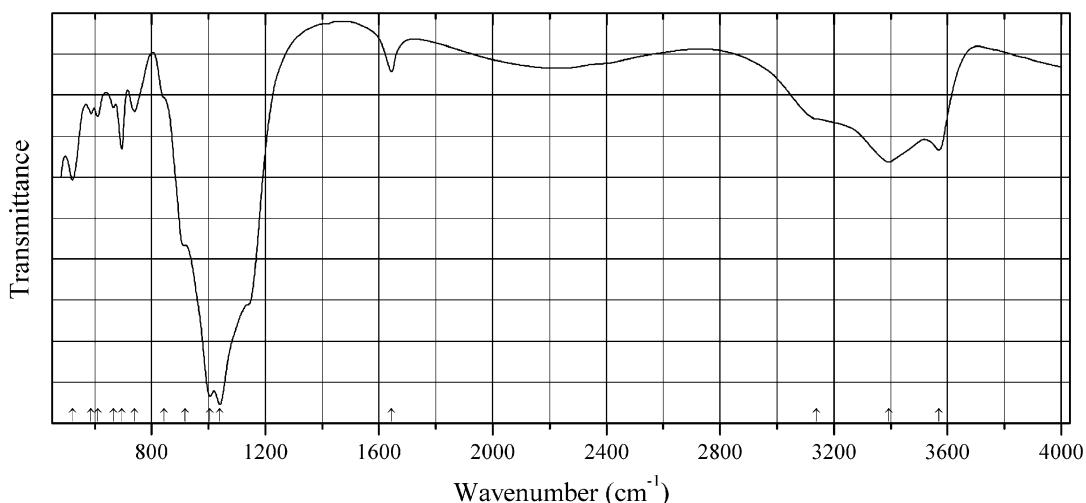
**Description:** Pale yellow zones of the two grains obtained from an American mineral collector.

Erroneously described as “schüllerite.” The crystal structure is solved. Triclinic, space group  $P-1$ ,  $a = 5.396(1)$ ,  $b = 7.071(1)$ ,  $c = 10.226(2)$  Å,  $\alpha = 99.73(3)^\circ$ ,  $\beta = 99.55(3)^\circ$ ,  $\gamma = 90.09(3)^\circ$ ,  $V = 379.1(2)$  Å³,  $Z = 1$ .  $D_{\text{calc}} = 3.879$  g/cm³. Structurally related to schüllerite. The empirical formula is  $(\text{Ba}_{1.57}\text{Sr}_{0.14}\text{K}_{0.14})(\text{Na}_{1.10}\text{Ca}_{0.43}\text{Mn}_{0.30}\text{Fe}_{0.17})(\text{Fe}_{0.88}\text{Mg}_{0.79}\text{Na}_{0.33})(\text{Ti}_{1.67}\text{Fe}_{0.21}\text{Nb}_{0.09}\text{Zr}_{0.02}\text{Al}_{0.01})\text{Si}_{3.95}\text{O}_{15.93}\text{F}_{2.07}$ . The Mössbauer spectrum given by Sokolova et al. (2013) cannot be used for precise determination of the  $\text{Fe}^{2+}$ : $\text{Fe}^{3+}$  ratio because of a strong scatter of experimental points. Consequently, the existence of a Mg-dominant site is questionable.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission using an IR microscope and a diamond micro compression cell.

**Source:** Sokolova et al. (2013).

**Wavenumbers (cm⁻¹):** 995sh, 967s, 860s, 675w.

**TiSi329 Hydroterskite**  $\text{Na}_2\text{ZrSi}_6\text{O}_{12}(\text{OH})_6$ 

**Origin:** Saint-Amable sill, Demix-Varennes quarry, near Varennes, Québec, Canada (type locality).

**Description:** Short prismatic crystals from the association with aegirine, analcime, an astrophyllite-group mineral, cataleite, a eudialyte-group mineral, fluorite, monazite, natrolite, and a rinkite-group species. Holotype sample. The crystal structure is solved. Orthorhombic, space group *Pnca*,  $a = 13.956(6)$ ,  $b = 14.894(7)$ ,  $c = 7.441(4)$  Å,  $V = 1546.8(20)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 2.57$  g/cm<sup>3</sup>. Optically biaxial (−),  $\alpha = 1.562(2)$ ,  $\beta = 1.567(2)$ ,  $\gamma = 1.571(2)$ ,  $2V = 86(3)^\circ$ . The empirical formula (after excluding of trace components) is (Na<sub>1.54</sub>K<sub>0.01</sub>Ca<sub>0.07</sub>Ce<sub>0.01</sub>La<sub>0.05</sub>)<sub>(Zr<sub>0.74</sub>Ti<sub>0.09</sub>Nb<sub>0.05</sub>Th<sub>0.005</sub>Fe<sub>0.08</sub>Mn<sub>0.06</sub>Al<sub>0.01</sub>)Si<sub>6.09</sub>O<sub>12</sub>(OH)<sub>5.96</sub>F<sub>0.035</sub>. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 7.427 (56) (020), 6.638 (48) (011), 6.327 (47) (210), 5.093 (49) (220), 4.123 (55) (031), 3.716 (53) (002, 040), 3.482 (51) (321), 3.322 (100) (022), 3.283 (80) (202, 240), 3.158 (54) (420), 3.091 (50) (411), 2.625 (48) (042), 2.544 (57) (402).</sub>

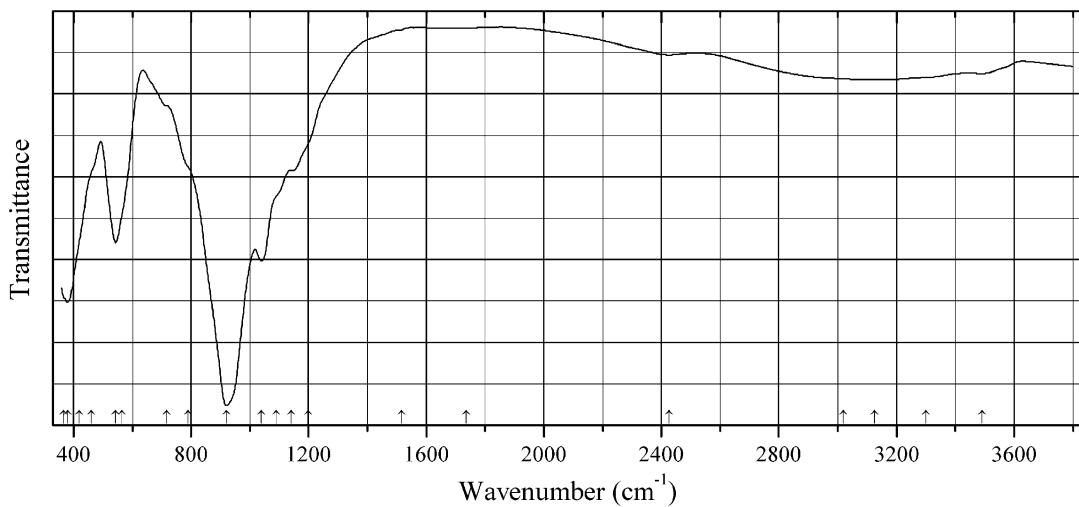
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission using adiamond-anvil cell microsampling device.

**Source:** Grice et al. (2015).

**Wavenumbers (cm<sup>−1</sup>):** 3569, 3393, 3138sh, 1644, 1139sh, 1040s, 1005s, 917sh, 843sh, 740, 695, 665w, 610w, 587w, 521.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### TiSi330 Betalomonosovite Na<sub>2</sub>□<sub>4</sub>Na<sub>2</sub>Ti<sub>2</sub>Na<sub>2</sub>Ti<sub>2</sub>(Si<sub>2</sub>O<sub>7</sub>)<sub>2</sub>[PO<sub>3</sub>(OH)][PO<sub>2</sub>(OH)<sub>2</sub>]O<sub>2</sub>(OF)



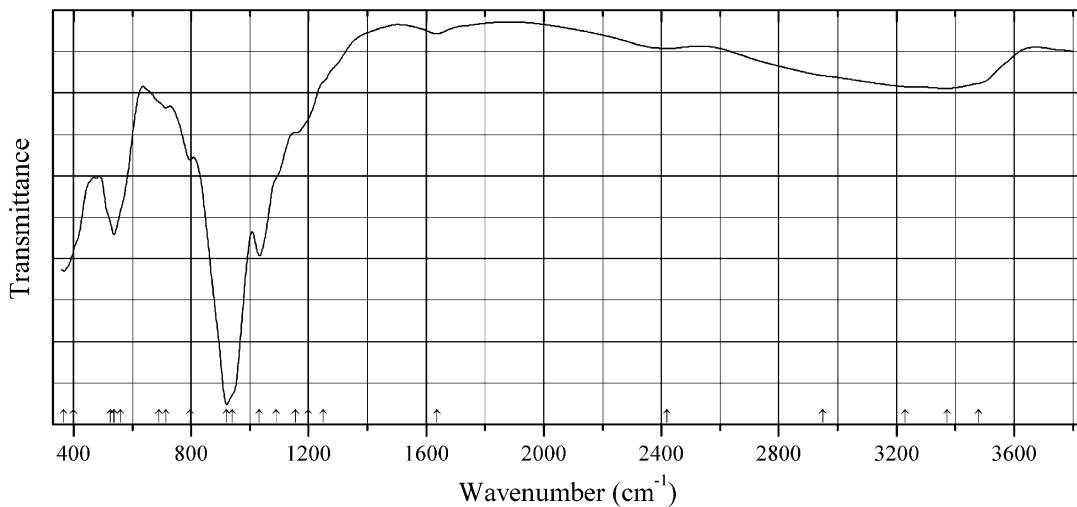
**Origin:** Vostochnyi (Eastern) apatite mine, Khibiny alkaline complex, Kola Peninsula, Russia.

**Description:** Yellow tabular crystals from the association with lamprophyllite, pectolite, aegirine, and eudialyte. The crystal structure is solved. Triclinic, space group *P-1*,  $a = 5.3185(3)$ ,  $b = 14.1333(9)$ ,  $c = 14.4147(8)$  Å,  $\alpha = 101.934(3)^\circ$ ,  $\beta = 96.040(3)^\circ$ ,  $\gamma = 90.120(3)^\circ$ ,  $V = 1053.89(10)$  Å<sup>3</sup>,  $Z = 1$ . The empirical formula is (electron microprobe): (Na<sub>5.40</sub>Ca<sub>0.50</sub>)<sub>(Ti<sub>3.22</sub>Fe<sup>3+</sup><sub>0.43</sub>Mg<sub>0.10</sub>Mn<sub>0.09</sub>Nb<sub>0.07</sub>)Si<sub>4.00</sub>P<sub>1.97</sub>O<sub>21.15</sub>(OH)<sub>4.85</sub>. The crystal-chemical formula is {Na<sub>1.49</sub>(Ti<sub>1.45</sub>Fe<sup>3+</sup><sub>0.55</sub>)O<sub>2.47</sub>(OH)<sub>1.63</sub>} {Na<sub>0.81</sub>Ca<sub>0.27</sub>Mn<sub>0.06</sub>(Ti<sub>1.84</sub>Mg<sub>0.10</sub>Nb<sub>0.06</sub>)[Si<sub>2</sub>O<sub>7</sub>]<sub>2</sub>} {Na<sub>3.22</sub>Ca<sub>0.22</sub>Mn<sub>0.03</sub>[P<sub>2.00</sub>O<sub>5.62</sub>(OH)<sub>2.38</sub>]}.</sub>

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>−1</sup>):** 3490, 3300sh, 3126, 3020, 2427w, 1736w, 1517w, 1200sh, 1140, 1090sh, 1040s, 921s, 790sh, 718w, 565sh, 543s, 460sh, 420sh, 380s, (367).

**Note:** The spectrum was obtained by N.V. Chukanov.

**TiSi331 Betalomonosovite**  $\text{Na}_2\square_4\text{Na}_2\text{Ti}_2\text{Na}_2\text{Ti}_2(\text{Si}_2\text{O}_7)_2[\text{PO}_3(\text{OH})][\text{PO}_2(\text{OH})_2]\text{O}_2(\text{OF})$ 

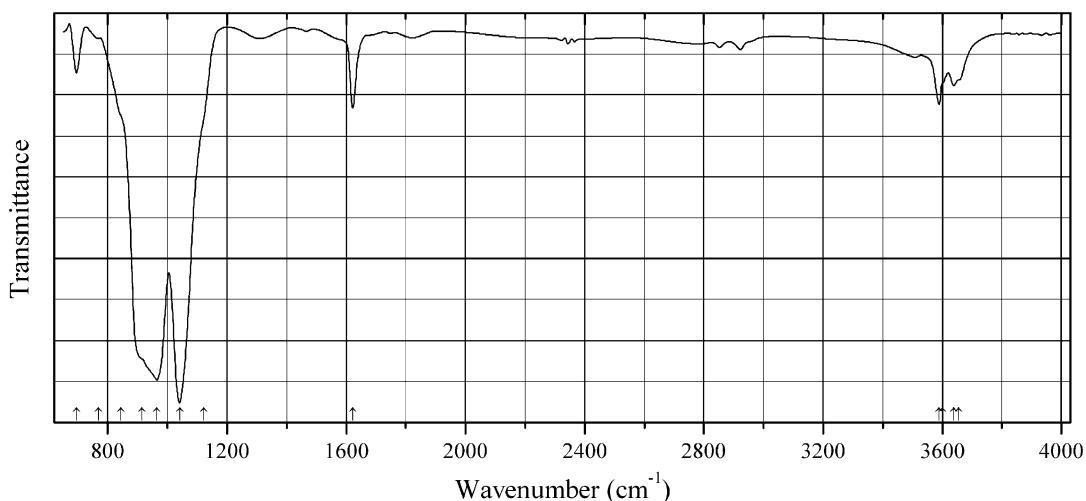
**Origin:** Olenii Ruchei (Reindeer Creek) open pit of the Olenii Ruchei apatite mine, Niorkpakhk Mt., Khibiny alkaline complex, Kola Peninsula, Russia.

**Description:** Beige lamellae crystals from the association with microcline, aegirine, and lamprophyllite. The crystal structure is solved. Triclinic, space group *P*-1,  $a = 5.30090(18)$ ,  $b = 14.1460(4)$ ,  $c = 14.4435(4)$  Å,  $\alpha = 103.3862(15)^\circ$ ,  $\beta = 90.4128(17)^\circ$ ,  $\gamma = 90.4128(17)^\circ$ ,  $V = 1046.21(6)$  Å<sup>3</sup>,  $Z = 1$ . The empirical formula is (electron microprobe):  $(\text{Na}_{4.40}\text{Ca}_{0.52}\text{K}_{0.01})(\text{Ti}_{3.14}\text{Fe}^{3+}_{0.41}\text{Mg}_{0.12}\text{Nb}_{0.11}\text{Mn}_{0.10})(\text{Si}_{3.98}\text{Al}_{0.02})\text{P}_{1.94}\text{O}_{19.91}(\text{OH})_{6.06}$ . The crystal-chemical formula is  $\{\text{Na}_{1.04}(\text{Ti}_{1.42}\text{Fe}^{3+}_{0.46}\text{Mn}_{0.12})\text{O}_{1.60}(\text{OH})_{2.40}\}\{\text{Na}_{1.03}\text{Ca}_{0.22}(\text{Ti}_{1.74}\text{Mg}_{0.16}\text{Nb}_{0.10})[\text{Si}_2\text{O}_7]_2\}\{\text{Na}_{2.33}\text{Ca}_{0.24}[\text{P}_{2.00}\text{O}_{4.80}(\text{OH})_{3.20}]\}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3480sh, 3373, 3230sh, 2950sh, 2420w, 1636w, 1250sh, 1200sh, 1156, 1090sh, 1033s, 940sh, 921s, 798, 714w, 690sh, 560sh, 538s, 525sh, 400sh, 367s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**TiSi332 Bulgakite**  $\text{Li}_2(\text{Ca},\text{Na})\text{Fe}^{2+}_7\text{Ti}_2(\text{Si}_4\text{O}_{12})_2\text{O}_2(\text{OH})_4(\text{F},\text{O})(\text{H}_2\text{O})_2$ 

**Origin:** Dara-i Pioz glacier, Dara-i Pioz alkaline massif, Tien Shan Mts., Tajikistan (type locality).

**Description:** Brownish orange grains from the association with amphibole, quartz, feldspar, brannockite, sogdianite, bafertisite, albite, and titanite. Holotype sample. A member of the astrophyllite supergroup. The crystal structure is solved. Triclinic, space group  $P\bar{1}$ ,  $a = 5.374(1)$  Å,  $b = 11.965(2)$  Å,  $c = 11.65(3)$  Å,  $\alpha = 113.457(8)^\circ$ ,  $\beta = 94.533(8)^\circ$ ,  $\gamma = 103.08(1)^\circ$ ,  $V = 657.5(8)$  Å<sup>3</sup>,  $Z = 1$ .  $D_{\text{meas}} = 3.30(2)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 3.326$  g/cm<sup>3</sup>. Optically biaxial (+),  $\alpha = 1.695(3)$ ,  $\beta = 1.711(2)$ ,  $\gamma = 1.750(3)$ ,  $2V = 70(5)^\circ$ . The empirical formula is  $(\text{Li}_{0.94}\text{K}_{0.91}\text{Rb}_{0.12}\text{Cs}_{0.03})(\text{Ca}_{0.60}\text{Na}_{0.40})(\text{Fe}_{5.34}\text{Mn}_{1.32}\text{Li}_{0.25}\text{Mg}_{0.05}\text{Na}_{0.04}\text{Zn}_{0.02})(\text{Ti}_{1.82}\text{Sn}_{0.10}\text{Nb}_{0.05}\text{Zr}_{0.04})[(\text{Si}_{7.78}\text{Al}_{0.24})\text{O}_{24}]\text{O}_{2.30}(\text{OH})_4\text{O}_{0.30} \cdot 0.94\text{H}_2\text{O}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 10.54 (100) (001), 3.50 (100) (003), 2.578 (100) (130), 2.783 (90) (1–42), 1.576 (68) (3–51, –3–22), 2.647 (55) (–211).

**Kind of sample preparation and/or method of registration of the spectrum:** Absorption. Kind of sample preparation is not indicated.

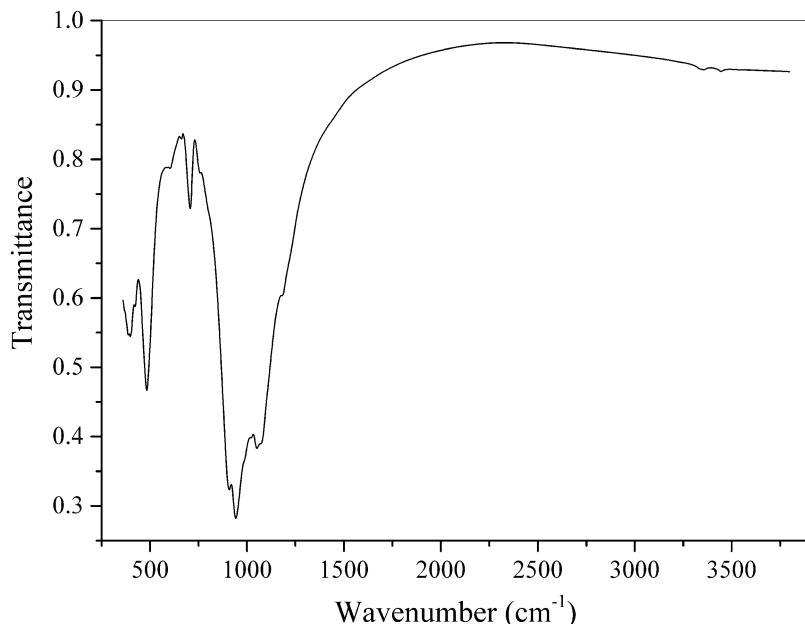
**Source:** Agakhanov et al. (2016b).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3655sh, 3639w, 3600sh, 3589, 1622, 1122sh, 1041s, 965s, 915sh, 844sh, 768sh, 695.

**Note:** Based on chemical data, the simplified formula of bulgakite should be  $\text{LiK}(\text{Ca},\text{Na})\text{Fe}^{2+}7\text{Ti}_2(\text{Si}_4\text{O}_{12})_2\text{O}_2(\text{OH})_4(\text{F},\text{O})(\square,\text{H}_2\text{O})_2$ . The wavenumbers were partly determined by us based on spectral curve analysis of the published IR spectrum. The band position denoted by Agakhanov et al. (2016b) as 940 cm<sup>-1</sup> actually corresponds to a strong peak with absorption maximum at 965 cm<sup>-1</sup> and a shoulder at 915 cm<sup>-1</sup>. The IR band at 695 cm<sup>-1</sup> is erroneously assigned to Si–O-stretching vibrations. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1041, 910s, 785sh, 733s, 660s, 569s, 420, 395, 367, 258, 233, 170, 133.

### TiSi333 Catapleiite heating product $\text{Na}_6\text{Zr}_3[\text{Si}_9\text{O}_{27}]$



**Origin:** Artificial.

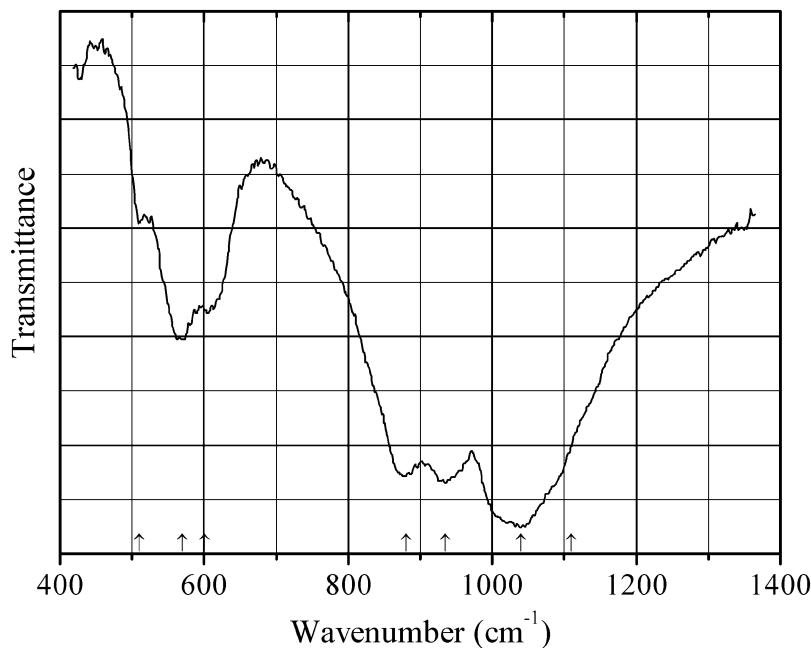
**Description:** Product of heating (from room temperature to 950 °C at a rate of 5 °C/min) of a catapleiite crystal from Aikuavenchorr Mt., Khibiny alkaline complex, Kola peninsula, Murmansk region, Russia. The crystal structure is solved. Hexagonal, space group  $P6_3/mcm$ ,  $a = 11.5901(9)$ ,  $c = 9.9546(9)$  Å,  $V = 1158.05(16)$  Å<sup>3</sup>. The structure is based on the heteropolyhedral framework which principally differs from that of catapleiite and is built by isolated [ZrO<sub>6</sub>] octahedra connected with each other by nine-membered rings [Si<sub>9</sub>O<sub>27</sub>] formed by SiO<sub>4</sub> tetrahedra.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3446w, 3356w, 3345sh, 1181, 1070sh, 1051s, 1019, 942s, 912s, 760w, 707, 660w, 599w, 483, 424, 400, 390.

**Note:** The spectrum was obtained by N.V. Chukanov. The bands in the range from 3300 to 3600 cm<sup>-1</sup> may correspond to adsorbed water.

### PSi11 Calcium orthophosphate orthosilicate Ca<sub>5</sub>(PO<sub>4</sub>)<sub>2</sub>(SiO<sub>4</sub>)



**Origin:** Synthetic.

**Description:** Obtained by sintering of compacted mixture of calcium hydrogen phosphate, calcium carbonate, and silicon oxide. Characterized by powder X-ray diffraction data. Hexagonal.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

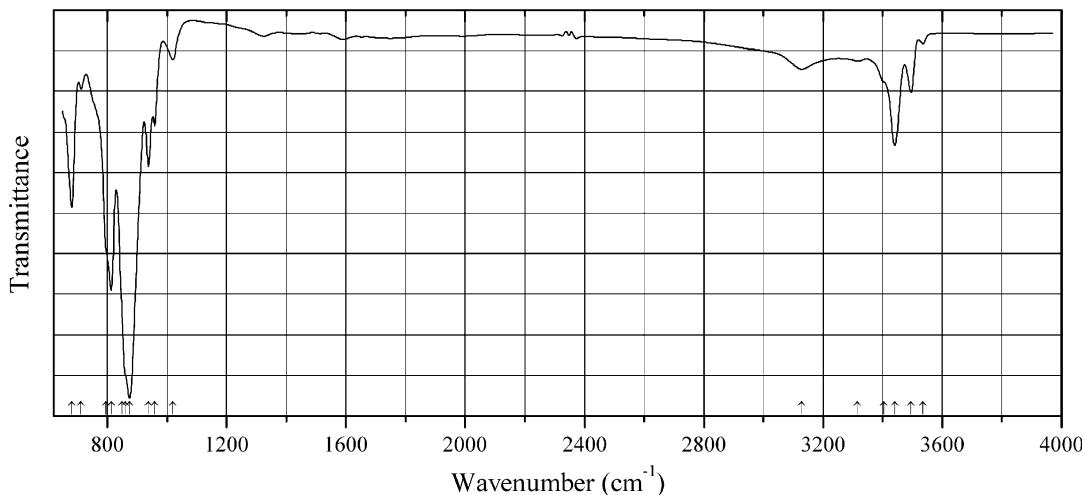
**Source:** Lugo et al. (2015).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1110sh, 1040s, 935s, 880s, 601, 570, 510.

**Note:** The wavenumber  $935 \text{ cm}^{-1}$  is erroneously indicated by Lugo et al. (2015) as  $960 \text{ cm}^{-1}$ . In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1084, 1058, 963s, 857s, 642, 587, 439, 435, 402, 297w, 218.

**AsSi14 Wiklundite**  $\text{Pb}_2(\text{Mn}^{2+},\text{Zn})_3(\text{Fe}^{3+},\text{Mn}^{2+})_2(\text{Mn}^{2+},\text{Mg})_{19}(\text{As}^{3+}\text{O}_3)_2[(\text{Si},\text{As}^{5+})\text{O}_4]_6(\text{OH})_{18}\text{Cl}_6$



**Origin:** Långban deposit, Bergslagen ore region, Filipstad district, Värmland, Sweden (type locality).

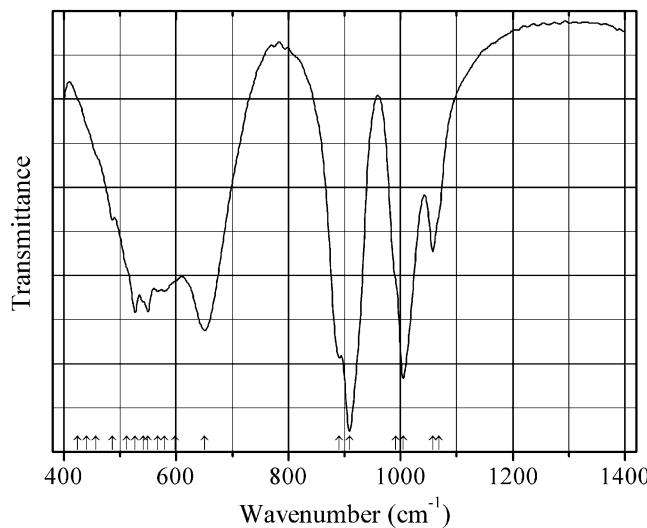
**Description:** Brown radiating aggregates from the association with tephroite, mimetite, turneaurite, johnbaumite, jacobsite, barite, native lead, filipstadite, and parwelite. Holotype sample. The crystal structure is solved. Rhombohedral, space group  $R-3c$ ,  $a = 8.257(2)$ ,  $c = 126.59(4) \text{ \AA}$ ,  $V = 7474(6) \text{ \AA}^3$ ,  $Z = 6$ .  $D_{\text{calc}} = 4.072 \text{ g/cm}^3$ . Optically uniaxial (−). The Mössbauer spectrum contains only one quadrupole doublet corresponding to  $\text{Fe}^{3+}$ . The empirical formula is  $\text{Pb}_{2.04}\text{Mn}_{21.23}\text{Fe}^{3+}_{1.76}\text{Zn}_{0.30}\text{Mg}_{0.23}\text{Ca}_{0.05}\text{Al}_{0.04}\text{Si}_{5.85}\text{As}_{2.37}\text{O}_{30}(\text{OH})_{18.10}\text{Cl}_{5.90}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ ,  $\text{\AA}$  ( $I$ , %)] are: 4.740 (40), 4.128 (83), 4.062 (58), 3.561 (40), 3.098 (81), 2.882 (100), 2.806 (90).

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of a single crystal.

**Source:** Cooper et al. (2016c).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3536w, 3496, 3441, 3404sh, 3316w, 3128w, 1020w, 959, 938, 875s, 861sh, 848sh, 813s, 795sh, 712w, 681.

**Note:** The presence of  $\text{Mn}^{2+}$  in the  $\text{Fe}^{3+}$ -dominant site  $M(1)$  with the mean  $M(1)-\text{O}$  distance of  $2.06 \text{ \AA}$  is questionable.

**USi11 Potassium uranium(V) sorosilicate  $K_3(U_3O_6)(Si_2O_7)$** 

**Origin:** Synthetic.

**Description:** Dark red needle crystals synthesized hydrothermally KOH, KF, UO<sub>3</sub>, and SiO<sub>2</sub> (in the molar ratio K:U:Si:F = 15:1:2:10) at 600 °C for 5 days. Characterized by powder X-ray diffraction data. The crystal structure contains an uranate column formed by corner-sharing UO<sub>6</sub> octahedra.

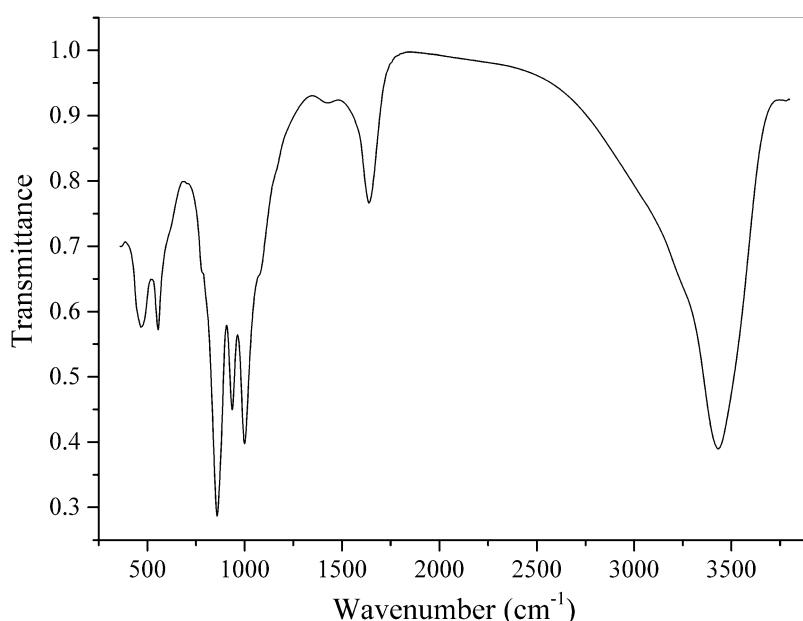
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Lin et al. (2008).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1068sh, 1057, 1005s, 991sh, 909s, 891s, 651s, 598sh, 579, 567, 550, 541, 527, 512sh, 487, 457sh, 441sh, 425sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (for Raman bands indicated by the authors,  $\text{cm}^{-1}$ ):** 972, 924, 888, 770, 570, 361, 232.

**USi12 Swamboite-(Nd)  $Nd_{0.333}[(UO_2)(SiO_3OH)] \cdot 2.5H_2O$** 

**Origin:** Swambo Hill (Swambo Mine), Kambove District, Katanga (Shaba), Democratic Republic of Congo (type locality).

**Description:** Yellow acicular crystals. Investigated by A.V. Kasatkin. Characterized by single-crystal X-ray diffraction data and qualitative electron microprobe analyses. Monoclinic,  $a = 6.70(4)$ ,  $b = 7.010(7)$ ,  $c = 8.86(2)$  Å,  $\beta = 102.2(3)^\circ$ ,  $V = 407(3)$  Å<sup>3</sup>.

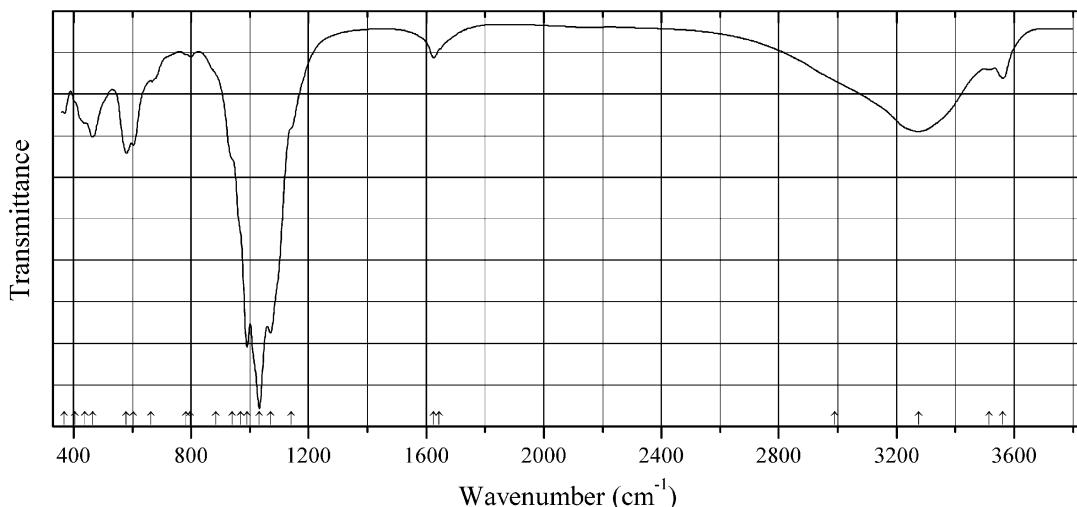
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3433s, 3250sh, 1638, (1427w), 1150sh, 1075sh, 1000s, 936s, 859s, 785sh, 610sh, 556, 471.

**Note:** The spectrum was obtained by N.V. Chukanov. The spectrum is very close to that of uranophane.

## 2.8 Phosphides and Phosphates

**P652 Zincoberaunite**  $ZnFe^{3+} \cdot 5(PO_4)_4(OH)_5 \cdot 6H_2O$



**Origin:** Hagendorf South granitic pegmatite, Hagendorf, Bavaria, Germany (type locality).

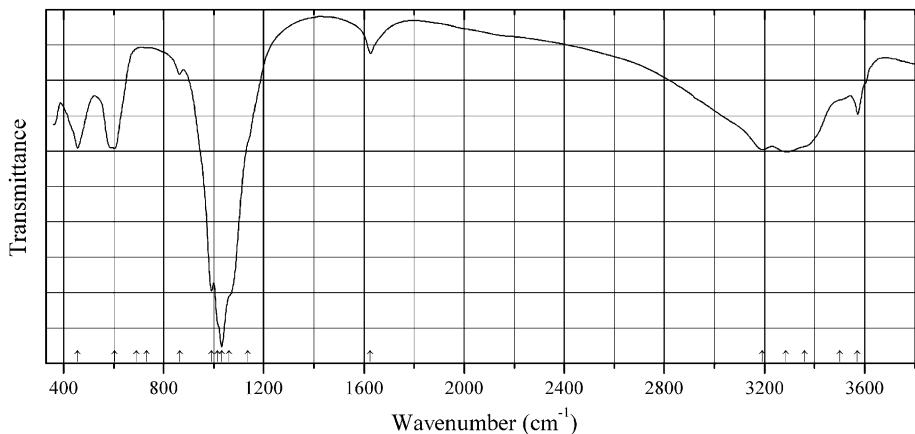
**Description:** Greenish-gray radial aggregates from the association with feldspar, quartz, jungite, phosphophyllite, and mitridatite. Holotype sample. The crystal structure is solved. Monoclinic, space group  $C2/c$ ,  $a = 20.837(2)$ ,  $b = 5.1624(4)$ ,  $c = 19.250(1)$  Å,  $\beta = 93.252(5)^\circ$ ,  $V = 2067.3(3)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 2.92$  g/cm<sup>3</sup>. Optically biaxial (-),  $\alpha = 1.745(5)$ ,  $\beta = 1.760(5)$ ,  $\gamma = 1.770(5)$ ,  $2V = 80(5)^\circ$ . The empirical formula is  $(Zn_{0.83}Ca_{0.08}Mg_{0.06})_{\sum 0.97}(Fe^{3+}_{4.88}Al_{0.16})_{\sum 5.04}(PO_4)_{4.09}(OH)_{4.78} \cdot 5.86H_2O$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 10.37 (100) (200), 9.58 (32) (002), 7.24 (26) (20-2), 4.817 (22) (111), 4.409 (13) (112), 3.483 (14) (11-4, 600), 3.431 (14) (404), 3.194 (15) (006, 31-4), 3.079 (33) (314).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3562, 3515w, 3276, 2990sh, 1645sh, 1625, 1140sh, 1070s, 1032s, 990s, 970sh, 940sh, 885sh, 798w, 782w, 665sh, 603, 580, 466, 440sh, 405sh, 368.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P653 Beraunite**  $\text{Fe}^{2+}\text{Fe}^{3+}_5(\text{PO}_4)_4(\text{OH})_5 \cdot 6\text{H}_2\text{O}$



**Origin:** Levaäniemi mine, Svappavaara, Kiruna district, Lappland, Sweden.

**Description:** Black spherulites from the association with cacoxyne. Al-bearing variety. Investigated by A.V. Kasatkin. The empirical formula is (electron microprobe):  $\text{Fe}_{5.26}\text{Al}_{0.74}(\text{PO}_4)_{4.00}(\text{OH})_5 \cdot 6\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

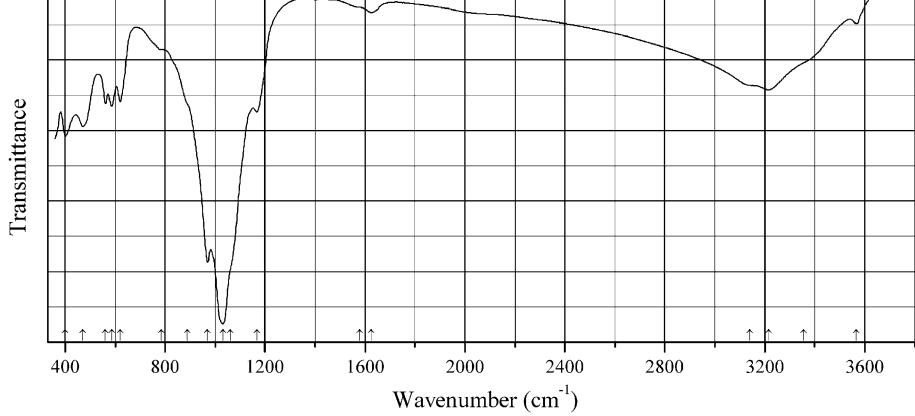
**Wavenumbers ( $\text{cm}^{-1}$ ):** 3572, 3500sh, 3360sh, 3286, 3192, 1626, 1135sh, 1060sh, 1031s, 1015sh,

991s, 866, (733w), 604, 690sh, 456.

**Note:** The spectrum was obtained by N

Figure 11. The spectrum was obtained by the TGA technique.

## **Fes4 Natroferriferite NaFe<sub>5</sub>(FO<sub>4</sub>)<sub>4</sub>(OH)<sub>6</sub>·2H<sub>2</sub>O**



**Origin:** Chino open pit, near Santa Rita, New Mexico, USA.

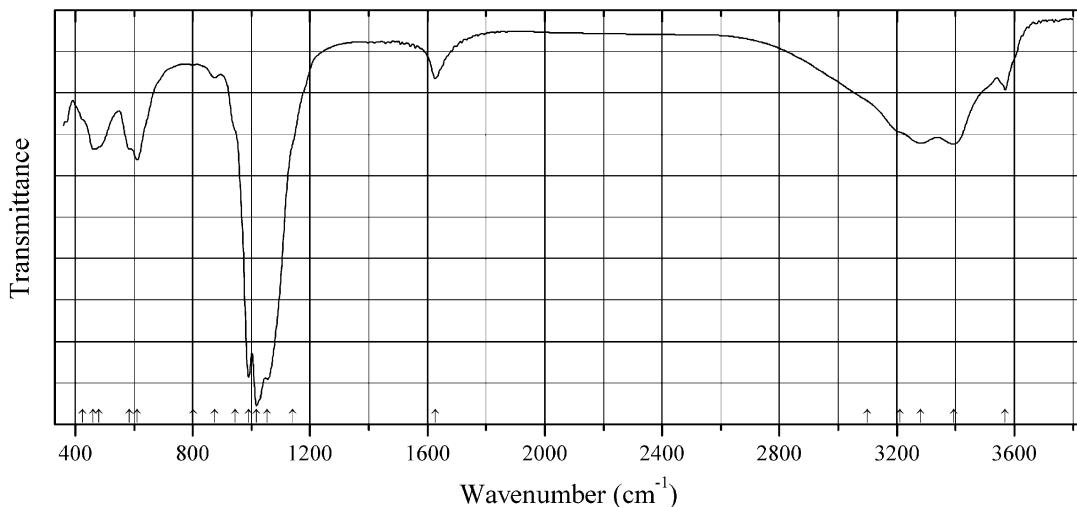
**Description:** Black spherulites with greenish-blue streak. Investigated by A.V. Kasatkin. The empirical formula is (electron microprobe):  $\text{Na}_{0.93}\text{Ca}_{0.15}\text{Fe}_{5.50}\text{Al}_{0.42}(\text{PO}_4)_{4.00}(\text{OH})_6 \cdot 2\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3567w, 3355sh, 3215, 3140, 1625w, 1580sh, 1167s, 1060sh, 1031s, 970s, 890sh, 786w, 620, 586, 561, 471s, 401s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P655 Tvrďite**  $\text{Fe}^{2+}\text{Fe}^{3+}_2\text{Al}_3(\text{PO}_4)_4(\text{OH})_5(\text{H}_2\text{O})_4 \cdot 2\text{H}_2\text{O}$



**Origin:** Hagendorf South pegmatite, Cornelia mine, Hagendorf, Waidhaus, Upper Palatinate, Bavaria, Germany.

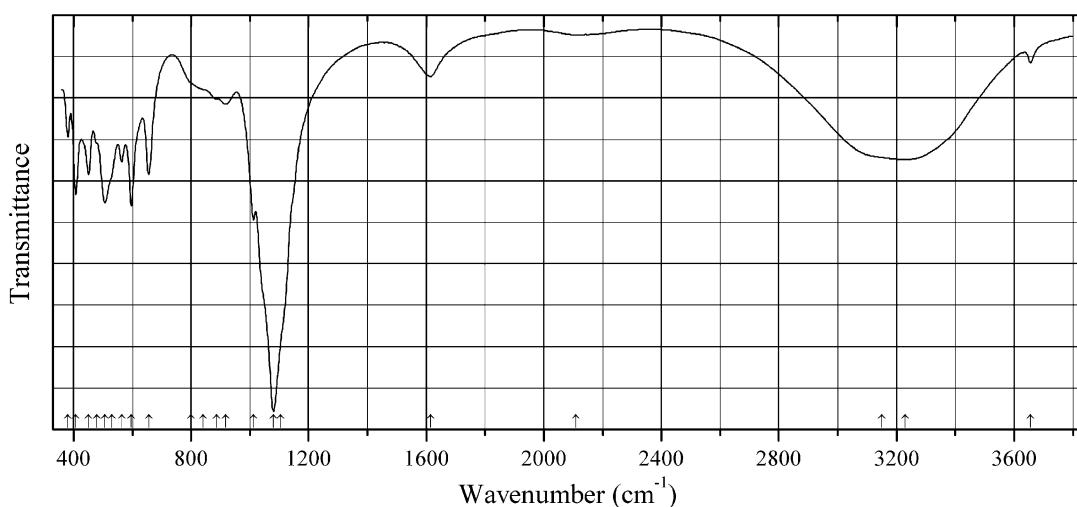
**Description:** Greenish-gray radial-fibrous aggregates. Al-deficient variety. The empirical formula is (electron microprobe):  $\text{Ca}_{0.05-0.08}\text{Zn}_{0.34-0.50}\text{Mn}_{0.04-0.07}\text{Mg}_{0-0.05}\text{Fe}_{3.85-3.99}\text{Al}_{1.44-1.66}\text{Cr}_{0.06}(\text{PO}_4)_4(\text{OH})_5(\text{H}_2\text{O})_4 \cdot 2\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3569, 3394, 3280, 3210sh, 3100sh, 1627, 1140sh, 1054s, 1018s, 990s, 945sh, 874, 802w, 610, 585sh, 480sh, 460, 425sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P656 Minyulite**  $\text{KAl}_2(\text{PO}_4)_2(\text{F},\text{OH}) \cdot 4\text{H}_2\text{O}$



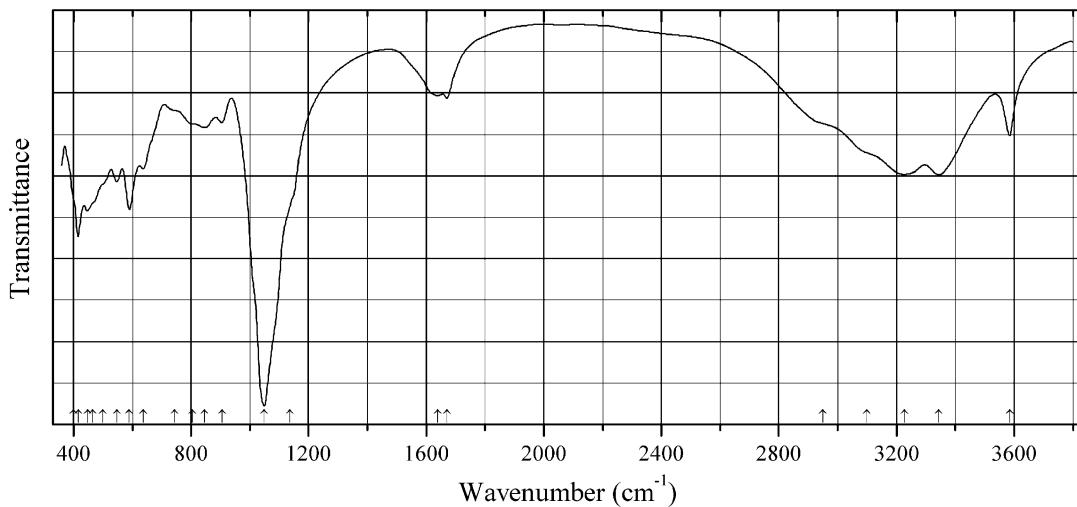
**Origin:** Cerro Mejillones, Mejillones Peninsula, Mejillones, Antofagasta, II Region, Chile.

**Description:** A F-rich sample. Investigated by I.V. Pekov.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3656w, 3229 (broad), 3150sh, 2110w (broad), 1615, 1105sh, 1080s, 1013s, 917, 886, 840sh, 800sh, 656s, 597s, 564, 530sh, 507, 480sh, 451s, 408s, 381.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P657 Variscite-4O**  $\text{Al}(\text{PO}_4)_2\text{H}_2\text{O}$ 

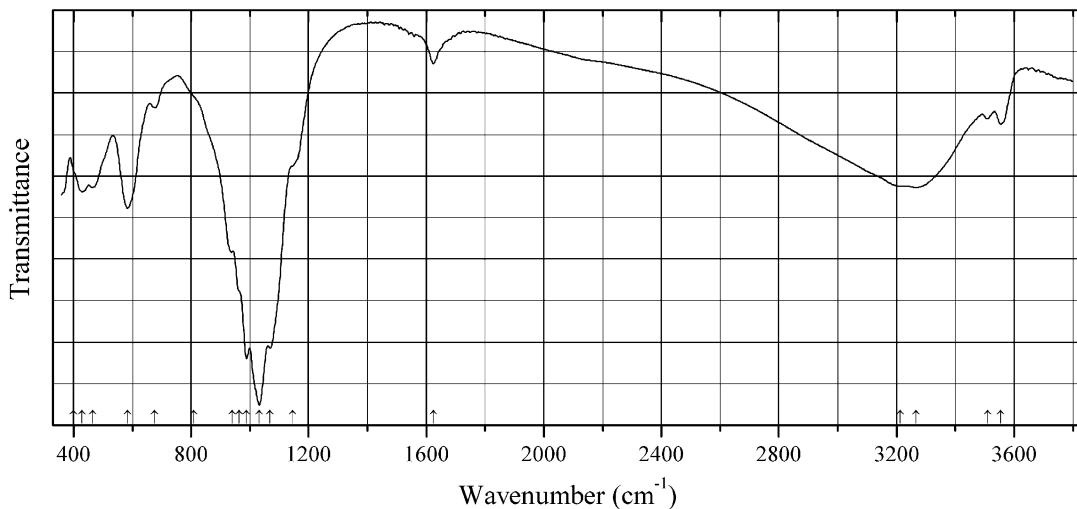
**Origin:** Cerro Mejillones, Mejillones Peninsula, Mejillones, Antofagasta, II Region, Chile.

**Description:** Colorless crystals from the association with gypsum and minyulite. Investigated by I.V. Pekov. Characterized by single-crystal X-ray diffraction data. Orthorhombic,  $a = 9.675(4)$ ,  $b = 9.893(4)$ ,  $c = 17.203(9)$  Å,  $V = 1647(1)$  Å<sup>3</sup>. The empirical formula is (electron microprobe):  $\text{Al}_{1.00}(\text{PO}_4)_{1.00}\cdot 2\text{H}_2\text{O}$

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3585, 3344s, 3228s, 3100sh, 2950sh, 1670, 1639, 1135sh, 1049s, 905, 846, 804, 745sh, 637, 590s, 547, 500sh, 465sh, 448s, 416s, 405sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P658 Beraunite**  $\text{Fe}^{2+}\text{Fe}^{3+}_5(\text{PO}_4)_4(\text{OH})_5\cdot 6\text{H}_2\text{O}$ 

**Origin:** Hagendorf South pegmatite, Cornelia mine, Hagendorf, Waidhaus, Upper Palatinate, Bavaria, Germany.

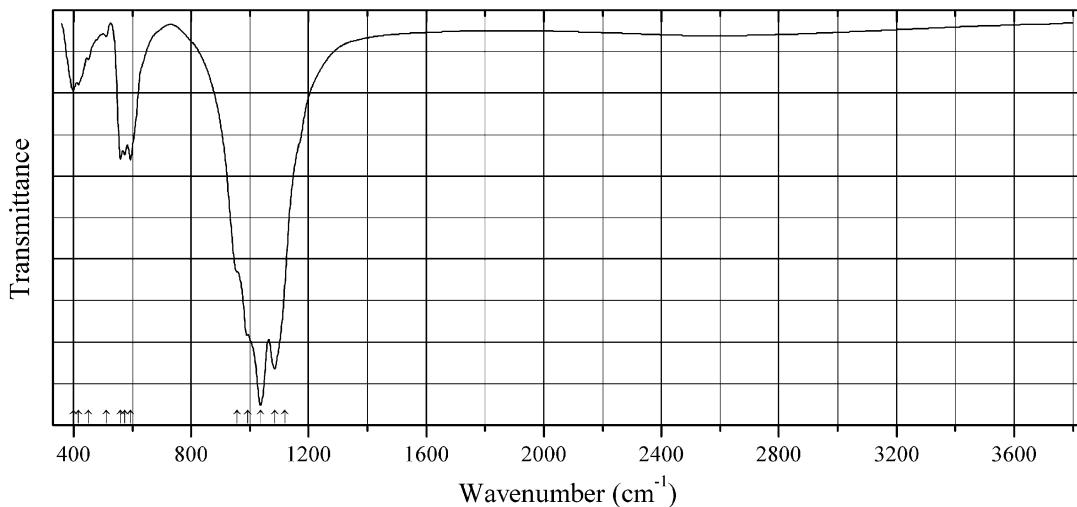
**Description:** Black radial aggregates. A Mn-bearing variety. The empirical formula is (electron microprobe):  $\text{Fe}_{5.44}\text{Mn}_{0.49}\text{Zn}_{0.07}(\text{PO}_4)_{4.00}(\text{OH})_5\cdot 6\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3554, 3510, 3265, 3213, 1625, 1145sh, 1069s, 1032s, 989s, 965sh, 940s, 810sh, 677, 584s, 465, 430, 400sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P659 Manitobaite**  $\text{Na}_{16}\text{Mn}^{2+}_{25}\text{Al}_8(\text{PO}_4)_{30}$



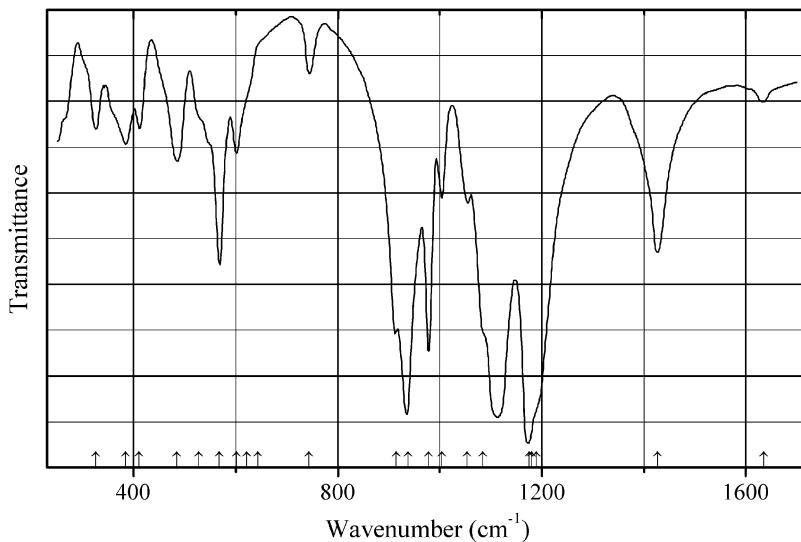
**Origin:** Cross Lake, Manitoba, Canada (type locality).

**Description:** Green grain. A fragment of holotype kindly granted by A.V. Kasatkin. The crystal structure is solved. Monoclinic, space group  $Pc$ ,  $a = 13.4516(15)$ ,  $b = 12.5153(16)$ ,  $c = 26.661(3)$  Å,  $\beta = 101.579(10)^\circ$ ,  $V = 4397.1(6)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{meas}} = 3.621(6)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 3.628$  g/cm<sup>3</sup>. Optically biaxial (−),  $\alpha = 1.682(1)$ ,  $\beta = 1.692(1)$ ,  $\gamma = 1.697(1)$ ,  $2V = 78.1(6)^\circ$ . The empirical formula is  $\text{Na}_{15.55}\text{Ca}_{1.47}\text{Mg}_{0.88}\text{Fe}^{2+}_{4.19}\text{Mn}^{2+}_{18.78}\text{Zn}_{0.32}\text{Al}_{6.54}\text{Fe}^{3+}_{1.05}\text{P}_{30.08}\text{O}_{120}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1120sh, 1084s, 1036s, 993s, 957, 594, 574, 560, 511w, 450, 416, 400.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P660 Ammonium vanadyl pyrophosphate**  $\alpha\text{-}(\text{NH}_4)_2(\text{VO})_3(\text{P}_2\text{O}_7)_2$ 

**Origin:** Synthetic.

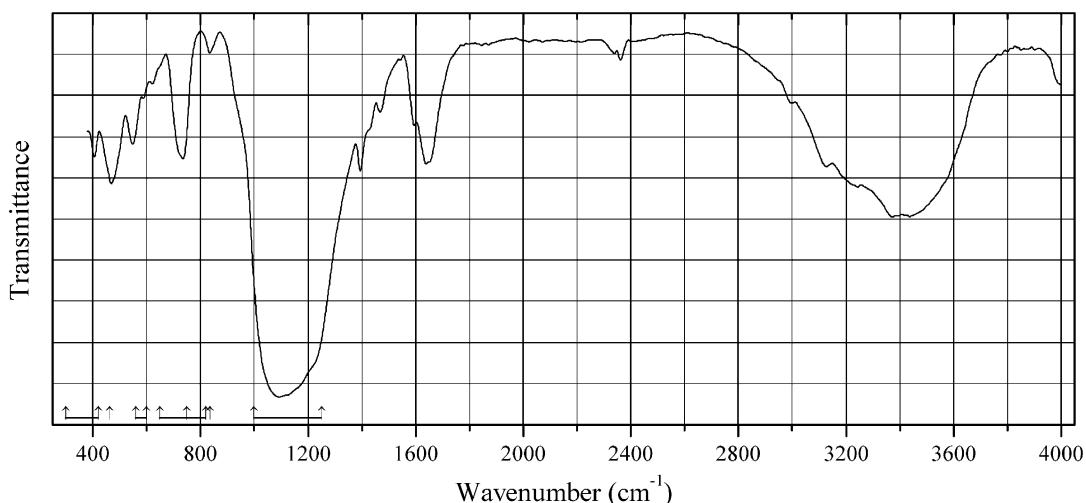
**Description:** Prepared from the mixture of  $\text{V}_2\text{O}_5$  and  $(\text{NH}_4)_2(\text{HPO}_4)$  which was firstly heated up to 200 °C, homogenized and further heated at 325 °C for 2 h in air. Orthorhombic, space group *Pnma*,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Baran and Rabe (1999).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3262 (broad), 1635w, 1427, 1189sh, 1175s, 1180s, 1085sh, 1054w, 1114s, 1004, 978s, 938s, 915w, 744, 643, 622sh, 601, 568s, 548sh, 527sh, 485, 411w, 385, 326.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**P661 Aluminium phosphate hydrate**  $\text{Al}(\text{PO}_4)\cdot n\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Ce-doped mesoporous material synthesized by the hydrothermal method, starting from aluminium hydroxide, 85% phosphoric acid, hydrated ceriumchloride and di-isopropylamine as an organic template agent. The empirical formula is  $\text{Ce}_{0.04}\text{Al}_{0.97}\text{P}_{1.01}\text{O}_{4.04} \cdot n\text{H}_2\text{O}$ . Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

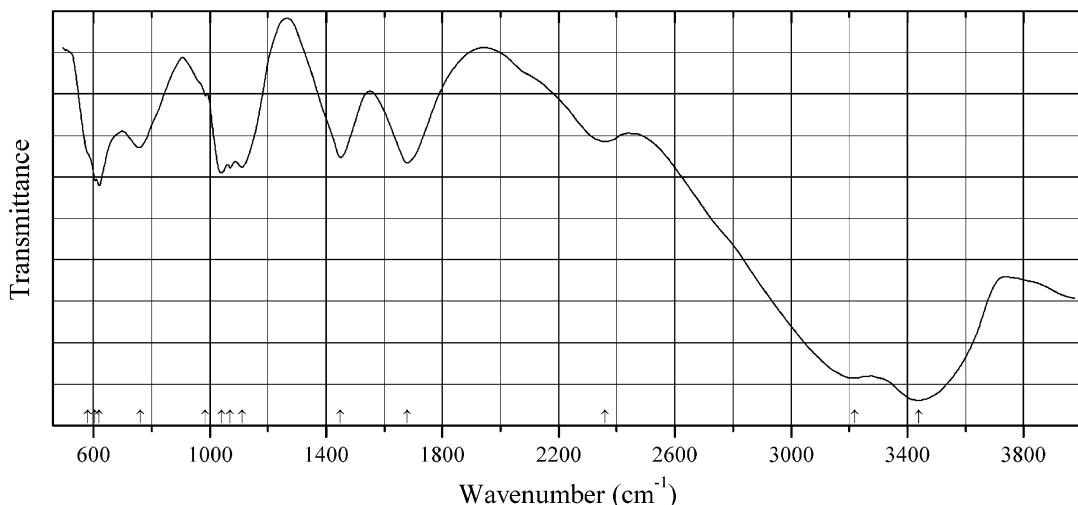
**Source:** Souza de Araujo et al. (1997).

**Wavenumbers (cm<sup>-1</sup>):** 1250–1000 (broad), 835, 820–650, 750–650, 600–560, 464, 420–300.

**Note:** The material was described as an anhydrous phosphate, but bands above 1550 cm<sup>-1</sup> indicate the presence of H<sub>2</sub>O molecules.

### P662 Struvite Cd analogue

**Ammonium cadmium phosphate hexahydrate**  $\text{Cd}(\text{NH}_4)(\text{PO}_4) \cdot 6\text{H}_2\text{O}$



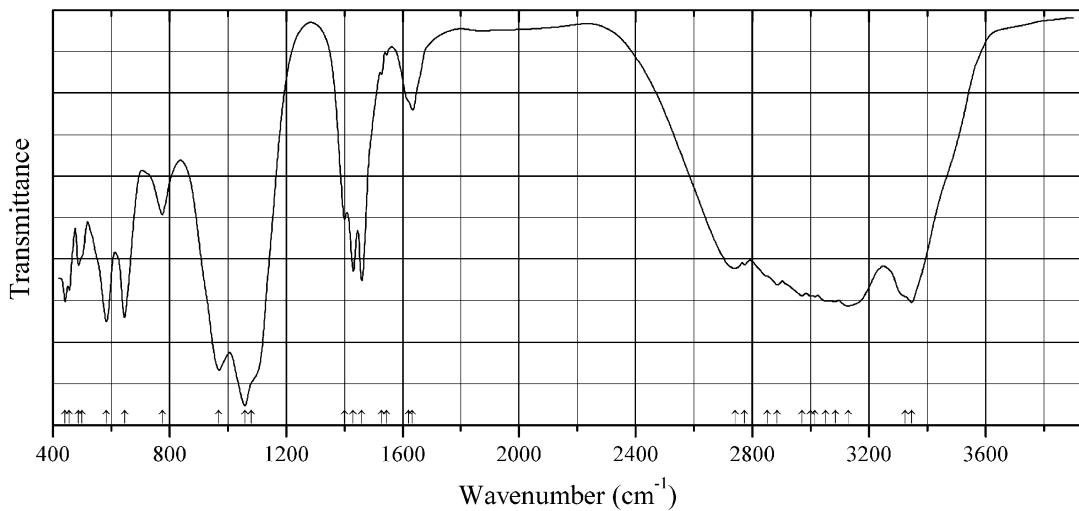
**Origin:** Synthetic.

**Description:** Obtained by slow evaporation at ordinary temperatures from the aqueous equimolar solutions of ammonium dihydrogen phosphate and cadmium sulfate. Structurally related to struvite. Orthorhombic,  $a = 13.882$ ,  $b = 12.249$ ,  $c = 11.395$  Å. Characterized by thermal and powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Ravikumar et al. (2002).

**Wavenumbers (cm<sup>-1</sup>):** 3440s, 3220s, 2360, 1680s, 1450s, 1110s, 1070s, 1040s, 985, 760, 620s, 605, 580sh.

**P663 Ammonium iron(II) phosphate hydrate** ( $\text{NH}_4\text{Fe}(\text{PO}_4)\cdot\text{H}_2\text{O}$ )

**Origin:** Synthetic.

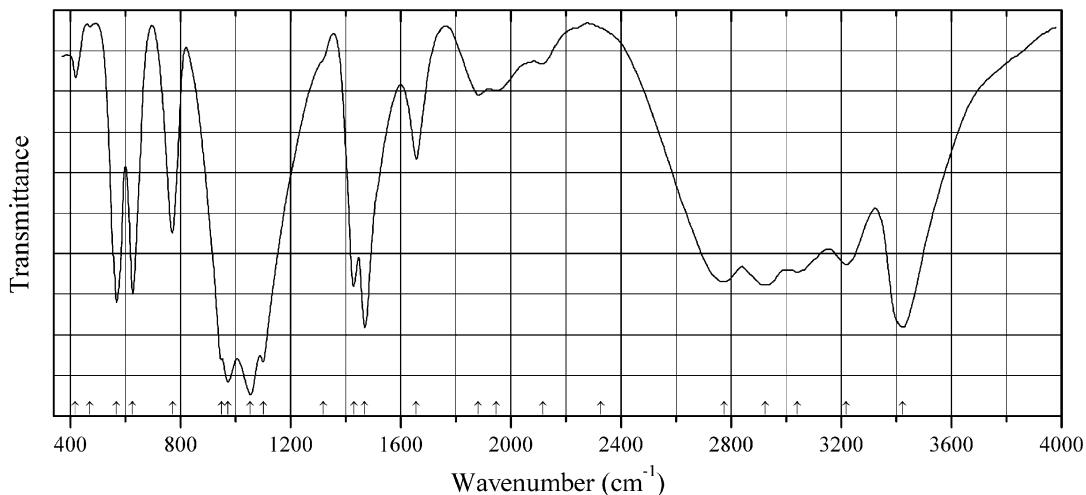
**Description:** White crystals obtained from the equimolar mixture of  $(\text{NH}_4)_3(\text{PO}_4)\cdot 3\text{H}_2\text{O}$  and  $\text{FeSO}_4\cdot 7\text{H}_2\text{O}$  ground in the presence of the surfactant PEG-400 and heated at 40 °C for 48 h. Characterized by powder X-ray diffraction data. Orthorhombic, space group  $Pmm2_1$ ,  $a = 5.660$ ,  $b = 8.825$ ,  $c = 4.826 \text{ \AA}$ ,  $V = 241 \text{ \AA}^3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Yuan et al. (2008).

**Wavenumbers (cm<sup>-1</sup>):** 3347, 3325sh, 3130, (3085), (3052), (3014), (3000), (2970), (2886), (2850sh), (2773), 2740, 1634, 1620sh, 1545, 1528, 1460, 1431, 1400, 1081sh, 1058s, 970s, 775, 646, 584, 500sh, 488, 457, 442.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**P664 Ammonium magnesium phosphate** ( $\text{NH}_4\text{Mg}(\text{PO}_4)\cdot\text{H}_2\text{O}$ )

**Origin:** Synthetic.

**Description:** Obtained by adding 0.5 M solution of  $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$  to an excess of saturated  $(\text{NH}_4)_2\text{HPO}_4$  solution. Characterized by thermal analysis and powder X-ray diffraction data.

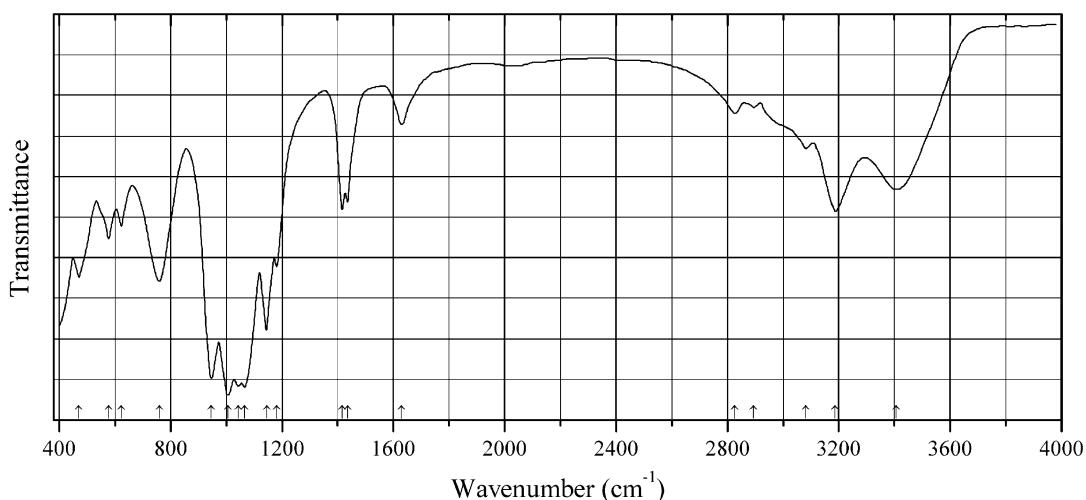
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Sronsri et al. (2014).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3424s, 3218, 3040, 2924, 2775, 2327w, 2118, 1948, 1882, 1657, 1470s, 1430, 1319sh, 1102s, 1055s, 974s, 949sh, 772, 627s, 568s, 472w, 419.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

#### P665 Ammonium titanophosphate $(\text{NH}_4)_2\text{Ti}_2\text{O}(\text{HPO}_4)(\text{PO}_4)_2$ ?



**Origin:** Synthetic.

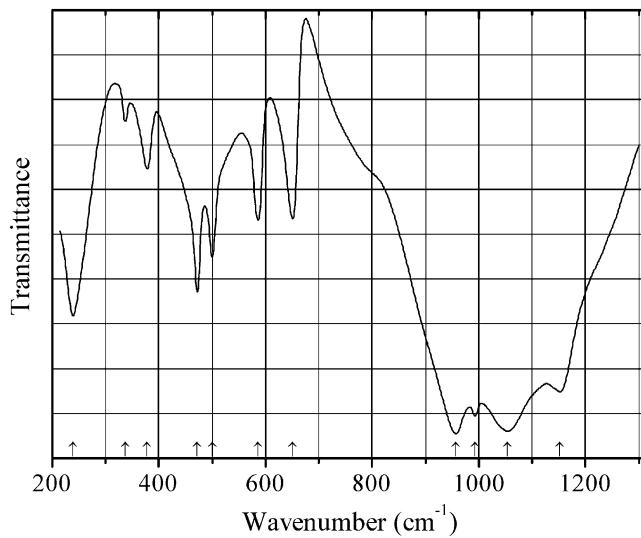
**Description:** Synthesized hydrothermally from  $\text{Ti}(\text{SO}_4)_2$ ,  $\text{H}_3(\text{PO}_4)_3$ , and ammonia solution at 200 °C for several hours. Characterized by powder X-ray diffraction data and thermal analysis.

**Kind of sample preparation and/or method of registration of the spectrum:** No data.

**Source:** Li et al. (2004b).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3407, 3187, 3081w, 2894w, 2826w, 1630, 1436, 1417, 1181, 1145s, 1067s, 1044s, 1006s, 947, 760, 624, 578, 471.

**Note:** The formula is questionable and is to be checked.

**P666 Antimony(III) phosphate SbPO<sub>4</sub>**

**Origin:** Synthetic.

**Description:** Prepared in the reaction of antimony with freshly prepared metaphosphoric acid at high temperatures. Characterized by powder X-ray diffraction data. Monoclinic, space group  $P2_1/m$ ,  $Z = 2$ .

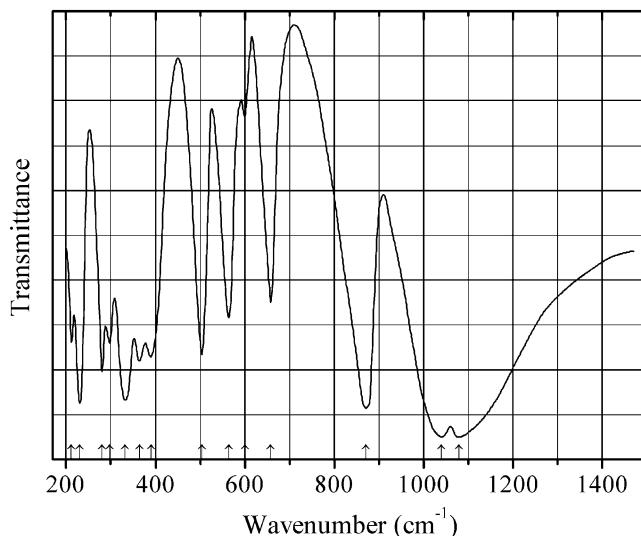
**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

**Source:** Brockner, and Hoyer (2002).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1152s, 1054s, 993s, 957s, 651, 586, 500, 472, 378, 337w, 239.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1054, 977, 937w, 623, 584, 548w, 478, 356s.

**P667 Antimony(V) oxophosphate SbO(PO<sub>4</sub>)**

**Origin:** Synthetic.

**Description:** Monoclinic, space group  $C2c$ ,  $a = 6.791(1)$ ,  $b = 8.033(1)$ ,  $c = 7.046(1)$  Å,  $\beta = 115.90$  (1)°,  $Z = 4$ . The crystal structure consists of chains of corner shared distorted octahedra linked together by  $\text{PO}_4$  tetrahedra.

**Kind of sample preparation and/or method of registration of the spectrum:** See Husson et al. (1988b).

**Source:** Husson et al. (1988a).

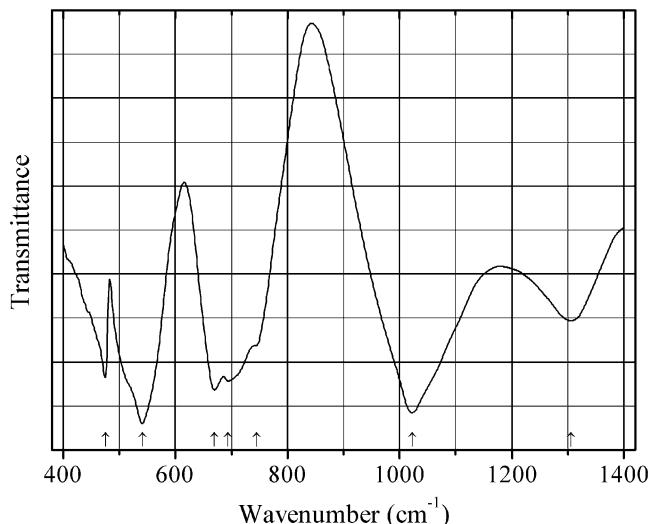
**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1080s, 1040s, 872s, 658, 600w, 564, 504, 390, 364, 332s, 297, 280, 231s, 212.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1122, 1060w, 1050, 1010, 788, 585s, 528s, 460w, 417, 375, 312s, 278, 197, 152, 135, 117w.

### P668 Minjiangite $\text{BaBe}_2(\text{PO}_4)_2$

#### Barium beryllium phosphate $\text{BaBe}_2(\text{PO}_4)_2$



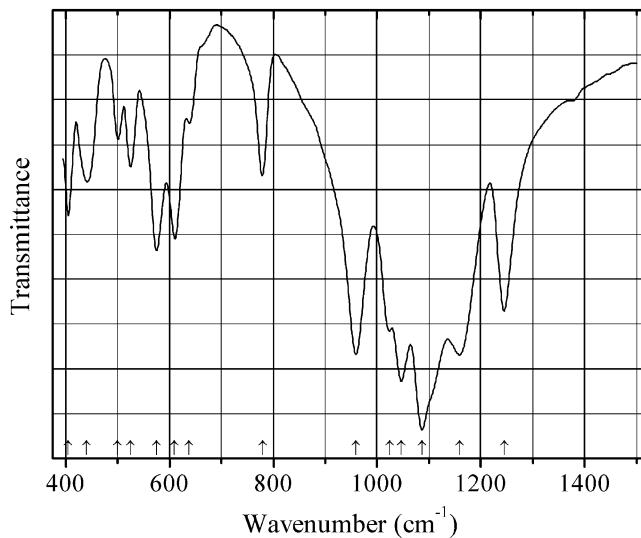
**Origin:** Synthetic.

**Description:** Colorless crystals synthesized hydrothermally from  $\text{BeO}$ ,  $\text{Ba}(\text{OH})_2 \cdot 8\text{H}_2\text{O}$ , and  $\text{H}_3\text{PO}_4$  (85%) at 200 °C for 7 days. The crystal structure is based on double layers of tetrahedra, which contain both Be and P in a 1:1 ratio. The Ba atoms are located in regular 12-coordinated polyhedra and connect two successive double layers. Hexagonal, space group  $P6/mmm$ ,  $a = 5.028(1)$ ,  $c = 7.466(1)$  Å,  $V = 162.51(1)$  Å<sup>3</sup>,  $Z = 1$ .  $D_{\text{calc}} = 3.507$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Dal Bo et al. (2014).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1305, 1022s, 745sh, 694, 670s, 541s, 475.

**P669 Barium chromium pyrophosphate  $\text{BaCr}_2(\text{P}_2\text{O}_7)_2$** 

**Origin:** Synthetic.

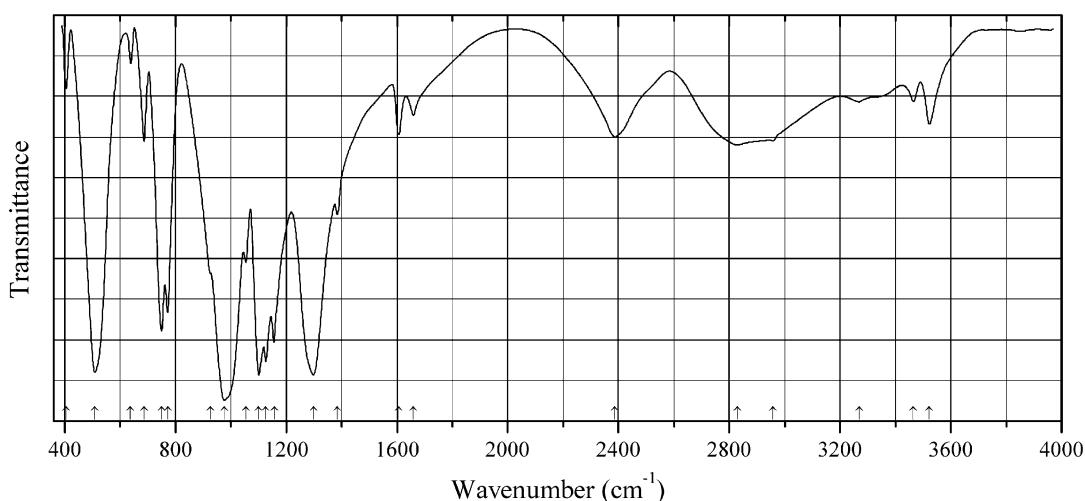
**Description:** Green solid synthesized by the conventional solid-state reaction technique, by heating stoichiometric mixture of  $\text{BaCO}_3$ ,  $\text{Cr}_2\text{O}_3$ , and  $(\text{NH}_4)(\text{H}_2\text{PO}_4)$  up to 1200 °C. Characterized by powder X-ray diffraction data. Triclinic, space group  $P-1$ ,  $a = 6.1408(5)$ ,  $b = 6.1898(4)$ ,  $c = 7.8027(6)$  Å,  $\alpha = 96.692(5)^\circ$ ,  $\beta = 101.686(5)^\circ$ ,  $\gamma = 105.542(4)^\circ$ ,  $V = 275.19(4)$  Å<sup>3</sup>,  $Z = 1$ .  $D_{\text{meas}} = 2.39(3)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 2.391$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Tao et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 1245, 1160s, 1087s, 1047, 1024, 960s, 780, 638w, 610, 575, 525, 500, 440, 405.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**P670 Barium sodium cyclotriphosphate hydrate  $\text{BaNa}(\text{P}_3\text{O}_9)\cdot 3\text{H}_2\text{O}$** 

**Origin:** Synthetic.

**Description:** Pink crystals obtained by adding barium nitrate to a saturated aqueous solution of sodium cyclotriphosphate in the stoichiometric ratio. The resulting mixture was left to stand at room temperature for 2 weeks. The crystal structure is solved. Triclinic, space group  $P\bar{1}$ ,  $a = 7.0350(3)$  Å,  $b = 9.0470(3)$  Å,  $c = 9.8800(2)$  Å,  $\alpha = 116.551(3)^\circ$ ,  $\beta = 95.932(2)^\circ$ ,  $\gamma = 74.088(3)^\circ$ ,  $V = 540.81(3)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 2.771$  g/cm<sup>3</sup>.

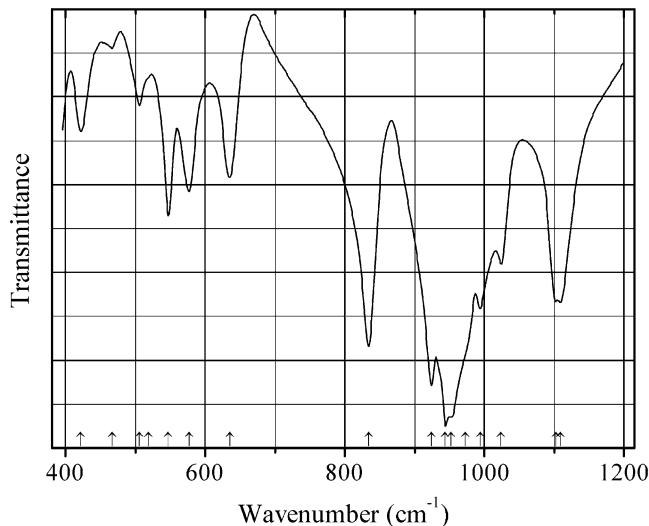
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Ezzaafrani et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 3522, 3465w, 3269w, 2959, 2829, 2387, 1659w, 1606, 1385, 1298s, 1157, 1126s, 1101s, 1055, 976s, 926sh, 772, 750, 687, 638w, 509s, 405w.

**Note:** The bands in the range from 2300 to 2900 cm<sup>-1</sup> indicate the presence of acid P-OH groups. Possibly, the correct formula is BaNa(HP<sub>3</sub>O<sub>9</sub>)(OH)·2H<sub>2</sub>O. This assumption could explain discrepancies between observed wavenumbers and those calculated according to the Libowitzky formula.

### P671 Barium vanadyl phosphate $\alpha$ -Ba(VO<sub>2</sub>)(PO<sub>4</sub>)



**Origin:** Synthetic.

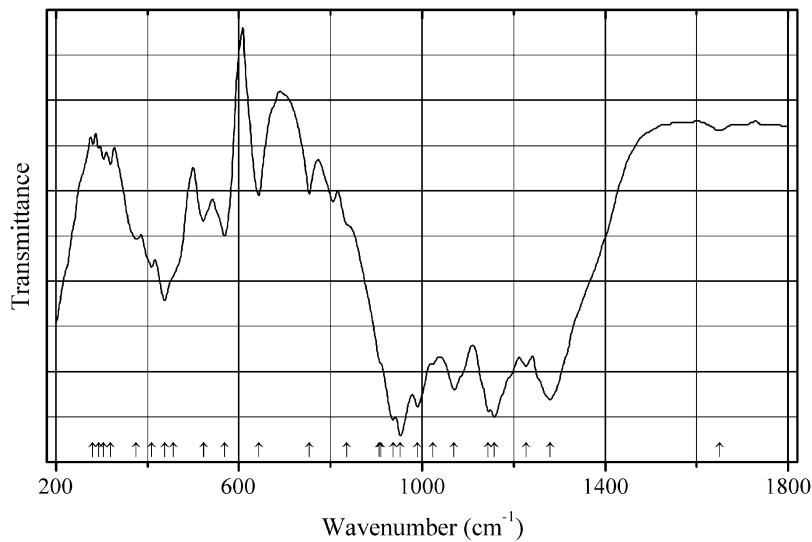
**Description:** Synthesized hydrothermally from V<sub>2</sub>O<sub>5</sub>, H<sub>3</sub>PO<sub>4</sub>, and BaCO<sub>3</sub>. Monoclinic, space group  $P2_1/c$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Borel et al. (2000).

**Wavenumbers (cm<sup>-1</sup>):** 1109, 1102, 1024, 994, 973sh, 952sh, 944s, 924s, 834s, 635, 577, 547, 518sh, 506, 467w, 421.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**P672  $\beta$ -Vanadyl pyrophosphate  $\beta$ -(VO)<sub>2</sub>(P<sub>2</sub>O<sub>7</sub>)**

**Origin:** Synthetic.

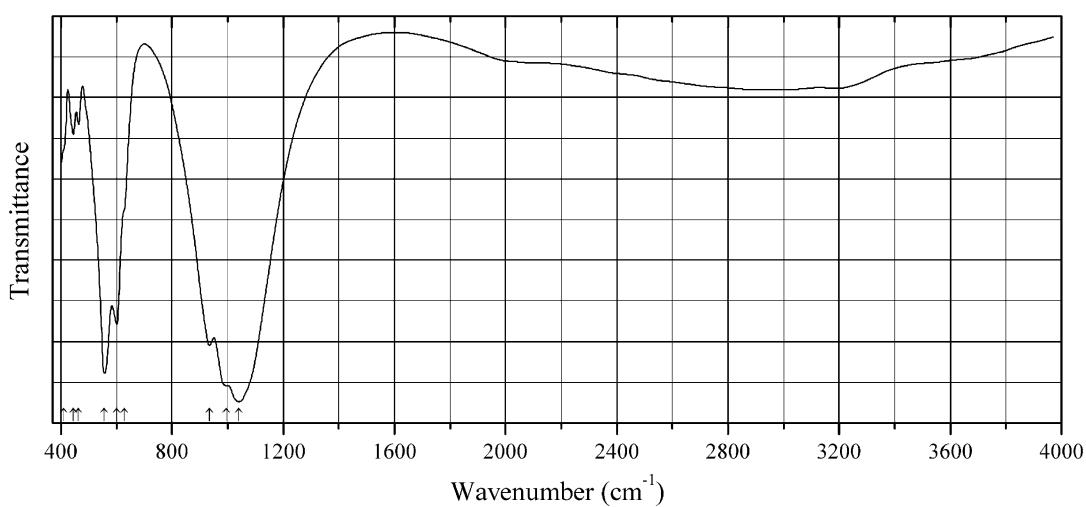
**Description:** Orthorhombic, space group *Pca2*.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Bordes et al. (1984).

**Wavenumbers (cm<sup>-1</sup>):** 1650w, 1280s, 1227, 1158s, 1145, 1070, 1024, 990, 953s, 937s, 910sh, 836sh, 906, 754, 643, 568, 523, 456sh, 438, 409, 376, 319w, 304w, 293w, 281w.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**P673 Bismuth(III) calcium oxophosphate BiCa<sub>4</sub>(PO<sub>4</sub>)<sub>3</sub>O**

**Origin:** Synthetic.

**Description:** Prepared by high temperature solid-state method, by stepwise heating stoichiometric mixture of  $\text{Bi}_2\text{O}_3$ ,  $\text{Ca}(\text{CO}_3)$ , and  $(\text{NH}_4)(\text{H}_2\text{PO}_4)$  up to 1050 °C. Characterized by powder X-ray diffraction data. Structurally related to apatite, space group  $P6_3/m$ .

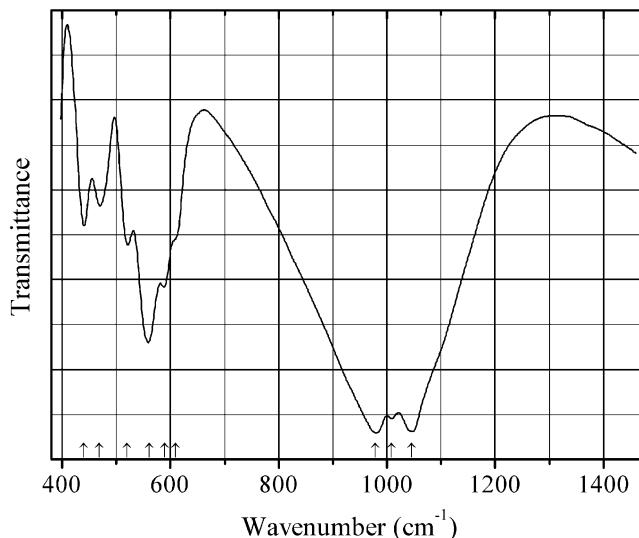
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Sumathi and Gopal (2015).

**Wavenumbers (cm<sup>-1</sup>):** 1041s, 995sh, 935s, 628sh, 602s, 557s, 464w, 445w, 409sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

#### P674 Bismuth(III) nickel oxophosphate $\text{BiNi}(\text{PO}_4)\text{O}$ $\text{BiNi}(\text{PO}_4)\text{O}$



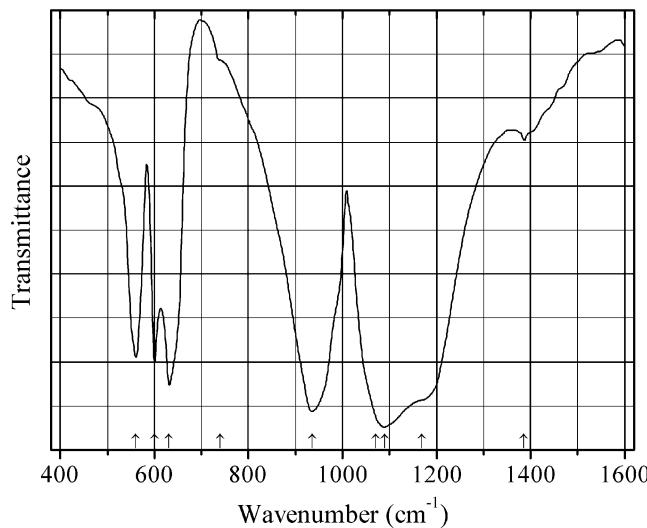
**Origin:** Synthetic.

**Description:** Prepared by solid-state reaction. Monoclinic,  $a = 7.1664(8)$ ,  $b = 11.206(1)$ ,  $c = 5.1732$  (6) Å,  $\beta = 107.281(6)$ °. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 4.727 (44) (-101), 4.338 (69) (120), 3.372 (70) (111), 2.850 (100) (-221), 2.568 (43) (131), 2.516 (41) (230).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Ketatni et al. (1999).

**Wavenumbers (cm<sup>-1</sup>):** 1046s, 1009s, 979s, 609sh, 590, 561s, 520, 468, 440.

**P675 Boron phosphate  $\text{BPO}_4$** 

**Origin:** Synthetic.

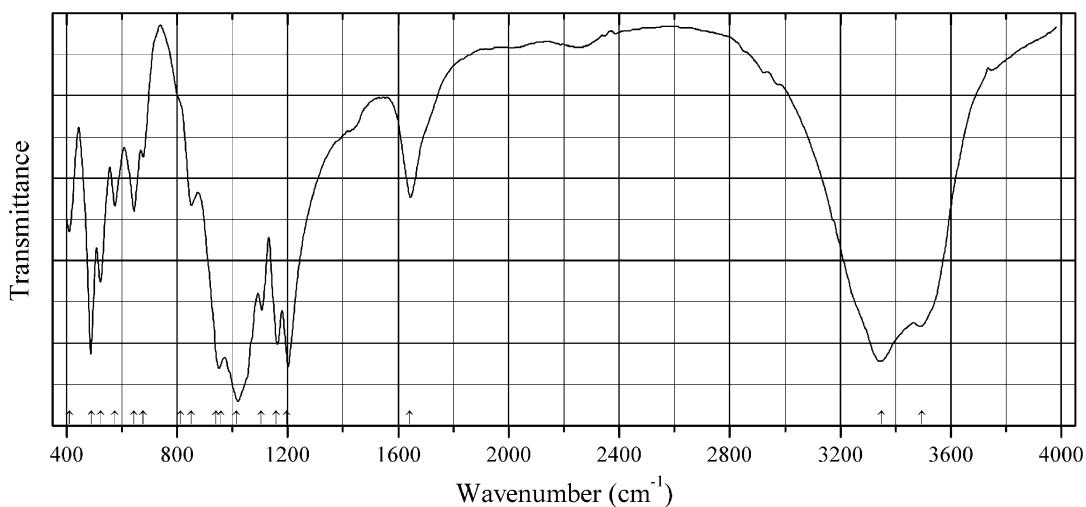
**Description:** Structurally related to cristobalite.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Osaka et al. (1984).

**Wavenumbers (cm⁻¹):** 1386w, 1168sh, 1090s, 1070sh, 935s, 739sh, 630, 600, 560.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**P676 Magnesium borophosphate  $(\text{H}_3\text{O})\text{Mg}(\text{BP}_2\text{O}_8)\cdot 3\text{H}_2\text{O}$** 

**Origin:** Synthetic.

**Description:** Synthesized from  $\text{MgCl}_2$ ,  $\text{B}_2\text{O}_3$ , and  $\text{H}_3\text{PO}_4$  in the presence of pyridine and  $\text{HCl}$ , under mild hydrothermal conditions (at  $170^\circ\text{C}$  for 3 days). The crystal structure is solved. Hexagonal, space group  $P6(1)22$ ,  $a = 9.4462(7)$ ,  $c = 15.759(2)$  Å,  $V = 1217.8(2)$  Å $^3$ ,  $Z = 6$ .  $D_{\text{calc}} = 2.439(3)$  g/cm $^3$ .

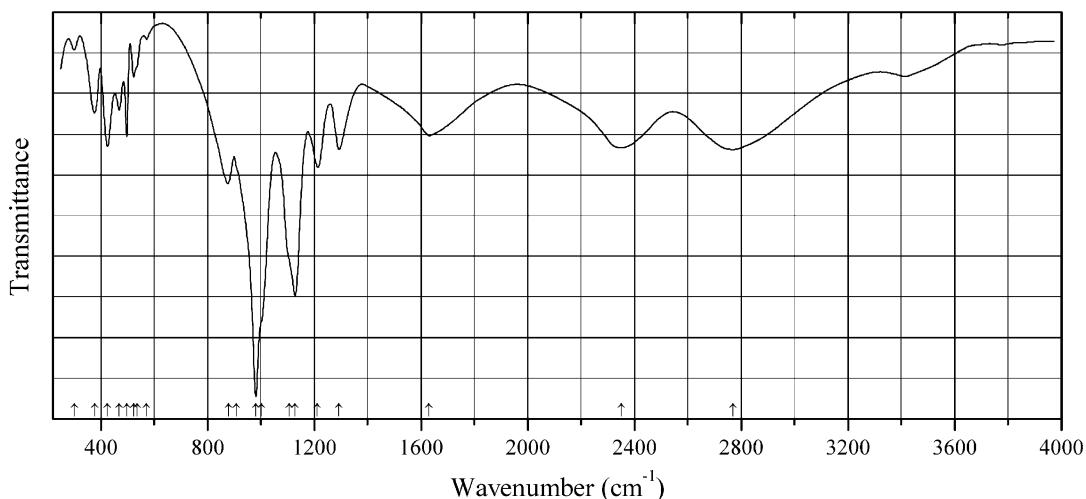
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Yang et al. (2011f).

**Wavenumbers (cm $^{-1}$ ):** 3494, 3348s, 1643, 1198s, 1159, 1105, 1016s, 959s, 940sh, 851, 812sh, 678w, 645, 576, 523, 491, 411.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### P677 Cesium acid (pentahydrogen) phosphate $\text{CsH}_5(\text{PO}_4)_2$



**Origin:** Synthetic.

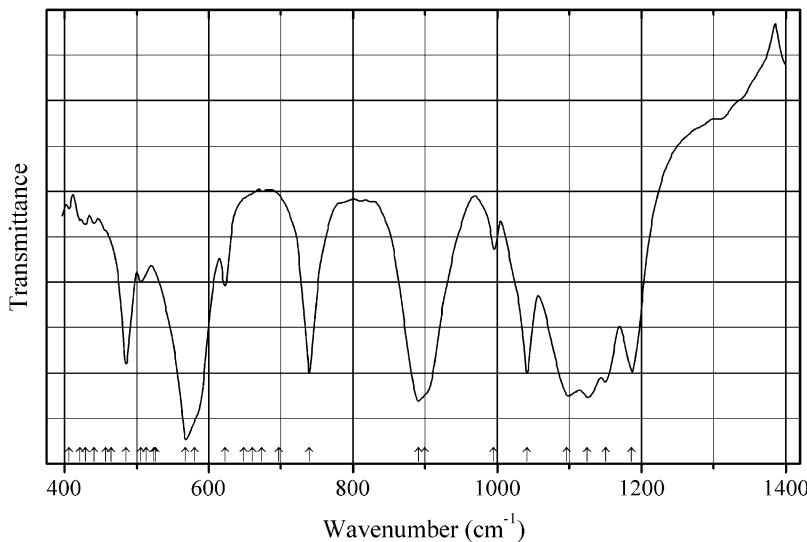
**Description:** Crystals grown from an aqueous solution of  $\text{Cs}_2\text{CO}_3$  and  $\text{H}_3\text{PO}_4$  (at the mole ratio 1:2) by evaporation at room temperature. Monoclinic, space group  $P2_1/c$ ,  $a = 10.879$ ,  $b = 7.768$ ,  $c = 9.526$  Å,  $\beta = 96.60^\circ$ ,  $Z = 4$ . Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Lavrova et al. (2006).

**Wavenumbers (cm $^{-1}$ ):** 3414w (broad), 2770 (broad), 2350 (broad), 1630 (broad), 1293, 1212, 1127s, 1105sh, 1001sh, 980s, 907, 878, 571w, 536sh, 497, 468, 425, 377, 300w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, a figure of the Raman spectrum is given.

**P678 Cesium manganese(II) pyrophosphate  $\text{Cs}_2\text{MnP}_2\text{O}_7$** 

**Origin:** Synthetic.

**Description:** Pink solid prepared from aqueous solutions of  $\text{Mn}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$ ,  $\text{CsCl}$ , and  $\text{NH}_4(\text{H}_2\text{PO}_4)$  as starting materials by heating resulting powder progressively from 200 to 700 °C with intermediate regrindings. The crystal structure is solved. Orthorhombic, space group  $Pnma$ ,  $a = 16.3398(3)$ ,  $b = 5.3872(1)$ ,  $c = 9.8872(2)$  Å,  $V = 870.33(3)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 3.775$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** Diffuse reflection of a mixture with KBr.

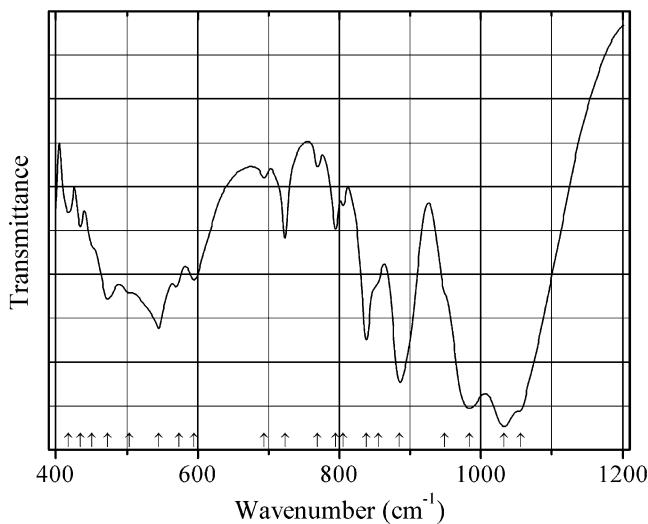
**Source:** Kaoua et al. (2013).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1186s, 1151s, 1125s, 1097s, 1041s, 995, 900sh, 891s, 740, 697sh, 674w, 661sh, 649sh, 623, 580sh, 568s, 525sh, 514sh, 506w, 485, 465sh, 457sh, 441w, 429w, 421w, 406w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The strong band at 891 cm<sup>-1</sup> and shoulder at 900 cm<sup>-1</sup> are indicated by Kaoua et al. (2013) as strong band at 896 cm<sup>-1</sup>. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1197w, 1165w, 1154w, 1142w, 1129, 1128w, 1107w, 1098w, 1081w, 1060w, 1041w, 1021s, 954w, 934w, 898w, 700s, 635w, 598w, 576w, 562, 536w, 521w, 498w, 466w, 428, 364, 327, 269w, 245w, 205, 202, 166w, 140w, 129w, 124w.

**P679 Cesium uranyl oxophosphate**  $\text{Cs}_3(\text{UO}_2)_2(\text{PO}_4)\text{O}_2$



**Origin:** Synthetic.

**Description:** Yellow crystals obtained in the reaction of triuranyl diphosphate tetrahydrate with a CsI flux at 750 °C. The crystal structure is solved. Monoclinic, space group  $C2/c$ ,  $a = 13.6261(13)$ ,  $b = 8.1081(8)$ ,  $c = 12.3983(12)$  Å,  $\beta = 114.61(12)^\circ$ ,  $V = 1245.41(20)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 2.684$  g/cm $^3$ .

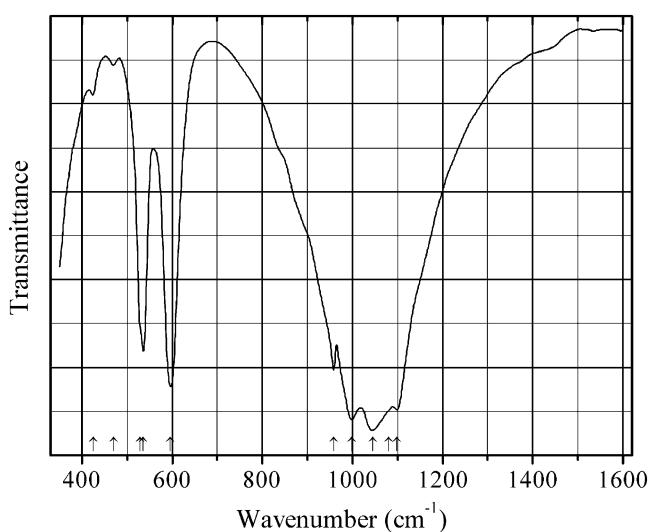
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

Source: Yagoubi et al. (2013).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1056sh, 1033s, 984s, 949sh, 885s, 855sh, 838, 805, 795, 769w, 723, 694w, 595, 574, 545, 504sh, 473, 451sh, 435w, 418w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**P680 Calcium chlorophosphate (“chlor-spodiosite”)**  $\text{Ca}_2(\text{PO}_4)\text{Cl}$



**Origin:** Synthetic.

**Description:** Crystals grown from melt by means of a reaction flux technique using  $\text{Ca}_3(\text{PO}_4)_2$  and  $\text{CaCl}_2$  as starting materials. Orthorhombic, space group  $Pbcm$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

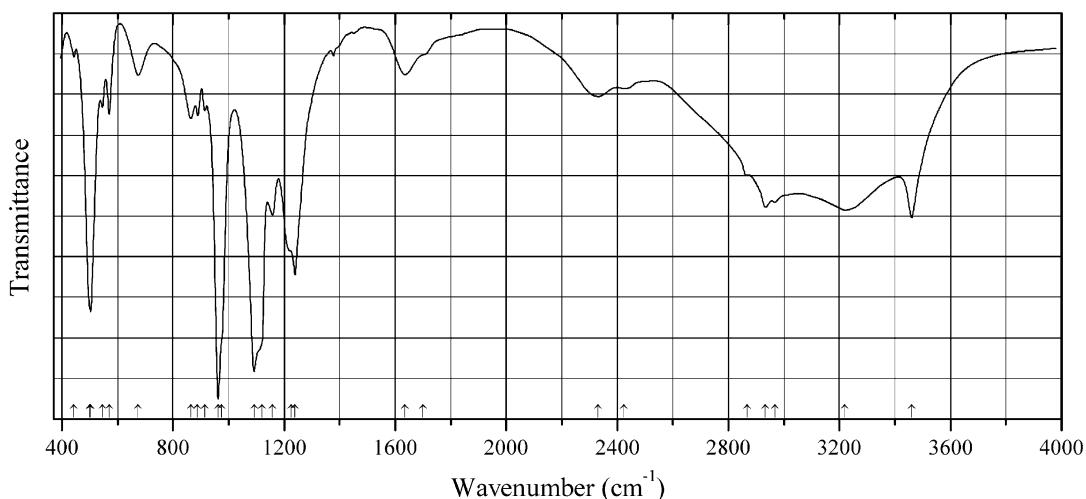
**Source:** Kowalczyk and Condrate Sr (1974).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1099s, 1080sh, 1046s, 999s, 959, 596, 536, 529sh, 471w, 425w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1077, 1063, 1048w, 1026w, 995, 958s, 627, 611, 551, 463, 397.

### P681 Calcium dihydropophosphate monohydrate $\text{Ca}(\text{H}_2\text{PO}_4)_2 \cdot \text{H}_2\text{O}$



**Origin:** Synthetic.

**Description:** Commercial reactant. Triclinic, space group  $P-1$ ,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Absorption. Kind of sample preparation is not indicated.

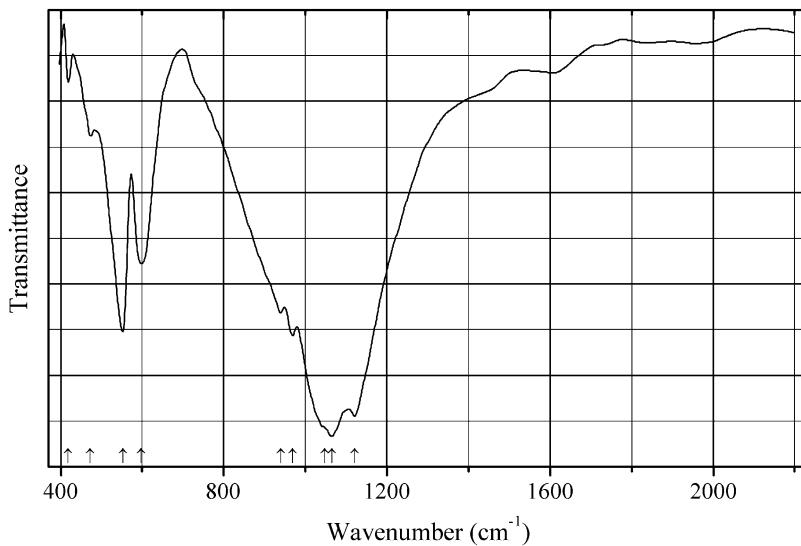
**Source:** Xu et al. (1998).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3461, 3220, 2967, 2934, 2868sh, 2423w, 2330, 1700sh, 1635w, 1239s, 1225sh, 1158, 1120sh, 1092s, 975sh, 962s, 914w, 888w, 864w, 675w, 570w, 545w, 504s, 500sh, 444w, 355, 250sh, 230.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 2810, 2386, 1217, 1159, 1112s, 1016, 988s, 956, 916s, 906, 580, 523, 499, 421, 366, 337, 251, 210, 170, 141, 124, 103, 85.

**P682 Calcium magnesium lanthanum phosphate  $\text{Ca}_8\text{MgLa}(\text{PO}_4)_7$**



**Origin:** Synthetic.

**Description:** Eu-doped sample synthesized in a solid-state reaction from the mixture of magnesium carbonate basic pentahydrate,  $\text{CaCO}_3$ ,  $(\text{NH}_4)_2\text{HPO}_4$ ,  $\text{La}_2\text{O}_3$ , and  $\text{Eu}_2\text{O}_3$ . Structurally related to whitlockite. Hexagonal, space group  $R\bar{3}c$ ,  $a = 10.38848$ ,  $c = 37.23035$  Å,  $V = 4017.89$  Å<sup>3</sup>. Characterized by powder X-ray diffraction data.

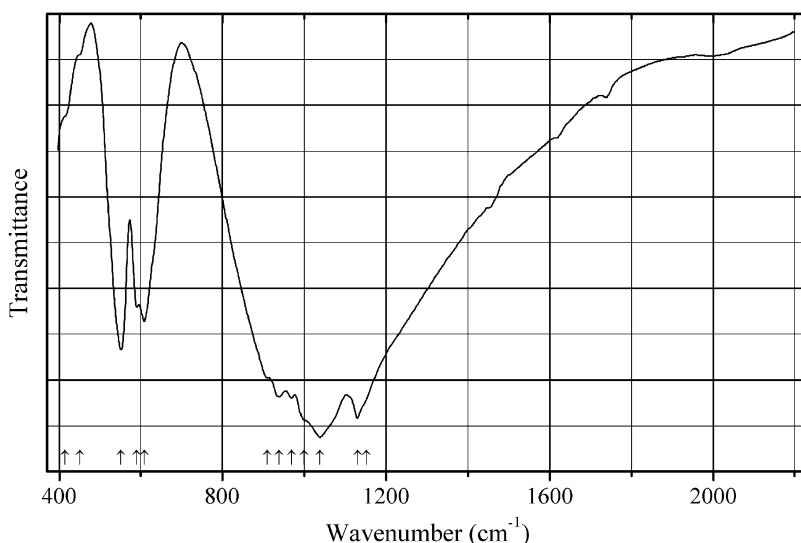
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Huang et al. (2009).

**Wavenumbers (cm<sup>-1</sup>):** 1121s, 1065s, 1047sh, 969, 939, 598, 552, 473w, 419w.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**P683 Calcium magnesium yttrium phosphate  $\text{Ca}_8\text{MgY}(\text{PO}_4)_7$**



**Origin:** Synthetic.

**Description:** Eu-doped sample synthesized in a solid-state reaction from a mixture of magnesium carbonate basic pentahydrate,  $\text{CaCO}_3$ ,  $(\text{NH}_4)_2\text{HPO}_4$ ,  $\text{Y}_2\text{O}_3$ , and  $\text{Eu}_2\text{O}_3$ . Structurally related to whitlockite. Hexagonal, space group  $R\bar{3}c$ ,  $a = 10.32966$ ,  $c = 36.94593$  Å,  $V = 3942.20$  Å<sup>3</sup>. Characterized by powder X-ray diffraction data.

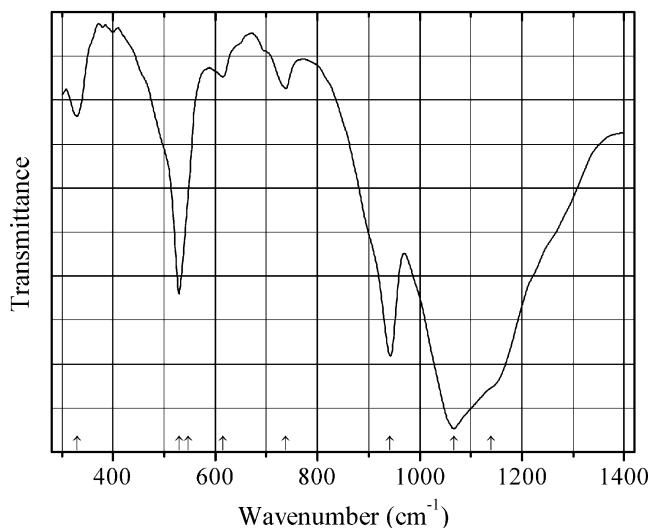
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Huang et al. (2009).

**Wavenumbers (cm<sup>-1</sup>):** 1151sh, 1130s, 1039s, 1000sh, 969s, 938s, 910sh, 608, 590, 551, 450sh, 415sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

#### P684 Cerium(IV) pyrophosphate $\text{CeP}_2\text{O}_7$



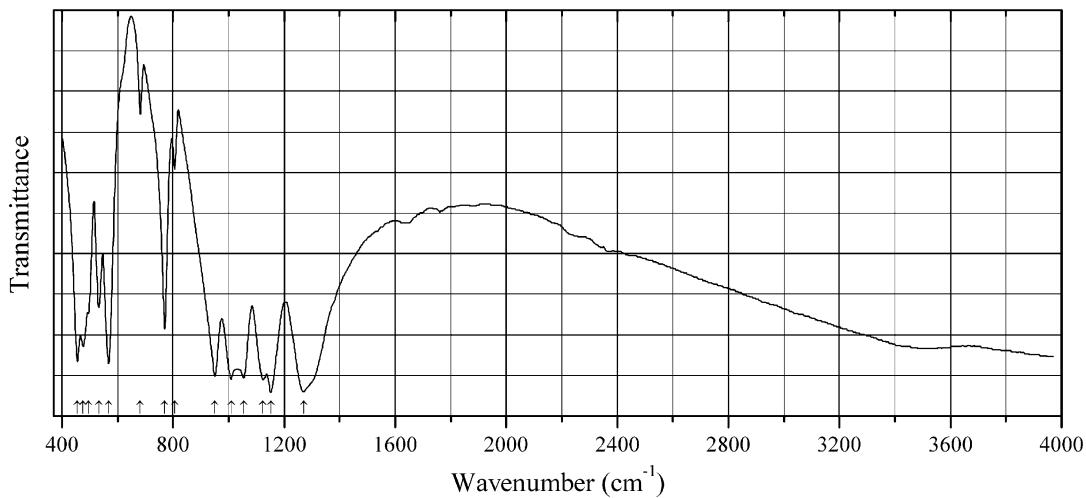
**Origin:** Synthetic.

**Description:** Obtained by adding aqueous solution of cerium(IV) sulfate to the solution of sodium pyrophosphate. Cubic,  $a = 8.607(4)$  Å. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 4.97 (30) (111), 4.31 (100) (200), 3.85 (15) (210), 3.51 (15) (211), 3.057 (28) (220), 2.599 (41) (311), 1.925 (17) (420).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Botto and Baran (1977).

**Wavenumbers (cm<sup>-1</sup>):** 1140sh, 1067s, 942s, 738w, 615w, 548sh, 530, 330.

**P685 Cerium(III) polyphosphate**  $\text{Ce}(\text{PO}_3)_3$ 

**Origin:** Synthetic.

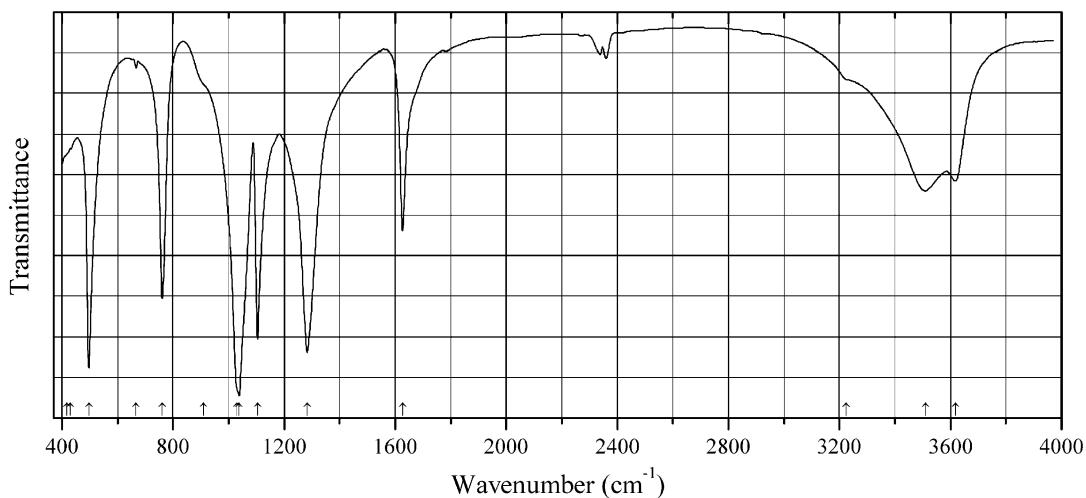
**Description:** Prepared from aqueous solutions of cerium(III) chloride and sodium cyclotriphosphate with subsequent annealing of the precipitate formed up to 1123 K. Orthorhombic, space group  $C222_1$ . The structure is based on infinite chains of  $\text{PO}_4$  tetrahedra.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Ternane et al. (2008).

**Wavenumbers (cm<sup>-1</sup>):** 1270s, 1152s, 1124s, 1055s, 1009s, 951s, 806, 770, 682w, 568, 532, 496, 476, 456.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**P686 Cerium metaphosphate trihydrate**  $\text{Ce}(\text{P}_3\text{O}_9)\cdot 3\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Prepared from aqueous solutions of cerium(III) chloride and sodium cyclotriphosphate. Hexagonal, space group  $P-6$ . The cyclotriphosphate anion  $P_3O_9^{3-}$  has a benitoite-type planar configuration.

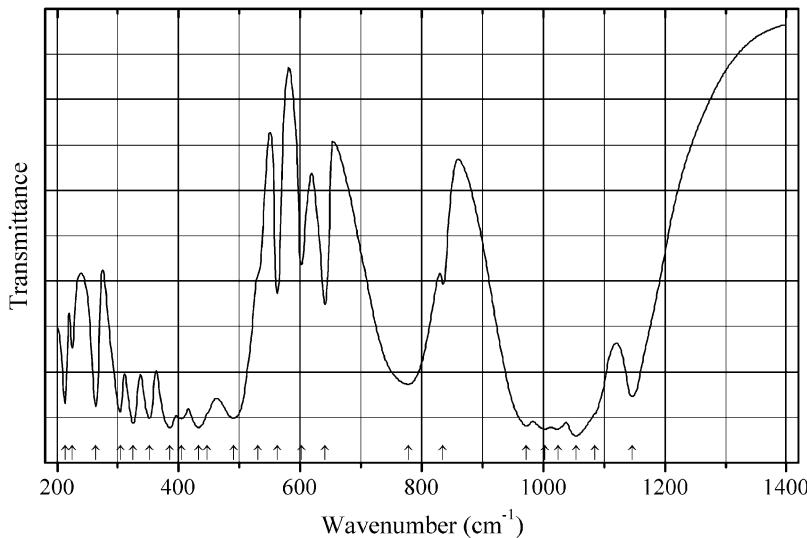
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Ternane et al. (2008).

**Wavenumbers (cm<sup>-1</sup>):** 3618, 3510, 3225sh, 1627, 1284s, 1105s, 1039s, 1029sh, 909sh, 761, (667w), 497s, 430sh, 417sh.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. Weak bands in the range from 2300 to 2400 cm<sup>-1</sup> and at 667 cm<sup>-1</sup> correspond to atmospheric CO<sub>2</sub>.

### P687 Copper tinanium oxyphosphate $\alpha\text{-CuTi}_2(\text{PO}_4)_2\text{O}_2$



**Origin:** Synthetic.

**Description:** Prepared by coprecipitation from aqueous solutions of Cu(NO<sub>3</sub>)<sub>2</sub>·3H<sub>2</sub>O and NH<sub>4</sub>(H<sub>2</sub>PO<sub>4</sub>) taken in stoichiometric quantities and ethanol solution of TiCl<sub>4</sub>. After evaporation of the solvent, the solid was stepwise heated up to 950 °C. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 7.5612(4)$ ,  $b = 7.0919(4)$ ,  $c = 7.4874(4)$  Å,  $\beta = 122.25(1)$ °,  $V = 339.55(6)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{meas}} = 3.71(2)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 3.729$  g/cm<sup>3</sup>. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 6.393 (30) (100), 4.746 (23) (110), 3.334 (27) (21–1), 3.307 (100) (11–2), 3.233 (49) (111), 3.198 (36) (200), 3.093 (40) (02–1), 2.585 (23) (22–1).

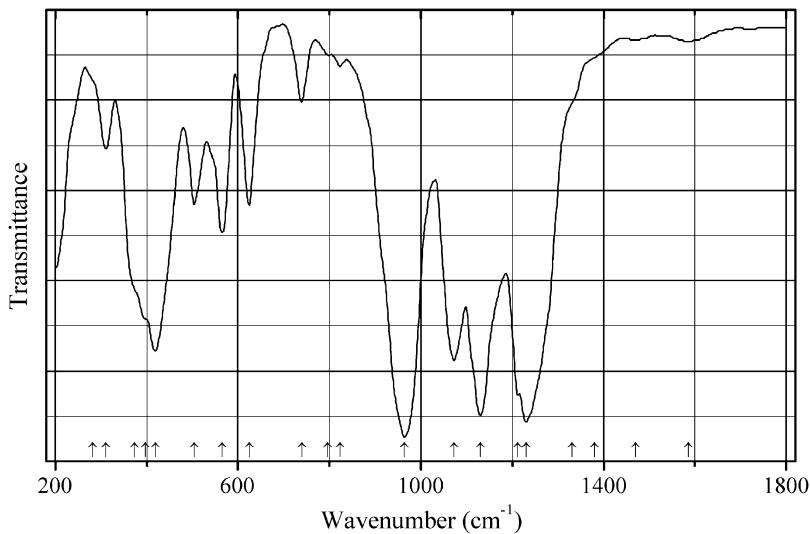
**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

**Source:** Benmokhtar et al. (2007a).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1146, 1085sh, 1054s, 1025s, 1003s, 972s, 835, 778, 641, 602, 562, 531sh, 490, 447sh, 433s, 405, 386s, 352, 325, 304, 264, 225, 213.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1119, 1069, 1057, 1036, 1026, 1007s, 986, 835, 732s, 571, 470, 445, 417, 392, 371, 353.

**P688  $\gamma$ -Vanadyl pyrophosphate  $\gamma$ -(VO)<sub>2</sub>(P<sub>2</sub>O<sub>7</sub>)**

**Origin:** Synthetic.

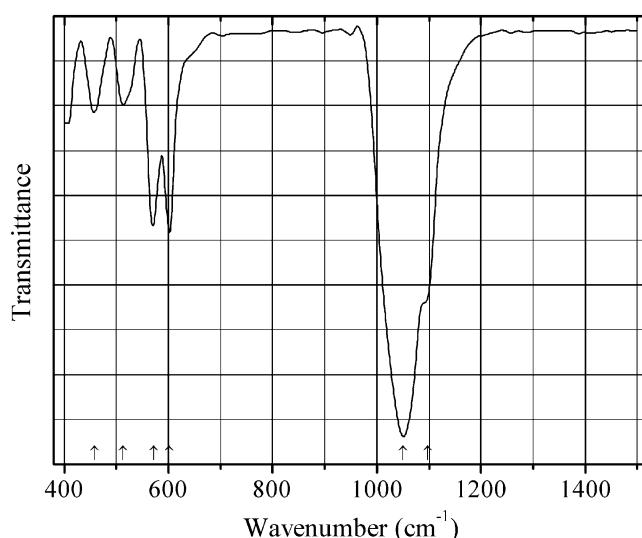
**Description:** Prepared by thermal decomposition of  $\gamma\text{-VOHPO}_4 \cdot 0.5\text{H}_2\text{O}$  at 750 °C for 3 h. Characterized by powder X-ray diffraction data. Orthorhombic, space group  $Pbc2_1$ ,  $a = 9.571$ ,  $b = 7.728$ ,  $c = 16.568$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Bordes et al. (1984).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1585w, 1471w, 1381sh, 1331sh, 1231s, 1213, 1130s, 1073, 964s, 824w, 797w, 740, 624, 565, 504, 419, 398sh, 373sh, 311, 282sh.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**P689 Lanthanum calcium oxophosphate LaCa<sub>4</sub>(PO<sub>4</sub>)<sub>3</sub>O**

**Origin:** Synthetic.

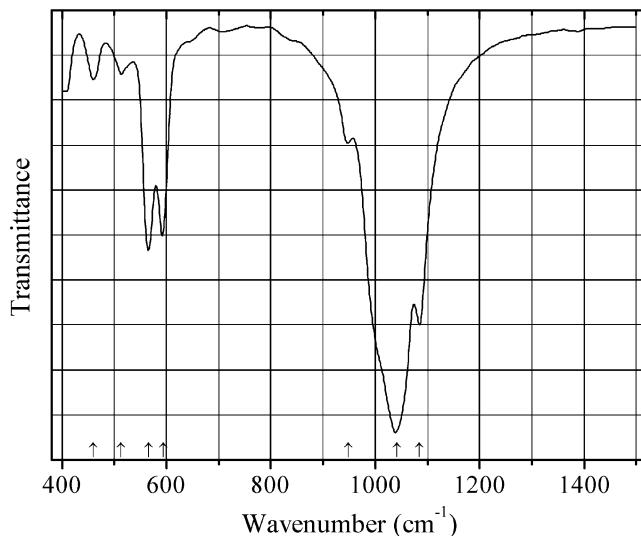
**Description:** Apatite-type compound synthesized by high-temperature solid-state reaction from a stoichiometric mixture of preheated  $\text{La}_2\text{O}_3$ ,  $\text{CaCO}_3$ , and  $(\text{NH}_4)(\text{H}_2\text{PO}_4)$ . Characterized by powder X-ray diffraction data. Hexagonal, space group  $P6_3$ ,  $a = 9.463(8)$ ,  $c = 6.92(1)$  Å,  $V = 536.64$  Å<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Buvaneswari and Varadaraju (2000).

**Wavenumbers (cm<sup>-1</sup>):** 1097sh, 1051s, 602, 572, 513, 459.

**P690 Lanthanum strontium oxophosphate**  $\text{LaSr}_4(\text{PO}_4)_3\text{O}$



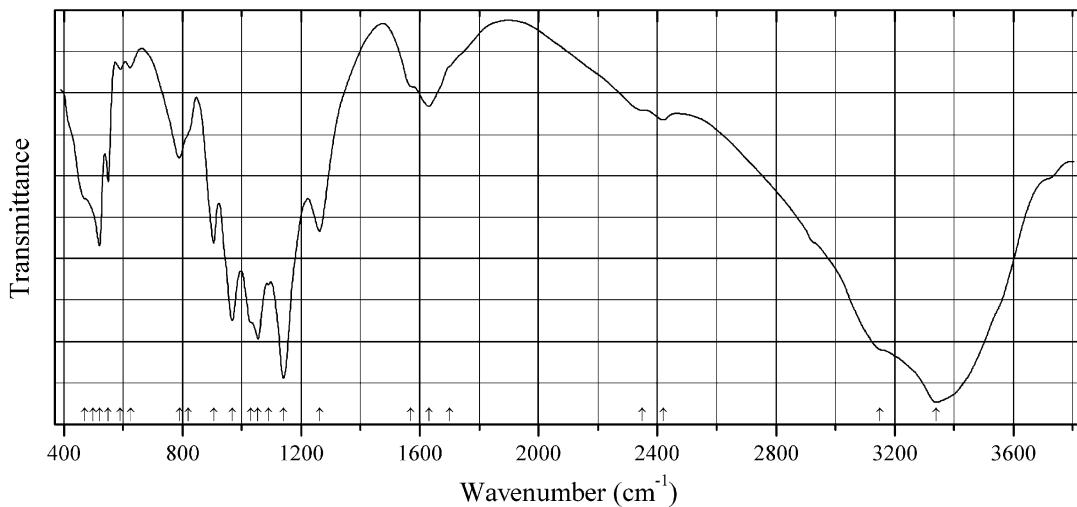
**Origin:** Synthetic.

**Description:** Apatite-type compound synthesized by high-temperature solid-state reaction from a stoichiometric mixture of preheated  $\text{La}_2\text{O}_3$ ,  $\text{SrCO}_3$ , and  $(\text{NH}_4)(\text{H}_2\text{PO}_4)$ . Characterized by powder X-ray diffraction data. Hexagonal, space group  $P6_3$ ,  $a = 9.71(1)$ ,  $c = 7.30(1)$  Å,  $V = 596.05$  Å<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Buvaneswari and Varadaraju (2000).

**Wavenumbers (cm<sup>-1</sup>):** 1085s, 1041s, 948sh, 591, 566, 513w, 460w.

**P691 Iron(II) acid phosphate hydrate  $\text{Fe}(\text{H}_2\text{PO}_4)_2 \cdot 2\text{H}_2\text{O}$** 

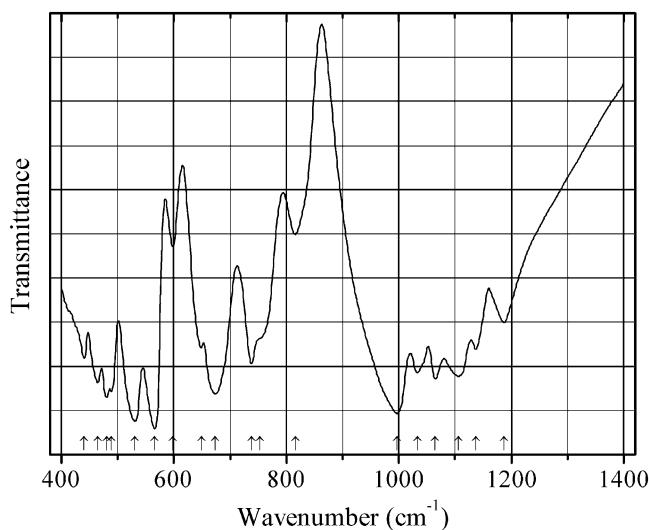
**Origin:** Synthetic.

**Description:** Synthesized from acidic phosphate solution containing 5–9 wt% FeO and 65 wt%  $\text{H}_3\text{PO}_4$  by a salting out procedure with ethyl alcohol. Monoclinic, space group  $P2_1/n$ ,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Koleva and Effenberger (2007).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3340s, 3150sh, 2420w, 2350w, 1700sh, 1630, 1568w, 1262, 1140s, 1090, 1055s, 1030sh, 968s, 905, 820, 790, 625w, 590w, 550, 520, 500, 470.

**P692 Lead beryllium phosphate hurlbutite-type  $\text{PbBe}_2(\text{PO}_4)_2$** 

**Origin:** Synthetic.

**Description:** Synthesized hydrothermally from BeO, H<sub>3</sub>PO<sub>4</sub> (85%), (NH<sub>4</sub>)(H<sub>2</sub>PO<sub>4</sub>), and Pb(NO<sub>3</sub>)<sub>2</sub> at 200 °C for 7 days. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 8.088(1)$ ,  $b = 9.019(1)$  Å,  $c = 8.391(1)$  Å,  $\beta = 90.12(1)^\circ$ ,  $V = 612.22(1)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 4.504$  g/cm<sup>3</sup>. Characterized by powder X-ray diffraction data.

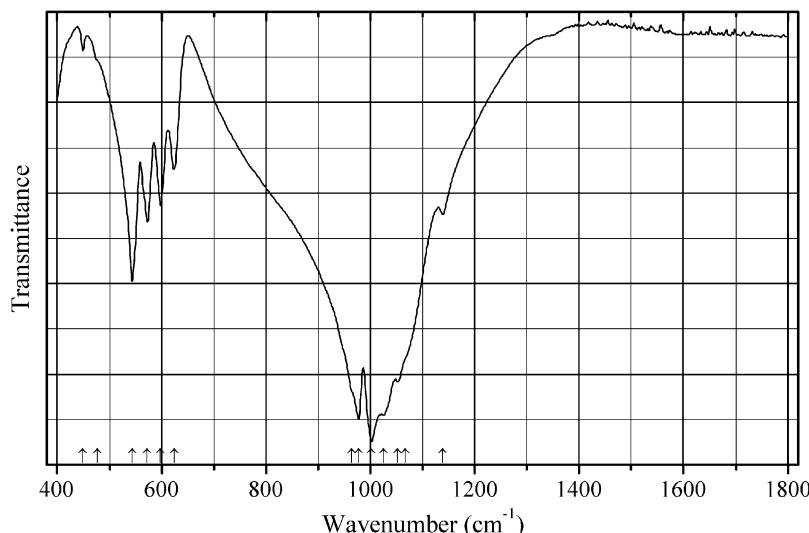
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Dal Bo et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 1187, 1137, 1106, 1065, 1033, 997s, 816, 753, 738, 674s, 649, 598, 566s, 531, 489, 481, 465, 441.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### P693 Lead iron(III) phosphate Pb<sub>3</sub>Fe<sub>2</sub>(PO<sub>4</sub>)<sub>4</sub>



**Origin:** Synthetic.

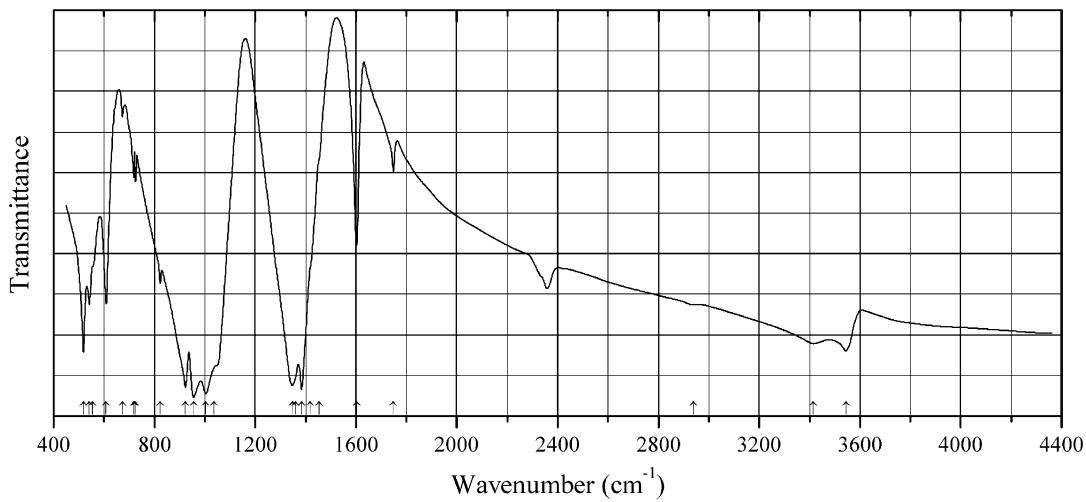
**Description:** Prepared from a stoichiometric mixture of Fe<sub>2</sub>O<sub>3</sub>, PbCO<sub>3</sub>, and (NH<sub>4</sub>)(H<sub>2</sub>PO<sub>4</sub>) by a ceramic technique. Characterized by elemental analysis, powder X-ray diffraction data, and Mössbauer spectrum. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 9.0065(6)$ ,  $b = 9.0574(6)$ ,  $c = 9.3057(6)$  Å,  $\beta = 116.880(4)^\circ$ ,  $V = 677.10(8)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 5.412$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Malakho et al. (2005).

**Wavenumbers (cm<sup>-1</sup>):** 1139, 1067sh, 1052s, 1025s, 1002s, 978s, 965sh, 624, 598, 573, 544, 477sh, 449w.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**P694 Lead phosphate nitrate hydrate  $\text{Pb}_2(\text{NO}_3)(\text{PO}_4) \cdot \text{H}_2\text{O}$** 

**Origin:** Synthetic.

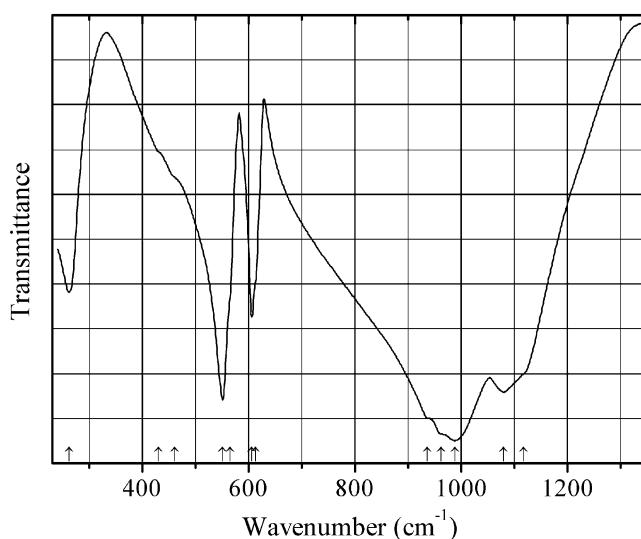
**Description:** Crystals grown by a sol-gel method in the presence of sodium metasilicate. Monoclinic, space group  $P2_1/c$ ,  $a = 19.511$ ,  $b = 7.37$ ,  $c = 10.994$  Å,  $\beta = 113^\circ$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission. **Source:** Vivekanandan et al. (1995).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3544, 3415, 2940sh, 1748w, 1603, 1453sh, 1419sh, 1384s, 1359sh, 1348s, 1037sh, 1004s, 955s, 923s, 823, 725w, 718w, 673, 608, 556sh, 542, 518.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 3500, 1653w, 1620w, 1370w, 1353, 1062s, 1044w, 1016s, 967, 947, 733, 722w, 617, 574w, 535w, 444w, 415, 392w, 239, 205w, 144, 125s, 96s, 75, 66.

**P695 Lead phosphate sulfate  $\text{Pb}_4(\text{PO}_4)_2(\text{SO}_4)$** 

**Origin:** Synthetic.

**Description:** Prepared by a solid-state reaction from a stoichiometric mixture of  $\text{Pb}_3(\text{CO}_3)_2(\text{OH})_2$ ,  $(\text{NH}_4)_2(\text{SO}_4)$ , and  $(\text{NH}_4)_2(\text{HPO}_4)$  in air at  $700^\circ\text{C}$  for several days. Cubic, space group  $I43d$ ,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

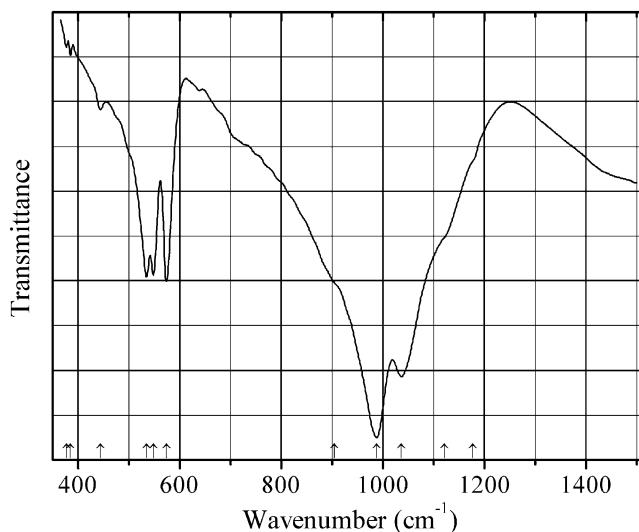
**Source:** Massaferro et al. (1999).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1118sh, 1080s, 989s, 936sh, 613sh, 606, 565sh, 551, 460sh, 430sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1120, 1085, 987s, 963sh, 944s, 609, 551, 459, 440, 430, 262.

### P696 Lead silver phosphate apatite-type $\text{Pb}_4\text{Ag}(\text{PO}_4)_3$



**Origin:** Synthetic.

**Description:** Prepared hydrothermally from a stoichiometric mixture of  $\text{Pb}_3(\text{PO}_4)_2$  and  $\text{Ag}_3(\text{PO}_4)$  at  $215^\circ\text{C}$  for 1 day. Hexagonal, space group  $P6_3/m$ ,  $a = 9.772(4)$ ,  $c = 7.210(3)$  Å. In the apatite-type structure,  $\text{Ag}^+$  ions concentrate in the column positions. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 4.238 (53) (200), 4.051 (53) (111), 3.202 (52) (210), 2.926 (100) (211), 2.904 (71) (112), 2.823 (72) (300).

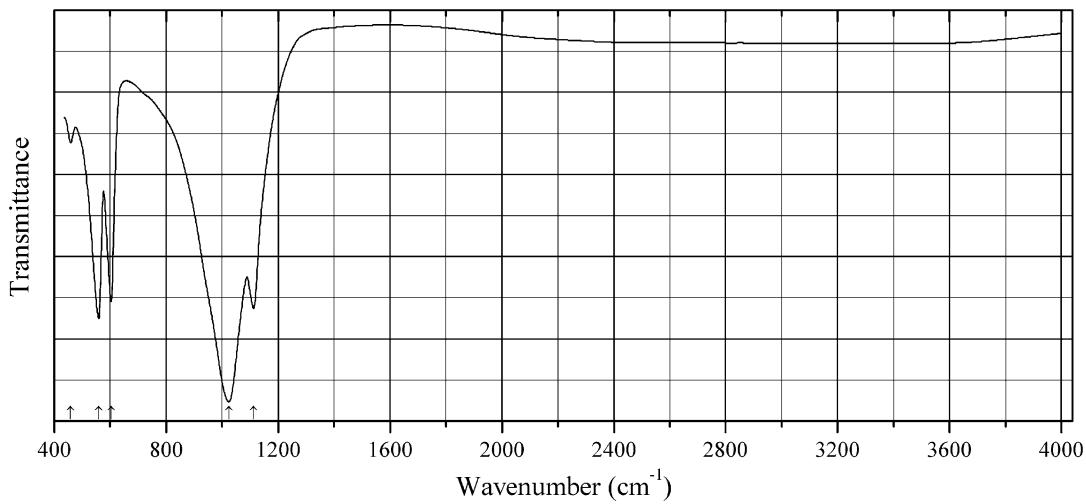
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Ternane et al. (2000).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1178sh, 1121sh, 1037s, 988s, 907sh, 574, 548, 535, 444w, 385w, 377w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1017, 963s, 933s, 577s, 558, 421, 388.

**P697 Lead sodium calcium phosphate apatite-type  $\text{Pb}_3\text{CaNa}(\text{PO}_4)_3$** 

**Origin:** Synthetic.

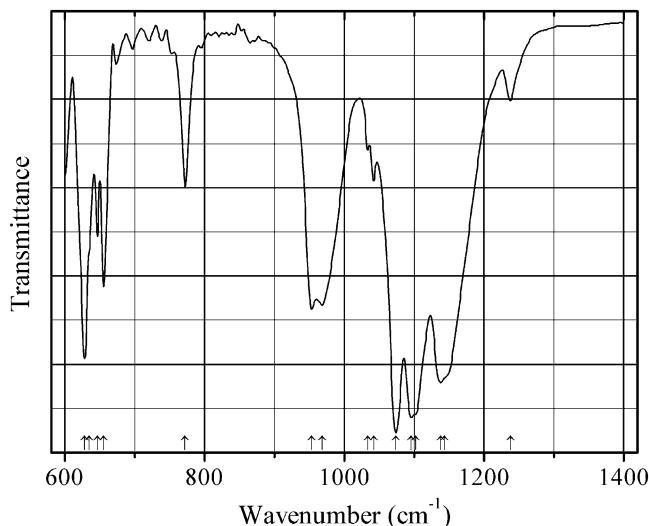
**Description:** Prepared by a solid-state reaction from a mixture of  $\text{Na}_2\text{CO}_3$ ,  $(\text{NH}_4)_2(\text{HPO}_4)$ ,  $\text{CaCO}_3$ , and  $\text{PbO}$  powders heated at 1073 K in air for 12 h and at 1173 K for 12 h. Characterized by powder X-ray diffraction data and chemical analysis. Hexagonal, space group  $P6_3/m$ ,  $a = 9.658(8)$ ,  $c = 7.081(6)$  Å,  $V = 572.01(8)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 5.63$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Naddari et al. (2003).

**Wavenumbers (cm<sup>-1</sup>):** 1113, 1024s, 604, 559, 459w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**P698 Lithium chromium pyrophosphate  $\text{LiCrP}_2\text{O}_7$** 

**Origin:** Synthetic.

**Description:** Prepared by solid-state reaction from a stoichiometric mixture of  $\text{Li}(\text{H}_2\text{PO}_4)$ ,  $\text{NH}_4(\text{H}_2\text{PO}_4)$ , and  $\text{CrCl}_3 \cdot 6\text{H}_2\text{O}$ , first at  $200^\circ\text{C}$  for 5 h, then at  $700^\circ\text{C}$  for 20 h, and finally at  $950^\circ\text{C}$  for 20 h with intermediate grindings and pelletizing. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2_1$ ,  $a = 4.7867(7)$ ,  $b = 8.0049(11)$ ,  $c = 6.9093(10)$  Å,  $\beta = 109.003(2)^\circ$ ,  $V = 250.32(6)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{calc}} = 3.090$  g/cm $^3$ .

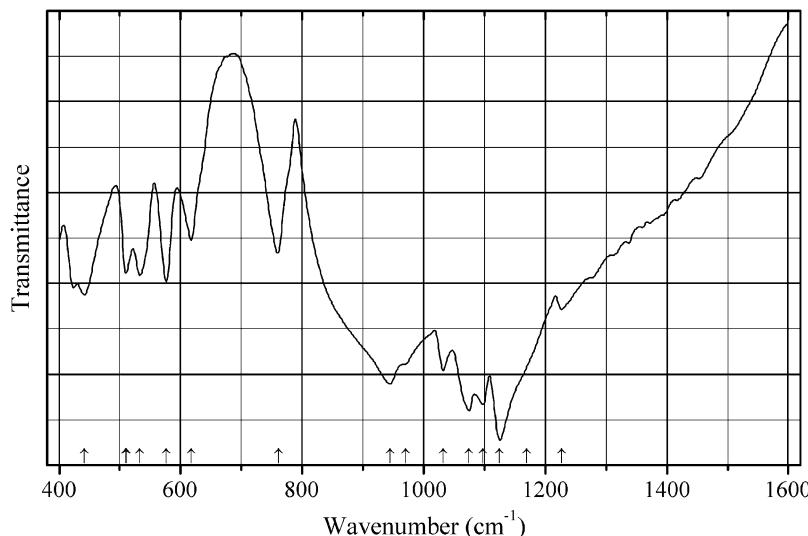
**Kind of sample preparation and/or method of registration of the spectrum:** The spectrum was recorded using a Pike MIRacle micrometer pressure clamp.

**Source:** Pachoud et al. (2013).

**Wavenumbers (cm $^{-1}$ ):** 1238w, 1144sh, 1138s, 1102sh, 1096s, 1074s, 1042w, 1034w, 968, 953, 772, 655, 646, 634sh, 628s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### P699 Lithiumiron(III) pyrophosphate $\text{LiFe}^{3+}(\text{P}_2\text{O}_7)$



**Origin:** Synthetic.

**Description:** Obtained from Li and Fe nitrates, and  $(\text{NH}_4)_2(\text{HPO}_4)$  by the co-precipitation method with subsequent heating of the obtained precipitate up to  $750^\circ\text{C}$  with several intermediate grindings. Monoclinic space group  $P2_1$ ,  $Z = 4$ .

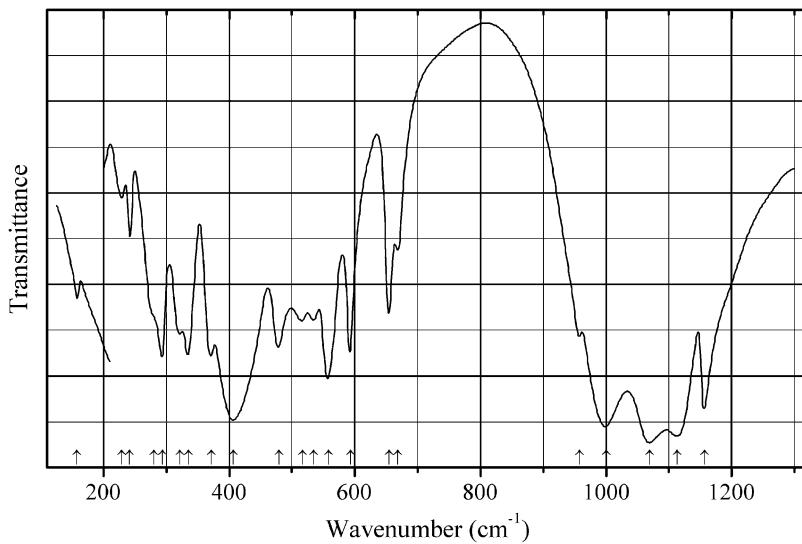
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Parajón-Costa et al. (2013).

**Wavenumbers (IR, cm $^{-1}$ ):** 1227, 1170sh, 1125s, 1098s, 1075s, 1032, 970sh, 945s, 761, 618, 577, 533, 510, 442.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 1122s, 1105s, 1073s, 1037, 975, 941, 767, 761, 618, 559, 537, 520, 512, 448, 427, 415.

**P700 Lithium magnesium phosphate olivine-type  $\text{LiMg}(\text{PO}_4)$** 

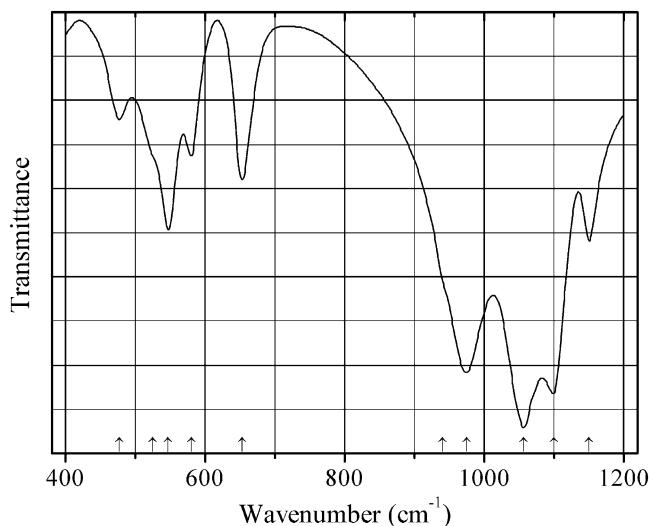
**Origin:** Synthetic.

**Description:** White solid synthesized by solid-state reaction between  $\text{Li}_2\text{CO}_3$ ,  $\text{MgO}$ , and  $(\text{NH}_4)_2(\text{HPO}_4)$  at 800 °C for 4 days. Orthorhombic, space group  $Pnma$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KI and polyethylene discs. Transmission.

**Source:** Paques-Ledent and Tarte (1974).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1157s, 1113s, 1070s, 1000s, 958, 669, 655, 593, 558s, 535, 517, 479, 407s, 372, 335, 322, 294, 280, 242, 229w, 158w.

**P701 Lithium nickel phosphate triphylite-type  $\text{LiNi}(\text{PO}_4)$** 

**Origin:** Synthetic.

**Description:** Synthesized by a solid-state reaction technique from the stoichiometric mixture of  $\text{Li}_2\text{CO}_3$ ,  $(\text{NH}_4)_2(\text{HPO}_4)$ , and  $\text{NiO}$  at 773 K for 48 h. Characterized by powder X-ray diffraction data. Orthorhombic, space group  $Pnma$ ,  $a = 10.0252(7)$ ,  $b = 5.8569(5)$ ,  $c = 4.6758(4)$  Å,  $V = 274.546$  Å<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** Absorption. Kind of sample preparation is not indicated.

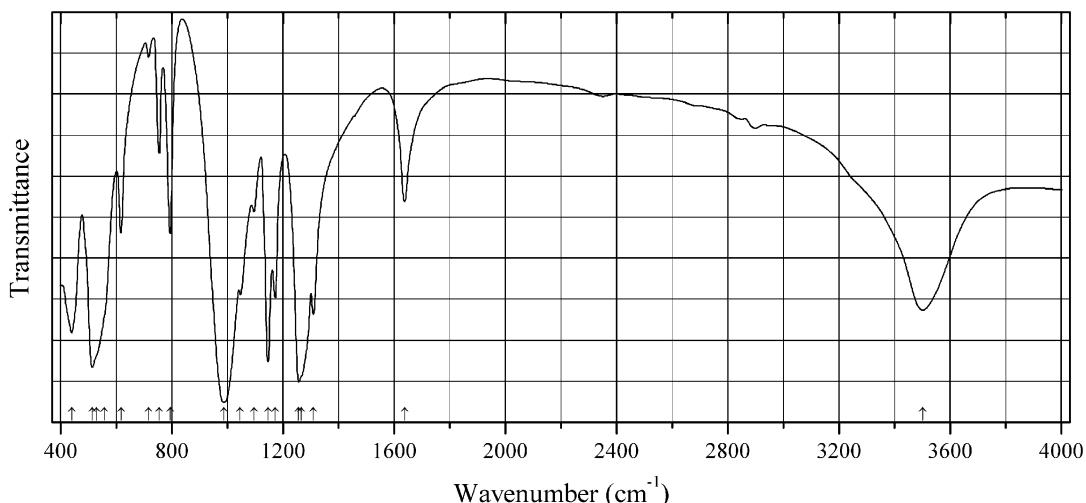
**Source:** Bechir et al. (2014).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1150, 1100s, 1057s, 975, 940sh, 653, 580, 547, 525sh, 477.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1085, 1070, 1009s, 946s, 637, 597w, 590, 575w, 460w, 320w, 300, 280, 252w, 233w, 170, 165, 116w.

#### P702 Lithium cyclo-hexaphosphate trihydrate $\text{Li}_6\text{P}_6\text{O}_{18} \cdot 3\text{H}_2\text{O}$



**Origin:** Synthetic.

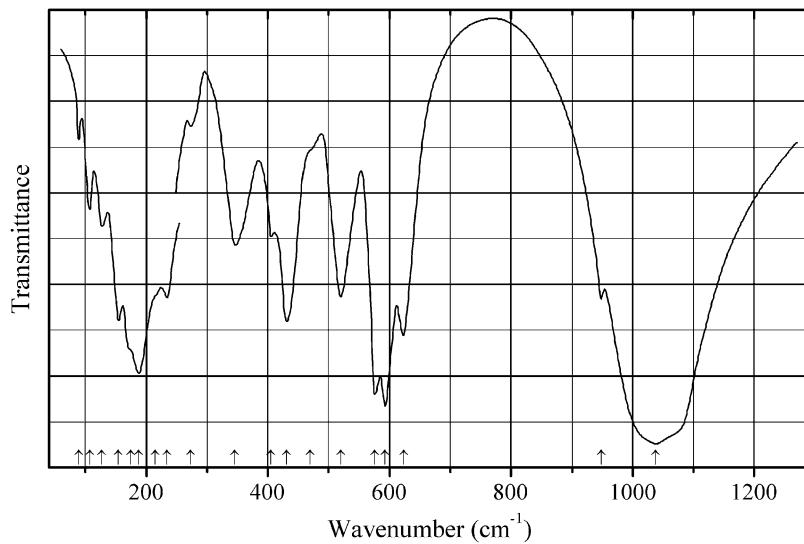
**Description:** Acicular crystals grown by a hydrothermal method from the solution of  $\text{Li}_6\text{P}_6\text{O}_{18} \cdot 6\text{H}_2\text{O}$  in the methanol-water (2:1 vol.) mixture. Trigonal, space group  $R-3m$ ,  $a = 15.7442(2)$ ,  $c = 12.5486$  (2) Å,  $V = 2693.8$  Å<sup>3</sup>,  $Z = 6$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Houlbert et al. (2004), Toumi et al. (1998).

**Wavenumbers (cm<sup>-1</sup>):** 3501, 1637, 1309, 1267sh, 1257s, 1173, 1146, 1096, 1047, 987s, 794, 755, 716w, 617, 558sh, 530sh, 514, 440.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**P703 Lithium strontium orthophosphate LiSr(PO<sub>4</sub>)**

**Origin:** Synthetic.

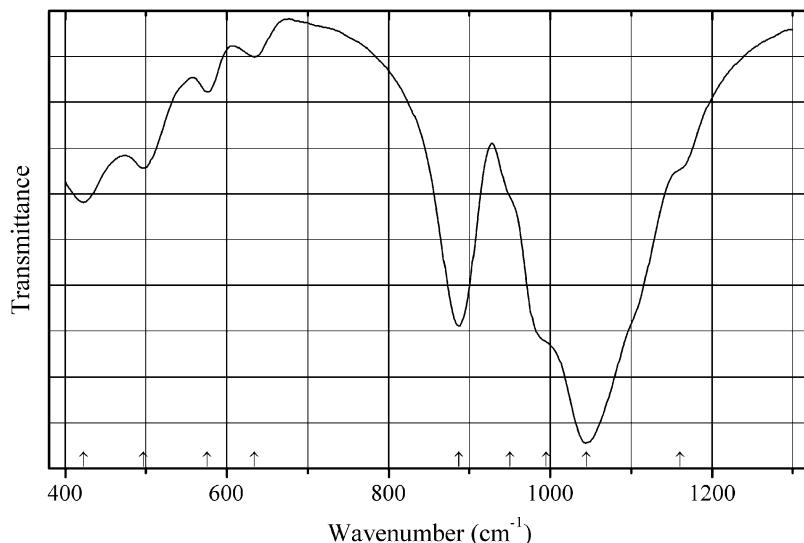
**Description:** Synthesized by a solid-state reaction between Li<sub>2</sub>CO<sub>3</sub>, SrCO<sub>3</sub>, and (NH<sub>4</sub>)<sub>2</sub>(HPO<sub>4</sub>) at 950 °C for 1 week, with several intermediate mixings and grindings. Characterized by powder X-ray diffraction data. Monoclinic (?). Structurally related to RbLi(SO<sub>4</sub>).

**Kind of sample preparation and/or method of registration of the spectrum:** Pressed discs. Transmission.

**Source:** Paques-Ledent (1978).

**Wavenumbers (cm<sup>-1</sup>):** 1038s, 948, 623, 593s, 576s, 520, 469sh, 431, 405, 346, 273w, 234, 215sh, 188s, 174sh, 154, 127, 107, 89w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**P704 Lithium vanadyl phosphate  $\alpha$ -Li(VO)(PO<sub>4</sub>)**

**Origin:** Synthetic.

**Description:** Synthesized from  $V_2O_5$ ,  $LiOH$ , and  $H_3PO_4$  in the ratio  $Li:V:P = 5:1:5$  via intermediate vanadyl oxalate by a microwave-assisted solvothermal method. Characterized by powder X-ray diffraction data. Triclinic,  $a = 6.7872(3)$ ,  $b = 7.2152(2)$ ,  $c = 7.8861(3)$  Å,  $\alpha = 89.904(2)^\circ$ ,  $\beta = 88.578(2)^\circ$ ,  $\gamma = 62.835(3)^\circ$ ,  $V = 343.46(2)$  Å<sup>3</sup>.

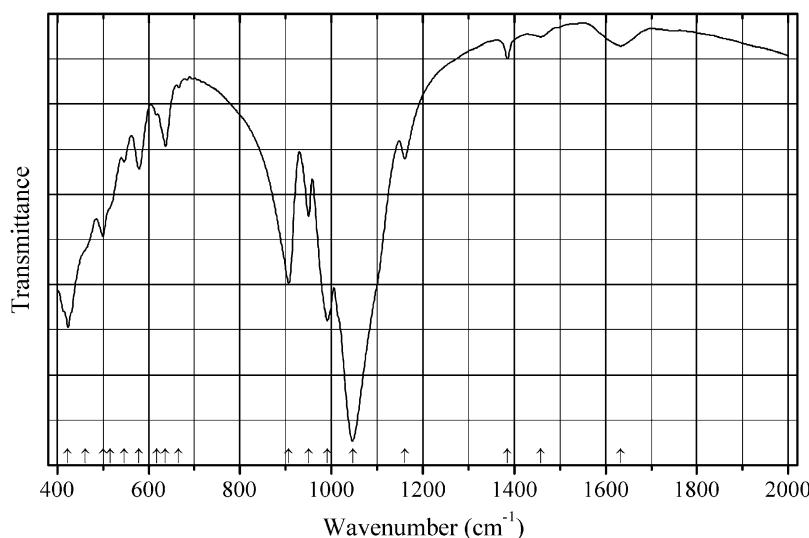
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Harrison and Manthiram (2013).

**Wavenumbers (cm<sup>-1</sup>):** 1160sh, 1045s, 995sh, 950sh, 887s, 634w, 576w, 497, 423.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

#### P705 Lithium vanadyl phosphate $Li(VO)(PO_4)$



**Origin:** Synthetic.

**Description:** Synthesized using  $LiAc \cdot 2H_2O$ ,  $V_2O_5$ ,  $(NH_4)(H_2PO_4)$ , and citric acid as the starting reagents. After evaporation the solvent, the product was sintered at 600 °C. Characterized by powder X-ray diffraction data. Triclinic,  $a = 6.731(5)$ ,  $b = 7.202(4)$ ,  $c = 7.923(2)$  Å,  $\alpha = 89.859(8)^\circ$ ,  $\beta = 91.261(5)^\circ$ ,  $\gamma = 116.891(10)^\circ$ ,  $V = 342.507$  Å<sup>3</sup>,  $Z = 4$ .

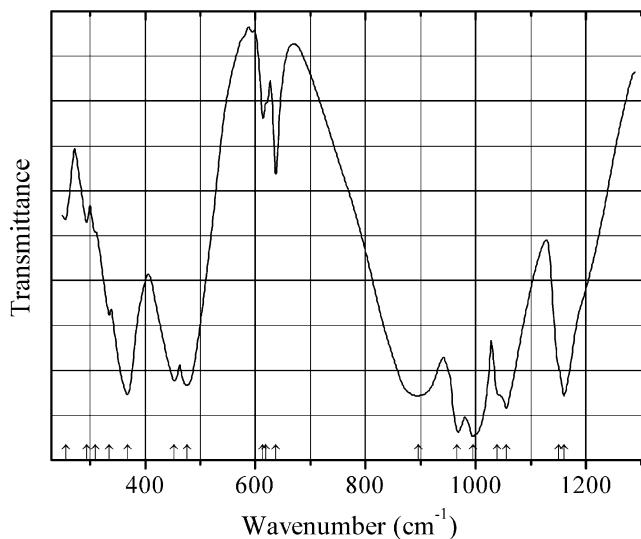
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Yang et al. (2008b).

**Wavenumbers (cm<sup>-1</sup>):** 1633w, 1458w, 1385w, 1161, 1047s, 991s, 950, 907s, 666, 637, 617, 579, 546, 516sh, 500, 461sh, 423s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The band at 1385 cm<sup>-1</sup> may correspond to  $NO_3^-$  admixture in KBr. The band at 1633 cm<sup>-1</sup> corresponds to adsorbed (?) water.

## P706 Lithium vanadyl phosphate $\beta$ -LiVOPO<sub>4</sub>



**Origin:** Synthetic.

**Description:** Prepared by a hydrothermal method. Characterized by powder X-ray diffraction data.

Orthorhombic, space group  $Pnma$ ,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Baran et al. (1994).

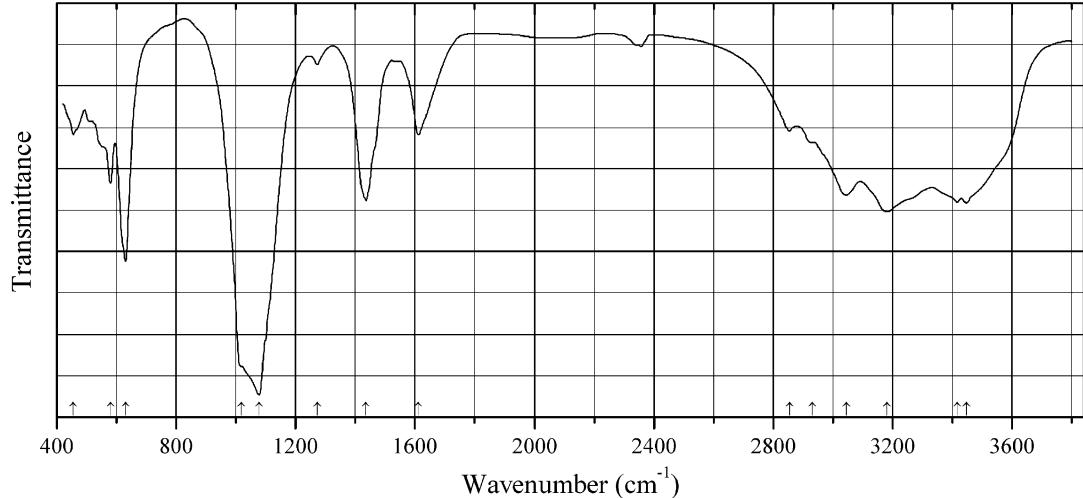
### Wavenumbers (IR, $\text{cm}^{-1}$ ):

Note: In the cited paper, Raman spectrum is given.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1104, 1077, 1062, 1025, 1005, 979, 936, 884s, 629, 468, 429, 363, 332, 322, 310, 266, 250.

## P707 Lithium zinc phosphate monohydrate $\alpha$ -LiZn(PO<sub>4</sub>)·H<sub>2</sub>O



**Origin:** Synthetic.

**Description:** Prepared from  $\text{LiH}_2(\text{PO}_4) \cdot \text{H}_2\text{O}$  and  $\text{ZnSO}_4 \cdot 7\text{H}_2\text{O}$  in the presence of  $(\text{NH}_4)(\text{HCO}_3)$  and polyethylene glycol. Characterized by powder X-ray diffraction data. Orthorhombic,  $a = 10.51848$  (8),  $b = 8.12715(6)$ ,  $c = 5.02215(5)$  Å.

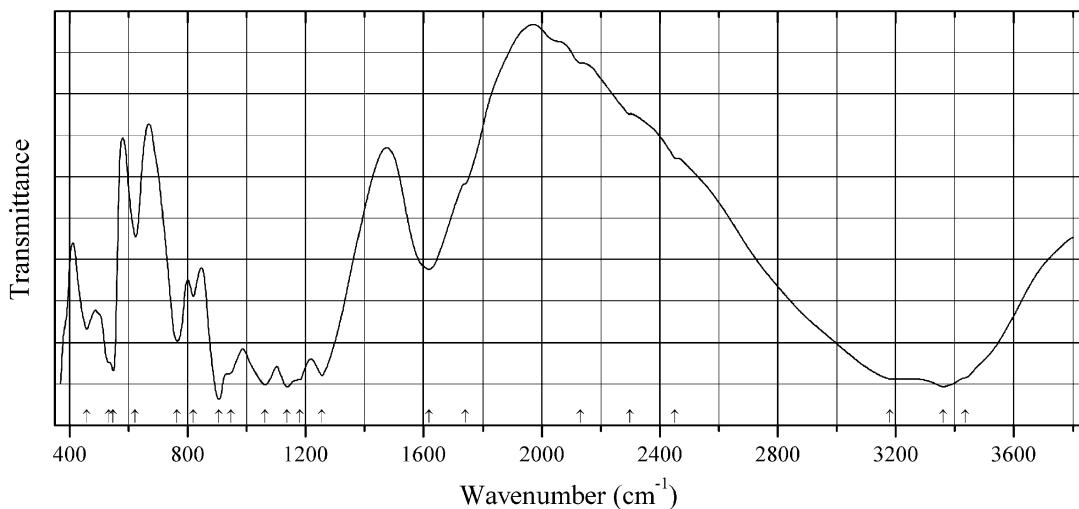
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Liao et al. (2009).

**Wavenumbers (cm<sup>-1</sup>):** 3447, 3417, 3182, 3045, 2932sh, 2854w, 1612, 1436, 1272w, 1079s, 1018, 630s, 580, 455.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, the wavenumber 455 cm<sup>-1</sup> is erroneously indicated as 415 cm<sup>-1</sup>. The bands in the range from 2800 to 3000 cm<sup>-1</sup> correspond to the admixture of an organic substance. The band at 1436 cm<sup>-1</sup> may correspond to a carbonate.

### P708 Magnesium acid phosphate hydrate $\text{Mg}(\text{H}_2\text{PO}_4)_2 \cdot 2\text{H}_2\text{O}$



**Origin:** Synthetic.

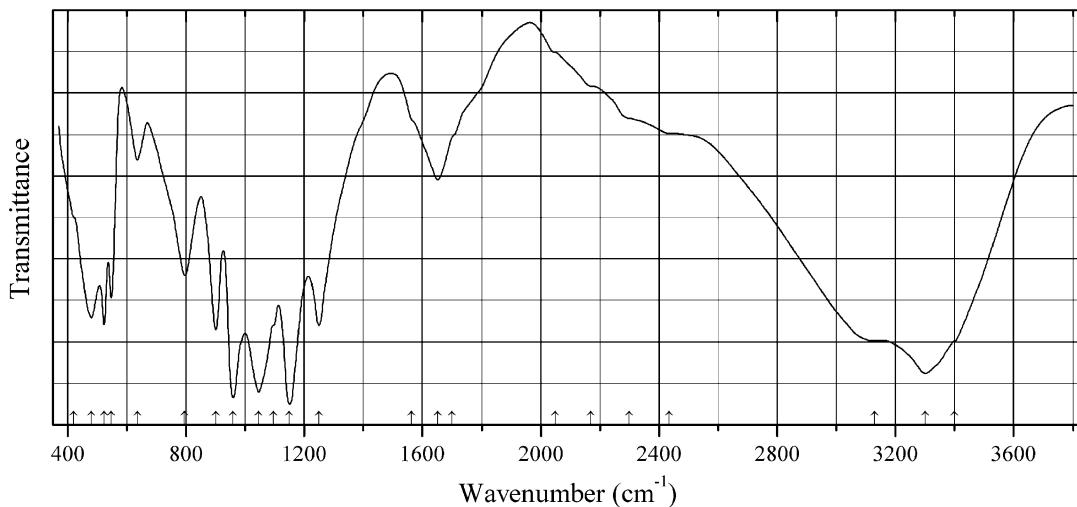
**Description:** Obtained by salting out with acetone from MgO solution in 65 wt%  $\text{H}_3\text{PO}_4$ . Monoclinic, space group  $P2_1/n$ ,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Koleva and Effenberger (2007).

**Wavenumbers (cm<sup>-1</sup>):** 3435sh, 3360, (3180sh), 2450w, 2300w, 2130w, 1740sh, 1618, 1256s, 1180s, 1138s, 1063s, 946sh, 906s, 820, 765, 623, 548, 533sh, 458.

**Note:** Unlike structurally investigated Ni, Zn, and Cd analogues (Koleva and Effenberger 2007), bands of acid OH groups in the range 2200–2500 cm<sup>-1</sup> are anomalously weak.

**P709 Manganese acid phosphate hydrate  $Mn(H_2PO_4)_2 \cdot 2H_2O$** 

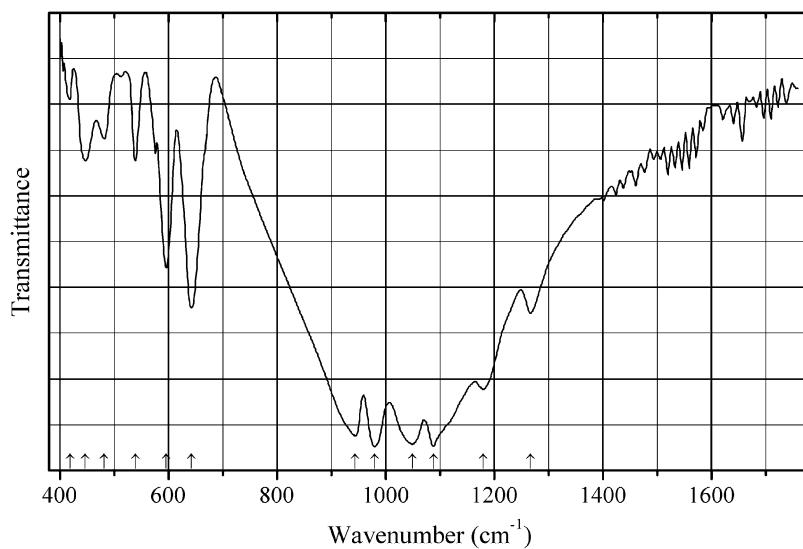
**Origin:** Synthetic.

**Description:** Obtained by salting out with acetone from MnO solution in 65 wt% H<sub>3</sub>PO<sub>4</sub>. Monoclinic, space group  $P2_1/n$ ,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Koleva and Effenberger (2007).

**Wavenumbers (cm<sup>-1</sup>):** 3400sh, 3300s, 3130sh, 2435sh, 2300sh, 2170w, 2050w, 1700sh, 1652, 1562sh, 1250, 1150s, 1095sh, 1046s, 960s, 900, 795, 637w, 547, 523, 480, 420.

**P710 Manganese(II) titanium orthophosphate  $MnTi_4(PO_4)_6$** 

**Origin:** Synthetic.

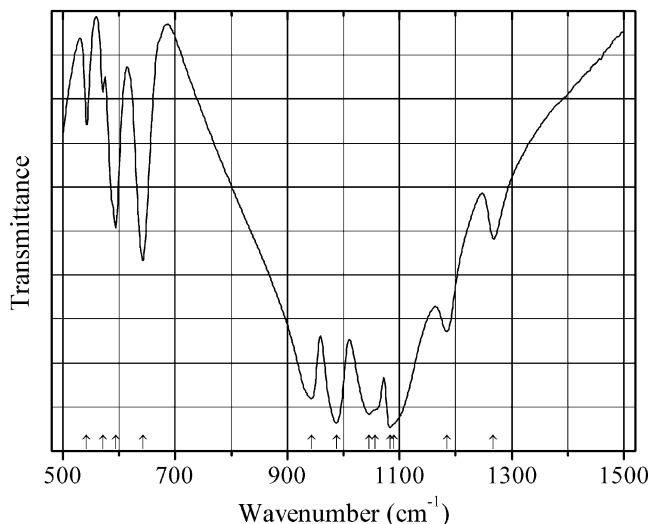
**Description:** Orange crystals obtained hydrothermally from  $\text{TiCl}_4$ , Mn, and  $\text{H}_3\text{PO}_4$  in the presence of  $\text{H}_2\text{O}_2$ , at 250 °C for 20 days. The crystal structure is solved. Hexagonal, space group *R*-3,  $a = 8.51300(10)$ ,  $c = 21.0083(3)$  Å,  $V = 1318.52(3)$  Å<sup>3</sup>,  $Z = 6$ .  $D_{\text{meas}} = 2.39(3)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 3.083$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Essehli et al. (2009).

**Wavenumbers (cm<sup>-1</sup>):** 1267, 1180, 1089s, 1049s, 980s, 944s, 642, 596, 539w, 482, 447w, 419.

### P711 Manganese(II) titanium phosphate $\text{MnTi}_4(\text{PO}_4)_6$ $\text{MnTi}_4(\text{PO}_4)_6$



**Origin:** Synthetic.

**Description:** Prepared from the stoichiometric mixture of  $\text{MnCO}_3$ ,  $\text{TiO}_2$ , and  $(\text{NH}_4)(\text{H}_2\text{PO}_4)$  using a solid-state reaction technique. Characterized by powder X-ray diffraction data. Hexagonal, space group *R*-3.

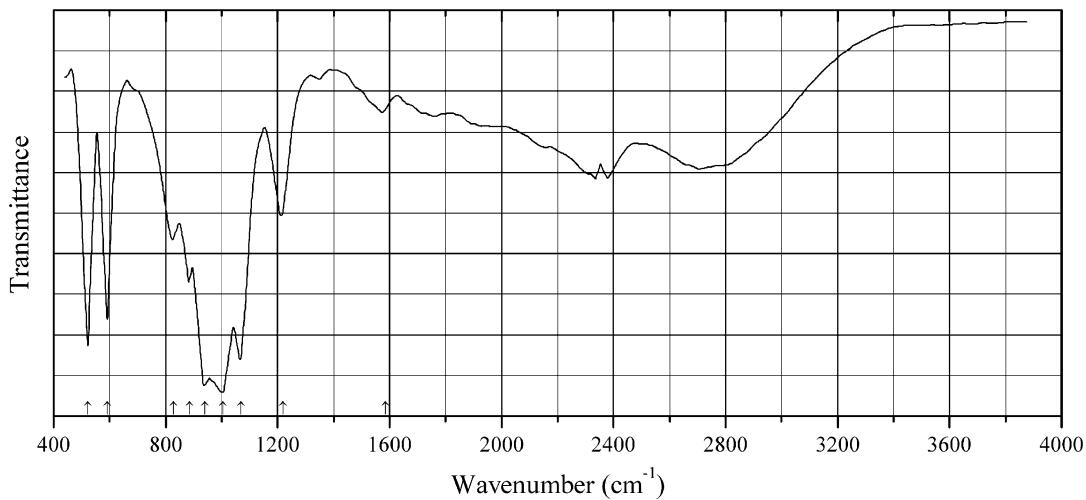
**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

**Source:** Pikl et al. (1998).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1267, 1185, 1090sh, 1083s, 1057sh, 1046s, 988s, 944s, 643, 594, 571w, 542, 441, 382, 360, 319s, 283w, 264w, 255w, 186w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1221w, 1091, 1083, 1050, 1034s, 1005, 976s, 939s, 696, 654, 604, 537, 454, 445, 438, 358, 350, 313, 285, 271, 259, 241, 199w.

**P712 Mercury(I) acid phosphate** ( $\text{Hg}_2\text{)(H}_2\text{PO}_4\text{)(PO}_4$ )

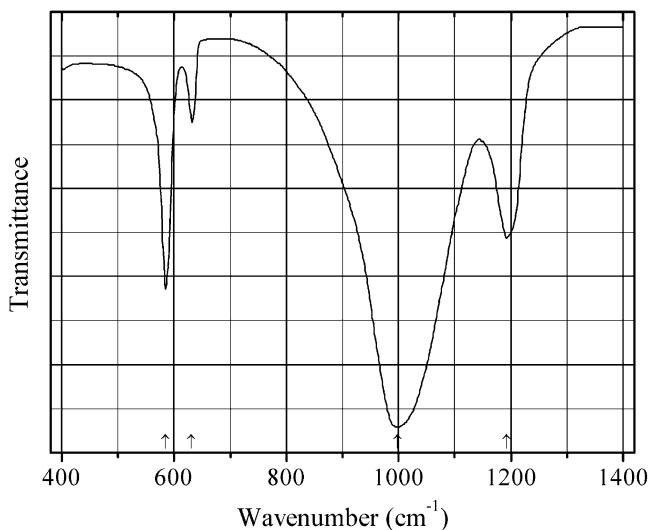
**Origin:** Synthetic.

**Description:** White precipitate obtained by adding a solution of  $\text{Hg}_2(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$  with minor  $\text{HNO}_3$  to excess of diluted orthophosphoric acid. The crystal structure is solved. Monoclinic, space group  $C2/c$ ,  $a = 9.597(2)$ ,  $b = 12.673(2)$ ,  $c = 7.976(1)$  Å,  $\beta = 110.91(1)^\circ$ ,  $V = 906.2(2)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 7.296$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Weil (2000).

**Wavenumbers (cm<sup>-1</sup>):** 1585w, 1218, 1069s, 1005s, 940s, 886, 829, 592s, 523s.

**P713 Molybdyl phosphate**  $\alpha\text{-}(\text{MoO})(\text{PO}_4)$ 

**Origin:** Synthetic.

**Description:** Obtained from the melt prepared from ammonium paramolybdate and H<sub>3</sub>PO<sub>4</sub> at 950 °C. Tetragonal, space group *P4/n*, *Z* = 2.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

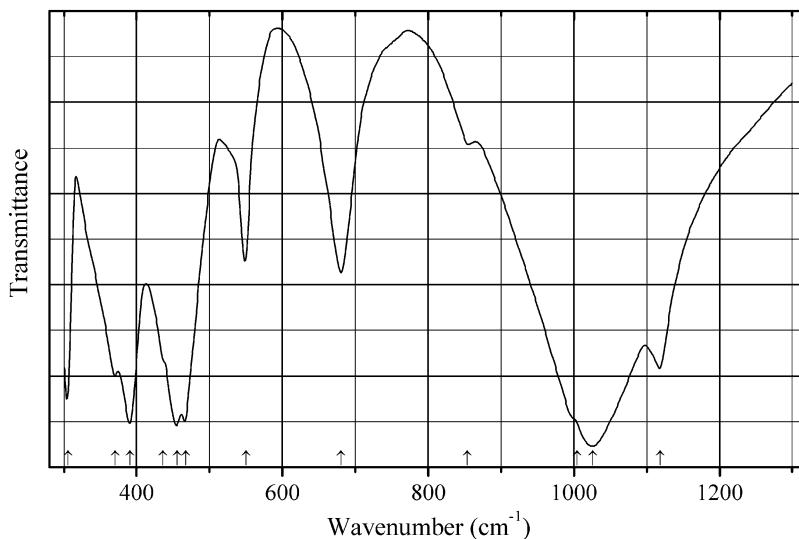
**Source:** Stranford and Condrate Sr (1984b).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1193, 998s, 631w, 585.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1079, 1013s, 947s, 621, 607, 447, 361, 292.

#### P714 Nickel vanadyl phosphate hydrate Ni(VO)(PO<sub>4</sub>)<sub>2</sub>·4H<sub>2</sub>O



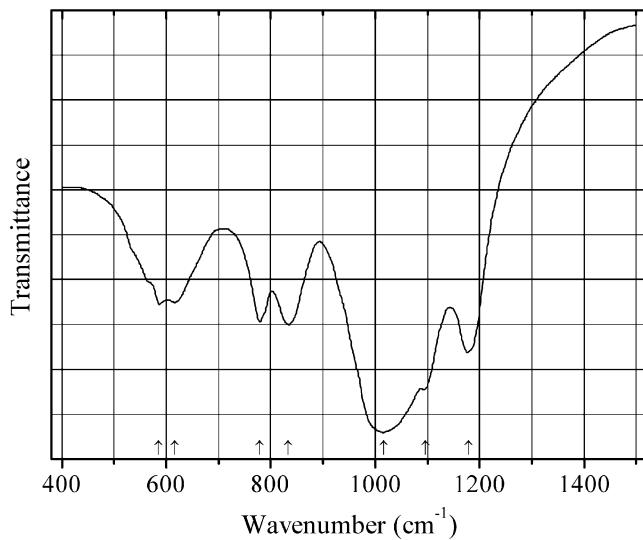
**Origin:** Synthetic.

**Description:** Tetragonal. The structure is based on VPO<sub>5</sub> layers linked by NiO<sub>6</sub> octahedra. V has fivefold coordination.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Baran et al. (1995).

**Wavenumbers (cm<sup>-1</sup>):** 3505sh, 3347, 3302s, 3070sh, 1687, 1558w, 1119, 1026s, 1005sh, 854w, 681, 550, 467s, 455s, 436sh, 391s, 370, 306, 289, 255, 227, 190.

**P715 Niobylphosphate  $\beta$ -(NbO)(PO<sub>4</sub>)**

**Origin:** Synthetic.

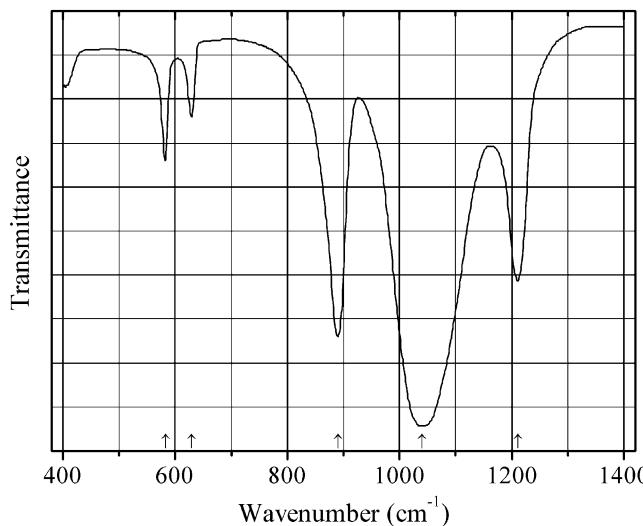
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Stranford and Condrate Sr (1984b).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1179, 1096, 1017s, 833, 779, 616, 585.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1120, 1097, 1022, 990, 969, 834, 785, 632, 609, 599, 583, 530, 442, 416, 383, 363, 347, 311, 288, 276, 241, 212, 177, 140, 115, 95, 80.

**P716 Niobyl phosphate  $\alpha$ -NbPO<sub>5</sub>**

**Origin:** Synthetic.

**Description:** Tetragonal, space group  $P4/n$ ,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

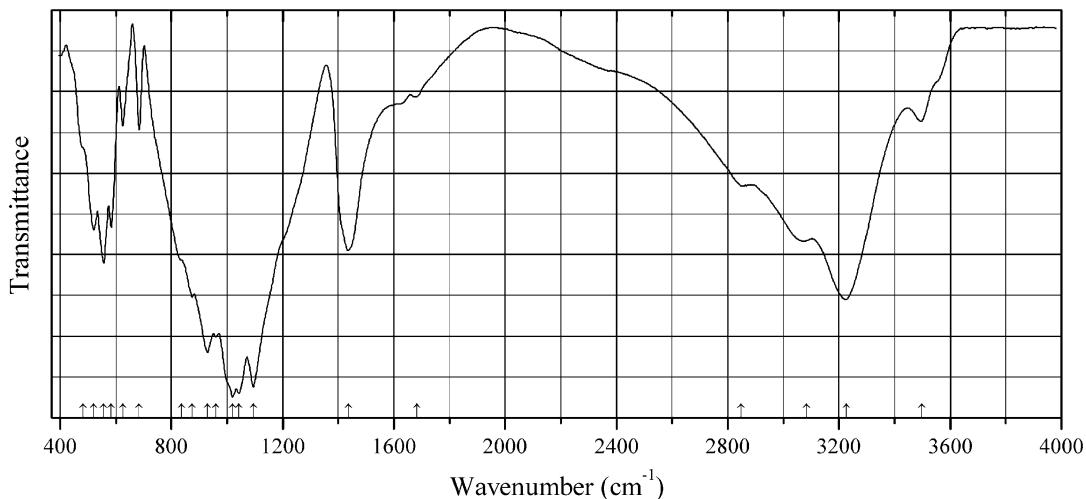
**Source:** Stranford and Condrate Sr (1984b).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1211, 1040s, 891s, 629, 583.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1113, 1014s, 984s, 800, 612, 467, 458, 376, 288, 200, 177, 160, 111.

### P717 Ammonium manganese(II) borophosphate $[\text{NH}_4]_4[\text{Mn}_9\text{B}_2(\text{OH})_2(\text{HPO}_4)_4(\text{PO}_4)_6]$



**Origin:** Synthetic.

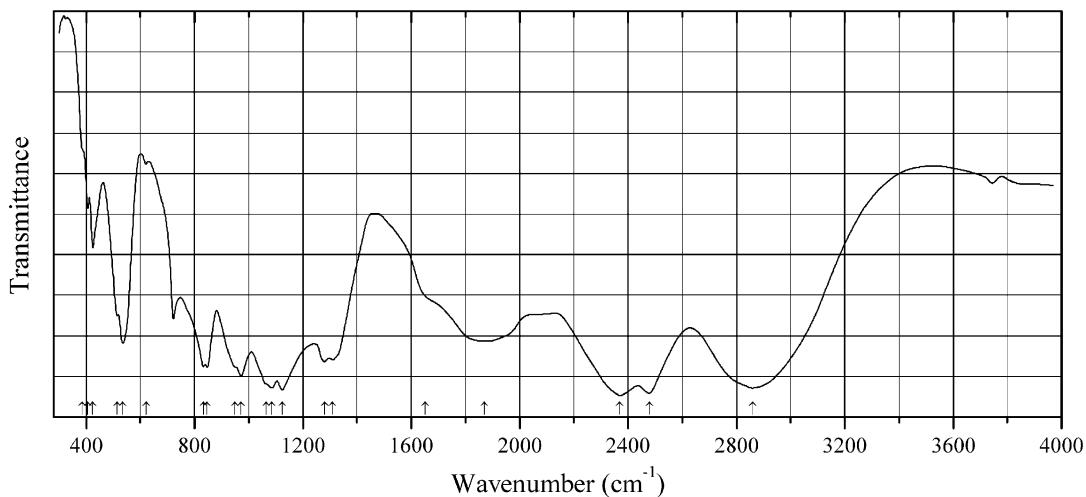
**Description:** Pink stick-like crystals prepared hydrothermally from  $\text{Mn}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$ ,  $\text{H}_3\text{BO}_3$ , and  $(\text{NH}_4)_2(\text{HPO}_4)$  at 200 °C for 5 days. Monoclinic, space group  $C2/c$ ,  $a = 32.603(7)$ ,  $b = 10.617(2)$ ,  $c = 10.718(2)$  Å,  $\beta = 108.26(3)^\circ$ ,  $V = 3523.2(12)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 2.971$  g/cm<sup>3</sup>. In the crystal structure, layers  $[\text{Mn}_9(\text{OH})_2(\text{HPO}_4)_4(\text{PO}_4)_6]$  are connected by B atoms having tetrahedral coordination to form 3D framework.  $\text{Mn}^{2+}$  has five- and sixfold coordination.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Yang et al. (2006).

**Wavenumbers (cm<sup>-1</sup>):** 3498, 3226s, 3084, 2848, 1684w, 1437, 1096s, 1044s, 1021s, 960, 930s, 875, 837sh, 685, 626, 583, 557, 521, 482sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**P718 Potassium acid phosphate  $K_2(HPO_4)$** 

**Origin:** Synthetic.

**Description:** Prepared by slow evaporation of aqueous solution of a commercial sample at 60 °C. Orthorhombic, space group  $Pna2_1$ ,  $Z = 12$ .

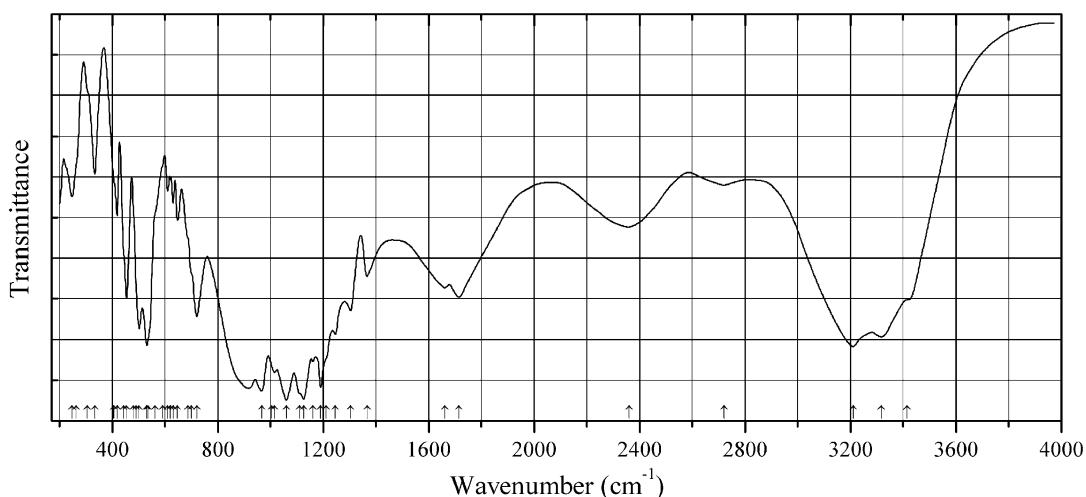
**Kind of sample preparation and/or method of registration of the spectrum:** Nujol and Fluorolube mulls. Transmission.

**Source:** Hadrich et al. (2001).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 2860s, 2480s, 2370s, 1870, 1650sh, 1310, 1280, 1124s, 1085s, 1065sh, 972s, 950sh, 847s, 832s, 622, 535, 515sh, 425, 407, 385sh.

**Note:** The band at  $\sim 720 \text{ cm}^{-1}$  corresponds to Nujol. The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1129w, 1119w, 1111w, 1100w, 1081w, 1066w, 1000, 969s, 946s, 856, 839sh, 828w, 587w, 571w, 559, 547, 534, 511w, 427w, 405w, 389, 382sh.

**P719 Potassium acid pyrophosphate hydrate  $K_3(HP_2O_7)\cdot 3H_2O$** 

**Origin:** Synthetic.

**Description:** Prepared in the reaction between a concentrated aqueous solution of potassium pyrophosphate and equimolar quality of acetic acid at 0–5 °C. Monoclinic, space group  $P2_1/c$ ,  $Z = 4$ .

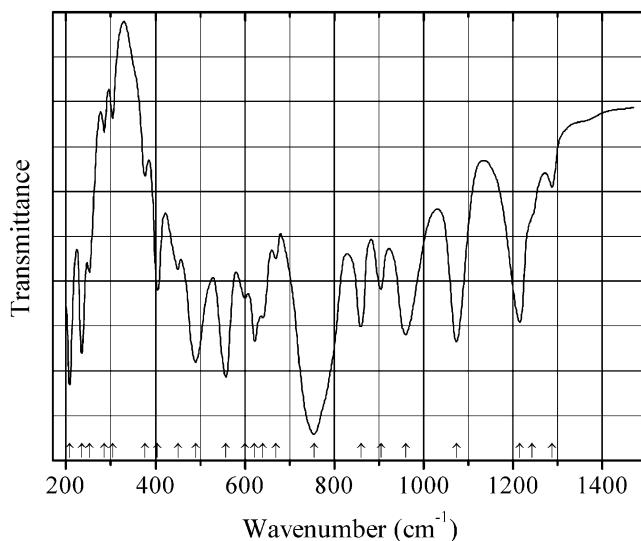
**Kind of sample preparation and/or method of registration of the spectrum:** Nujol and hexachlorobutadiene mulls. Transmission.

**Source:** Sarr and Diop (1984).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3414, 3316s, 3210s, 2720w, 2360 (broad), 1714, 1660, 1366, 1304, 1246, 1210sh, 1190s, 1160, 1125s, 1110sh, 1060s, 1015, 1005, 966s, 932–870s (broad), 720, 700sh, 686sh, 648w, 630w, 620w, 610w, 590sh, 562sh, 536sh, 531, 502, 480sh, 454, 444sh, 418, 407sh, 334, 306sh, 264sh, 247.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

#### P720 Potassium antimony(V) oxophosphate $\text{K}_5\text{Sb}_5\text{P}_2\text{O}_{20}$



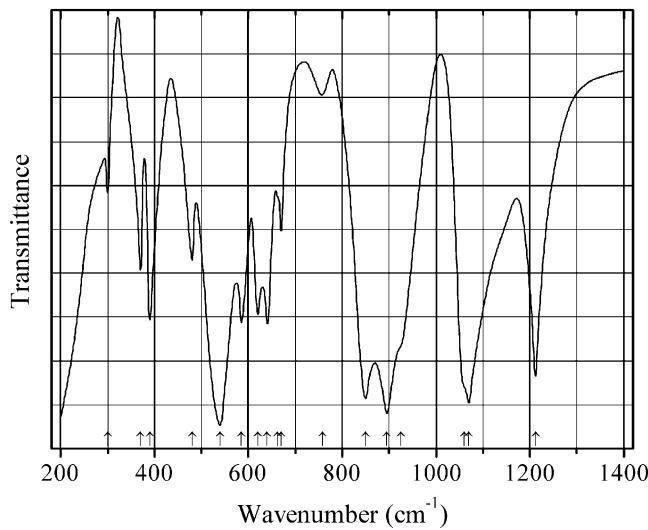
**Origin:** Synthetic.

**Source:** Husson et al. (1984).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1288w, 1244sh, 1216s, 1074s, 960s, 905, 860, 755s, 670, 640, 622s, 601w, 558s, 490s, 450, 405, 376, 304, 285, 252, 235s, 208s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1240, 1180, 1070, 975, 821w, 775w, 647s, 599s, 566w, 543, 507, 489, 472, 440w, 380w, 339s, 322, 267, 215w, 161, 108sh, 74.

**P721 Potassium antimony oxophosphate**  $K_2Sb(PO_4)O_2$ 

**Origin:** Synthetic.

**Description:** Obtained by a solid-state reaction technique. The crystal structure is solved. Orthorhombic, space group  $Pnma$ ,  $a = 9.429(4)$ ,  $b = 5.891(3)$ ,  $c = 11.030(5)$  Å,  $V = 612.72$  Å $^3$ ,  $Z = 4$ .  $D_{\text{meas}} = 3.50(5)$  g/cm $^3$ ,  $D_{\text{calc}} = 3.53$  g/cm $^3$ .

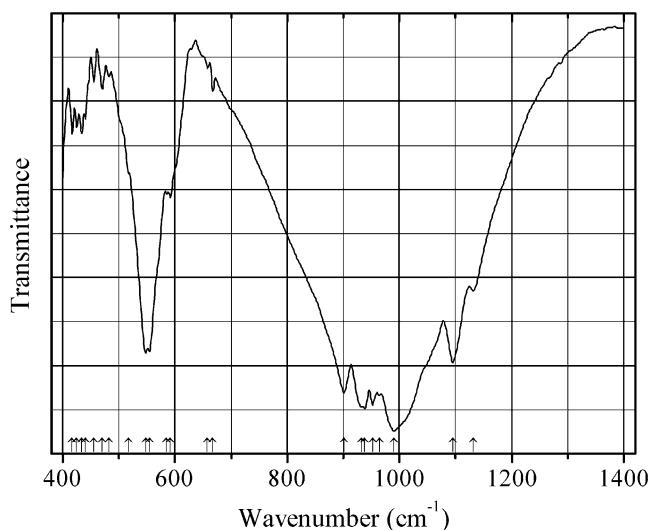
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Botto and Garcia (1989).

**Wavenumbers (IR, cm $^{-1}$ ):** 1212s, 1070s, 1060sh, 925sh, 895s, 850s, 758w, 670, 662sh, 640, 620, 585, 540s, 480, 390, 370, 300w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 1190, 1071s, 653s, 620w, 600, 545s, 537sh, 508w, 496w, 487w, 473w, 434w, 326, 308, 266s.

**P722 Potassium bismuth(III) phosphate**  $K_3Bi_2(PO_4)_3$ 

**Origin:** Synthetic.

**Description:** Prepared by crystallization from the melt obtained by heating stoichiometric mixture of  $K_2CO_3$ ,  $Bi_2O_3$ , and  $(NH_4)(H_2PO_4)$  to 1223 K. Characterized by powder X-ray diffraction data. Orthorhombic, possibly isostructural with  $Na_3Bi_2(PO_4)_3$ .

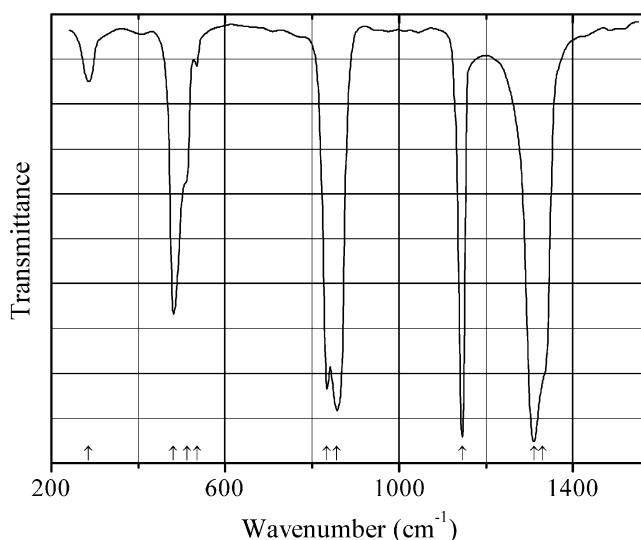
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Mariappan et al. (2005).

**Wavenumbers ( $cm^{-1}$ ):** 1132, 1095s, 990s, 964s, 952s, 938s, 933sh, 901s, (667w), (658w), 592, 585, 555s, 548s, (517), (482w), (470w), (455w), (440w), (434w), (425w), (417w).

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

### P723 Potassium difluorophosphate $K(PO_2F_2)$



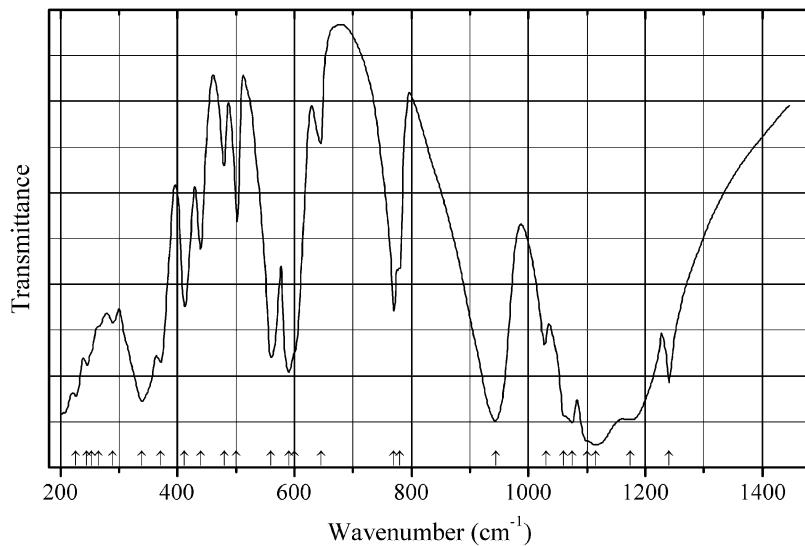
**Origin:** Synthetic.

**Description:** Obtained from a melt prepared from  $KPF_6$  and  $KPO_3$ . Orthorhombic (?).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Bühler and Bues (1961).

**Wavenumbers ( $cm^{-1}$ ):** 1330sh, 1311s, 1145s, 857s, 834, 535w, 512sh, 481, 286w.

**P724 Potassium iron pyrophosphate KFe(P<sub>2</sub>O<sub>7</sub>)**

**Origin:** Synthetic.

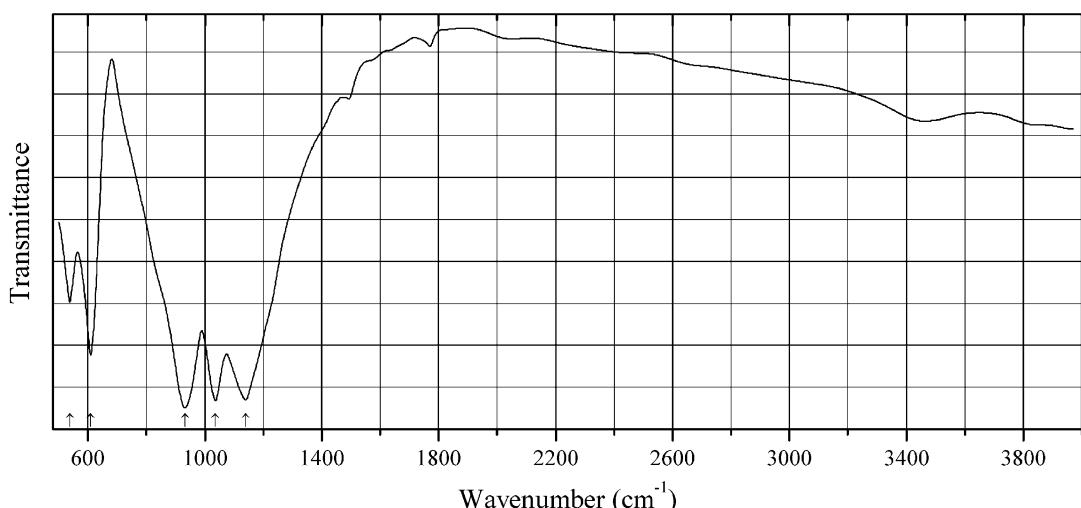
**Description:** Obtained by evaporation of an aqueous solution containing a stoichiometric mixture of KNO<sub>3</sub>, Fe(NO<sub>3</sub>)<sub>3</sub>, and (NH<sub>4</sub>)<sub>2</sub>(HPO<sub>4</sub>) followed by stepwise heating up to 750 °C with intermediate grindings. Monoclinic, space group P2<sub>1</sub>/c, *a* = 7.3523, *b* = 9.9875, *c* = 8.1872 Å, β = 106.499°, V = 576.45 Å<sup>3</sup>, Z = 4. Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Belkouch et al. (1995).

**Wavenumbers (cm<sup>-1</sup>):** 1240s, 1175s, 1115s, 1100sh, 1075s, 1060sh, 1030, 945s, 780sh, 770, 645w, 600sh, 590, 560, 500, 480, 440, 412, 371, 339s, 289, 265sh, 252sh, 245, 226.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**P725 Potassium lead borophosphate KPb(BP<sub>2</sub>O<sub>8</sub>)**

**Origin:** Synthetic.

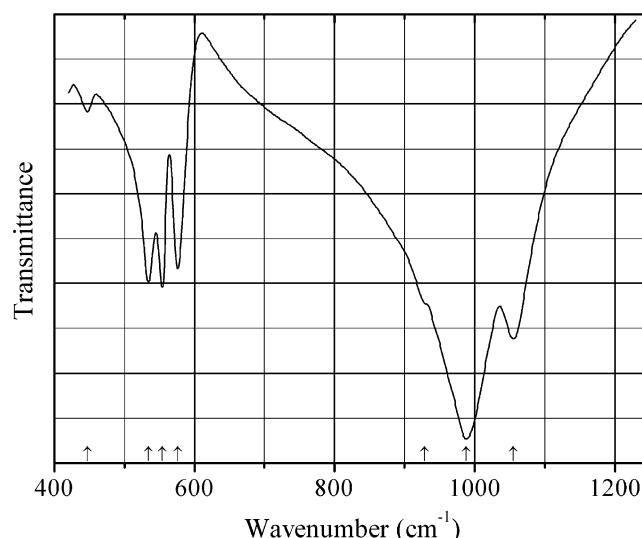
**Description:** Colorless crystals grown by the top seed growth method from a  $K_2O-PbO-B_2O_3-P_2O_5$  system. The melt was kept at 880 °C for 24 h and then cooled first to 865 °C at a rate of 0.5 °C/min and thereafter to 861 °C within 20 h. Characterized by powder X-ray diffraction data. The crystal structure is solved. Tetragonal, space group  $I-42d$ ,  $a = 7.1464(7)$ ,  $c = 13.8917(16)$  Å,  $V = 709.46(13)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 4.185$  g/cm<sup>3</sup>. The structure contains 12-membered rings, in which 6  $PO_4$  tetrahedra and 6  $BO_4$  tetrahedra are linked by O atoms.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Li et al. (2013).

**Wavenumbers (cm<sup>-1</sup>):** 1139s, 1036s, 932s, 610, 538.

#### P726 Potassium lead phosphate $KPb_4(PO_4)_3$



**Origin:** Synthetic.

**Description:** Prepared in a solid-state reaction, by heating a mixture of  $PbO$ ,  $K_2CO_3$ , and  $(NH_4)_2(HPO_4)$  first to 500 °C, and thereafter (after intermediate grinding) at 700 °C for 48 h. Characterized by powder X-ray diffraction data. Hexagonal, space group  $P6_3/m$ ,  $a = 9.8276(3)$ ,  $c = 7.3010(4)$  Å,  $V = 610.67(2)$  Å<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

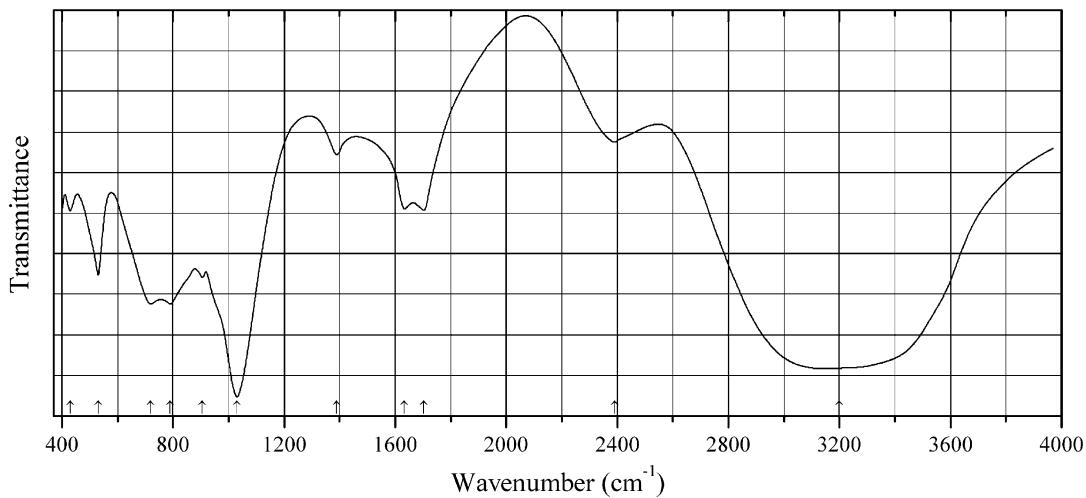
**Source:** Azrour et al. (2011).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1055s, 988s, 928sh, 576, 554, 534, 447w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1025, 976, 959s, 933s, 583s, 558, 418, 389, 235sh, 204, 159w, 130s.

**P727 Potassium magnesium acid phosphate hydrate  $KMg_2H(PO_4)_2 \cdot 15H_2O$**



**Origin:** Synthetic.

**Description:** Prepared by the precipitation reaction between  $MgSO_4$  and  $K_2(HPO_4)$  solutions. Characterized by powder X-ray diffraction data. Triclinic,  $a = 6.2908$ ,  $b = 12.2451$ ,  $c = 6.5551 \text{ \AA}$ ,  $\alpha = 93.64^\circ$ ,  $\beta = 89.14^\circ$ ,  $\gamma = 94.73^\circ$ .

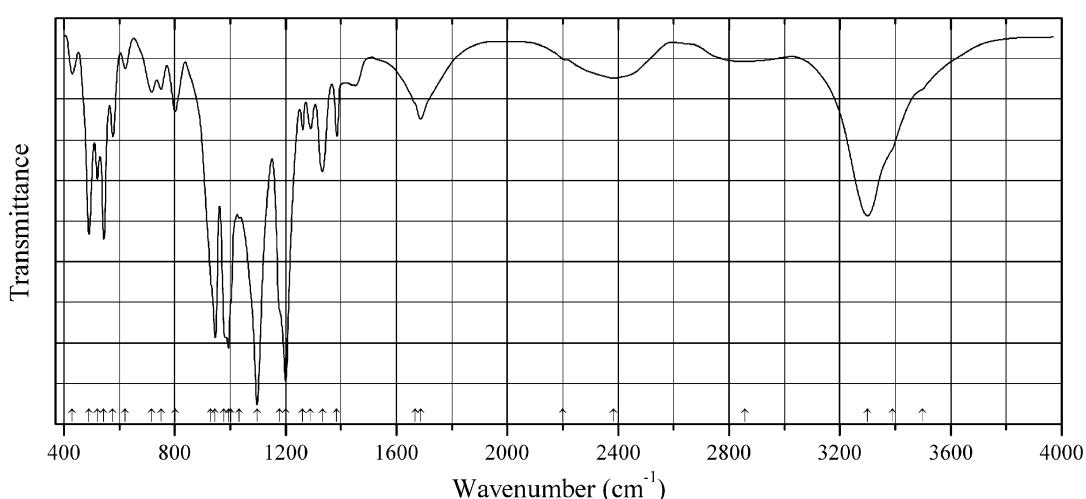
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc and Nujol mull. Transmission.

**Source:** Koleva et al. (2015).

**Wavenumbers (cm⁻¹):** 3200s, 2390, 1704, 1633, 1390w, 1031s, 905, 790s, 720s, 530, 429w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**P728 Potassium magnesium acid pyrophosphate hydrate  $KMg_{0.5}(H_2P_2O_7) \cdot H_2O$**



**Origin:** Synthetic.

**Description:** Prepared in the reaction of aqueous solutions of  $\text{MgCl}_2$  and  $\text{K}_4\text{P}_2\text{O}_7$  in the presence of HCl. The crystal structure is solved. Triclinic, space group  $P-1$ ,  $a = 6.8565(2)$ ,  $b = 7.3621(3)$ ,  $c = 7.6202(3)$  Å,  $\alpha = 81.044(2)^\circ$ ,  $\beta = 72.248(2)^\circ$ ,  $\gamma = 83.314(3)^\circ$ ,  $V = 360.90(2)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{calc}} = 2.257$  g/cm $^3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

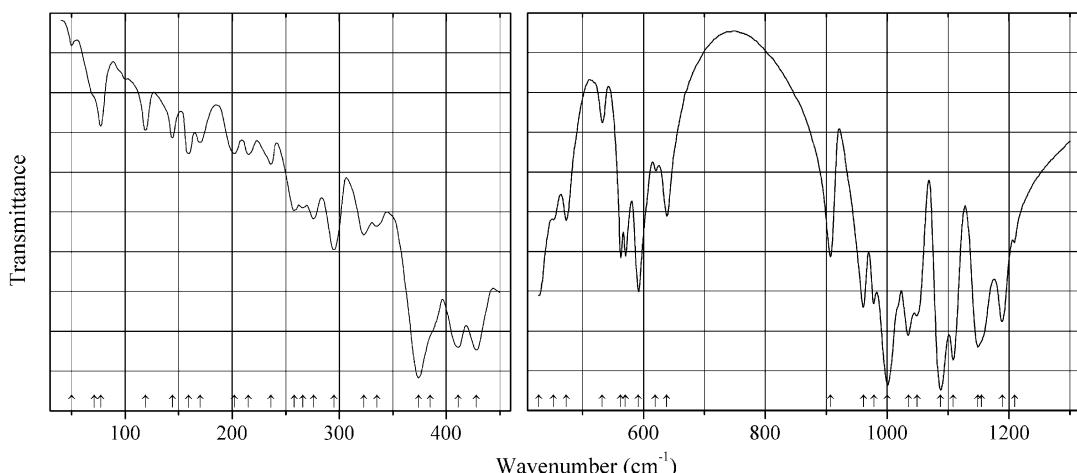
**Source:** Harcharras et al. (2003).

**Wavenumbers (IR, cm $^{-1}$ ):** 3498sh, 3389sh, 3299, 2858, 2383 (broad), 2201, 1687, 1669sh, 1385w, 1333, 1290, 1262, 1200s, 1179sh, 1097s, 1033s, 1002sh, 994s, 978sh, 946s, 931sh, 802, 751, 717, 622w, 577, 544, 520, 491, 431w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 3484w, 3387, 3318, 3281s, 2787w, 2405w, 2176w, 1705w, 1605w, 1332w, 1278w, 1217s, 1165, 1121, 1115w, 1081, 1048s, 1023, 992, 955w, 900w, 763s, 729, 589s, 555, 534, 512, 472, 452, 409s, 381, 373s, 365, 339, 311, 300s, 245.

### P729 Potassium magnesium orthophosphate $\text{KMg}_4(\text{PO}_4)_3$ $\text{KMg}_4(\text{PO}_4)_3$



**Origin:** Synthetic.

**Description:** Obtained from  $\text{K}_2\text{WO}_4$ - $\text{WO}_3$  flux containing  $\text{K}(\text{H}_2\text{PO}_4)$  and  $\text{MgO}$  in the molar ratio 2:1. The crystal structure is solved. Orthorhombic, space group  $Pnmm$ ,  $a = 16.361(3)$ ,  $b = 9.562(19)$ ,  $c = 6.171(12)$  Å,  $V = 965.4(3)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 2.898$  g/cm $^3$ .

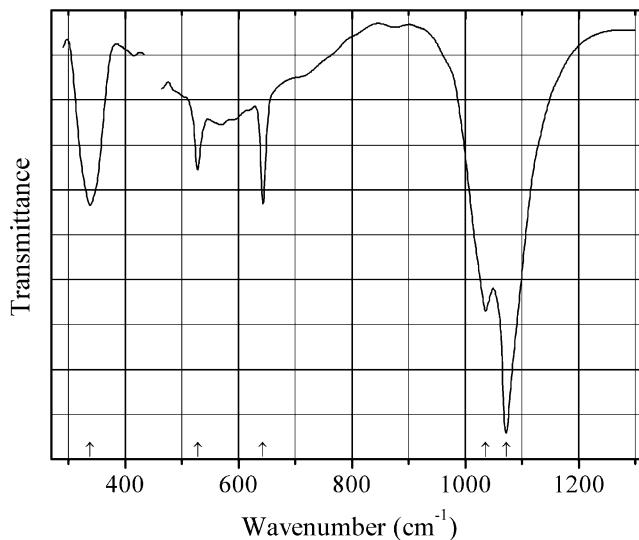
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc (400–1500 cm $^{-1}$ ) and Nujol mull (30–500 cm $^{-1}$ ). Absorption.

**Source:** Tomaszewski et al. (2005).

**Wavenumbers (IR, cm $^{-1}$ ):** 1209w, 1189, 1155sh, 1149s, 1108s, 1087s, 1049s, 1035s, 1000s, 978, 961, 907, 638, 619, 591, 570, 562, 532, 473, 452, 428, 411, 385sh, 374, 335, 323, 295, 276, 266, 258, 236w, 215w, 202w, 170w, 159w, 144w, 119w, 77w, 71sh, 50w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, polarized Raman spectra are given.

**Wavenumbers (Raman, [z(xx)-z] polarization, cm $^{-1}$ ):** 1152w, 1141w, 1103w, 1086, 1079, 1016s, 982s, 956, 636, 624w, 604w, 589w, 565, 550w, 509w, 471w, 415, 298w, 283, 275w, 253w, 156, 132.

**P730 Potassium magnesium yttrium phosphate (xenotime-type)  $KMgY(PO_4)_2$** 

**Origin:** Synthetic.

**Description:** Obtained from stoichiometric amounts of  $(NH_4)_2(HPO_4)$ ,  $K_2CO_3$ ,  $MgO$ , and  $Y_2O_3$ , with  $NH_4Cl$  as a flux, first at  $850\text{ }^{\circ}\text{C}$  for several hours, and thereafter (after adding  $KCl$  and grinding) at  $650\text{--}850\text{ }^{\circ}\text{C}$  for 2 days, with subsequent washing with cold water. Characterized by powder X-ray diffraction data and elemental analysis. Tetragonal, space group  $I4_1/AMD$ ,  $a = 6.886$ ,  $c = 6.025\text{ \AA}$ ,  $Z = 2$ .  $D_{\text{meas}} = 3.940\text{ g/cm}^3$ ,  $D_{\text{calc}} = 3.983\text{ g/cm}^3$ .

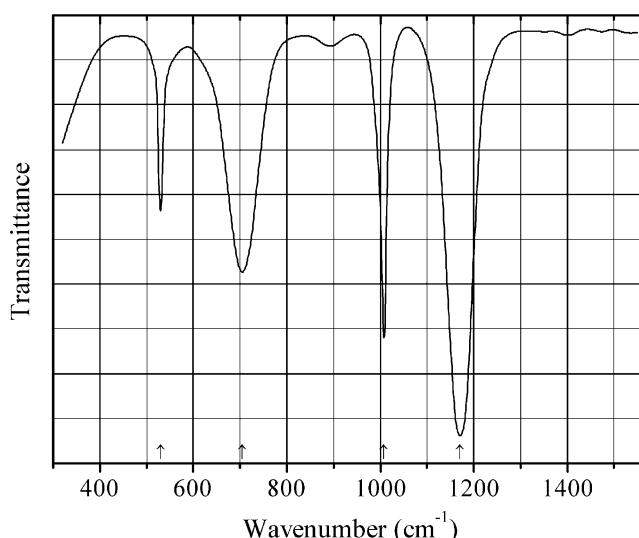
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Shao-Long et al. (1996).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1072s, 1036s, 643, 528, 338.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1061s, 1030, 1004s, 669, 659w, 590, 569w, 553w, 533w, 488, 338, 305s, 225w, 205, 195, 165, 92w, 85w.

**P731 Potassium monofluorophosphate  $K_2(PO_3F)$** 

**Origin:** Synthetic.

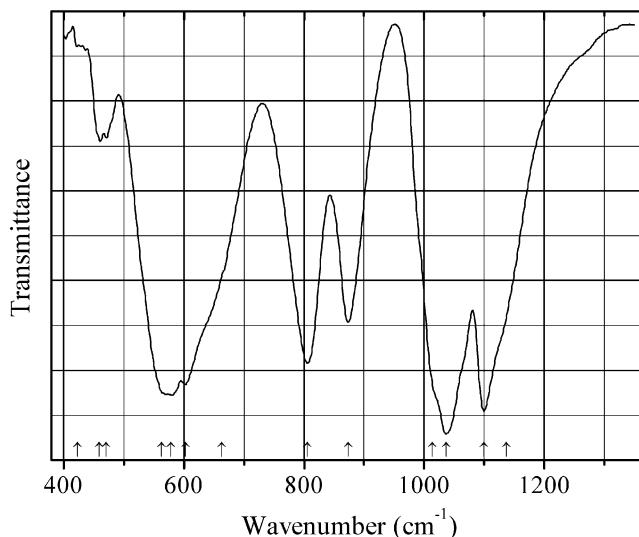
**Description:** Obtained from the melt containing KF and  $\text{KPO}_3$ . Orthorhombic,  $a = 7.554$ ,  $b = 5.954$ ,  $c = 10.171 \text{ \AA}$ ,  $V = 457 \text{ \AA}^3$ ,  $Z = 4$  (Payen et al. 1979).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Bühler and Bues (1961).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1170s, 1008s, 705s, 530.

### P732 Potassium niobium oxophosphate $\text{K}_3\text{Nb}_5\text{O}_{11}(\text{PO}_4)_2$



**Origin:** Synthetic.

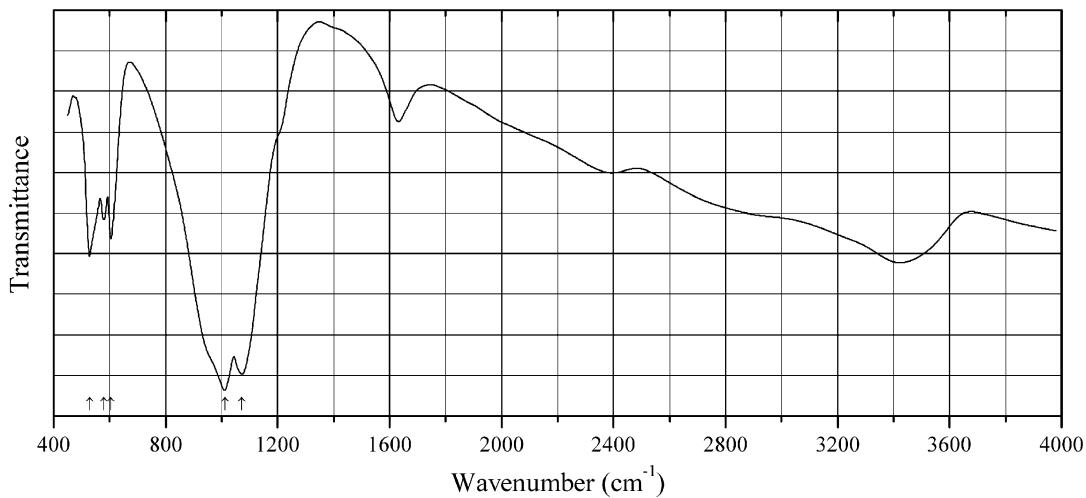
**Description:** Prepared in the cation exchange reaction between  $\text{Ti}_3\text{Nb}_5\text{O}_{11}(\text{PO}_4)_2$  and excess of KCl at  $460^\circ\text{C}$  for 24 h. Characterized by powder X-ray diffraction data and electron microprobe analysis.

Trigonal, space group  $R-3c$ ,  $a = 13.002(7)$ ,  $c = 53.742(3) \text{ \AA}$ ,  $V = 7868(13) \text{ \AA}^3$ ,  $Z = 18$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Fakhfakh et al. (2003).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1136sh, 1099s, 1036s, 1013sh, 874, 806, 663sh, 603, 579s, 563s, 471, 460, 424w.

**P733 Potassium tin orthophosphate  $KSn_4(PO_4)_3$** 

**Origin:** Synthetic.

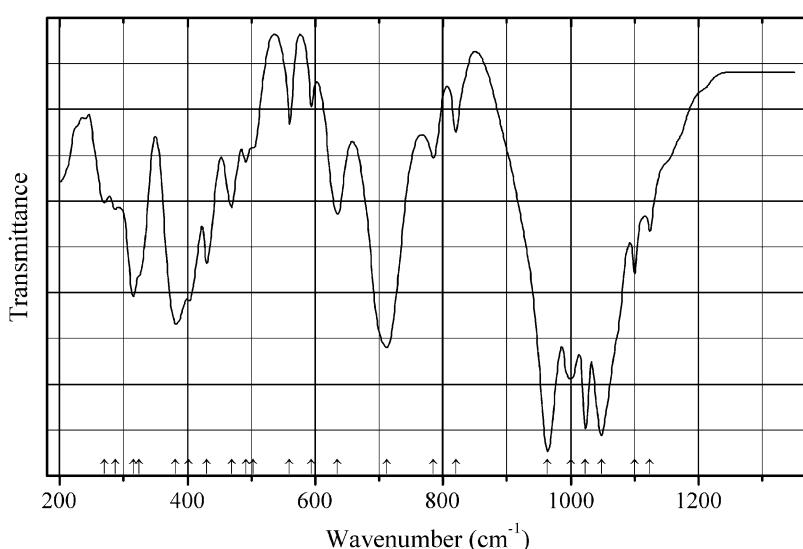
**Description:** Synthesized hydrothermally from  $SnCl_2$  and  $K(H_2PO_4)$  at  $170\text{ °C}$  for 3 days. Characterized by powder X-ray diffraction data. The crystal structure is solved. Trigonal, space group  $R\bar{3}c$ ,  $a = 9.7124(11)$ ,  $c = 24.363(3)$  Å,  $V = 1990.3(4)$  Å $^3$ ,  $Z = 6$ .  $D_{\text{calc}} = 3.999$  g/cm $^3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Bontchev and Moore (2004).

**Wavenumbers (cm $^{-1}$ ):** 1073s, 1012s, 604, 579, 529.

**Note:** Bands above  $1400\text{ cm}^{-1}$  indicate that the sample was contaminated with a compound containing acid OH groups and  $H_2O$  molecules.

**P734 Potassium titanium oxophosphate  $KTi(PO_4)O$** 

**Origin:** Synthetic.

**Description:** Orthorhombic, space group  $Pn2_1a$ . The structure contains distorted  $TiO_6$  octahedra whereas  $PO_4$  tetrahedra are stated as being undistorted. However the strong band at  $964\text{ cm}^{-1}$  indicates that  $PO_4$  tetrahedra are actually distorted.

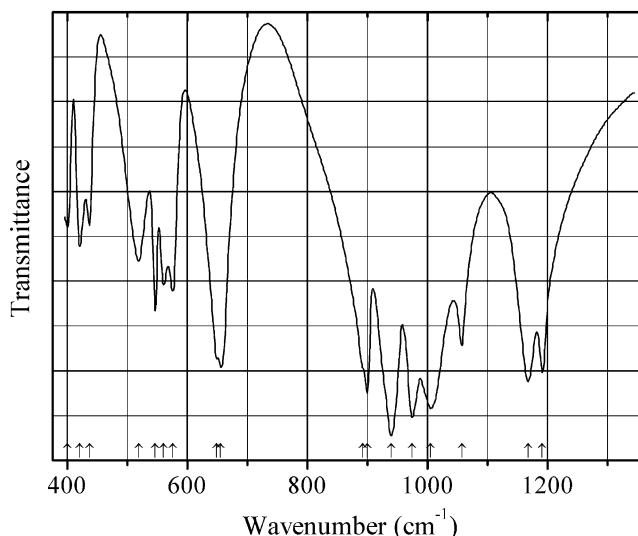
**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull. Transmission.

**Source:** Jacco (1986).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1124, 1100, 1048s, 1023s, 1000s, 964s, 820, 785, 712s, 635, 594w, 560, 503sh, 492, 469, 430, 402, 381s, 324sh, 315, 287, 270.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### P735 Potassiumvanadyl phosphate $K_2(VO_2)(PO_4)$



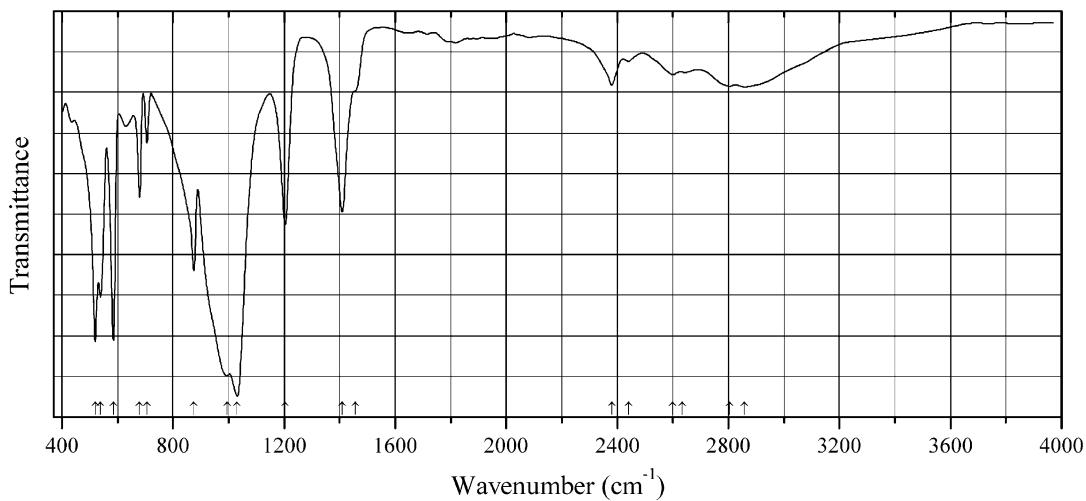
**Origin:** Synthetic.

**Description:** Yellow crystals prepared from the powders of  $NH_4VO_3$ ,  $(NH_4)_2(HPO_4)$ , and  $KNO_3$  mixed in the molar ratio 1:1:2 and heated first at  $350\text{ }^\circ C$  for 2 h and thereafter for  $440\text{ }^\circ C$  for 1 h. The crystal structure is solved. Monoclinic, space group  $P2_1/n$ ,  $a = 6.863(2)$ ,  $b = 13.479(5)$ ,  $c = 7.505(1)$  Å,  $\beta = 111.02(10)^\circ$ ,  $V = 648.0(3)$  Å<sup>3</sup>,  $Z = 4$ . Vanadium has fivefold coordination with two short V–O distances.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Korthuis et al. (1993).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1191s, 1167s, 1057, 1005s, 974s, 939s, 899s, 892sh, 655s, 648, 575, 560, 546, 518, 436, 420, 400.

**P736 Potassium ytterbium acid orthoborate acid orthophosphate  $K_3Yb[BO(OH)_2]_2(HPO_4)_2$** 

**Origin:** Synthetic.

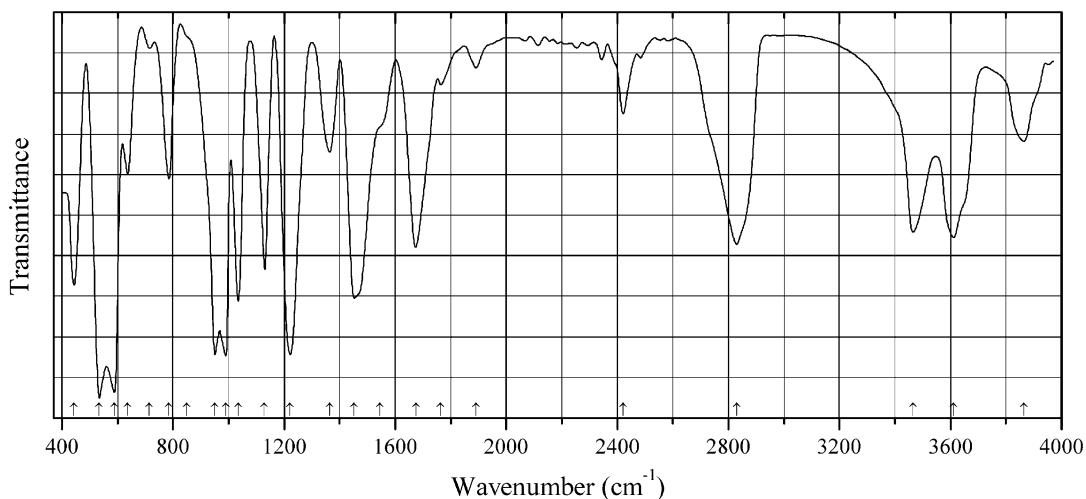
**Description:** Prepared hydrothermally from Yb<sub>2</sub>O<sub>3</sub> preliminarily dissolved in concentrated HCl, K<sub>2</sub>B<sub>4</sub>O<sub>7</sub>·4H<sub>2</sub>O, and K<sub>2</sub>HPO<sub>4</sub> (with the molar ratio K:Yb:B:P = 18:1:8:7) at 453 K for 5 days. Characterized by electron microprobe analyses. The crystal structure is solved. Trigonal, space group *R*-3, *a* = 5.6809(2), *c* = 36.594(5) Å, *V* = 1022.8(2) Å<sup>3</sup>, *Z* = 3. *D*<sub>calc</sub> = 2.942 g/cm<sup>3</sup>. In B-centered triangles, O atoms and OH groups are disordered.

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of a powdered sample.

**Source:** Zhou et al. (2011).

**Wavenumbers (cm<sup>-1</sup>):** 2859, 2805, 2635sh, 2600w, 2441w, 2380, 1456sh, 1409, 1204, 1031s, 994s, 875, 706, 680, 585s, 538, 520s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**P737 Potassium zinc acid pyrophosphate hydrate  $K_2Zn(H_2P_2O_7)_2 \cdot 2H_2O$** 

**Origin:** Synthetic.

**Description:** The crystal structure is solved. Orthorhombic, space group  $Pnma$ ,  $a = 9.901(17)$ ,  $b = 11.071(14)$ ,  $c = 13.65(4)$  Å,  $V = 1496$  Å $^3$ ,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

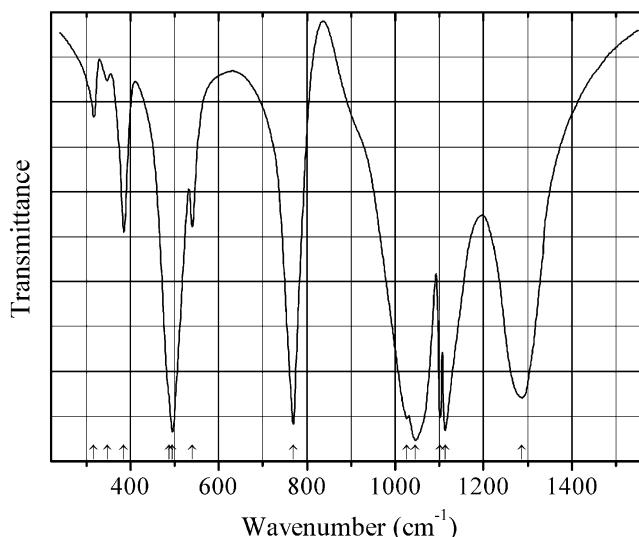
**Source:** Khaoulaf et al. (2012).

**Wavenumbers (IR, cm $^{-1}$ ):** 3864, 3612, 3466, 2829, 2421, 1891w, 1764w, 1676, 1545sh, 1453, 1363, 1222s, 1129, 1036, 990s, 951s, 850sh, 785, 715w, 637, 589s, 534s, 444.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 3544, 3401s, 3300, 2750, 2316w, 1787w, 1665w, 1312, 1190s, 1136, 1070s, 1006, 918, 755s, 823w, 609s, 609s, 572, 524w, 464s, 416s, 389, 341s, 314w, 267s.

### P738 Potassium zinc cyclotriphosphate benitoite-type KZn(P<sub>3</sub>O<sub>9</sub>)



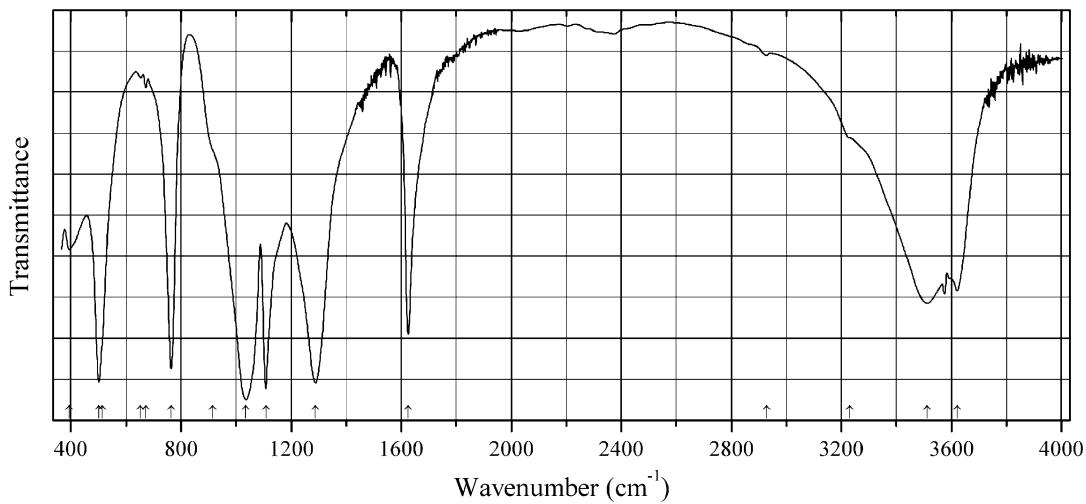
**Origin:** Synthetic.

**Description:** Synthesized by solid-state reaction techniques from a stoichiometric mixture of (NH<sub>4</sub>)<sub>2</sub>PO<sub>4</sub>, KHCO<sub>3</sub>, and ZnO (or ZnCO<sub>3</sub>) at 600 °C with several intermediate grindings. Characterized by powder X-ray diffraction data. Hexagonal, isostructural with benitoite.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Tarte et al. (1987).

**Wavenumbers (cm $^{-1}$ ):** 1287s, 1113s, 1102s, 1046s, 1027s, 769s, 540, 495s, 487sh, 385, 347w, 317.

**P739 Praseodymium cyclotriphosphatetrihydrate**  $\text{Pr}(\text{P}_3\text{O}_9)\cdot 3\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Prepared by mixing  $\text{PrCl}_3\cdot 6\text{H}_2\text{O}$  and  $\text{Na}_3\text{P}_3\text{O}_9$  0.1 M aqueous solutions in a 1:1 ratio. The crystal structure is solved. Hexagonal, space group *P*-6,  $a = 6.7677(4)$ ,  $c = 6.0501(4)$  Å,  $V = 239.98(3)$  Å<sup>3</sup>,  $Z = 1$ .  $D_{\text{calc}} = 2.988$  g/cm<sup>3</sup>.

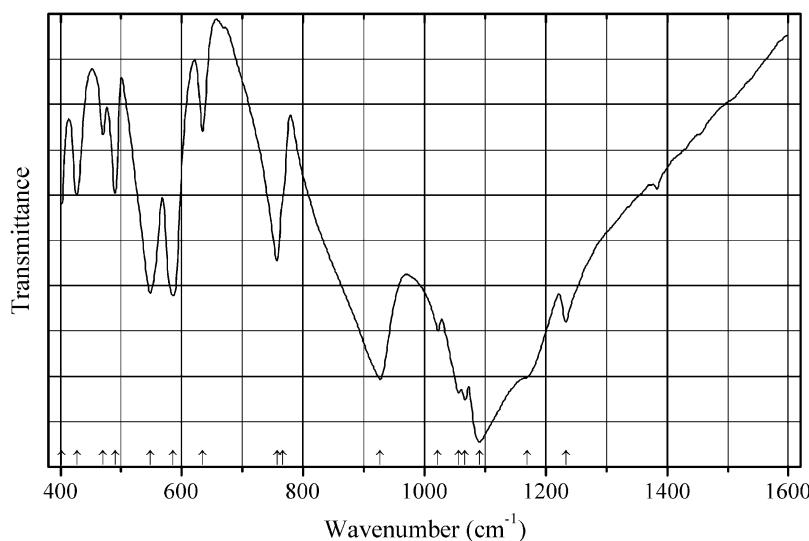
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Jouini et al. (2006).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3620, 3512, 3230sh, (2928), 1626, 1289s, 1108s, 1036s, 915sh, 764s, (672), (653), (514), 501s, 394.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The wavenumber 1289 cm<sup>-1</sup> is erroneously indicated by Jouini et al. (2006) as 1298 cm<sup>-1</sup>. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1248s, 1176s, 1103, 900, 656s, 662, 481, 357s, 306s, 269, 202w, 169, 131, 78.

**P740 Rubidium iron(III) pyrophosphate**  $\text{RbFe}^{3+}(\text{P}_2\text{O}_7)$ 

**Origin:** Synthetic.

**Description:** Prepared from aqueous solutions of corresponding nitrates and  $(\text{NH}_4)_2(\text{HPO}_4)$  using a co-precipitation method, with subsequently heating precipitate at  $750^\circ\text{C}$  at 15–20 h. Characterized by powder X-ray diffraction data. Triclinic, space group  $P\bar{2}_1/c$ ,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

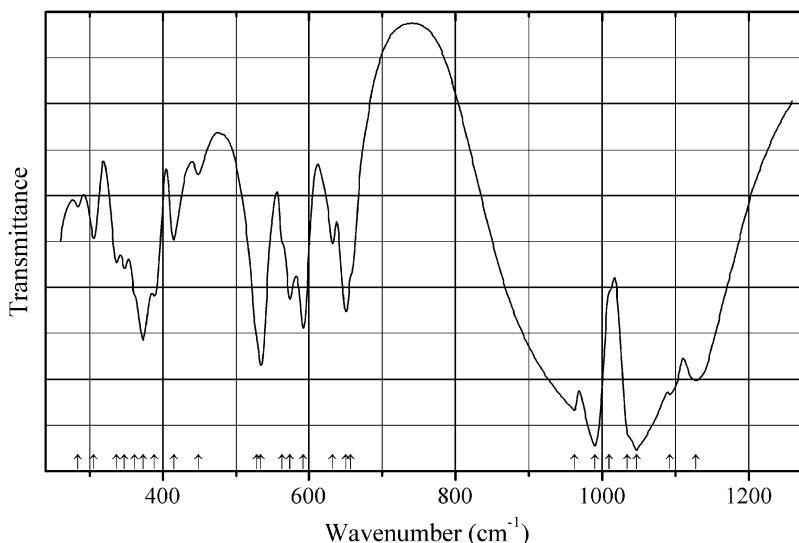
**Source:** Parajón-Costa et al. (2013).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1233, 1170sh, 1091s, 1067s, 1057s, 1022, 927s, 766sh, 757, 634, 586, 548, 490, 470, 427, 402.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1156s, 1119s, 1094s, 1066s, 908, 765, 640, 598, 574, 548, 473, 431, 406.

#### P741 Rubidium vanadyl phosphate $\text{Rb}(\text{VO})(\text{PO}_4)$



**Origin:** Synthetic.

**Description:** Obtained by heating pelletized mixture of  $\text{Rb}_4\text{V}_2\text{O}_7$ ,  $\text{V}_2\text{O}_3$ , and  $\text{P}_2\text{O}_5$  in a molar ratio of 1:1:2 at  $785^\circ\text{C}$ . Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group  $P\bar{2}_12_12_1$ ,  $Z = 4$ . The structure contains square pyramidal  $\text{VO}_5$  groups (with one short V–O bond of  $1.579\text{ \AA}$ ) and tetrahedral  $\text{PO}_4$  units.

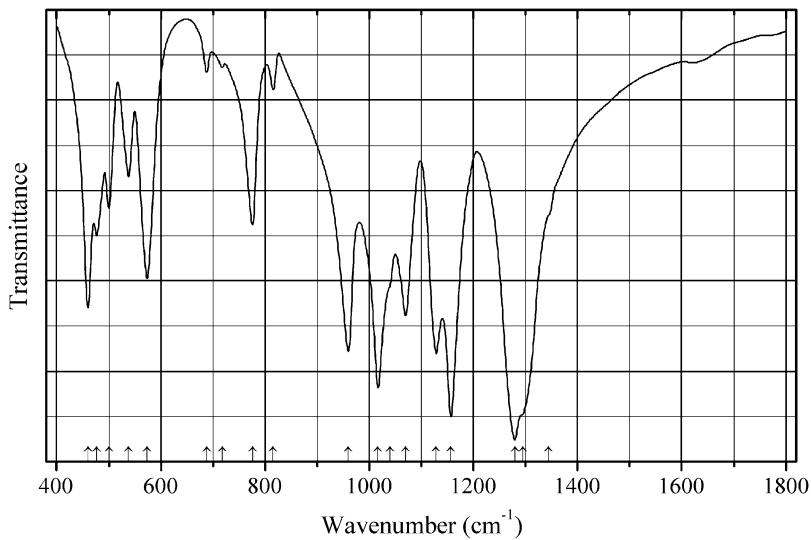
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Baran et al. (1996).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1128s, 1093s, 1047s, 1035sh, 1010sh, 990s, 962s, 657sh, 650, 632, 592, 574, 563, 534s, 529sh, 449w, 415, 389, 373, 362sh, 348, 337, 306, 284w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1149, 1125, 1094, 1077, 1045, 1005s, 964, 664, 630, 593, 560, 523, 450, 405, 351, 320, 285s.

**P742 Samarium metaphosphate Sm(PO<sub>3</sub>)<sub>3</sub>**

**Origin:** Synthetic.

**Description:** Synthesized from the mixture of Sm<sub>2</sub>O<sub>3</sub> and (NH<sub>4</sub>)(H<sub>2</sub>PO<sub>4</sub>) heated successively at 170, 240, 350, 440, and 550 °C for 24 h. Characterized by powder X-ray diffraction data. Orthorhombic, space group *C222*<sub>1</sub>.

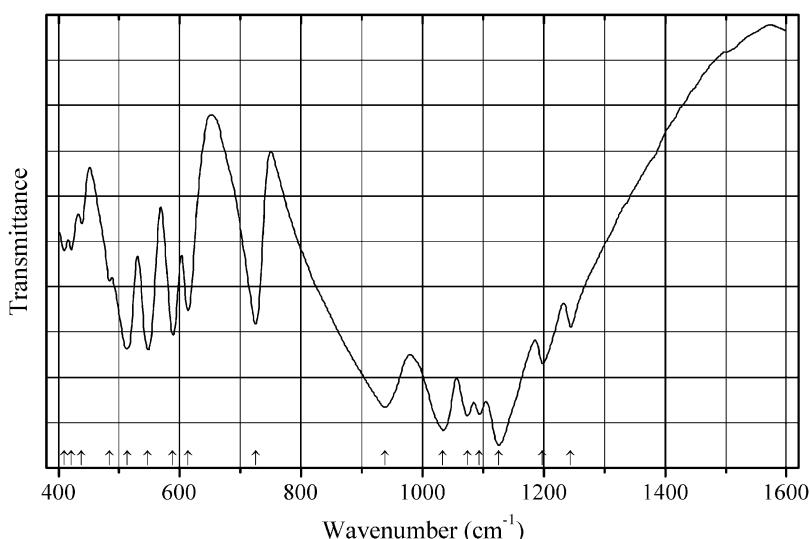
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Ilieva et al. (2001).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1345sh, 1295sh, 1280s, 1157s, 1129, 1070, 1040sh, 1017s, 960s, 816w, 776, 718w, 688w, 574, 538, 500, 477, 460.

**Note:** In the cited paper, IR and Raman spectra of Ga, In, Y, Sm, Gd, and Dy metaphosphates are given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1305, 1270s, 1200s, 1170, 1131, 1093, 1064, 983, 753, 720, 692s, 580, 565, 538, 501, 469, 405, 366, 350, 326, 294, 276, 250, 230, 145.

**P743 Silver iron(III) pyrophosphate AgFe<sup>3+</sup>(P<sub>2</sub>O<sub>7</sub>)**

**Origin:** Synthetic.

**Description:** Obtained by heating precipitate obtained in the reaction between aqueous solutions of Ag and Fe nitrates and  $(\text{NH}_4)_2(\text{HPO}_4)$  at 750 °C for 15–20 h with several grindings. Monoclinic,  $a = 9.566(4)$ ,  $b = 8.001(2)$ ,  $c = 7.325(2)$  Å,  $\beta = 111.86(1)$ °.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

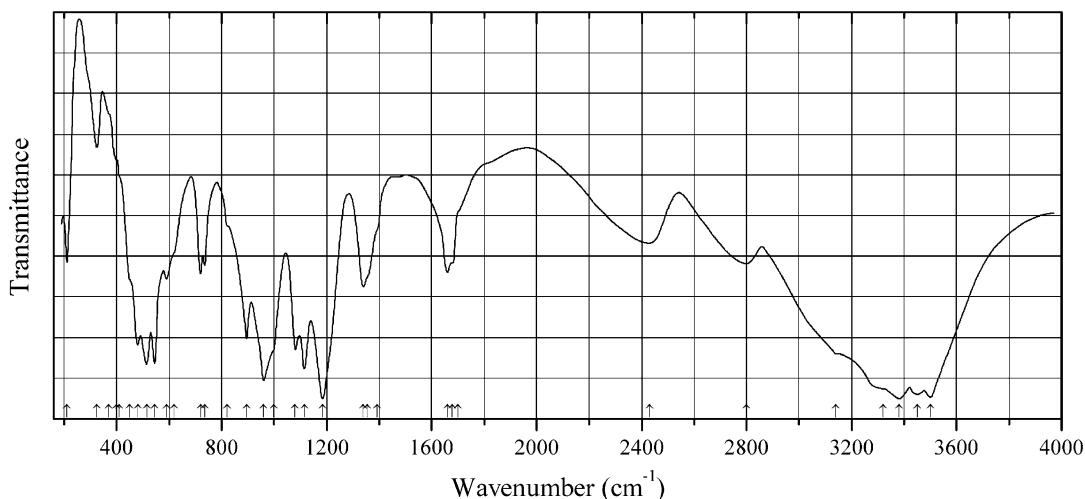
**Source:** Parajón-Costa et al. (2013).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1244, 1198, 1126s, 1094s, 1074s, 1034s, 939s, 725, 613, 588, 547, 513, 484, 438w, 421w, 409w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1225, 1136, 1105s, 1084s, 1050, 1038, 1020, 933, 741, 625, 569, 535w, 511, 490, 443, 415w, 400w.

#### P744 Sodium acid pyrophosphate hydrate $\text{Na}_3(\text{HP}_2\text{O}_7) \cdot 9\text{H}_2\text{O}$



**Origin:** Synthetic.

**Description:** Needle-like crystals obtained at 0 °C by crystallization from an aqueous solution containing stoichiometric amounts of  $\text{H}_4\text{P}_2\text{O}_7$  and NaOH. Monoclinic, space group  $P2_1/c$ ,  $Z = 4$ .

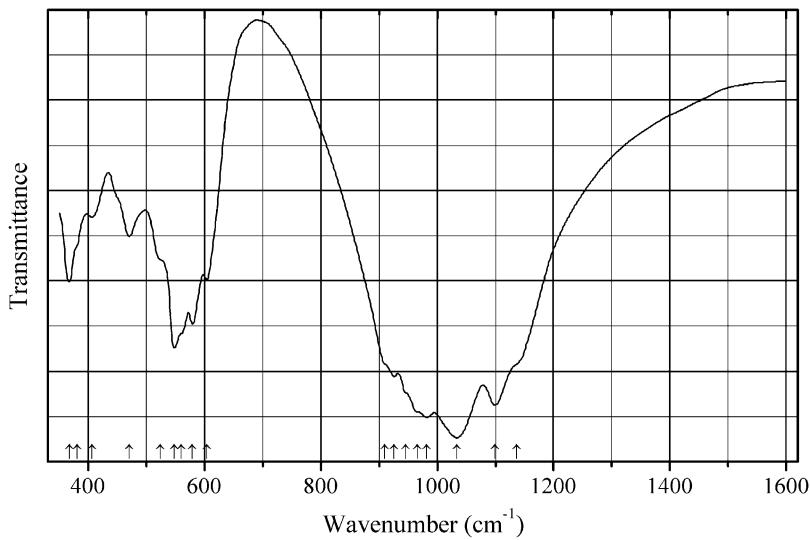
**Kind of sample preparation and/or method of registration of the spectrum:** Nujol or hexachlorobutadiene mull. Transmission.

**Source:** Sarr and Diop (1987).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3500s, 3450s, 3380s, 3320sh, 3140sh, 2800, 2430, 1700, 1680, 1660, 1392sh, 1356sh, 1340, 1185s, 1115s, 1080, 1000sh, 960s, 895, 820sh, 735, 720, 620, 590, 545s, 515s, 480s, 450sh, 410sh, 400sh, 370sh, 325, (211).

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 3507, 3436, 3376, 3325, 2807w, 2360w, 1713w, 1670w, 1426w, 1351w, 1328w, 1189, 1102s, 1088, 1070, 976, 963, 945w, 940w, 732sh, 726, 552w, 529w, 488, 451w, 426w.

**P745 Sodium gadolinium oxophosphate**  $\text{Na}_2\text{GdO}(\text{PO}_4)_2$ 

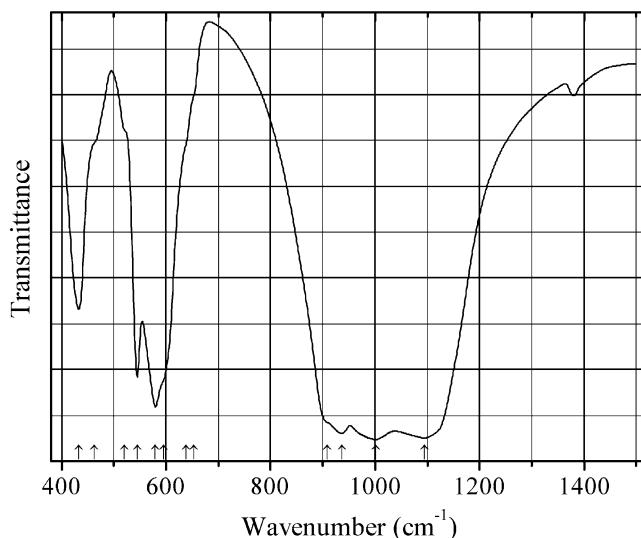
**Origin:** Synthetic.

**Description:** Obtained in the solid-state reaction between  $\text{Gd}_2\text{O}_3$  and  $\text{Na}_4\text{P}_2\text{O}_7$ . Characterized by powder X-ray diffraction data. Orthorhombic, space group  $Pmm2$  (?),  $a = 14.709(6)$ ,  $b = 10.661(4)$ ,  $c = 13.081(6)$  Å. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 14.6929 (30) (100), 6.4964 (60) (002), 3.1178 (43) (231), 2.9417 (45) (500), 2.7821 (100) (323), 2.6547 (50) (040).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Gönen et al. (2000), Uztetik-Amour and Kizilyalli (1995).

**Wavenumbers (cm⁻¹):** 1136sh, 1099s, 1034s, 982s, 965sh, 945sh, 926s, 909sh, 604, 579, 560sh, 548, 523sh, 470, 406w, 381, 367.

**P746 Sodium iron(II) iron(III) phosphate alluaudite-type**  $\text{Na}_2\text{Fe}^{2+} \text{Fe}^{3+}(\text{PO}_4)_3$ 

**Origin:** Synthetic.

**Description:** Synthesized hydrothermally from stoichiometric quantities of  $\text{NaH}_2\text{PO}_4 \cdot \text{H}_2\text{O}$ ,  $\text{FePO}_4$ , and  $\text{FeO}$  at  $400^\circ\text{C}$  for 7 days. Characterized by powder X-ray diffraction data. Monoclinic, space group  $C2/c$ ,  $a = 11.849(2)$ ,  $b = 12.539(1)$ ,  $c = 6.486(1)$  Å,  $\beta = 114.51(1)^\circ$ ,  $V = 876.8(1)$  Å $^3$ ,  $Z = 4$ .

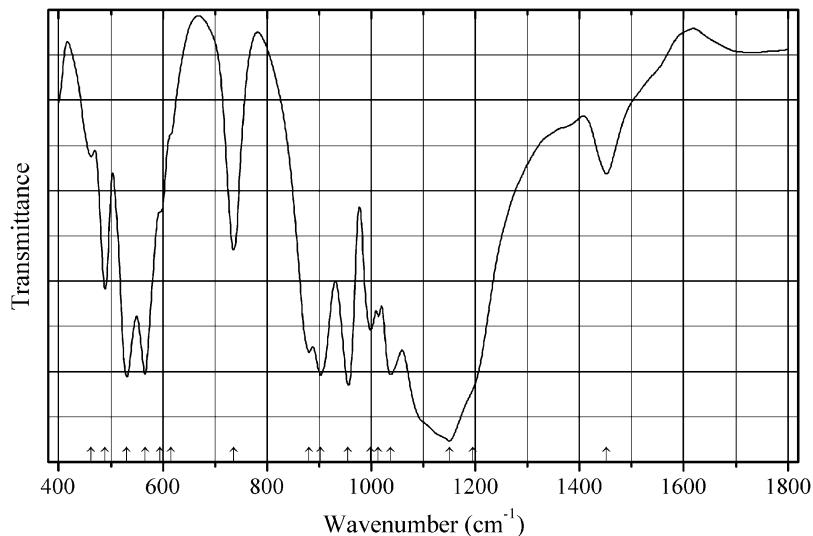
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Hatert et al. (2005).

**Wavenumbers (cm $^{-1}$ ):** 1094s, 1001s, 936s, 909sh, 653sh, 638sh, 595sh, 580s, 545, 520sh, 463sh, 433.

**Note:** A weak band between 1370 and 1380 cm $^{-1}$  may correspond to the  $\text{NO}_3^-$  impurity.

#### P747 Sodium iron(II) pyrophosphate $\text{Na}_2\text{Fe}(\text{P}_2\text{O}_7)$



**Origin:** Synthetic.

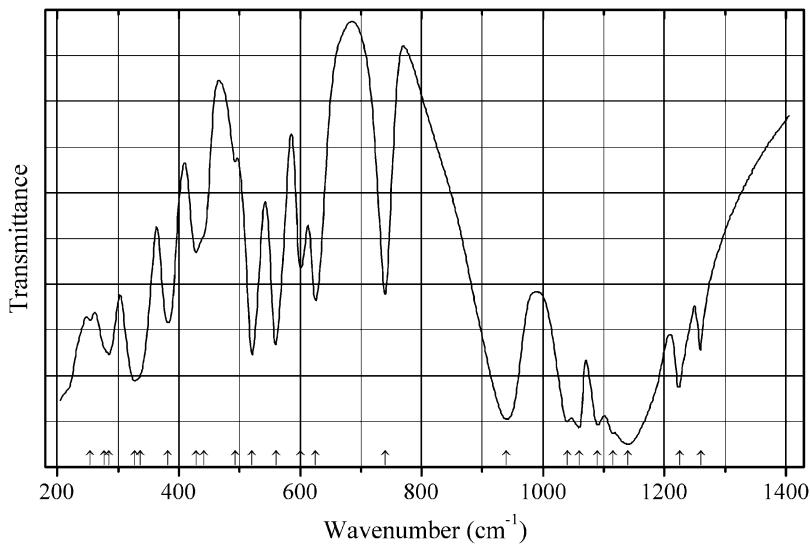
**Description:** Synthesized by a solid-state route from a mixture containing stoichiometric molar amounts of  $\text{Na}(\text{HCO}_3)$ ,  $\text{Fe}(\text{C}_2\text{O}_4) \cdot 2\text{H}_2\text{O}$ , and  $(\text{NH}_4)_2\text{HPO}_4$  at  $600^\circ\text{C}$  for 12 h in a reducing atmosphere. Characterized by powder X-ray diffraction data and Mössbauer spectrum. Triclinic, space group  $P-1$ ,  $a = 6.4415(3)$ ,  $b = 9.4576(4)$ ,  $c = 11.0076(5)$  Å,  $\alpha = 64.685(2)^\circ$ ,  $\beta = 85.989(3)^\circ$ ,  $\gamma = 73.033(3)^\circ$ ,  $V = 578.64(4)$  Å $^3$ .  $\text{Fe}^{2+}$  occupies two independent sites.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Barpanda et al. (2014).

**Wavenumbers (cm $^{-1}$ ):** 1452w, 1196sh, 1150s, 1038s, 1014, 999, 956s, 903s, 881, 736, 616sh, 595sh, 566s, 531s, 489, 462.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. The band at 1452 cm $^{-1}$  may correspond to the admixture of a carbonate.

**P748 Sodium iron(III) pyrophosphate NaFe(P<sub>2</sub>O<sub>7</sub>)**

**Origin:** Synthetic.

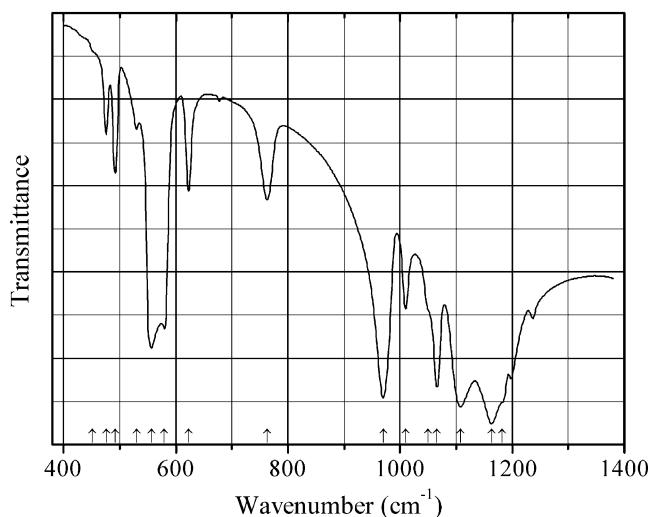
**Description:** Synthesized by stepwise heating of a solid obtained by evaporation of an aqueous solution containing a stoichiometric mixture of NaNO<sub>3</sub>, Fe(NO<sub>3</sub>)<sub>3</sub>·nH<sub>2</sub>O, and (NH<sub>4</sub>)<sub>2</sub>(HPO<sub>4</sub>) first at 120 °C for 24 h, thereafter at 320 °C (to decompose NH<sub>4</sub>NO<sub>3</sub>) and finally, after grinding, at 750 °C for 16 h. Monoclinic, space group P2<sub>1</sub>/c, *a* = 7.3244, *b* = 7.9045, *c* = 9.5745 Å, β = 111.858°, *V* = 514.5 Å<sup>3</sup>, *Z* = 4.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Belkouch et al. (1995).

**Wavenumbers (cm<sup>-1</sup>):** 1260, 1225, 1140s, 1115sh, 1090s, 1060s, 1040s, 940s, 740, 625, 600, 560, 520, 493w, 442sh, 428, 382, 336sh, 327, 285, 277sh, 254.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**P749 Sodium lanthanum pyrophosphate NaLaP<sub>2</sub>O<sub>7</sub>**

**Origin:** Synthetic.

**Description:** Crystals obtained by heating a mixture containing 3 g of  $\text{Na}_3\text{P}_3\text{O}_9$  and 0.5 g of  $\text{La}_2\text{O}_3$ , first at 1000 °C for 20 days and thereafter at 600 °C for 10 h. The crystal structure is solved. Orthorhombic, space group  $Pnma$ ,  $a = 8.645(2)$ ,  $b = 5.317(1)$ ,  $c = 12.737(2)$  Å,  $V = 585.5(2)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 3.810$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

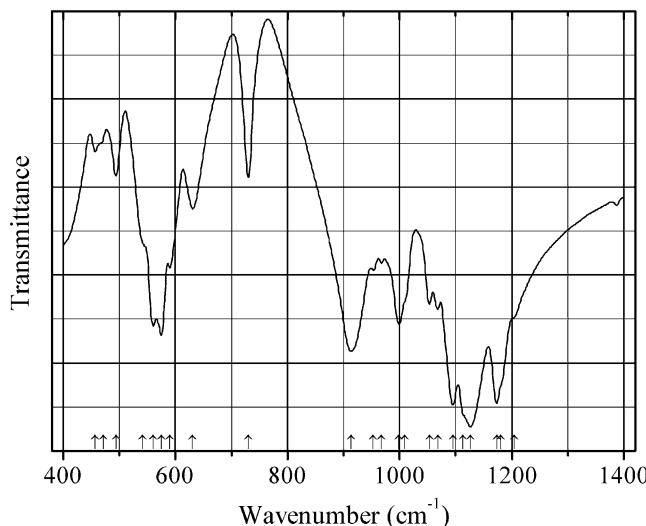
**Source:** Férid and Horchani-Naifer (2004).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1182sh, 1163s, 1108s, 1066s, 1050sh, 1010, 970s, 763, 623, 580, 557s, 530, 492, 476, 451sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1152, 1132, 1086, 1072s, 1005, 939, 778s, 618, 580, 535, 523w, 486, 463, 367w, 324, 305w, 251, 221.

**P750 Sodium magnesium orthophosphate pyrophosphate**  $\text{Na}_4\text{Mg}_3(\text{PO}_4)_2(\text{P}_2\text{O}_7)$   
 $\text{Na}_4\text{Mg}_3(\text{PO}_4)_2(\text{P}_2\text{O}_7)$



**Origin:** Synthetic.

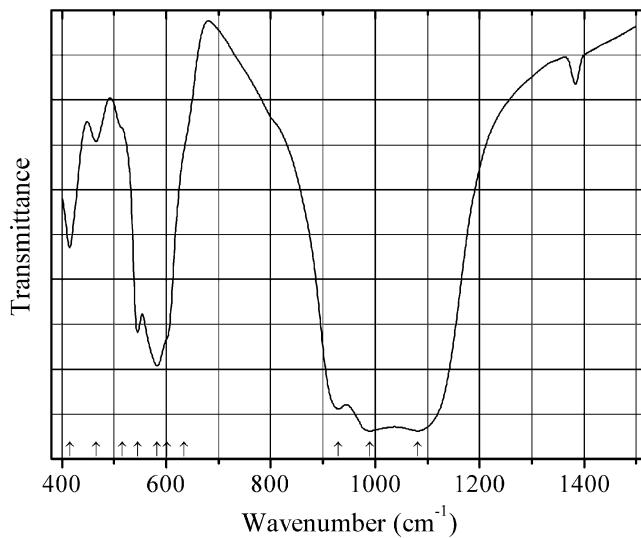
**Description:** Crystals grown from the melt of a mixture of  $\text{Na}_2\text{CO}_3$ ,  $\text{MgO}$ , and  $(\text{NH}_4)(\text{H}_2\text{PO}_4)$  in the molar ratio Na:Mg:P = 4:3:4, by stepwise heating the mixture at 200, 500, and 900 °C followed by cooling down to 400 °C at the rate of 10 °C/h. Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group  $Pn2_1a$ ,  $a = 17.985(2)$ ,  $b = 6.525(9)$ ,  $c = 10.511(1)$  Å,  $V = 1233.58(18)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 2.847$  g/cm<sup>3</sup>. The structure is based on a 3D framework  $[\text{Mg}_3\text{P}_2\text{O}_{13}]$  formed by  $\text{PO}_4^{3-}$  and  $\text{P}_2\text{O}_7^{4-}$  groups and  $\text{MgO}_6$  octahedra.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Essehl et al. (2010).

**Wavenumbers (cm<sup>-1</sup>):** 1205sh, 1180sh, 1173s, 1126s, 1113sh, 1095s, 1068, 1053, 1009sh, 999s, 968, 953, 914s, 730, 631, 590, 575s, 561s, 542sh, 494, 471sh, 457w.

**P751 Sodium manganese(II) iron(III) phosphate alluaudite-type**  $\text{Na}_2\text{Mn}^{2+}\text{Fe}^{3+}(\text{PO}_4)_3$



**Origin:** Synthetic.

**Description:** Synthesized hydrothermally from stoichiometric quantities of  $\text{NaH}_2\text{PO}_4 \cdot \text{H}_2\text{O}$ ,  $\text{FePO}_4$ , and  $\text{MnO}$  at  $400^\circ\text{C}$  for 7 days. Characterized by powder X-ray diffraction data. Monoclinic, space group  $C2/c$ ,  $a = 12.024(4)$ ,  $b = 12.629(6)$ ,  $c = 6.515(3)$  Å,  $\beta = 114.58(4)^\circ$ ,  $V = 899.6(5)$  Å $^3$ ,  $Z = 4$ .

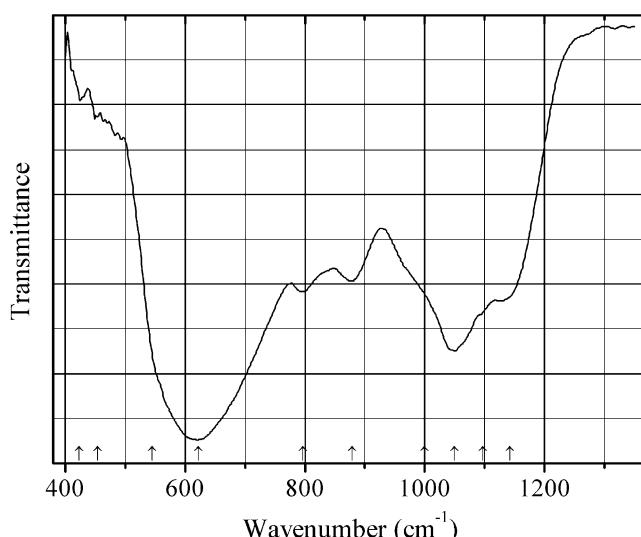
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Hatert et al. (2005).

**Wavenumbers (cm<sup>-1</sup>):** 1082s, 990s, 930s, 634sh, 602s, 583, 545, 516sh, 466w, 415.

**Note:** A weak band between 1370 and 1380 cm $^{-1}$  may correspond to the  $\text{NO}_3^-$  impurity.

**P752 Sodium niobium oxophosphate**  $\text{Na}_3\text{Nb}_5\text{O}_{11}(\text{PO}_4)_2$



**Origin:** Synthetic.

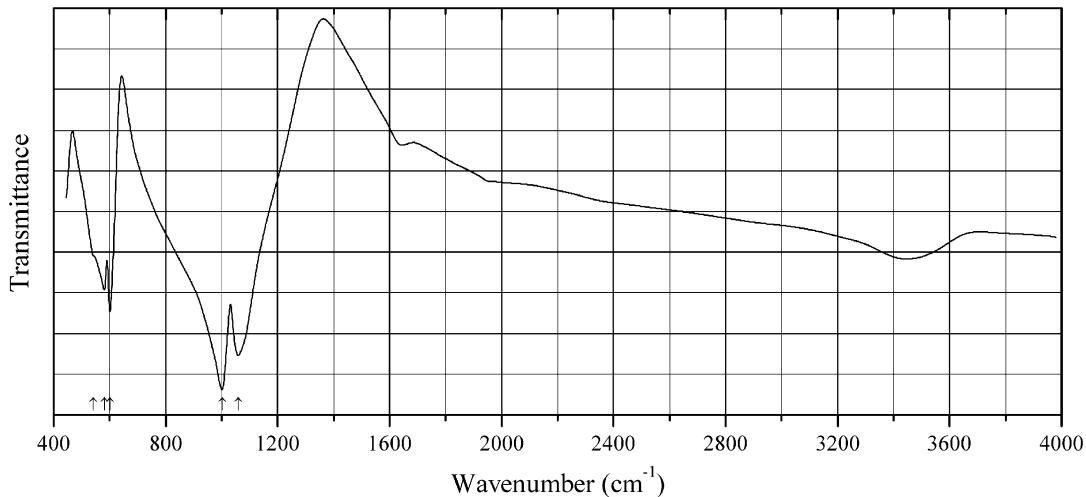
**Description:** Prepared in the cation exchange reaction between  $\text{Ti}_3\text{Nb}_5\text{O}_{11}(\text{PO}_4)_2$  and excess of KCl at 460 °C for 24 h. Characterized by powder X-ray diffraction data and electron microprobe analysis. Trigonal, space group  $R-3c$ ,  $a = 12.979(3)$ ,  $c = 53.613(2)$  Å,  $V = 7822(7)$  Å<sup>3</sup>,  $Z = 18$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Fakhfakh et al. (2003).

**Wavenumbers (cm<sup>-1</sup>):** 1142, 1097sh, 1050s, 999sh, 879, 797, 622s, 545, (454w), (424w).

### P753 Sodium tin orthophosphate $\text{NaSn}_4(\text{PO}_4)_3$



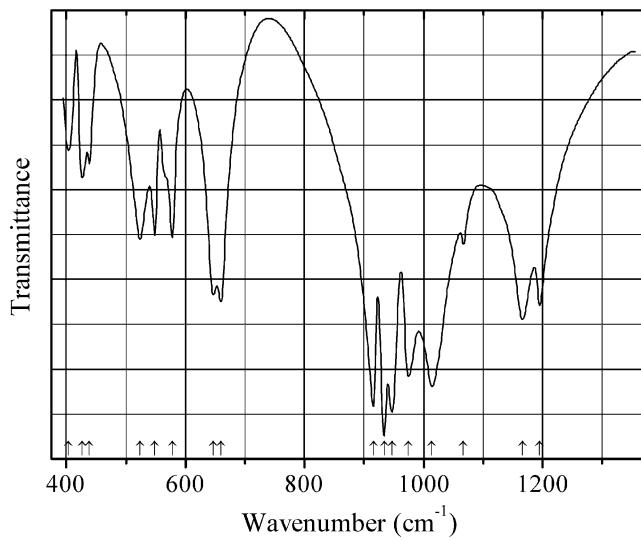
**Origin:** Synthetic.

**Description:** Prepared hydrothermally from  $\text{SnCl}_2$ ,  $\text{NaOH}$ , and  $\text{H}_3\text{PO}_4$  at 170 °C for 3 days. Characterized by powder X-ray diffraction data. The crystal structure is solved. Trigonal, space group  $R3c$ ,  $a = 9.5508(13)$ ,  $c = 24.083(3)$  Å,  $V = 1902.4(4)$  Å<sup>3</sup>,  $Z = 6$ .  $D_{\text{calc}} = 4.099$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Bontchev and Moore (2004).

**Wavenumbers (cm<sup>-1</sup>):** 1059s, 1002s, 601, 581, 543sh.

**P754 Sodium vanadyl phosphate  $\text{Na}_2(\text{VO}_2)(\text{PO}_4)$   $\text{Na}_2(\text{VO}_2)(\text{PO}_4)$** 

**Origin:** Synthetic.

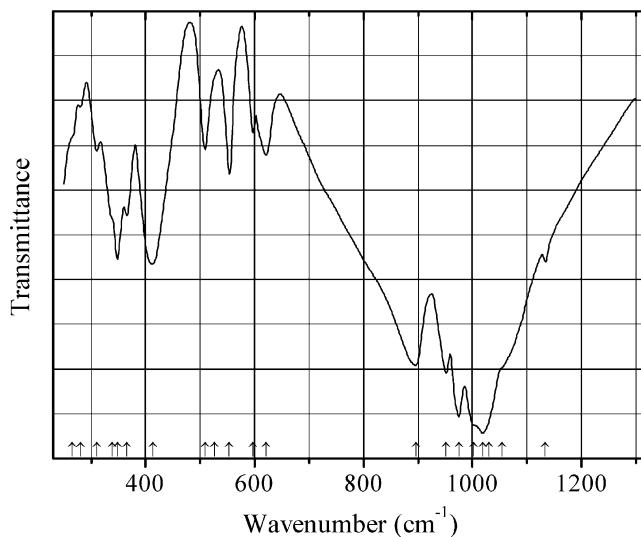
**Description:** Prepared by heating a mixture of  $\text{NH}_4\text{VO}_3$ ,  $(\text{NH}_4)_2(\text{HPO}_4)$ , and  $\text{KNO}_3$  in the molar ratio 1:1:2, first at 350 °C for 2 h and thereafter at 440 °C for 1 h. The crystal structure is solved. Monoclinic, space group  $P2_1/n$ ,  $a = 6.1805(7)$ ,  $b = 12.436(1)$ ,  $c = 7.386(1)$  Å,  $\beta = 107.00(1)$ °,  $V = 542.9(1)$  Å<sup>3</sup>,  $Z = 4$ . Vanadium has fivefold coordination with two short V–O bonds.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Korthuis et al. (1993).

**Wavenumbers (cm<sup>-1</sup>):** 1195, 1166, 1067, 1014s, 975s, 947s, 934s, 916s, 660, 647, 578, 565sh, 549, 524, 439, 427, 404.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**P755 Sodium vanadyl phosphate  $\text{Na}(\text{VO})\text{PO}_4$   $\text{Na}(\text{VO})\text{PO}_4$** 

**Origin:** Synthetic.

**Description:** Prepared hydrothermally. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $Z = 4$ . Vanadium has octahedral coordination.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

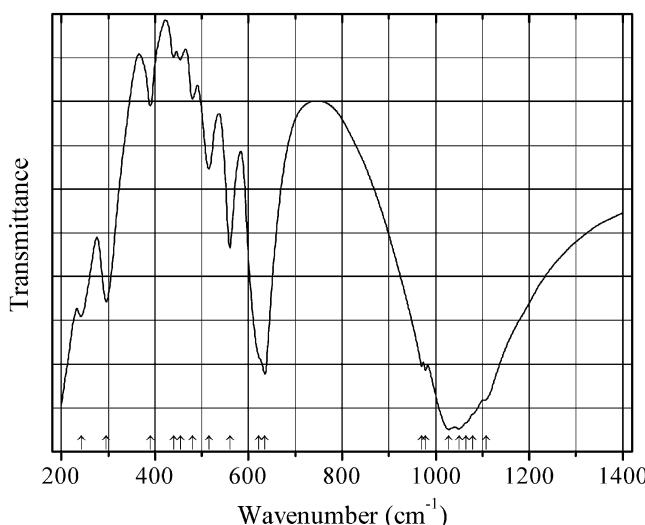
**Source:** Baran et al. (1994).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1134, 1055sh, 1030sh, 1019s, 1002sh, 975s, 952s, 896s, 621, 597w, 554, 527sh, 509, 413, 366, 348, 339sh, 310w, 281w, 265sh.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1025, 1012sh, 1000, 970, 930, 878s, 620, 600, 388, 340, 319, 268.

#### P756 Sodium zinc orthophosphate $\text{NaZn}(\text{PO}_4)$



**Origin:** Synthetic.

**Description:** Single crystals obtained from a  $\text{Na}_2\text{MoO}_4$  flux, decreasing the temperature. Monoclinic, space group  $P2_1/n$ ,  $Z = 12$ . Structurally related to beryllonite.

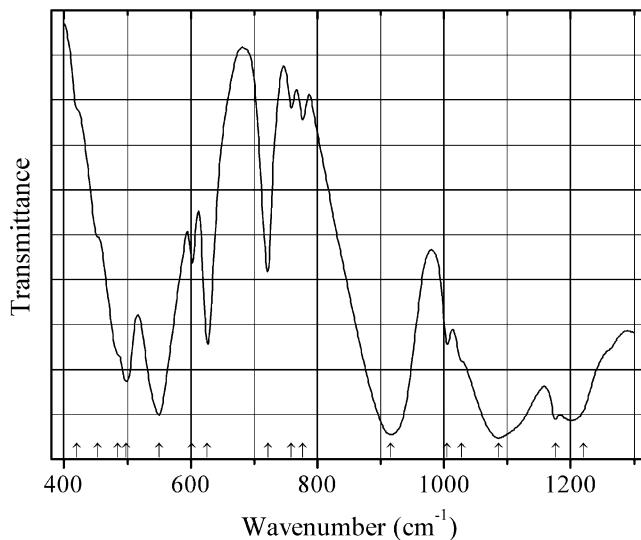
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Botto and Vassallo (1989).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1108sh, 1080sh, 1065sh, 1050s, 1028s, 978, 970, 635s, 622sh, 560, 515, 480, 454w, 440w, 390, 296, 242.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1096, 1066w, 1036, 1029, 1023, 975s, 969s, 634w, 564w, 505w, 384, 378, 222w.

**P757 Sodium zinc pyrophosphate  $\text{Na}_2\text{ZnP}_2\text{O}_7$** 

**Origin:** Synthetic.

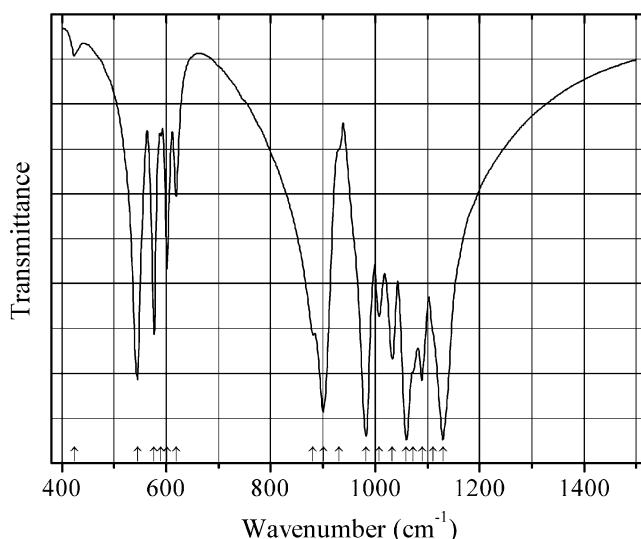
**Description:** Synthesized by heating stoichiometric quantities of  $\text{Na}_2\text{CO}_3$ ,  $\text{ZnO}$ , and  $(\text{NH}_4)_2(\text{HPO}_4)$  first at 523 K and then at 623 K. Characterized by powder X-ray diffraction data. The crystal structure is solved. Tetragonal, space group  $P4_2/n$ ,  $a = 21.771$ ,  $c = 10.285$  Å. The structure is based on  $[\text{ZnP}_2\text{O}_7]$  layers.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Chouaib et al. (2011).

**Wavenumbers (cm<sup>-1</sup>):** 1220s, 1176s, 1086s, 1028sh, 1005, 916s, 777w, 759w, 722, 626, 602, 550s, 498s, 485sh, 453sh, 420sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**P758 Strontium iron phosphate whitlockite-related  $\text{Sr}_9\text{Fe}(\text{PO}_4)_7$** 

**Origin:** Synthetic.

**Description:** Prepared by heating a mixture of  $\text{SrCO}_3$ ,  $\text{Fe}_2\text{O}_3$ , and  $(\text{NH}_4)(\text{H}_2\text{PO}_4)$  with a weight ratio of 9:0.5:7, first at 900 K, and thereafter at 1370 K for 120 h with several intermediate grindings. Characterized by Mössbauer spectroscopy and powder X-ray diffraction data. The crystal structure is solved from powder neutron diffraction data. Monoclinic, space group  $C2/c$ ,  $a = 14.4971(2)$ ,  $b = 10.6005(13)$ ,  $c = 17.9632(3)$  Å,  $\beta = 112.5053(9)^\circ$ ,  $V = 2550.28(7)$  Å<sup>3</sup>,  $Z = 4$ .

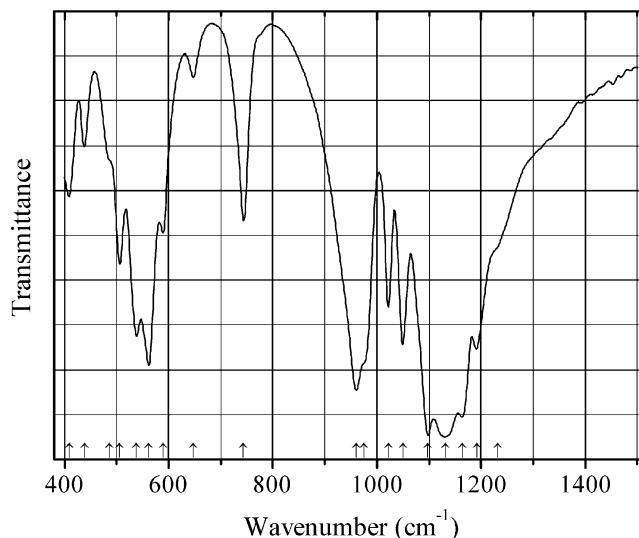
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Belik et al. (2005).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1130s, 1111sh, 1090s, 1072sh, 1060s, 1033, 1008, 983s, 931w, 901s, 881, 619, 601, 590, 577, 545s, 424w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, a figure of the Raman spectrum is given.

#### P759 Strontium magnesium pyrophosphate $\text{SrMgP}_2\text{O}_7$



**Origin:** Synthetic.

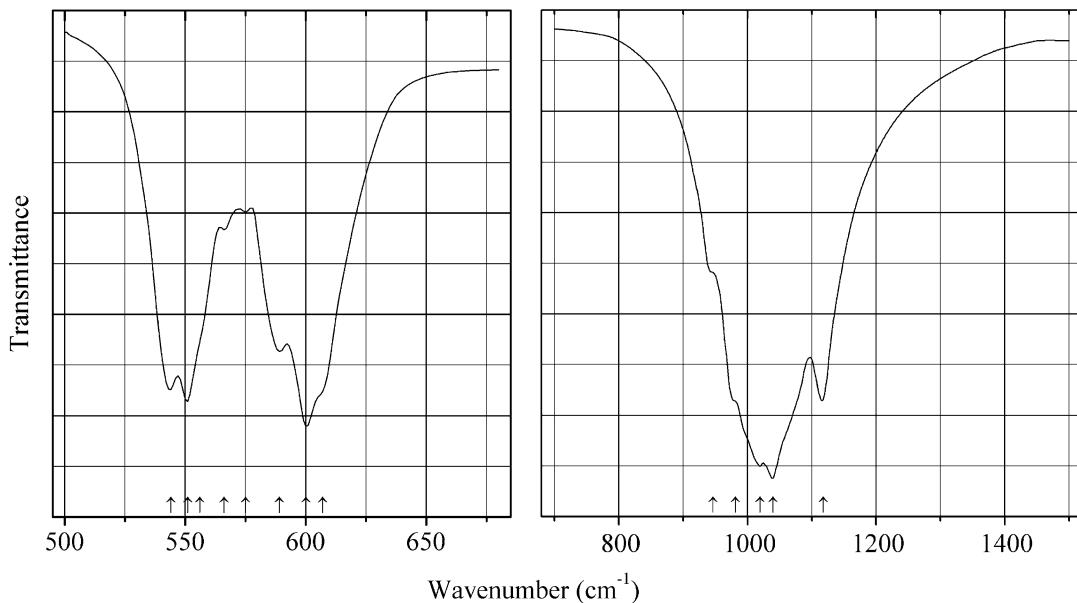
**Description:** Prepared by stepwise heating a mixture of  $\text{SrCO}_3$ ,  $\text{MgCO}_3$ , and  $(\text{NH}_4)(\text{H}_2\text{PO}_4)$ , taken in stoichiometric amounts, at 500, 700, and 900 °C, for 5 h at each temperature, with intermediate grindings. Monoclinic,  $a = 5.309$ ,  $b = 8.299$ ,  $c = 12.68$  Å,  $\beta = 90.6^\circ$ ,  $V = 558.64$  Å<sup>3</sup> (see JCPDS card No. 49-1027).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Velchuri et al. (2011b).

**Wavenumbers (cm<sup>-1</sup>):** 1232sh, 1192, 1164s, 1132s, 1098s, 1050, 1022, 975sh, 960s, 744, 647w, 589, 562, 538, 506, 486sh, 439, 409.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**P760 Calcium strontium orthophosphate whitlockite-type  $\text{Ca}_2\text{Sr}(\text{PO}_4)_2$** 


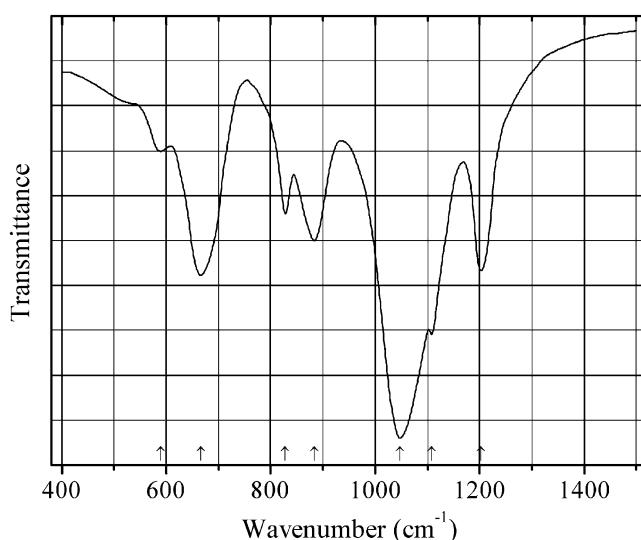
**Origin:** Synthetic.

**Description:** Prepared by heating a mixture of  $\text{CaCO}_3$ ,  $\text{Ce}_2\text{P}_2\text{O}_7$ , and  $\text{Sr}_3(\text{PO}_4)_2$  at 1000 °C for 120 h with grinding every 30 h. Characterized by powder X-ray diffraction data. The crystal structure is solved. Trigonal, space group  $R\bar{3}c$ ,  $a = 10.5612(2)$ ,  $c = 38.0588(5)$  Å,  $V = 3676.32(9)$  Å<sup>3</sup>,  $Z = 21$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Belik et al. (2002).

**Wavenumbers (cm<sup>-1</sup>):** 1117s, 1039s, 1019s, 981sh, 946sh, 607sh, 600s, 589, 575w, 566w, 556sh, 551s, 544s.

**P761 Tantalum oxyphosphate  $\beta\text{-Ta}(\text{PO}_4)\text{O}$** 


**Origin:** Synthetic.

**Description:** Prepared by dehydration of a  $\text{Ta}(\text{PO}_4)\text{O}\cdot n\text{H}_2\text{O}$  precursor at 900 °C. For details of synthesis techniques see Hahn (1951). Monoclinic, space group  $P2_1$  (?).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

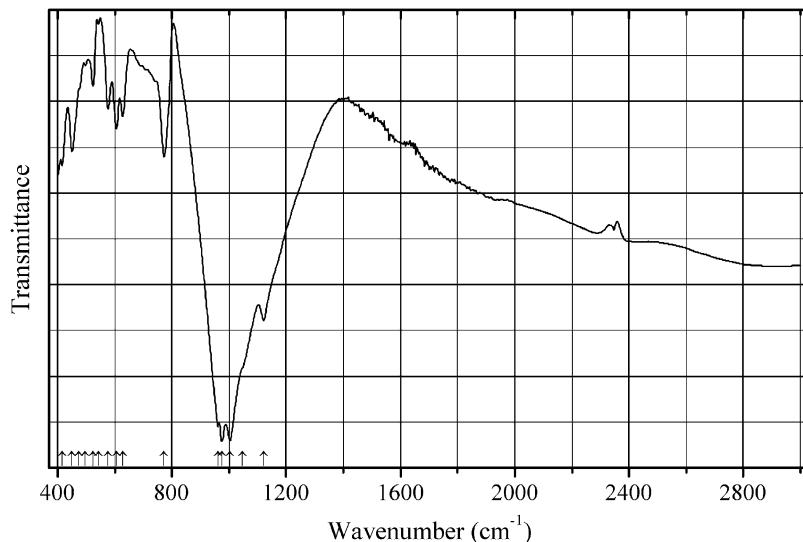
**Source:** Stranford and Condrate Sr (1984c, 1990).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1202, 1108, 1048s, 883, 828, 666, 589w.

**Note:** In the cited papers, Raman spectra are given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1135, 1107, 1041, 1019, 997, 882w, 810w, 671w, 636w, 616w, 606w, 593w, 558w, 471w, 425w, 412w, 384w, 366, 334, 287, 269, 236, 214, 176, 118.

### P763 Tellurium(IV) oxyphosphate $\text{Te}_2(\text{PO}_4)_2\text{O}$



**Origin:** Synthetic.

**Description:** Colorless crystals prepared by heating a mixture of  $\text{TeO}_2$  and  $\text{P}_4\text{O}_{10}$  at 550 °C for 24 h.

Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $Cc$ ,  $a = 5.3819(7)$ ,  $b = 13.6990(19)$ ,  $c = 9.5866(12)$  Å,  $\beta = 103.682(2)^\circ$ ,  $V = 686.73(16)$  Å<sup>3</sup>,  $Z = 4$ . Te has fivefold coordination.

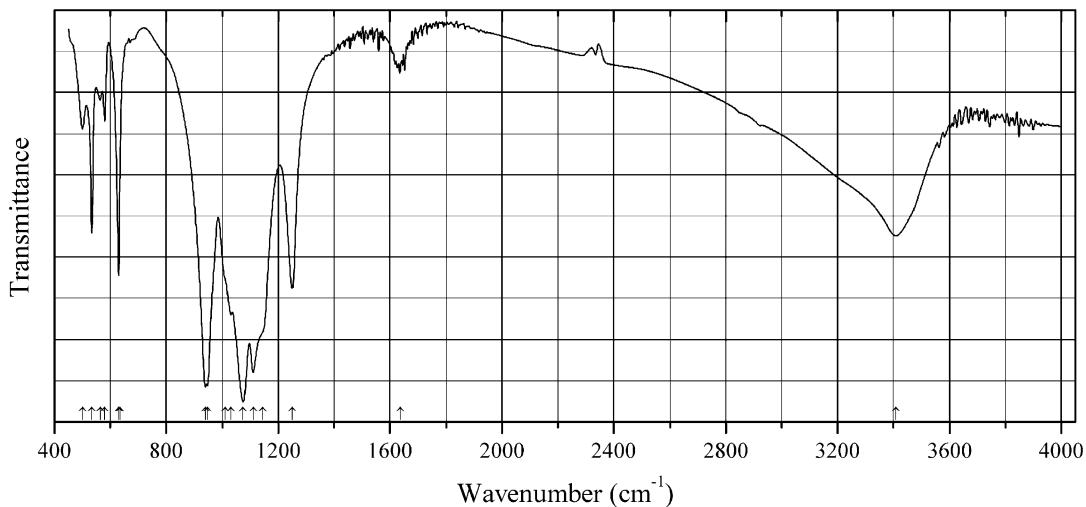
**Kind of sample preparation and/or method of registration of the spectrum:** A sample pressed between two KBr pellets (Authors' wording, maybe erroneous). Transmission.

**Source:** Kim et al. (2010a).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1121, 1047sh, 1004s, 975s, 961, 773, 628, 606, 577, 543w, 524, 498, 476sh, 451, (416).

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**P764 Thorium hydrogenphosphate**  $\text{Th}_2(\text{PO}_4)_2(\text{HPO}_4)\cdot\text{H}_2\text{O}$



**Origin:** Synthetic.

**Description:** Prepared hydrothermally from thorium nitrate and phosphorous acid at 190 °C for 7 days.

Characterized by powder X-ray diffraction data. The crystal structure is solved. Triclinic, space group  $P\bar{2}_1$ ,  $a = 6.7023(8)$  Å,  $b = 7.0150(8)$  Å,  $c = 11.184(1)$  Å,  $\beta = 107.242(4)^\circ$ ,  $Z = 2$ .

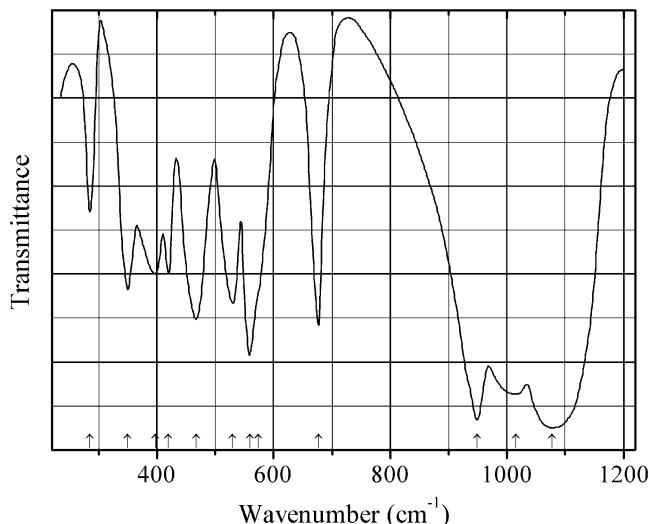
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Salvadó et al. (2005).

**Wavenumbers (cm<sup>-1</sup>):** 3410, 1636w, 1250, 1144sh, 1111s, 1075s, 1030, 1010sh, 947s, 940s, 635sh, 629, 580, 563w, 534, 500.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. Typical bands of P-OH groups (in the range 1800–3000 cm<sup>-1</sup>) are absent in the IR spectrum. However, in the IR spectrum of  $\text{Th}_2(\text{PO}_4)_2(\text{HPO}_4)\cdot\text{H}_2\text{O}$  given by Brandel et al. (2001) a weak band at 2400 cm<sup>-1</sup> is observed.

**P765 Titanium(III) orthophosphate**  $\text{Ti}(\text{PO}_4)$



**Origin:** Synthetic.

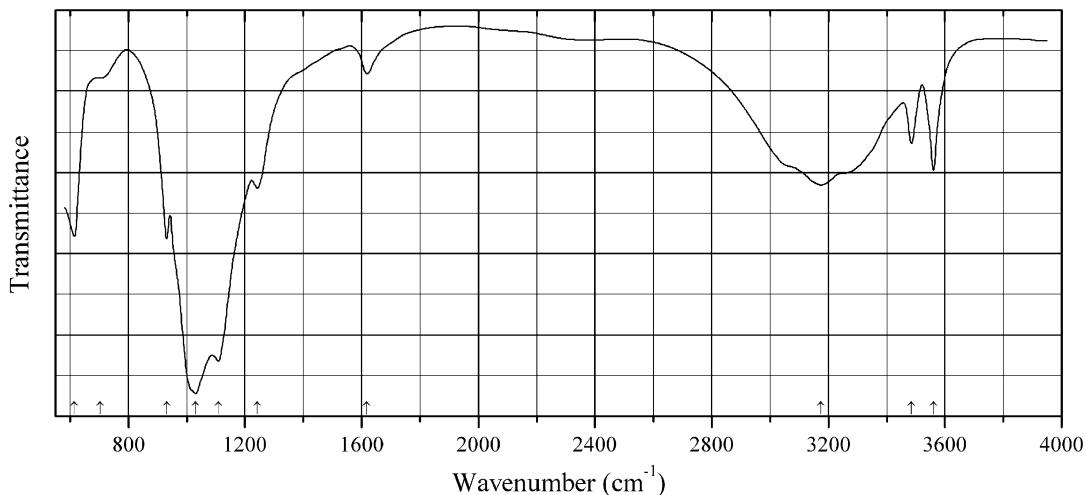
**Description:** Prepared by heating a mixture of  $\text{TiO}_2$  and  $(\text{NH}_4)_2(\text{HPO}_4)$  (in a molar ratio of 1.0:1.1) at 950 °C under reducing conditions (in argon gas, in the presence of iron wires and porous titanium metal). Orthorhombic, isostructural with  $\beta\text{-Cr}(\text{PO}_4)$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Baran et al. (1989).

**Wavenumbers (cm<sup>-1</sup>):** 1078s, 1015s, 949s, 677, 574sh, 559sh, 530, 467, 420, 397, 350, 285.

### P766 Titanium acid phosphate monohydrate $\alpha\text{-Ti}(\text{HPO}_4)_2\cdot\text{H}_2\text{O}$



**Origin:** Synthetic.

**Description:** Prepared in the reaction of a solution of  $\text{TiCl}_4$  in  $\text{HCl}(\text{aq})$  with an aqueous solution of phosphoric acid. Characterized by powder X-ray diffraction data. Monoclinic,  $a = 8.85(6)$ ,  $b = 5.21(3)$ ,  $c = 15.2(1)$  Å,  $\beta = 115.8^\circ$ .

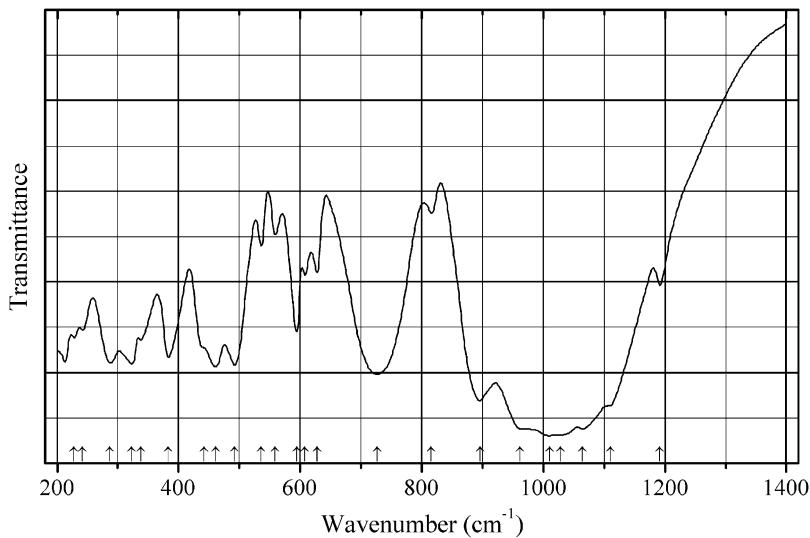
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Slade et al. (1997).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3561, 3484, 3175 (broad), 1617w, 1242, 1108s, 1029s, 932, 702w, 615.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 3559w, 3552, 3528, 3484, 3209, 3012, 1204, 1048sh, 1034sh, 1024s, 1016s, 975w, 588, 492w, 428, 329s, 233, 198, 181, 154w, 108w, 79w.

**P767 Titanium oxophosphate hydrate  $\text{Ti}_2(\text{PO}_4)_2\text{O}\cdot\text{H}_2\text{O}$** 

**Origin:** Synthetic.

**Description:** Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2_1$ ,  $a = 7.3735(12)$ ,  $b = 7.0405(10)$ ,  $c = 7.6609(10)$  Å,  $\beta = 121.48(2)^\circ$ ,  $V = 339.2(1)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{meas}} = 3.10$  g/cm $^3$ ,  $D_{\text{calc}} = 3.13$  g/cm $^3$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 4.795 (64) (−111), 4.688 (37) (110), 3.364 (33) (−112), 2.396 (56) (−222), 2.392 (56) (022), 2.344 (100) (220), 2.300 (39) (−312), 2.293 (38) (112), 1.682 (37) (−224).

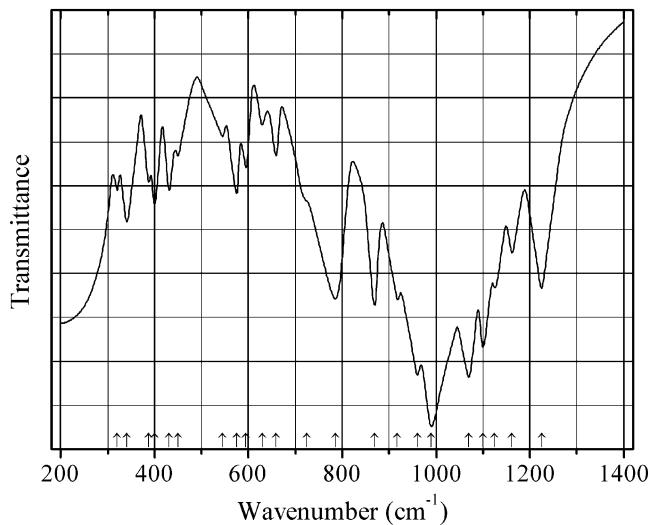
**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

**Source:** Benmokhtar et al. (2007b).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3256, 1651w, 1514w, 1192, 1110s, 1064s, 1028sh, 1010s, 962sh, 896s, 816w, 727s, 628, 608, 594, 559w, 536w, 492, 461, 442sh, 383, 338, 323, 287, 242, 228, 196, 130.

**Note:** In the cited paper, Raman spectrum is given.

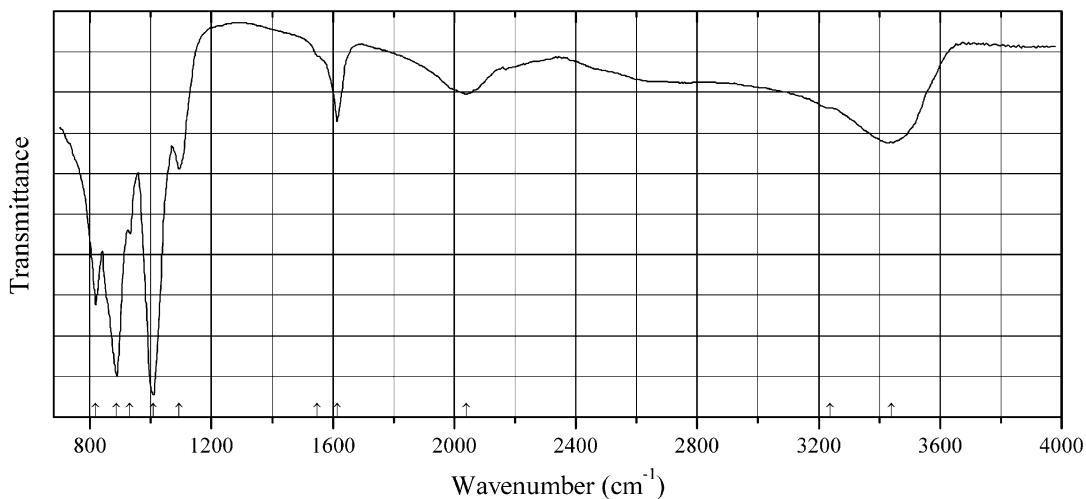
**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1087, 1050w, 1015sh, 1006s, 972sh, 904w, 681s, 642, 614, 601, 585, 536, 498, 451, 410, 376, 348, 323, 287, 268, 245s, 213.

**P768 Tungsten(VI) oxyphosphate**  $\text{W}_2\text{O}_3(\text{PO}_4)_2$ 

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1225, 1162, 1125, 1100, 1070, 990, 960, 918, 869, 785, 725sh, 659, 629, 595, 575, 545, 450, 431, 400, 388, 341, 320.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1210, 1170, 1110, 1090, 1020, 999, 995, 980, 950, 912, 857, 810, 715, 660, 640, 613, 580, 448, 432, 421, 407, 393, 380, 350, 320, 300, 278, 257, 242, 222, 205, 172.

**P769 Uranyl oxy-hydroxyphosphate**  $(\text{UO}_2)_3(\text{PO}_4)\text{O}(\text{OH}) \cdot 3\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Crystals prepared by hydrothermal treatment of crystals of natural albite with inclusions of natural phosphates with 0.1 M solution of uranyl nitrate. Characterized by electron microprobe analysis. The crystal structure is solved. Tetragonal, space group  $P4_2/mbc$ ,  $a = 14.015(1)$ ,  $c = 13.083(2)$  Å,  $V = 2575.6(4)$  Å $^3$ ,  $Z = 8$ .  $D_{\text{calc}} = 5.092$  g/cm $^3$ . The structure contains chains

composed of uranyl pentagonal and hexagonal bipyramids and phosphate tetrahedra linked via common edges.

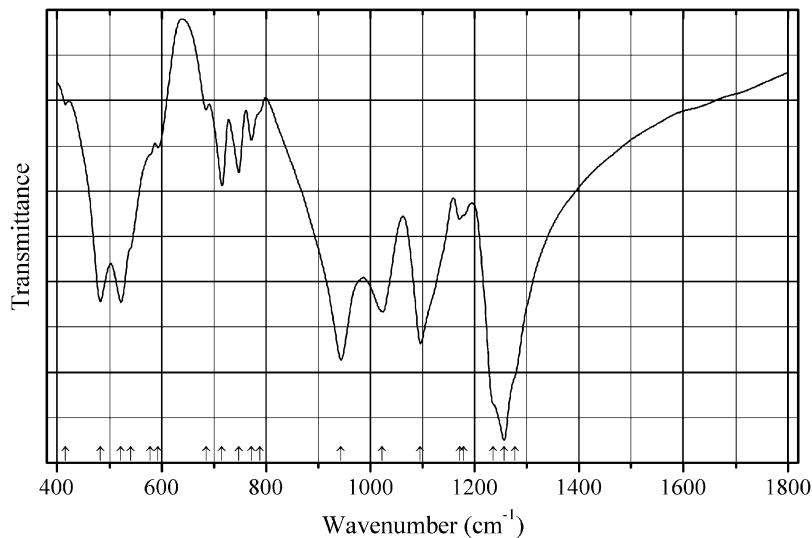
**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of a powdered sample.

**Source:** Burns et al. (2004).

**Wavenumbers (cm<sup>-1</sup>):** 3439, 3237sh, 2040, 1614, 1547sh, 1093, 1008s, 931, 887s, 818.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

#### P770 Yttrium metaphosphate Y(PO<sub>3</sub>)<sub>3</sub>



**Origin:** Synthetic.

**Description:** Prepared by stepwise heating a mixture of Y<sub>2</sub>O<sub>3</sub> and (NH<sub>4</sub>)(H<sub>2</sub>PO<sub>4</sub>) at 170, 240, 350, 440, and 550 °C. Monoclinic. Powder X-ray diffraction pattern corresponds to JCPDS card no. 42-0501.

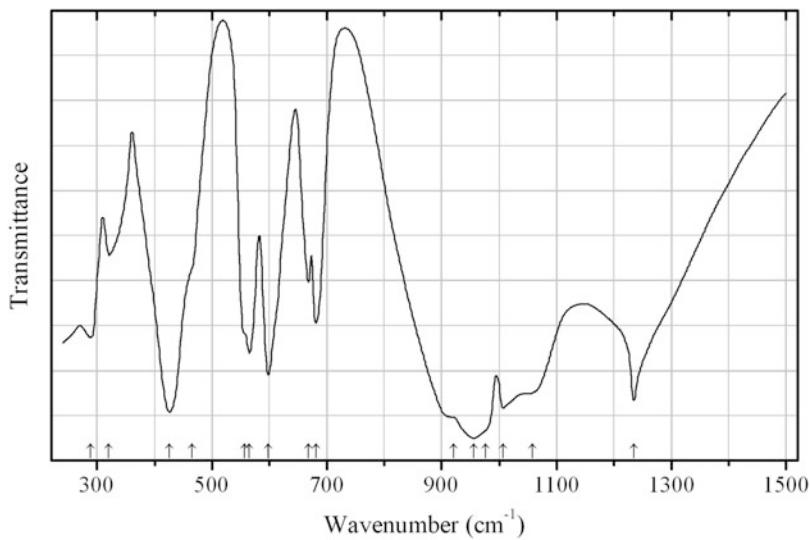
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Ilieva et al. (2001).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1277sh, 1256s, 1235sh, 1179sh, 1171w, 1096s, 1023s, 944s, 789sh, 772w, 748w, 716w, 685w, 593w, 579sh, 541sh, 522s, 483s, 416w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1237s, 1205s, 1171, 1123, 1095, 1055, 1000w, 726, 681s, 568w, 510, 493, 416, 374, 350, 302w, 273w, 250w, 188w.

**P771 Zinc vanadyl phosphate  $\text{Zn}_2(\text{VO})(\text{PO}_4)_2$** 

**Origin:** Synthetic.

**Description:** Prepared by heating a mixture of  $\text{ZnO}$ ,  $\text{VO}_2$ , and  $\text{P}_2\text{O}_5$ , taken in stoichiometric amounts, at  $850^\circ\text{C}$  for 2 days. Characterized by powder X-ray diffraction data. Tetragonal, space group  $I4\text{cm}$ ,  $a = 8.9227(13)$ ,  $c = 9.039(3)$  Å,  $Z = 4$ . The  $\text{Zn}^{2+}$  ions exhibit a square pyramidal coordination.

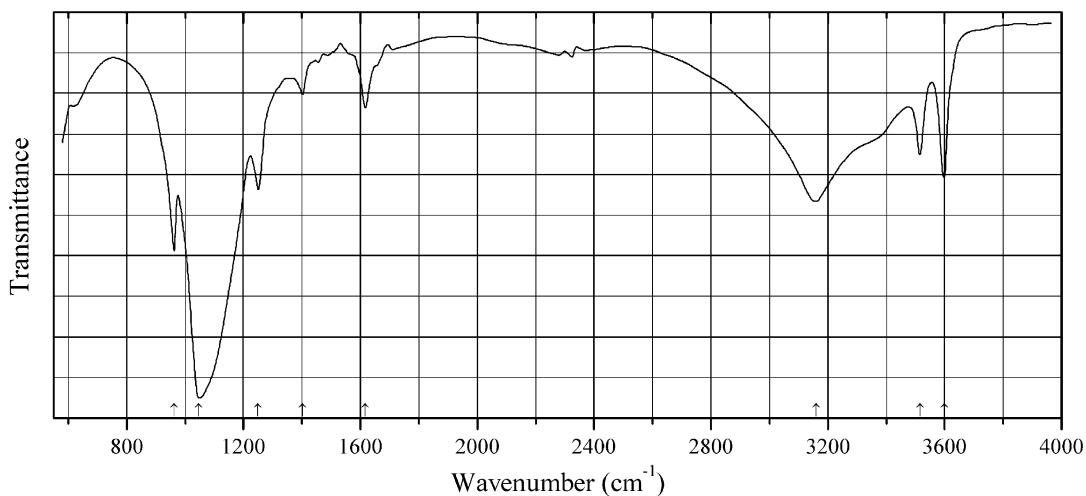
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Baran and Lii (1992).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1235s, 1058s, 1007s, 976sh, 956s, 921sh, 681, 668, 598, 565, 556sh, 465sh, 426s, 320, 288.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1125, 1067, 1010, 976s, 915, 662, 595, 570, 470sh, 430, 413, 325, 285, 248.

**P772 Zirconium acid phosphate monohydrate  $\alpha\text{-Zr}(\text{HPO}_4)_2 \cdot \text{H}_2\text{O}$** 

**Origin:** Synthetic.

**Description:** Characterized by DSC and powder X-ray diffraction data. Monoclinic,  $a \approx 9.06\text{--}9.07$ ,  $b \approx 5.26\text{--}5.31$ ,  $c \approx 16.0\text{--}16.3 \text{ \AA}$ ,  $\beta \approx 111^\circ$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Slade et al. (1997).

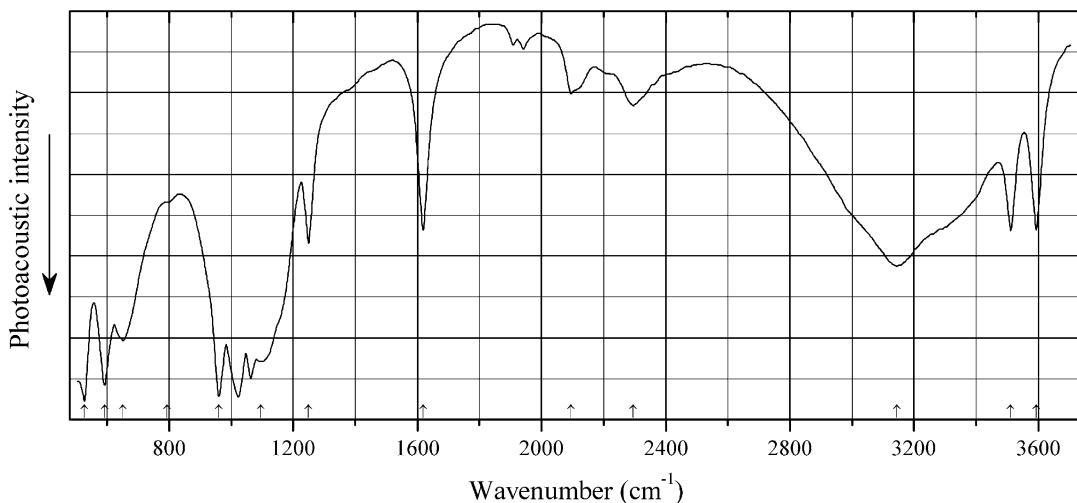
**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3598, 3515, 3159, 1617, 1401w, 1250, 1046s, 963.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 3914w, 3592w, 3515w, 3142w, 2751w, 1613w, 1145w, 1081, 1055s, 990, 964, 591, 540, 517w, 432, 418, 399, 294, 214, 186w, 157, 118w, 107, 79, 63, 55w.

**Note:** Bands of acid phosphate groups (in the range of  $2000\text{--}2400 \text{ cm}^{-1}$ ) are anomalously weak. However, distinct and stronger bands in this range are observed in the IR spectrum of  $\alpha\text{-Zr}(\text{HPO}_4)_2\cdot\text{H}_2\text{O}$  given by Casciola et al. (2007).

### P773 Zirconium acid phosphate monohydrate $\alpha\text{-Zr}(\text{HPO}_4)_2\cdot\text{H}_2\text{O}$



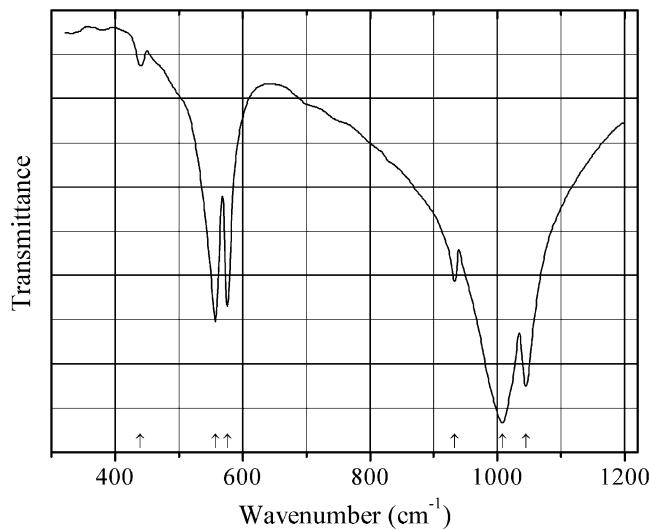
**Origin:** Synthetic.

**Description:** Prepared by the direct precipitation method in the presence of HF. Characterized by powder X-ray diffraction data. Monoclinic (see Slade et al. 1997).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Photoacoustic method of registration.

**Source:** Casciola et al. (2007).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3593, 3511, 3144 (broad), 2295w, 2094w, 1618, 1249, 1095s, (1062, 1024—artifacts), 960s, 793sh, 651, 592s, 527s.

**P774 Alforsite  $\text{Ba}_5(\text{PO}_4)_3\text{Cl}$** 

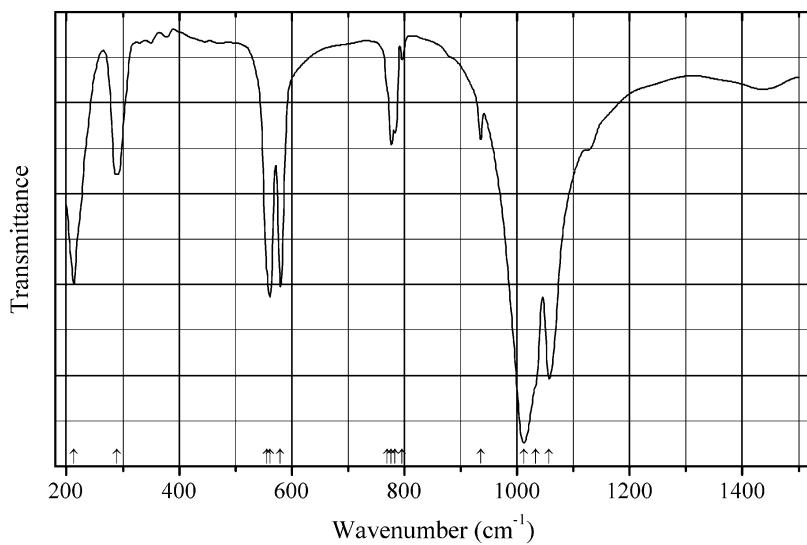
**Origin:** Synthetic.

**Description:** Hexagonal, space group  $P6_3/m$ ,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Baran and Aymonino (1972).

**Wavenumbers (cm<sup>-1</sup>):** 1045s, 1008s, 933, 576, 557, 440w.

**P775 Alforsite F-analogue  $\text{Ba}_5(\text{PO}_4)_3\text{F}$** 

**Origin:** Synthetic.

**Description:** Mn-doped sample obtained by repeated heating a mixture of  $\text{BaCO}_3$ ,  $\text{Mn}_2\text{O}_3$ ,  $\text{NH}_4\text{F}$ , and  $(\text{NH}_4)(\text{H}_2\text{PO}_4)$ , taken in appropriate amounts, at 1250 °C for 12 h. Characterized by powder X-ray diffraction data. The empirical formula is ( $Z = 1$ ):  $\text{Ba}_{10}[\text{P}_{0.95}\text{Mn}_{0.05}\text{O}_4]_6\text{F}_2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Dardenne et al. (1998).

**Wavenumbers (cm<sup>-1</sup>):** 1057s, 1033sh, 1012s, 935.5w, 796w, 783.5, 777, 769sh, 580, 561, 556sh, 290, (213).

**Note:** The bands in the range from 760 to 800 cm<sup>-1</sup> may correspond to  $[\text{MnO}_4]^{3-}$  vibrational modes.

#### P776 Ankoleite $\text{K}(\text{UO}_2)(\text{PO}_4) \cdot n\text{H}_2\text{O}$

**Origin:** Synthetic.

**Description:** Obtained from uranyl nitrate, potassium nitrate, and phosphoric acid mixed in stoichiometric proportions by a wet chemistry method at 60 °C for 4 days. Characterized by TG and powder X-ray diffraction data. Tetragonal, space group  $P4/ncc$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of a powdered sample.

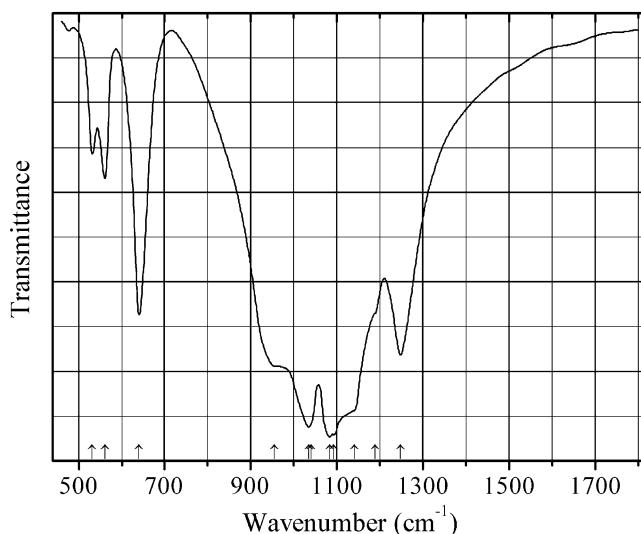
**Source:** Clavier et al. (2016).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3589, 3468, 3350, 3201, 2990, 1658, 1622, 1109, 1059, 985, 904, 866, 813, 666, 541, 529.

**Note:** The wavenumbers are taken from the table given in the cited paper. There are strong discrepancies between these values and the figure of the IR spectrum of ankoleite from this paper. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 3805w, 3498w, 3375w, 3237w, 3110w, 2786w, 1004s, 994s, 831s, 826s, 400, 291, 195, 173, 113, 108.

#### P777 Calcium iron(III) tin orthophosphate $\text{CaFeSn}(\text{PO}_4)_3$



**Origin:** Synthetic.

**Description:** Synthesized by a solid-state reaction technique from a mixture of  $\text{CaCO}_3$ ,  $\text{SnO}_2$ ,  $\text{Fe}_2\text{O}_3$ , and  $(\text{NH}_4)(\text{H}_2\text{PO}_4)$  taken in stoichiometric proportion. Trigonal, space group  $R-3c$ ,  $Z = 6$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

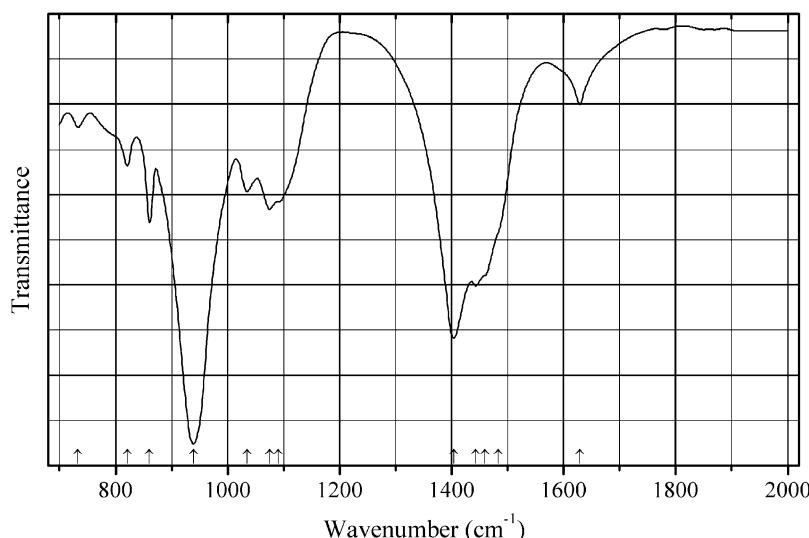
**Source:** Antony et al. (2011).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1248s, 1189sh, 1140sh, 1092sh, 1083s, 1041sh, 1035s, 954s, 641, 561, 532.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1213, 1106s, 1046sh, 999sh, 977sh, 784, 657, 600, 576, 486sh, 436s, 380w, 348, 309, 254sh, 226, 201, 145.

### P778 Jörgkellerite $(\text{Na}, \square)_3\text{Mn}^{3+}_3(\text{PO}_4)_2(\text{CO}_3)(\text{O}, \text{OH})_2 \cdot 5\text{H}_2\text{O}$



**Origin:** Oldoinyo Lengai volcano, Gregory Rift, northern Tanzania (type locality).

**Description:** Brown spherulites from the association with shortite, calcite, fluorite, magnetite, and khanneshite. Holotype sample. The crystal structure is solved. Trigonal, space group  $P-3$ ,  $a = 11.201(2)$ ,  $c = 10.969(2)$  Å,  $V = 1191.9(7)$  Å<sup>3</sup>,  $Z = 3$ .  $D_{\text{calc}} = 2.56$  g/cm<sup>3</sup>. Optically uniaxial (−),  $\omega = 1.700(2)$ ,  $\epsilon = 1.625(2)$ . The empirical formula is (electron microprobe, H<sub>2</sub>O and CO<sub>2</sub> calculated):  $(\text{Na}_{2.46}\text{K}_{0.28}\text{Ca}_{0.08}\text{Sr}_{0.04}\text{Ba}_{0.02})(\text{Mn}^{3+}_{2.39}\text{Fe}^{3+}_{0.56})(\text{PO}_4)_{1.95}(\text{SO}_4)_{0.05}(\text{CO}_3)[\text{O}_{1.84}(\text{OH})_{0.16}] \cdot 5\text{H}_2\text{O}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å (I, %) ( $hkl$ )] are: 10.970 (100) (001), 5.597 (15) (002), 4.993 (8) (111), 2.796 (14) (220), 2.724 (20) (004).

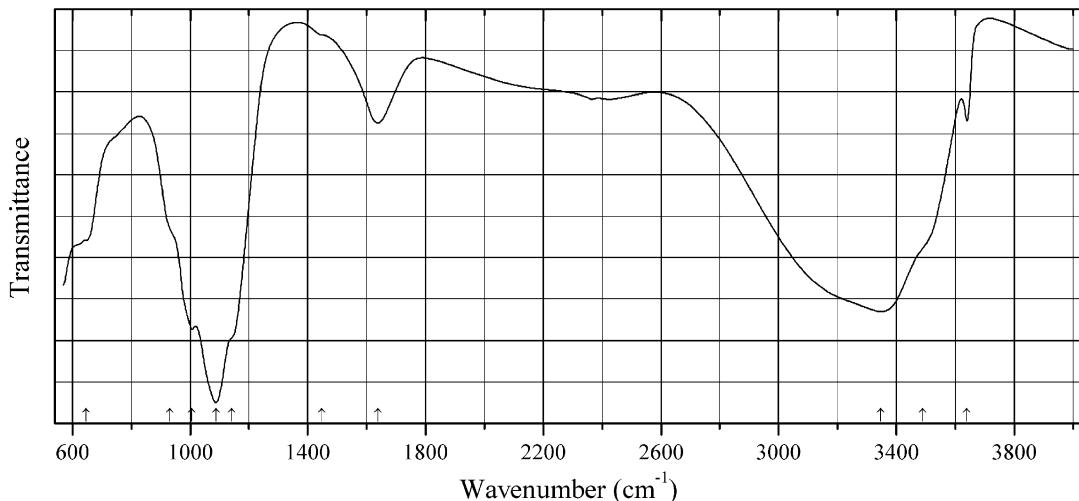
**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection using IR microscope.

**Source:** Zaitsev et al. (2017).

**Wavenumbers (cm<sup>-1</sup>):** 1629, 1483sh, 1459sh, 1443s, 1404s, 1091sh, 1075, 1035, 939s, 861, 821, 733w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The tentative assignment of the strongest band at 939 cm<sup>-1</sup> to phosphate groups made in the cited paper is questionable.

**P779 Ferrivauxite Fe<sup>3+</sup>Al<sub>2</sub>(PO<sub>4</sub>)<sub>2</sub>(OH)<sub>3</sub>·5H<sub>2</sub>O**



**Origin:** Llallagua tin deposit, Rafael Bustillo province, Potosí department, Bolivia (type locality).

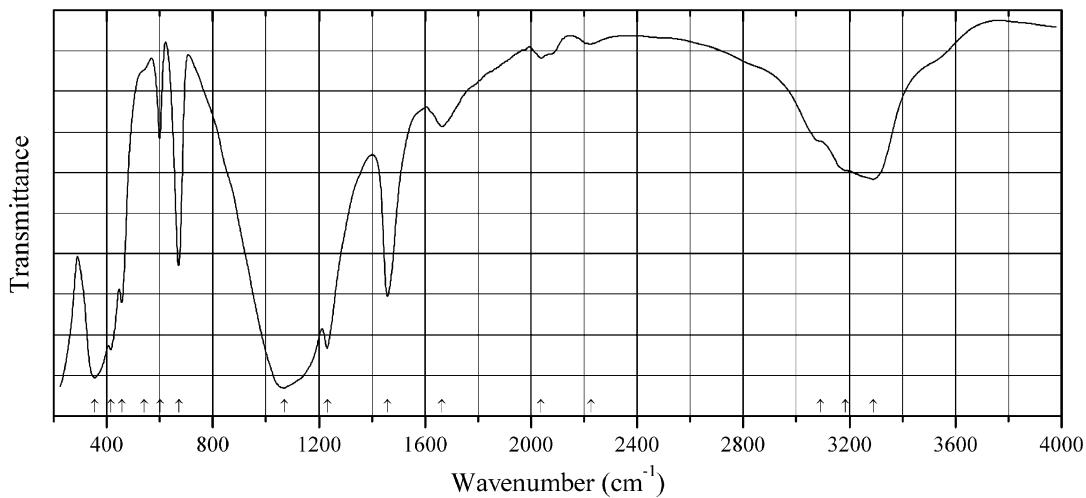
**Description:** Golden brown pseudomorphs after vauxite from the association with sigloite and crandallite. Holotype sample. The crystal structure is solved. Triclinic, space group *P*-1, *a* = 9.198(2), *b* = 11.607(3), *c* = 6.112(2) Å,  $\alpha$  = 98.237(9) $^\circ$ ,  $\beta$  = 91.900(13) $^\circ$ ,  $\gamma$  = 108.658(9) $^\circ$ , *V* = 609.7(5) Å<sup>3</sup>, *Z* = 2. *D*<sub>calc</sub> = 2.39 g/cm<sup>3</sup>. Optically biaxial (-),  $\alpha$  = 1.589(1),  $\beta$  = 1.593(1),  $\gamma$  = 1.596(1), 2*V* = 60(4) $^\circ$ . The empirical formula is (electron microprobe): Fe<sup>3+</sup><sub>0.94</sub>Mn<sub>0.01</sub>Al<sub>1.98</sub>P<sub>2.05</sub>O<sub>8</sub>(OH)<sub>3</sub>·5H<sub>2</sub>O. The strongest lines of the powder X-ray diffraction pattern [*d*, Å (*I*, %) (*hkl*)] are: 10.834 (100) (010), 8.682 (24) (100), 8.242 (65) (-110), 6.018 (28) (001), 5.918 (23) (110), 5.491 (30) (-120), 4.338 (26) (200), 2.898 (32) (300).

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. A diamond anvil microsample cell was used.

**Source:** Raade et al. (2016).

**Wavenumbers (cm<sup>-1</sup>):** 3640, 3490sh, 3348s, 1638, 1447sh, 1142sh, 1087s, 1007s, 932sh, 645sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**P780 Kosnarite NH<sub>4</sub>-analogue (NH<sub>4</sub>)Zr<sub>2</sub>(PO<sub>4</sub>)<sub>3</sub>**

**Origin:** Synthetic.

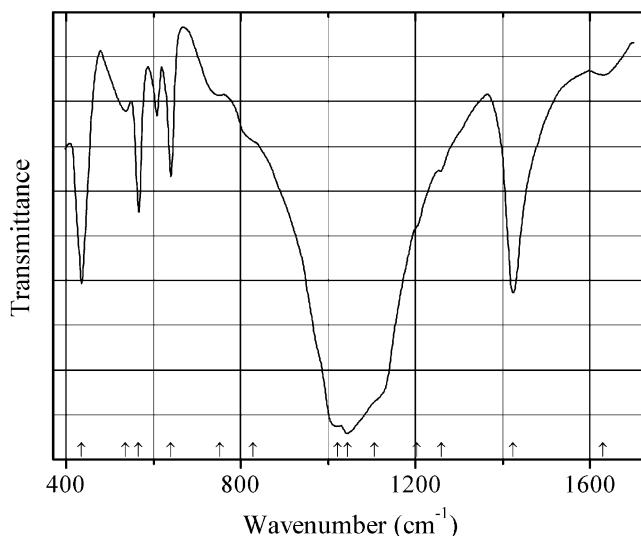
**Description:** Prepared hydrothermally. Rhombohedral,  $a = 8.676(1)$ ,  $c = 24.288(5)$  Å. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 6.394 (67) (102), 4.721 (72) (104), 4.340 (80) (110), 3.825 (92) (113), 3.194 (57) (204), 2.960 (100) (116).

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Clearfield et al. (1984).

**Wavenumbers (cm<sup>-1</sup>):** 3290, 3185sh, 3090sh, 2226w, 2037w, 1665, 1458, 1232s, 1069s, 672, 601, 541sh, 457, 416s, 356s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The band at 1665 cm<sup>-1</sup> indicates the presence of H<sub>2</sub>O molecules.

**P781 Kosnarite NH<sub>4</sub>-analogue cubic polymorph (NH<sub>4</sub>)Zr<sub>2</sub>(PO<sub>4</sub>)<sub>3</sub>**

**Origin:** Synthetic.

**Description:** Prepared by heating a mixture of  $\text{ZrO}_2$  and  $(\text{NH}_4)(\text{H}_2\text{PO}_4)$  at 608 K for 72 h. Cubic,  $a = 1.0186(3)$  Å. Contains minor admixture of rhombohedral  $(\text{NH}_4)\text{Zr}_2(\text{PO}_4)_3$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 5.893 (75) (111), 4.562 (100) (210), 4.164 (33) (211), 3.222 (86) (310), 3.072 (40) (311), 2.723 (75) (321), 1.895 (35) (520).

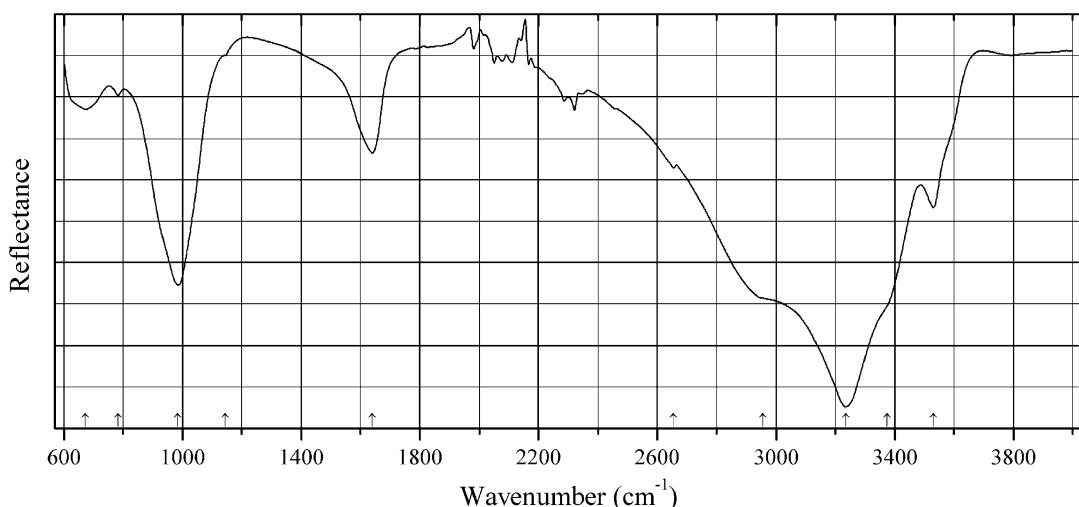
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Ono (1985).

**Wavenumbers (cm<sup>-1</sup>):** (1630w), 1424s, 1260w, 1203sh, 1107sh, 1044s, 1021s, 828sh, 752w, 640, 566, 536, 436s.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

### P782 Kummerite $\text{Mn}^{2+}\text{Fe}^{3+}\text{Al}(\text{PO}_4)_2(\text{OH})_2 \cdot 8\text{H}_2\text{O}$



**Origin:** Hagendorf South pegmatite, Cornelia mine, Hagendorf, Waidhaus, Upper Palatinate, Bavaria, Germany (type locality).

**Description:** Sprays or rounded aggregates of thin amber yellow laths from the association with Zn-and Al-bearing beraunite. Holotype sample. The crystal structure is solved. Triclinic, space group P-1,  $a = 5.316(1)$  Å,  $b = 10.620(3)$  Å,  $c = 7.118(1)$  Å,  $\alpha = 107.33(3)^\circ$ ,  $\beta = 111.22(3)^\circ$ ,  $\gamma = 72.22(2)^\circ$ ,  $V = 348.4(2)$  Å<sup>3</sup>,  $Z = 1$ .  $D_{\text{calc}} = 2.34$  g/cm<sup>3</sup>. Optically biaxial (-),  $\alpha = 1.565(5)$ ,  $\beta = 1.600(5)$ ,  $\gamma = 1.630(5)$ ,  $2V = 70(5)^\circ$ . The empirical formula is  $(\text{Mn}_{0.37}\text{Mg}_{0.27}\text{Zn}_{0.03}\text{Fe}^{2+}_{0.33})(\text{Fe}^{3+}_{1.06}\text{Al}_{0.94})(\text{PO}_4)_{1.91}(\text{OH})_{2.27} \cdot 7.73\text{H}_2\text{O}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 9.885 (100) (010), 6.47 (20) (001), 4.942 (30) (020), 3.988 (9) (-110), 3.116 (18) (1-20), 2.873 (11) (-121).

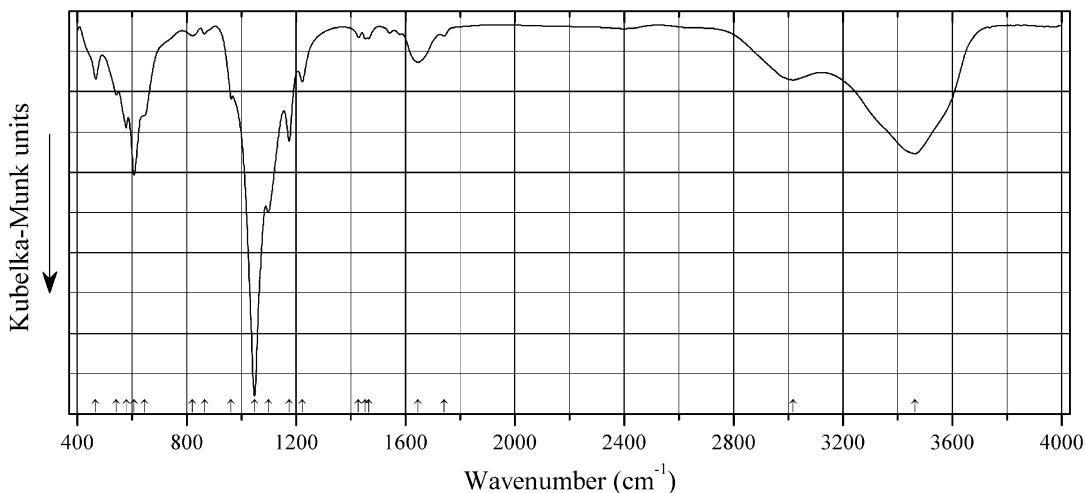
**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of an individual crystal.

**Source:** Grey et al. (2016a).

**Wavenumbers (cm<sup>-1</sup>):** 3530, 3375sh, 3235s, 2955sh, 2655, 1640, 1145sh, 985s, 783w, 674.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### P783 Krásnoite Ca<sub>3</sub>Al<sub>7.7</sub>Si<sub>3</sub>P<sub>4</sub>O<sub>22.9</sub>(OH)<sub>13.3</sub>F<sub>2</sub>·8H<sub>2</sub>O



**Origin:** Huber open pit, Krásno ore district, Czech Republic (type locality).

**Description:** Aggregates of colorless platy crystals. Holotype sample. Trigonal, space group  $P-3m1$ ,  $a = 6.9956(4)$ ,  $c = 20.200(2)$  Å,  $V = 856.09(9)$  Å<sup>3</sup>,  $Z = 3$ .  $D_{\text{meas}} = 2.48(4)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 2.476$  g/cm<sup>3</sup>. Optically uniaxial (+),  $\omega = 1.548(2)$ ,  $\epsilon = 1.549(2)$ . The empirical formula is Ca<sub>3</sub>Al<sub>7.7</sub>Si<sub>3</sub>P<sub>4</sub>O<sub>22.9</sub>(OH)<sub>12.1</sub>F<sub>2</sub>·8H<sub>2</sub>O. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 20.186 (97) (001), 6.736 (100) (003), 5.800 (67) (101, 011), 3.496 (60) (110), 2.8730 (87) (114, 11-4), 2.7633 (73) (203), 2.1042 (75) (109).

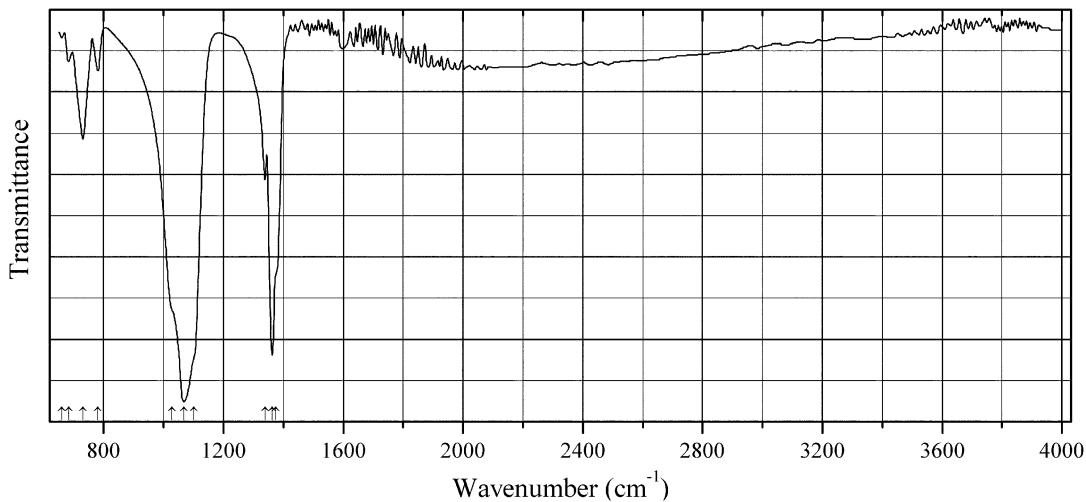
**Kind of sample preparation and/or method of registration of the spectrum:** Micro-diffuse reflectance of a mixture with KBr recalculated in Kubelka-Munk units.

**Source:** Mills et al. (2012b).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3463s, 3017, 174w1, 1645, 1465w, 1453w, 1429w, 1223, 1175, 1098, 1048s, 963, 865w, 820w, 647sh, 608s, 580, 542, 467.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers [Raman, cm<sup>-1</sup>, for the wavelengths 532 nm (785 nm)]:** 1425 (1422), (1289), 1190 (1196), 1091 (1091), 1032 (1032), 1009 (1007), 960 (962), 920 (920), 705 (706), 634 (638), 620 (621), 512 (508), 477 (460), 424 (430), 364 (363), 271, 190, 143.

**P784 Minjiangite  $\text{BaBe}_2(\text{PO}_4)_2$** 

**Origin:** Nanping No. 31 pegmatite, Fujian Province, southeastern China (type locality).

**Description:** White crystals from the association with montebrasite, quartz, muscovite, hydroxylapalite, and palermoite. Holotype sample. The crystal structure is solved. Hexagonal, space group  $P\bar{6}/mmm$ ,  $a = 5.029(1)$  Å,  $c = 7.466(1)$  Å,  $V = 163.52(1)$  Å $^3$ ,  $Z = 1$ .  $D_{\text{calc}} = 3.49$  g/cm $^3$ . Optically biaxial (+),  $\omega = 1.587(3)$ ,  $\epsilon = 1.602(2)$ . The empirical formula is  $(\text{Ba}_{0.99}\text{Ca}_{0.01})\text{Be}_{1.98}(\text{P}_{1.99}\text{Si}_{0.01})\text{O}_8$ .

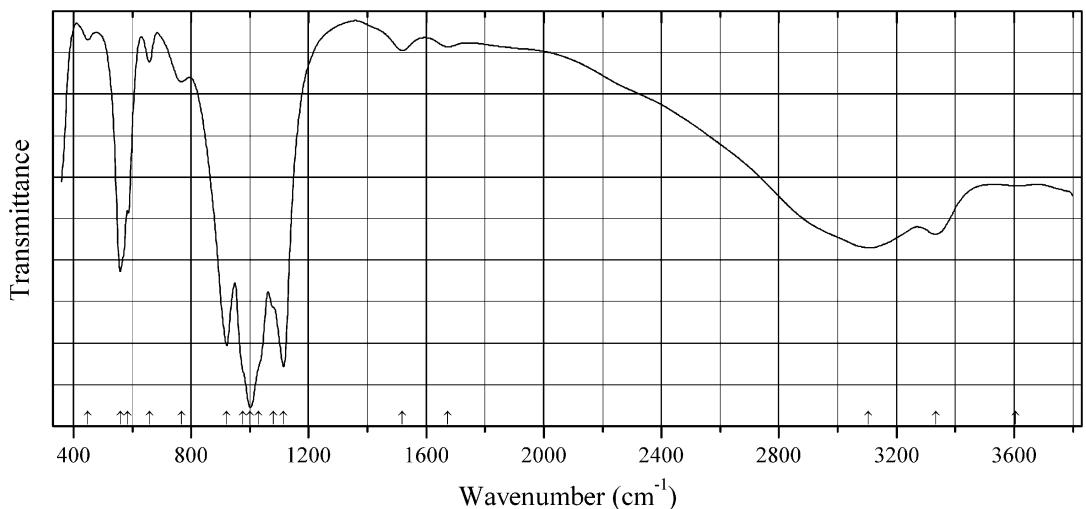
**Kind of sample preparation and/or method of registration of the spectrum:** Reflection.

**Source:** Rao et al. (2015).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1375s, 1363s, 1339s, 1101sh, 1068s, 1027sh, 781, 730, 683w, 660w.

**Note:** Possibly, an erroneous spectrum. In particular, assignment of the strong bands at 1375, 1363, and 1339  $\text{cm}^{-1}$  to Be–O-stretching vibrations (Rao et al. 2015) is questionable. Dal Bo et al. (2014) give another IR spectrum for the synthetic analogue of minjiangite. The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1233s, 1050s, 491, 478, 328w, 189w.

**P785 Xanthoxenite  $\text{Ca}_4\text{Fe}^{3+}(\text{PO}_4)_4(\text{OH})_2 \cdot 3\text{H}_2\text{O}$** 

**Origin:** Palermo No. 1 mine, Groton, Grafton Co., New Hampshire, USA.

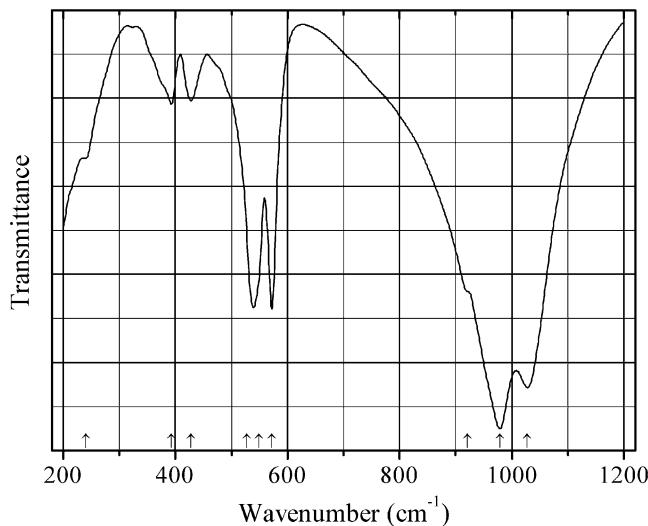
**Description:** Beige crust. Investigated by A.V. Kasatkin. The empirical formula is (electron microprobe):  $(\text{Ca}_{3.49}\text{Mn}_{0.49})\text{Fe}_{2.10}(\text{PO}_4)_{3.92}(\text{OH})_x \cdot n\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3605w, 3334, 3103s, 1674w, 1518w, 1115s, 1080sh, 1030sh, 1001s, 977sh, 921s, 767, 658w, 585, 559s, 448w.

**Note:** The spectrum was obtained by N.V. Chukanov.

#### P786 Oxypyromorphite $\text{Pb}_{10}(\text{PO}_4)_6\text{O}$



**Origin:** Synthetic.

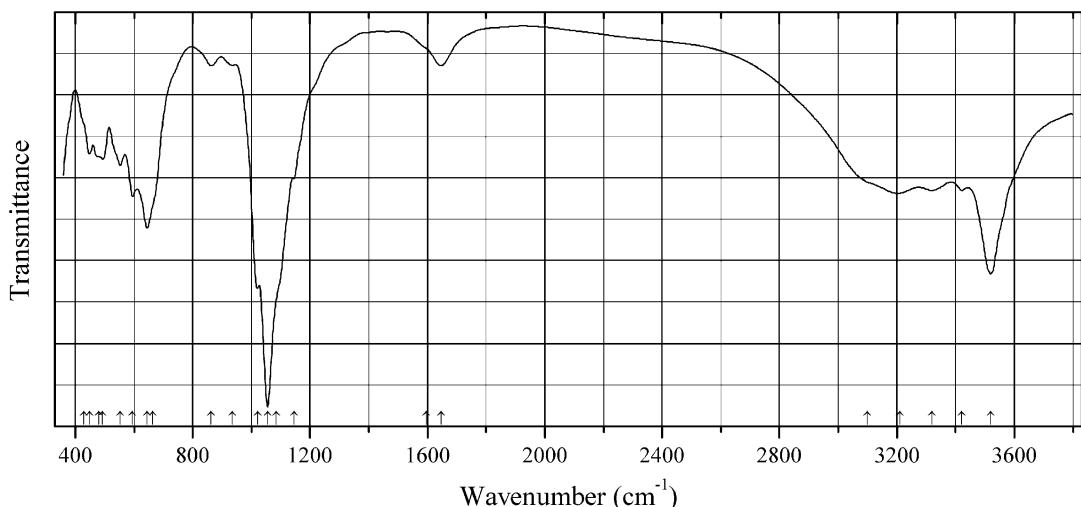
**Description:** Hexagonal, space group  $P6_3/m$  or  $P-6$ ,  $a = 9.826$ ,  $c = 7.431$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** RbI disc. Transmission.

**Source:** Engel (1973).

**Wavenumbers (cm<sup>-1</sup>):** 3560w, 1028s, 979s, 921sh, 572s, 549sh, 538s, 428, 393, 241.

#### P787 Fluorwavellite $\text{Al}_3(\text{PO}_4)_2(\text{OH})_2\text{F} \cdot 5\text{H}_2\text{O}$



**Origin:** Baturovskiy stone quarry, Chelyabinsk region, South Urals, Russia.

**Description:** Pale green radiated aggregate from the association with quartz and crandallite.

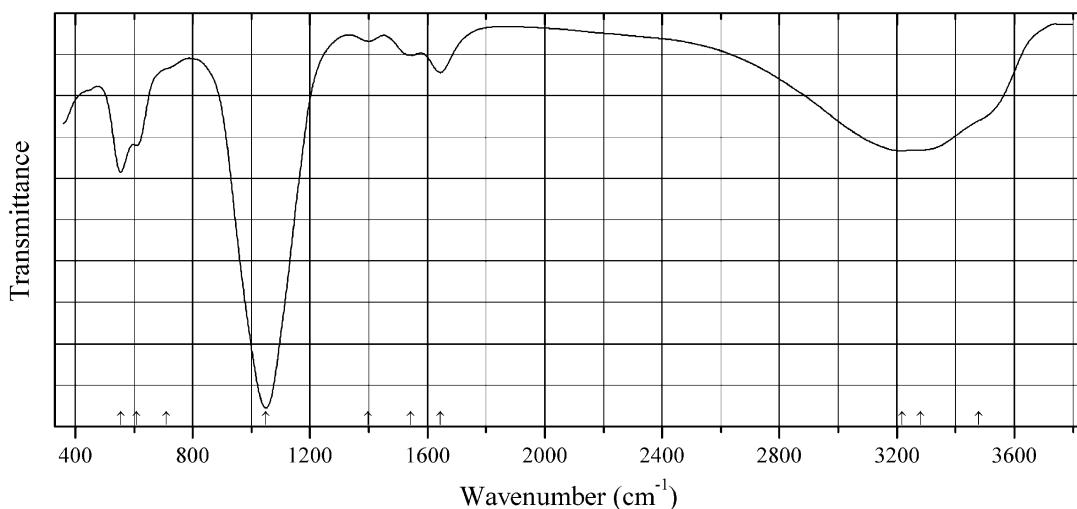
Investigated by A.V. Kasatkin. The empirical formula is (electron microprobe):  $\text{Al}_{2.96}(\text{PO}_4)_{2.04}\text{F}_{0.95}(\text{OH})_x \cdot n\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3519s, 3422, 3320, 3210, 3100sh, 1647, 1595sh, 1145, 1085sh, 1055s, 1022s, 934w, 863w, 665sh, 644s, 595, 552, 493, 479, 448, 430sh.

**Note:** Many samples regarded earlier as wavellite are actually fluorwavellite. The spectrum was obtained by N.V. Chukanov.

### P788 Smirnovskite $(\text{Th},\text{Ca})(\text{PO}_4) \cdot n\text{H}_2\text{O}$



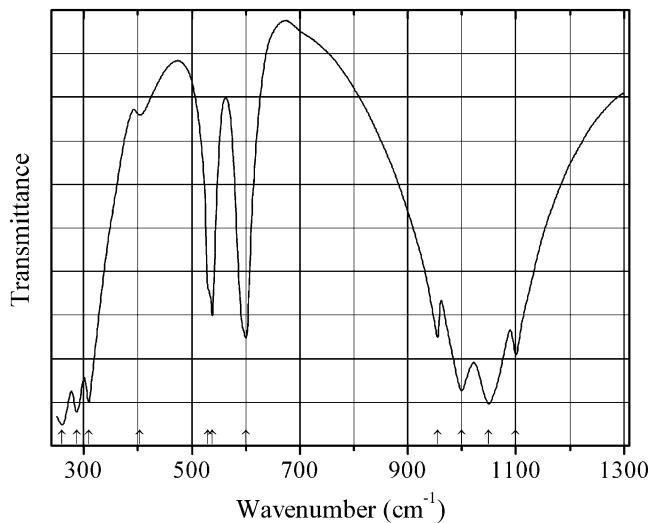
**Origin:** Etyka (Etykinskoe) Ta deposit, Baley district, Transbaikal area, Siberia, Russia.

**Description:** Dark red-brown grain. Investigated by A.V. Kasatkin. X-ray amorphous, metamict. The empirical formula is (electron microprobe):  $(\text{Th}_{0.84}\text{Ca}_{0.22}\text{Pb}_{0.02})(\text{PO}_4)_{0.93}(\text{H}_2\text{O},\text{OH})_x$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3480sh, 3280s, 3217s, 1645, 1543, 1398w, 1049s, 710sh, 608, 554s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P789 Goryainovite**  $\text{Ca}_2(\text{PO}_4)\text{Cl}$ 

**Origin:** Synthetic.

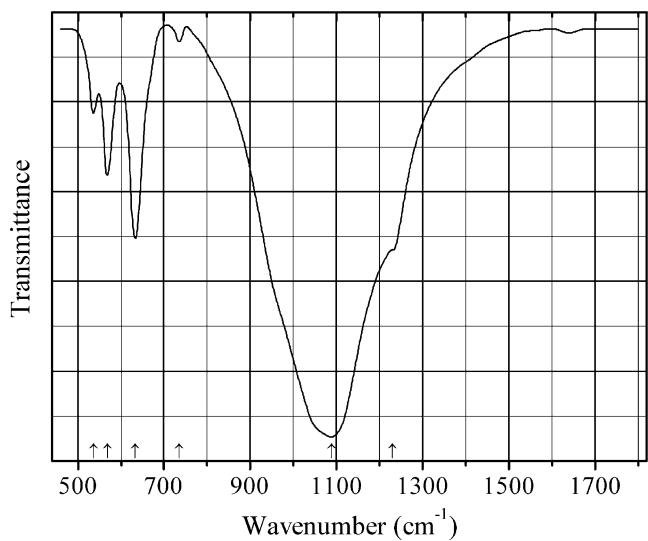
**Description:** Crystals grown from the melt using excess  $\text{CaCl}_2$  as flux (“chlorospodiosite”).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Banks et al. (1967).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1100, 1050s, 1000s, 955, 600, 538, 530sh, 404w, 309s, 287s, 260s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**P790 Sodium iron(III) tin orthophosphate**  $\text{Na}_2\text{FeSn}(\text{PO}_4)_3$ 

**Origin:** Synthetic.

**Description:** Powdery sample synthesized from  $\text{Na}_2\text{CO}_3$ ,  $\text{SnO}_2$ ,  $\text{Fe}_2\text{O}_3$ , and  $(\text{NH}_4)(\text{H}_2\text{PO}_4)$  by a solid-state reaction technique. Hexagonal, space group  $R-3C$ ,  $Z = 6$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

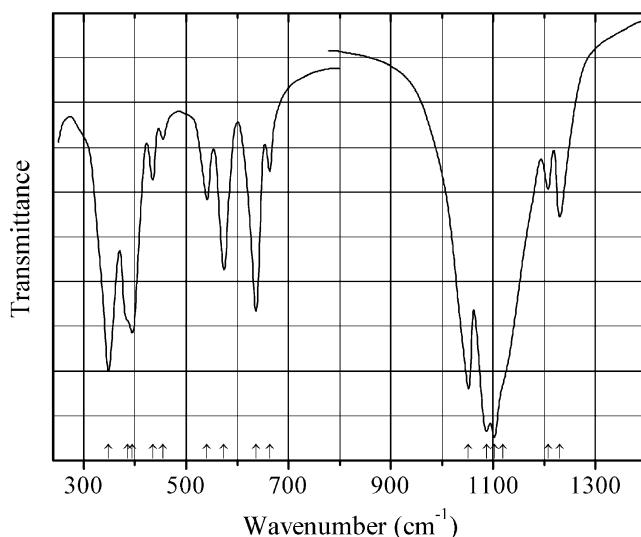
**Source:** Antony et al. (2011).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1230sh, 1088s, 735w, 633, 568, 536w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** (1250), 1042s, 571, 530, 449s, 416, 250, 220, 168.

## P791 Sodium tin phosphate $\text{NaSn}_2(\text{PO}_4)_3$



**Origin:** Synthetic.

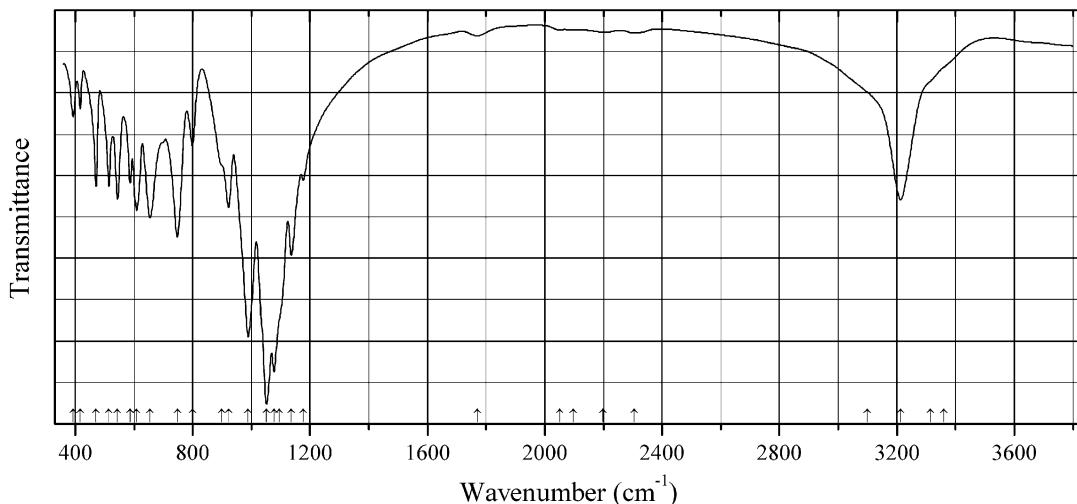
**Description:** Synthesized from  $\text{Na}_2\text{CO}_3$ ,  $\text{SnO}_2$ , and  $(\text{NH}_4)_2(\text{HPO}_4)$  by a solid-state reaction technique. Trigonal, space group  $R-3c$ .  $Z = 6$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission

Source: Tarte et al. (1986).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1230, 1207, 1119sh, 1102s, 1087s, 1052s, 663, 636, 574, 541, 455w, 435, 395s, 385sh, 348s

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**P792 Väyrynenite**  $\text{BeMn}^{2+}(\text{PO}_4)(\text{OH})$ 

**Origin:** Chalot (Chalotuy) Be-Ta pegmatite deposit, Onon district, Transbaikal area, Siberia, Russia.

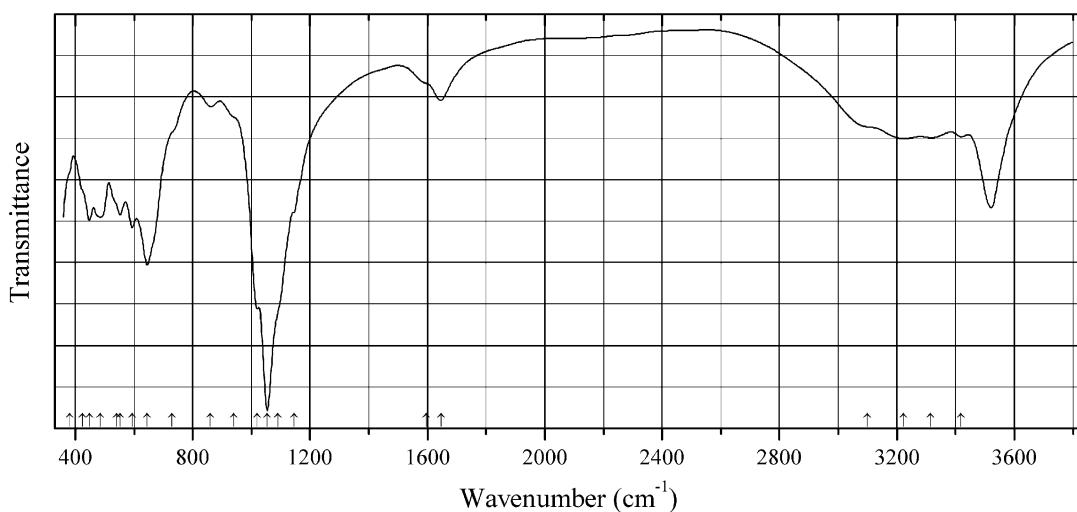
**Description:** Pink grains from the association with muraesite, eosphorite, and fluorapatite.

Investigated by I.S. Lykova. Characterized by single-crystal X-ray diffraction data. Monoclinic,  $a = 4.726(6)$ ,  $b = 14.525(16)$ ,  $c = 5.416(3)$ ,  $\beta = 102.81(8)^\circ$ ,  $V = 362.6(7) \text{ \AA}^3$ . The empirical formula is (electron microprobe):  $\text{Be}_{1.00}(\text{Mn}_{0.69}\text{Fe}_{0.22}\text{Mg}_{0.03}\text{Ca}_{0.03})_{\Sigma 0.97}\text{P}_{1.01}\text{O}_4(\text{OH})$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3360sh, 3315sh, 3213s, 3100sh, 2306w, 2199w, 2096w, 2050w, 1769w, 1177, 1136s, 1095sh, 1078s, 1051s, 989s, 922, 900sh, 799, 748s, 654, 609, 587, 544, 515, 471, 417, 393.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P793 Wavellite-(OH)**  $\text{Al}_3(\text{PO}_4)_2(\text{OH},\text{F})_2 \cdot 5\text{H}_2\text{O}$ 

**Origin:** Mauldin Mt. quarries, Arkansas, USA.

**Description:** White radiated aggregate from the association with quartz. OH-dominant sample.

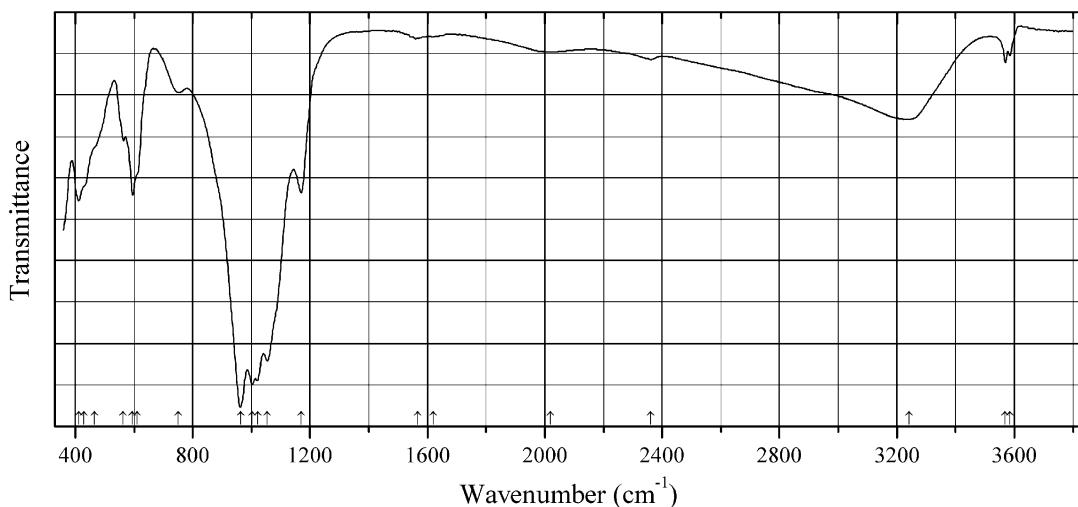
Investigated by A.V. Kasatkin. The empirical formula is (electron microprobe):  
 $\text{Al}_{2.95}(\text{PO}_4)_{2.08}(\text{OH},\text{H}_2\text{O})_2[(\text{OH})_{0.53}\text{F}_{0.47}] \cdot 5\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3223s, 3419, 3315, 3223, 3100, 1647, 1595sh, 1145, 1090sh, 1054s, 1021s, 940sh, 861w, 730sh, 645s, 593s, 552, 540sh, 486, 448, 425sh, 380sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P794 Rockbridgeite**  $\text{Fe}^{2+}\text{Fe}^{3+}_4(\text{P}\square_4)_3(\text{OH})_5$



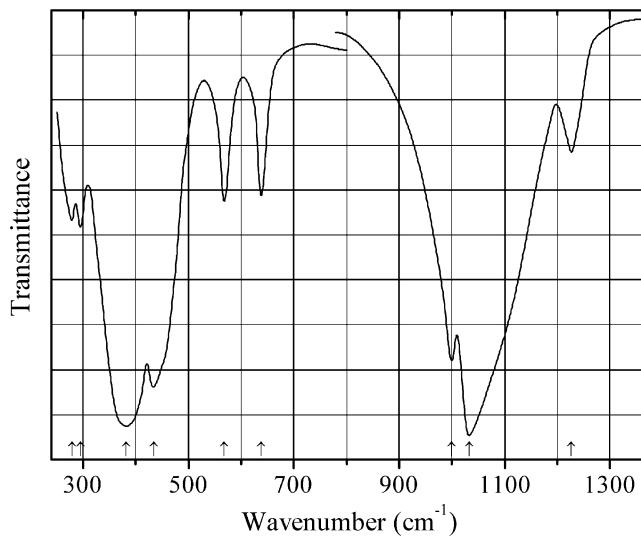
**Origin:** Kyz-Aul deposit, Naberezhnoe, Kerch Peninsula, Kerch iron-ore basin, Russia.

**Description:** Black crystalline crust from the association with leucophosphite. The empirical formula is (electron microprobe):  $(\text{Fe}_{0.93}\text{Mn}_{0.03}\text{Mg}_{0.02}\text{Ca}_{0.02})\text{Fe}_4(\text{PO}_4)_{2.98}(\text{SiO}_4)_{0.02}(\text{OH})_5$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å (I, %)] are: 6.97 (29), 4.847 (28), 4.659 (21), 3.603 (31), 3.460 (34), 3.405 (43), 3.198 (43), 3.198 (100), 2.428 (33).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3585, 3569, 3241, 2360w, 2020w, 1620sh, 1566w, 1170, 1054s, 1022s, 1003s, 963s, 752, 610sh, 595, 563, 465sh, 430sh, 412.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P795 Sodium titanium phosphate**  $\text{NaTi}_2(\text{PO}_4)_3$ 

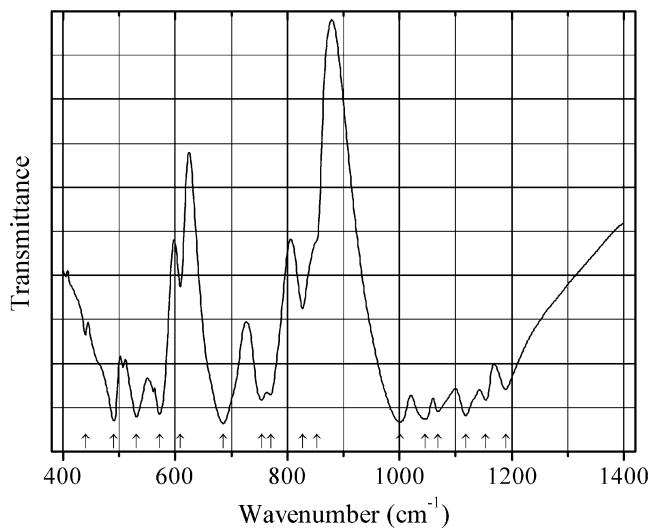
**Origin:** Synthetic.

**Description:** Synthesized from stoichiometric quantities of  $\text{Na}_2\text{CO}_3$ ,  $\text{TiO}_2$ , and  $(\text{NH}_4)_2(\text{HPO}_4)$  by conventional solid-state reaction techniques. Characterized by powder X-ray diffraction data. Hexagonal, space group  $R-3c$ ,  $Z = 6$

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Tarte et al. (1986).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1227, 1033s, 1000, 638, 568, 434, 382s, 295, 279.

**P796 Strontiohurlbutite**  $\text{SrBe}_2(\text{PO}_4)_2$ 

**Origin:** Synthetic.

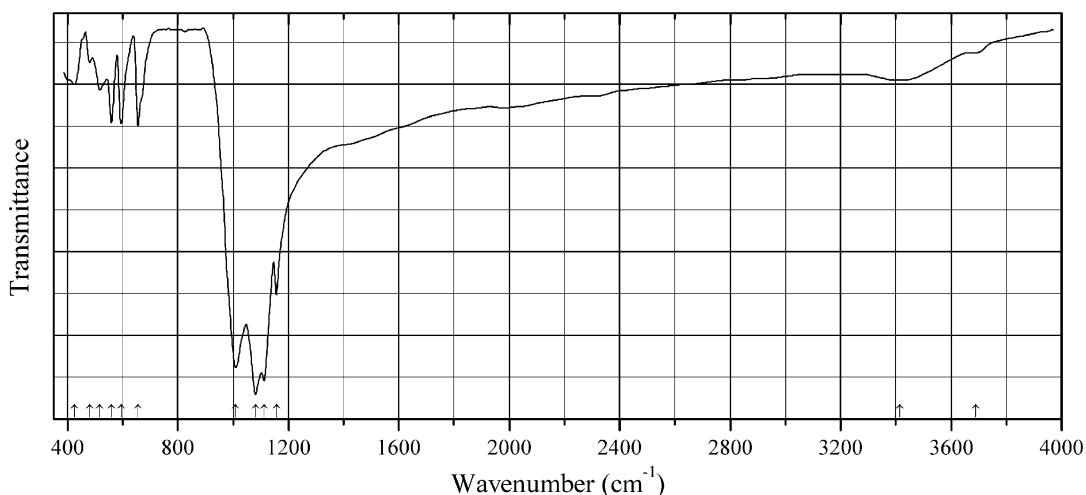
**Description:** Synthesized hydrothermally from BeO, H<sub>3</sub>PO<sub>4</sub>, and Sr(NO<sub>3</sub>)<sub>2</sub> at 200 °C for 7 days with subsequent rapid cooling. The crystal structure is solved. Monoclinic, space group *P2<sub>1</sub>/c*, *a* = 8.000 (1), *b* = 8.986(1), *c* = 8.418(1) Å,  $\beta$  = 90.22(1)°, *V* = 605.10(6) Å<sup>3</sup>, *Z* = 4. *D*<sub>calc</sub> = 3.244 g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Dal Bo et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 1189, 1153s, 1118s, 1068s, 1046s, 1001s, 853sh, 827, 770s, 754s, 686s, 609, 572s, 531s, 507, 491s, 440.

### P798 Triphylite Mg-analogue LiMg(PO<sub>4</sub>)



**Origin:** Synthetic.

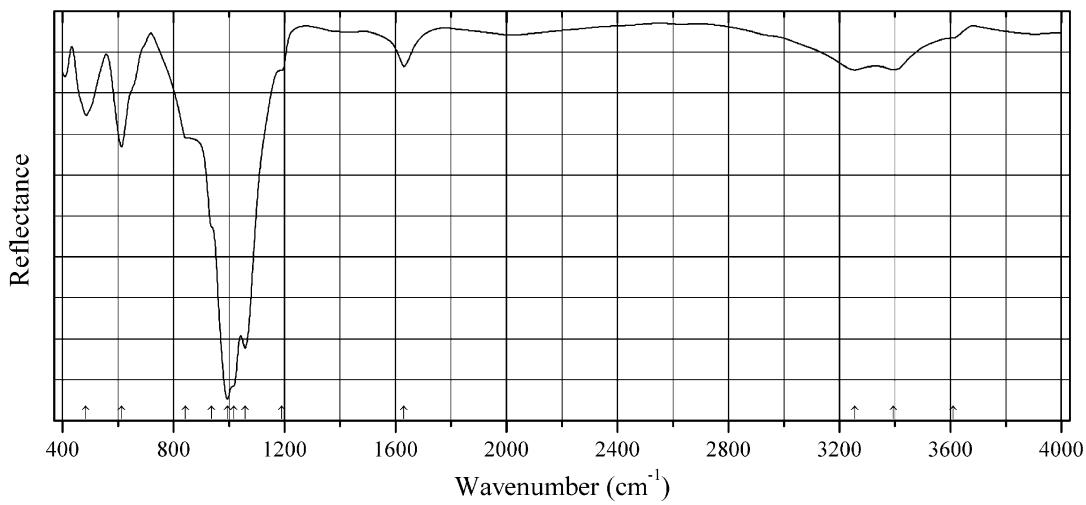
**Description:** Obtained in a solid-state reaction between (NH<sub>4</sub>)Mg(PO<sub>4</sub>)·H<sub>2</sub>O and Li<sub>2</sub>(CO<sub>3</sub>). Characterized by powder X-ray diffraction data. Orthorhombic, space group *Pmn21* (?), *a* = 10.114(4), *b* = 5.928(9), *c* = 4.666(1) Å, *V* = 279.813(3) Å<sup>3</sup>, *Z* = 2.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Sronsri et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 1157, 1112s, 1081s, 1009s, 655, 594, 559, 517, 480w, 425.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. Bands above 3200 cm<sup>-1</sup> may be due to adsorbed water.

**P799 Tvrďite**  $\text{Fe}^{2+}\text{Fe}^{3+}_2\text{Al}_3(\text{PO}_4)_4(\text{OH})_5(\text{H}_2\text{O})_4 \cdot 2\text{H}_2\text{O}$ 

**Origin:** Krásno, near Horní Slavkov, Czech Republic (type locality).

**Description:** Aggregates of olive-greyish-green acicular crystals from the association with quartz, Al-rich beraunite, fluorapatite, and pharmacosiderite. Holotype sample. The crystal structure is solved. Triclinic, space group  $C2/c$ ,  $a = 20.564$ ,  $b = 5.101(1)$ ,  $c = 18.883(4)$  Å,  $\beta = 93.68(3)^\circ$ ,  $V = 1976.7(7)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 2.834$  g/cm $^3$ . Optically biaxial (−),  $\alpha = 1.650(2)$ ,  $\beta = 1.671(1)$ ,  $\gamma = 1.677(1)$ ,  $2V = 56(1)^\circ$ . The empirical formula based on electron microprobe analyses is  $\text{Zn}_{0.52}\text{Fe}^{2+}_{0.50}\text{Fe}^{3+}_{2.21}\text{Al}_{2.75}(\text{PO}_4)_{3.86}(\text{AsO}_4)_{0.19}(\text{OH})_{4.60}\text{F}_{0.23} \cdot n\text{H}_2\text{O}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 10.227 (100) (200), 9.400 (6) (002), 7.156 (14) (20–2), 5.120 (7) (400), 3.416 (11) (600), 3.278 (6) (60–2), 2.562 (5) (800), 2.0511 (3) (10.0).

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of powdered mineral.

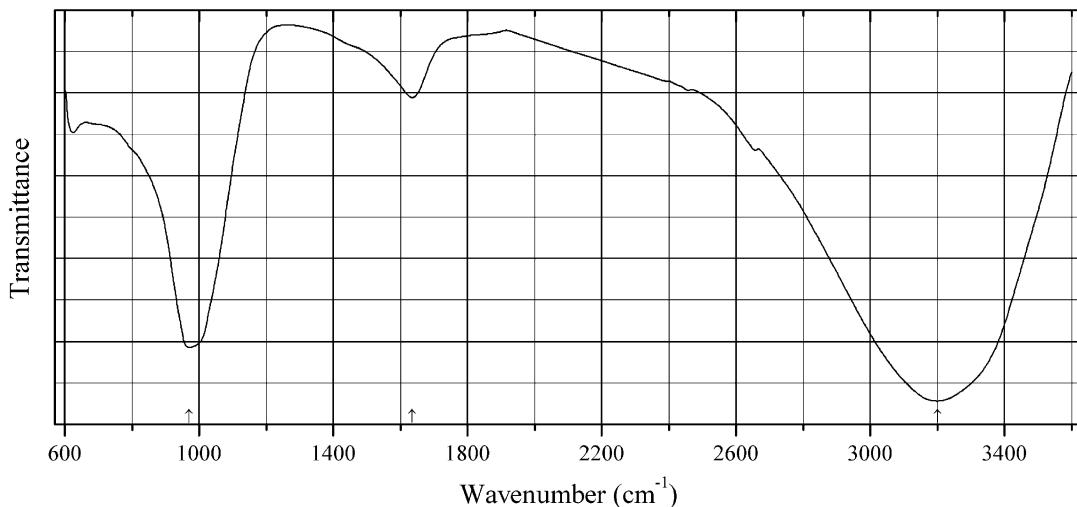
**Source:** Sejkora et al. (2016).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3610sh, 3394, 3255, 1631, 1191sh, 1058s, 1017sh, 994s, 936sh, 843sh, 613, 485.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1623, 1194, 1102, 1023s, 860s, 698, 637, 586, 496, 415, 303, 281, 233, 143.

**P800 Wilhelmgübelite**  $\text{ZnFe}^{2+}\text{Fe}^{3+}_3(\text{PO}_4)_3(\text{OH})_4 \cdot 7\text{H}_2\text{O}$



**Origin:** Hagendorf South pegmatite, Cornelia mine, Hagendorf, Waidhaus, Upper Palatinate, Bavaria, Germany (type locality).

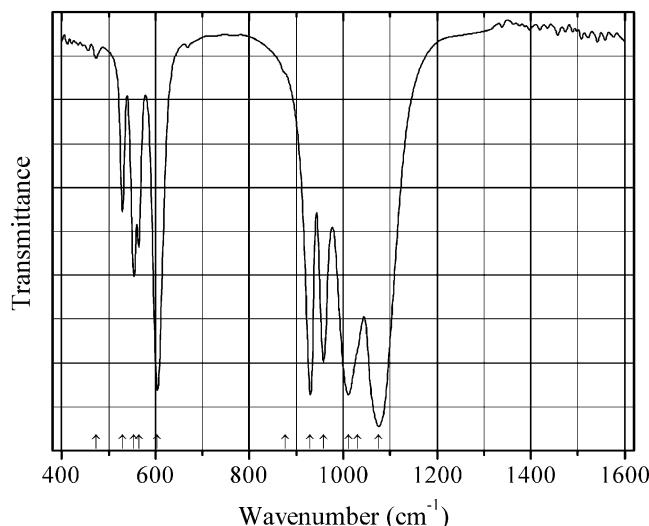
**Description:** Radiating sprays of needle-like rectangular laths from the association with steinmetzite, chalcophanite, jahnsite, mitridatite, albite, apatite, muscovite, and quartz. Holotype sample. The crystal structure is solved. Orthorhombic, space group  $Pmab$ ,  $a = 10.987(7)$ ,  $b = 25.378(13)$ ,  $c = 6.387(6)$  Å,  $V = 1781(2)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 2.82$  g/cm<sup>3</sup>. Optically biaxial (+),  $\alpha = 1.560(2)$ ,  $\beta = 1.669(2)$ ,  $\gamma = 1.718(2)$ ,  $2V = 63(1)$ °. The empirical formula is  $\text{Zn}_{1.50}\text{Mn}^{2+}_{0.27}\text{Fe}^{2+}_{0.60}\text{Fe}^{3+}_{2.33}(\text{PO}_4)_3(\text{OH})_{2.73} \cdot 8.27\text{H}_2\text{O}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 12.65 (100) (020), 8.339 (5) (120), 6.421 (14) (001), 6.228 (8) (011), 4.223 (30) (120) and 2.111 (7) (0.12.0).

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of powdered mineral.

**Source:** Grey et al. (2016c).

**Wavenumbers (cm<sup>-1</sup>):** 3200s, 1635, 970s.

**P801 Ximengite polymorph**  $\text{Bi}(\text{PO}_4)$



**Origin:** Synthetic.

**Description:** Obtained by heating trigonal  $\text{Bi}(\text{PO}_4)$  (ximengite) at 673 K for 5 h. Characterized by powder X-ray and neutron diffraction. Monoclinic, space group  $P2_1/n$ ,  $a = 6.7552(1)$ ,  $b = 6.9417(2)$ ,  $c = 6.4772(2)$  Å,  $\beta = 103.691(2)^\circ$ ,  $V = 295.10(1)$  Å $^3$ ,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

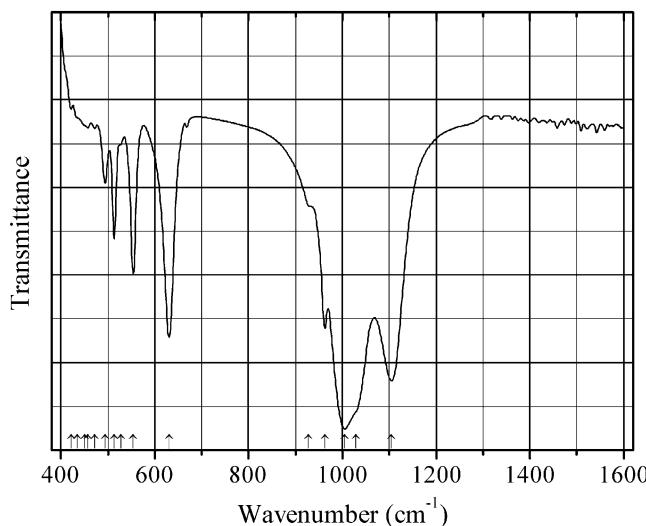
**Source:** Achary et al. (2013).

**Wavenumbers (IR, cm $^{-1}$ ):** 1076s, 1031sh, 1011s, 958s, 930s, 876sh, 604s, 564, 554, 529, 473w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 1050, 1039, 1021, 981, 970, 948, 926, 604, 598, 573, 557, 523, 496, 464, 457, 407, 388, 284, 273, 237, 230, 207, 183, 177, 170, 136, 131, 109, 97, 90, 70, 60, 51.

### P802 Ximengite polymorph $\text{Bi}(\text{PO}_4)$



**Origin:** Synthetic.

**Description:** Obtained by heating trigonal  $\text{Bi}(\text{PO}_4)$  (ximengite) at 973 K for 5 h. Characterized by powder X-ray and neutron diffraction data. Monoclinic, space group  $P2_1/m$ ,  $a = 4.8804(1)$ ,  $b = 7.0684(2)$ ,  $c = 4.7033(1)$  Å,  $\beta = 96.285(3)^\circ$ ,  $V = 161.27(1)$  Å $^3$ ,  $Z = 2$ .

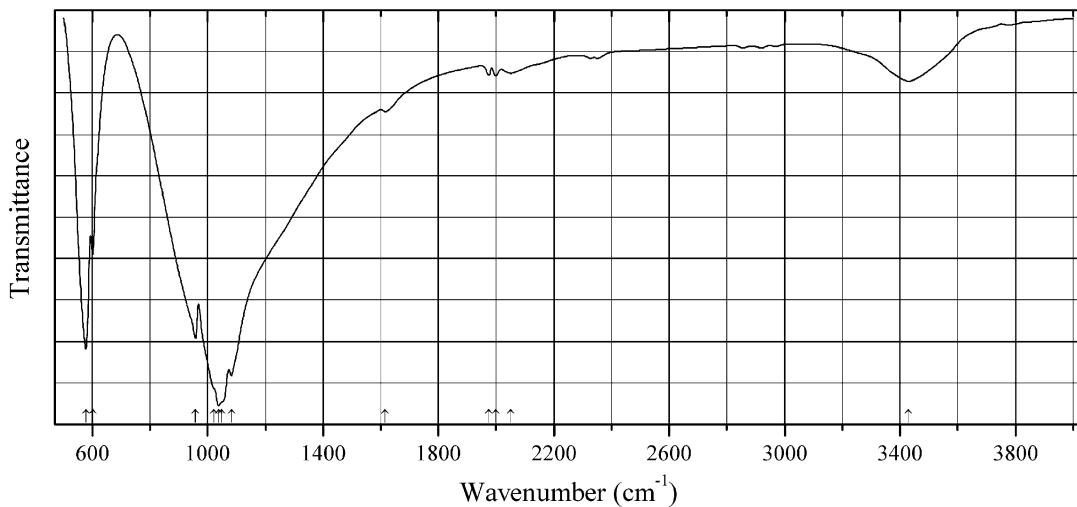
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Achary et al. (2013).

**Wavenumbers (IR, cm $^{-1}$ ):** 1105s, 1029sh, 1005s, 963, 928sh, 630s, 554, 527sh, 513, 494, 472w, 457w, 451sh, 434sh, 421w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 1046, 1038, 983, 966, 610, 557, 548, 486, 354, 244, 214, 171, 144, 136, 92, 69, 56.

**P803 Buchwaldite dimorph  $\text{NaCa}(\text{PO}_4)$** 

**Origin:** Synthetic.

**Description:** A sample doped with 1 mol%  $\text{Sm}^{3+}$  prepared by heating a stoichiometric mixture of  $(\text{NH}_4)(\text{H}_2\text{PO}_4)$ ,  $\text{Na}_2\text{CO}_3$ ,  $\text{CaCO}_3$ , and  $\text{Sm}_2\text{O}_3$  firstly at 185 °C for 2 h, then 714 °C for 1 h and finally at 950 °C for 3 h in air. Characterized by powder X-ray diffraction data. Orthorhombic, space group  $\text{Pn}2_1\text{a}$ ,  $a = 20.39$ ,  $b = 5.412$ ,  $c = 9.161$  Å.

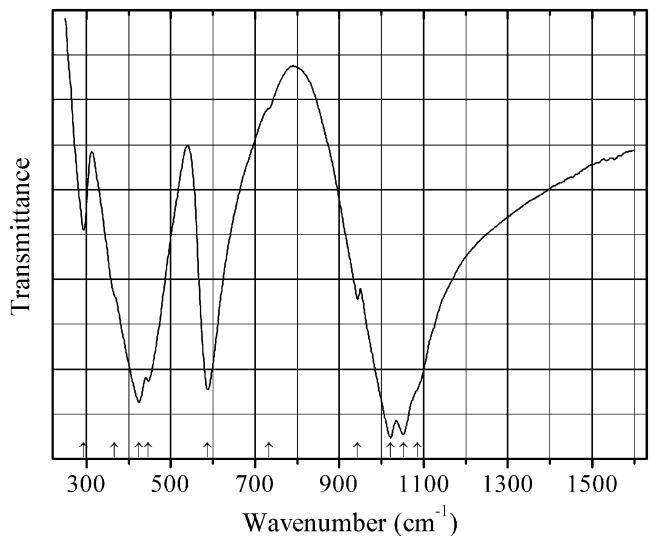
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Ratnam et al. (2014).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3430, 2050w, 2000w, 1975w, 1616w, 1082s, 1049sh, 1038s, 1022sh, 957s, 602, 578s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The bands at 3430 and 1616  $\text{cm}^{-1}$  correspond to the admixture of water molecules. For the IR spectrum of Eu-doped buchwaldite dimorph see also Grandhe et al. (2012). In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1158, 965s, 898.

**P804 Nalipoite**  $\text{NaLi}_2(\text{PO}_4)$ 

**Origin:** Synthetic.

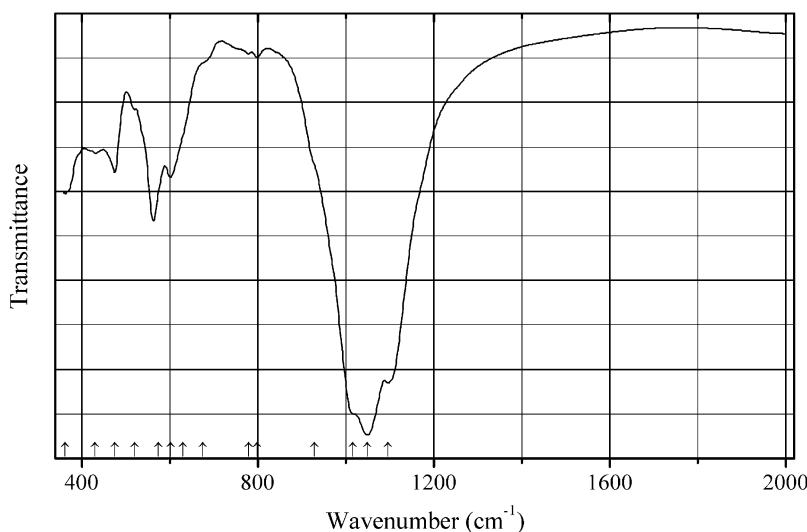
**Description:** Obtained by mixing aqueous solutions containing stoichiometric amounts of NaOH,  $\text{H}_3\text{PO}_4$ , and LiOH, followed by drying at 100 °C in air. Characterized by powder X-ray diffraction data. Orthorhombic, space group  $Pmn\bar{b}$ ,  $a = 6.8751(1)$ ,  $b = 9.9888(3)$ ,  $c = 4.9315(6)$  Å,  $V = 338.66(8)$  Å<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** López et al. (2014a).

**Wavenumbers (cm<sup>-1</sup>):** 1085sh, 1052s, 1022s, 944, 733sh, 588s, 447, 422s, 367sh, 293.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**P806 Fluorcarmoite-(BaNa)**  $\text{Ba}\square\text{Na}_2\text{Na}_2\square\text{CaMg}_{13}\text{Al}(\text{PO}_4)_{11}(\text{PO}_3\text{OH})\text{F}_2$ 

**Origin:** Costa Balzi Rossi, Magliolo, Savona, Liguria, Italy (type locality).

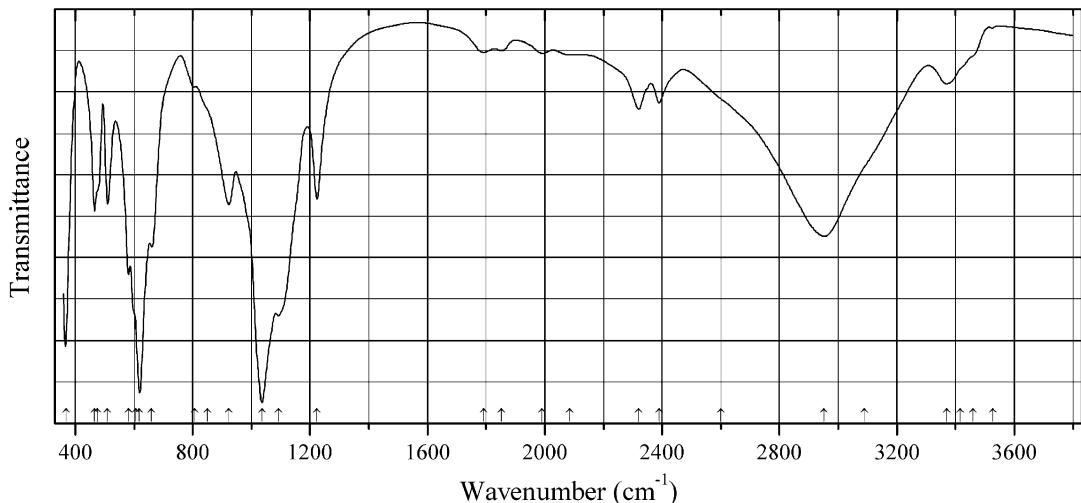
**Description:** Yellow grain.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 1097s, 1050s, 1017s, 930sh, 799w, 780w, 675sh, 630sh, 602, 574, 520w, 475, 430, 363.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P807 Florencite-(Nd) NdAl<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>(OH)<sub>6</sub>**



**Origin:** Svodovy area, Maldynyrd Ridge, Subpolar Urals, Russia.

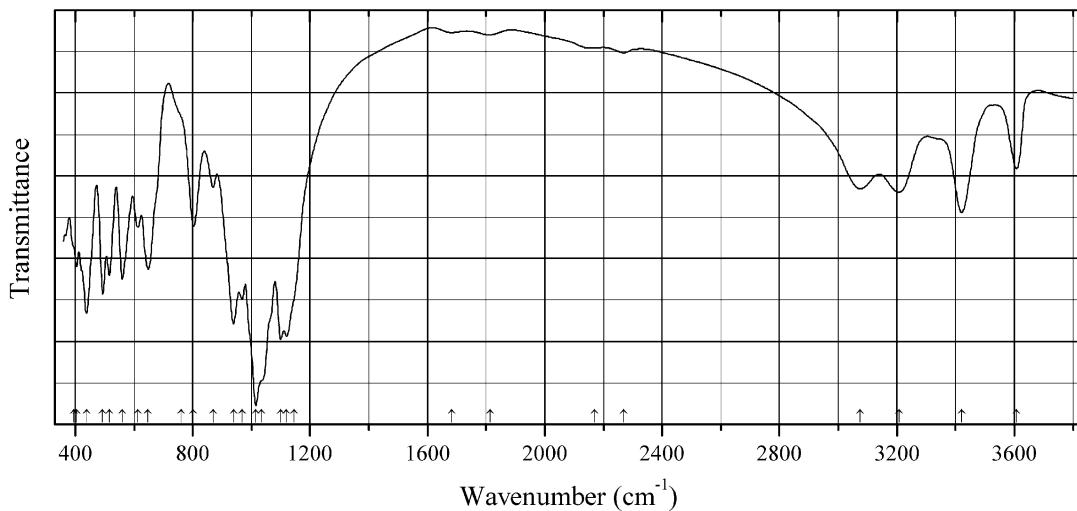
**Description:** Pink crystals from the association with xenotime-(Y) and quartz. The empirical formula is (electron microprobe): (Nd<sub>0.36</sub>Sm<sub>0.23</sub>Ce<sub>0.23</sub>La<sub>0.05</sub>Pr<sub>0.05</sub>Sr<sub>0.05</sub>Ca<sub>0.01</sub>)Al<sub>1.99</sub>Fe<sub>0.02</sub>(PO<sub>4</sub>)<sub>2.00</sub>(OH, H<sub>2</sub>O)<sub>6</sub>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3527w, 3460sh, 3415sh, 3370, 3090sh, 2951s, 2600sh, 2389, 2320, 2085w, 1991w, 1853w, 1792w, 1224, 1092s, 1036s, 923, 850sh, 806w, 660, 619s, 605sh, 581, 510, 475sh, 466, 368s.

**Note:** The bands in the range from 1700 to 2400 cm<sup>-1</sup> indicate the presence of acid phosphate groups.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P808 Lulzacite**  $\text{Sr}_2\text{Fe}^{2+} \text{Al}_4(\text{PO}_4)_4(\text{OH})_{10}$ 

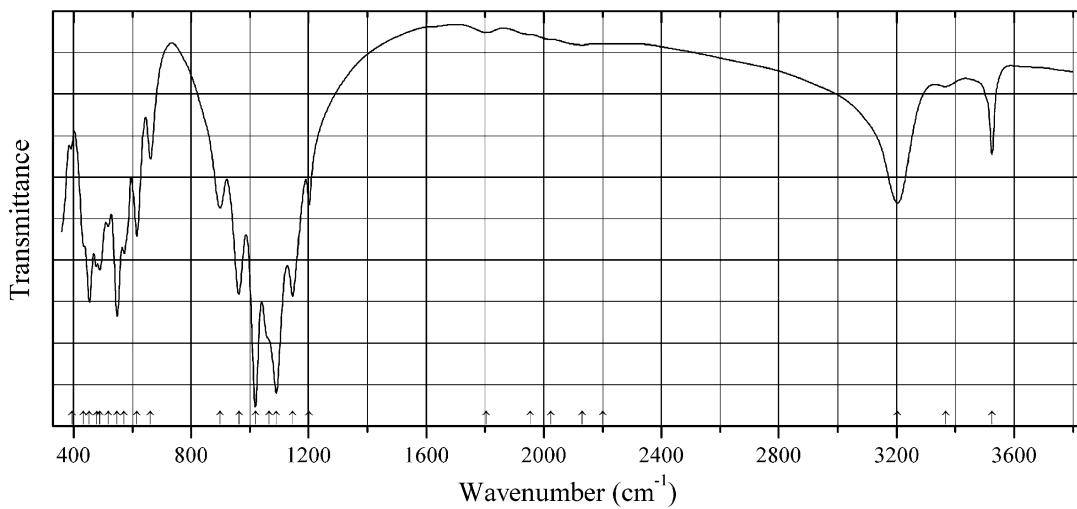
**Origin:** Bois-de-la-Roche quarry, Saint-Aubin-des-Châteaux, Loire-Atlantique, Pays de la Loire, France (type locality).

**Description:** Light greenish-gray columnar aggregate. The empirical formula is (electron microprobe):  $(\text{Sr}_{1.9}\text{Ca}_{0.1})(\text{Fe}_{1.9}\text{Mg}_{0.9}\text{Zn}_{0.1}\text{Mn}_{0.1})(\text{Al}_{3.7}\text{Fe}_{0.3})(\text{PO}_4)_{4.0}(\text{OH})_{10}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3607, 3422s, 3209, 3074, 2270w, 2170w, 1814w, 1683w, 1145sh, 1120s, 1099s, 1035sh, 1015s, 968, 939s, 869, 803, 760sh, 648, 613, 560, 516, 493, 438s, 404, 395sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P809 Penikisite**  $\text{BaMg}_2\text{Al}_2(\text{PO}_4)_3(\text{OH})_3$ 

**Origin:** Blow River, Yukon, Canada.

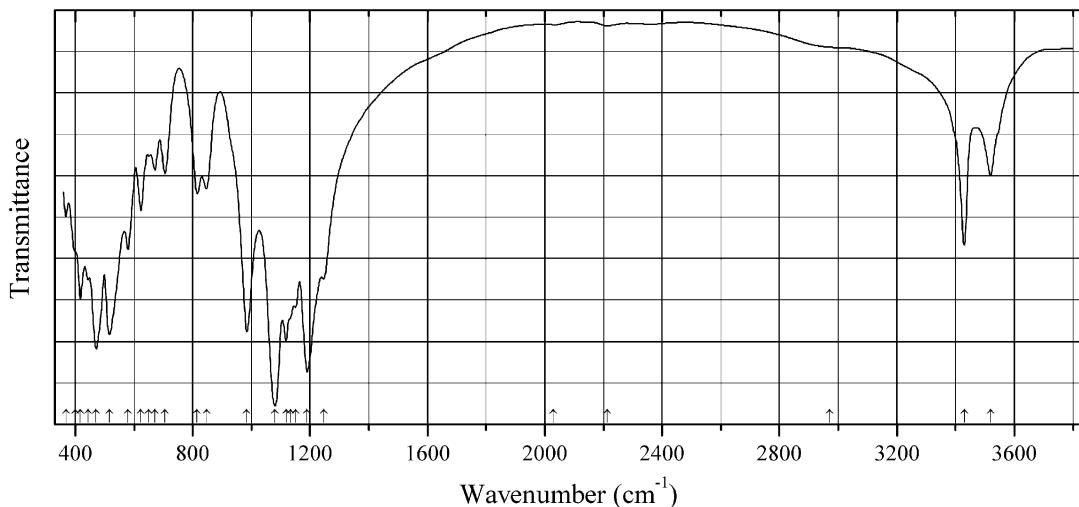
**Description:** Blue crystals. The empirical formula is (electron microprobe):  $\text{Ba}_{1.01}(\text{Mg}_{0.99}\text{Fe}_{0.92}\text{Mn}_{0.08})(\text{Al}_{1.84}\text{Fe}_{0.13}\text{Ti}_{0.03})(\text{PO}_4)_{3.00}(\text{OH})_3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3525, 3368w, 3203, 2200sh, 2130w, 2025w, 1953w, 1805w, 1202, 1146s, 1090s, 1065sh, 1019s, 963s, 899, 662, 616, 573, 548s, 519, 489, 480, 454s, 435sh, 395w.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P810 Trolleite  $\text{Al}_4(\text{PO}_4)_3(\text{OH})_3$**



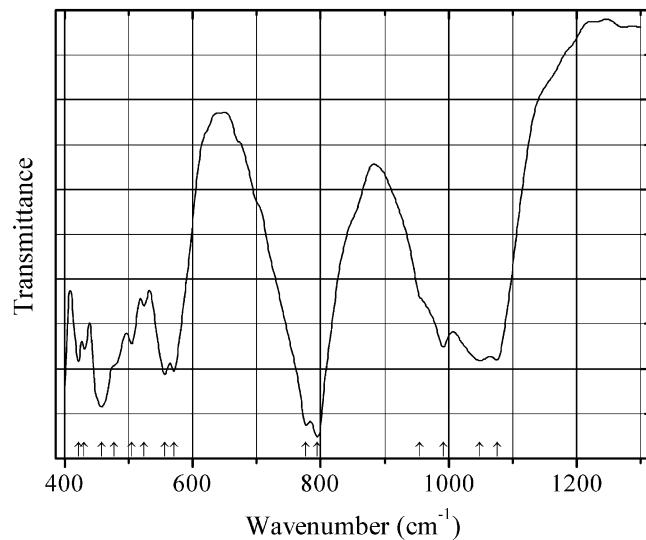
**Origin:** Hålsjöberg (Horrsjöberg), Torsby, Värmland, Sweden.

**Description:** Pale bluish-green grains from the association with scorzalite, kyanite, and rutil. Confirmed by the IR spectrum.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3519, 3430, 2970w, 2213w, 2030w, 1247, 1190s, 1150, 1133, 1118, 1081s, 984, 847, 815, 706, 671, 650w, 624, 580, 516s, 471s, 444, 417, 400sh, 369.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P811 Petitjeanite**  $\text{Bi}_3\text{O}(\text{PO}_4)_2(\text{OH})$ 

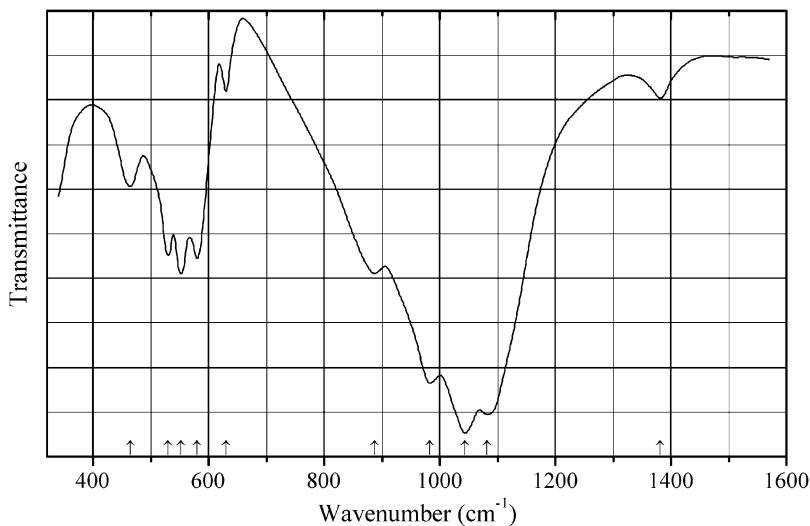
**Origin:** Schneeberg District, Erzgebirge (Ore Mts.), Saxony, Germany.

**Description:** Spherulitic crust. The empirical formula is (electron microprobe):  $(\text{Bi}_{2.85}\text{Pb}_{0.1}\text{Ca}_{0.1})(\text{PO}_4)_{0.9}(\text{AsO}_4)_{0.4}(\text{VO}_4)_{0.3})(\text{OH})$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1076s, 1049s, 992, 955sh, 795s, 777s, 570, 556, 523, 504, 477sh, 457s, 430, 421.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P812 Varulite**  $\text{NaCaMn}^{2+}(\text{PO}_4)_3$ 

**Origin:** Solleftea, Ångermanland, Sweden.

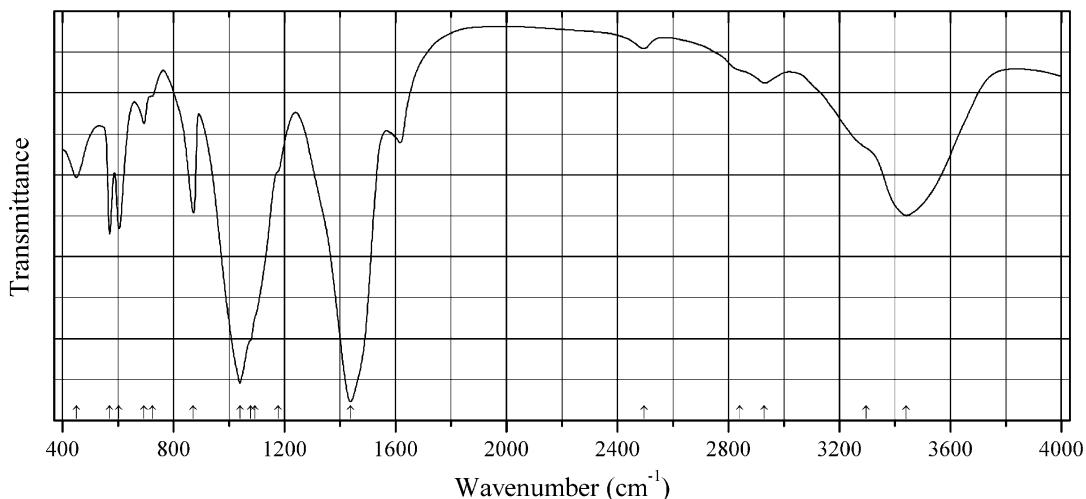
**Description:** Anhedral grains. Ca-deficient variety or analogue of varulite. The empirical formula is (electron microprobe):  $\text{Na}_{1.5}\text{Ca}_{0.3}\text{Mn}_{2.4}\text{Fe}_{0.8}(\text{PO}_4)_{3.0}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %)] are: 6.12 (90), 5.47 (40), 3.50 (70), 3.146 (100), 2.736 (100), 2.560 (30).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** (1382), 1082s, 1044s, 983s, 887, 630w, 580, 552s, 530, 465.

**Note:** The spectrum was obtained by N.V. Chukanov. The band at 1382 cm<sup>-1</sup> may correspond to an impurity.

#### P813 Daqingshanite-(Ce) $\text{Sr}_3\text{Ce}(\text{PO}_4)(\text{CO}_3)_3$



**Origin:** Bayan Obo deposit, Bayan Obo Mining District, Baotou Prefecture, Inner Mongolia, China (type locality).

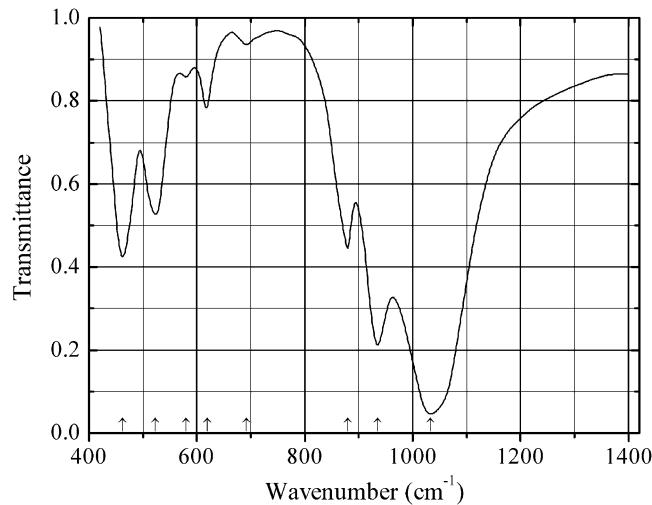
**Description:** Pale yellow crystals and grains from the association with benstonite, huntite, strontianite, pyrite, phlogopite, and monazite. Holotype sample. Trigonal,  $a = 10.058$ ,  $c = 9.225$  Å.  $D_{\text{meas}} = 3.81$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 3.71$  g/cm<sup>3</sup>. Optically uniaxial (-),  $\epsilon = 1.609$ ,  $\omega = 1.708$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %)] are: 3.95 (60), 3.16 (100), 2.52 (70), 2.110 (50), 2.040 (60), 1.941 (60).

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Ren et al. (1983).

**Wavenumbers (cm<sup>-1</sup>):** 2930, 2840, 2495w, 1617, 1438s, 1178sh, 1094sh, 1078sh, 1040s, 872, 724sh, 694, 604, 570, 450.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. Bands in the ranges 3000–4000 and 1600–1700 cm<sup>-1</sup> may be due to absorbed water.

**P814 Sodium calcium silicophosphate  $\text{Na}_2\text{Ca}_4(\text{PO}_4)_2\text{SiO}_4$  (apatite-type)  $\text{Na}_2\text{Ca}_4(\text{PO}_4)_2\text{SiO}_4$** 

**Origin:** Synthetic.

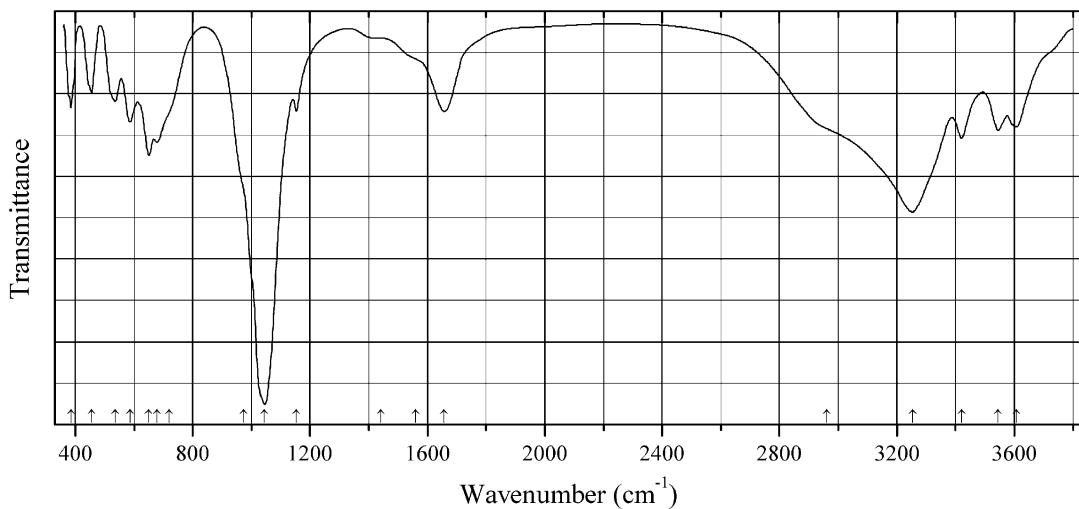
**Description:** Fine powder. Characterized by thermal and powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** Absorption. Kind of sample preparation is not indicated.

**Source:** Pirayesh and Nychka (2013).

**Wavenumbers (cm⁻¹):** 1033s, 935s, 879, 692w, 619, 580w, 523, 462.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**P815 Mangangordonite  $\text{Mn}^{2+}\text{Al}_2(\text{PO}_4)_2(\text{OH})_2 \cdot 8\text{H}_2\text{O}$** 

**Origin:** Foote Mine, Kings Mountain, Cleveland Co., North Carolina, USA (type locality).

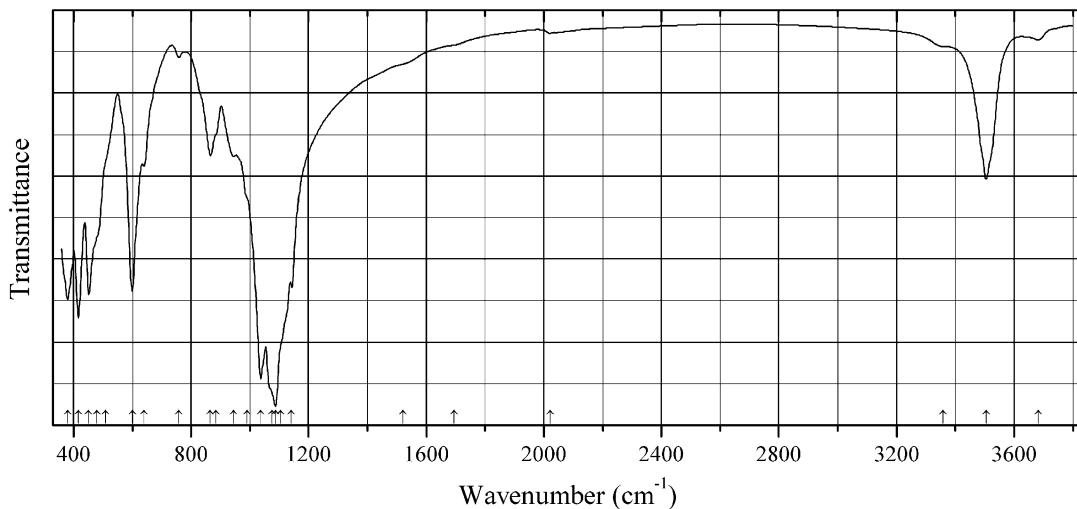
**Description:** Pale yellow prismatic crystals from the association with whiteite-(MnFeMg) and birnessite. The empirical formula is (electron microprobe):  $(\text{Mn}_{0.7}\text{Fe}_{0.2}\text{Mg}_{0.1})(\text{Al}_{0.8}\text{Fe}_{0.2})(\text{PO}_4)_{2.0}(\text{OH})_2 \cdot 8\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3607, 3545, 3420, 3253s, 2960sh, 1657, 1560sh, 1442w, 1157, 1045s, 975sh, 720sh, 679, 650s, 587, 536, 456, 386.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P817 Althausite  $\text{Mg}_4(\text{PO}_4)_2(\text{OH},\text{O})(\text{F},\square)$**



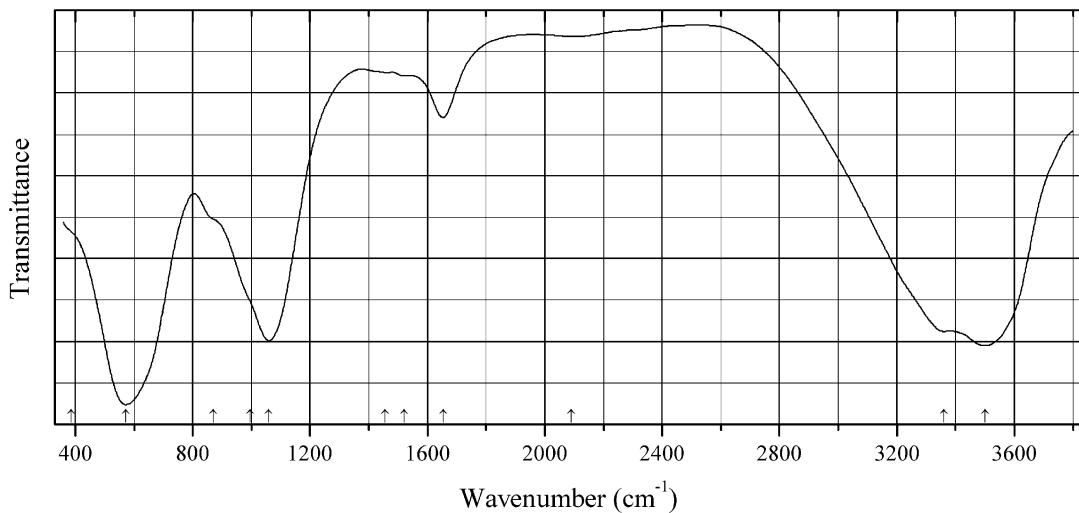
**Origin:** Tingelstadtfjern quarry, Modum, Buskerud, Norway (type locality).

**Description:** Brownish single-crystal grain. Confirmed by the IR spectrum.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3682w, 3505, 3359w, 2022w, 1695sh, 1520sh, 1142s, 1105sh, 1087s, 1075sh, 1037s, 990sh, 946, 885sh, 866, 759w, 639, 600s, 510sh, 480sh, 452s, 417s, 381s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P818 Cu,Al-hydroxyphosphate**  $\text{CuAl}_5(\text{PO}_4)(\text{OH})_{13}\text{F} \cdot n\text{H}_2\text{O}$ 

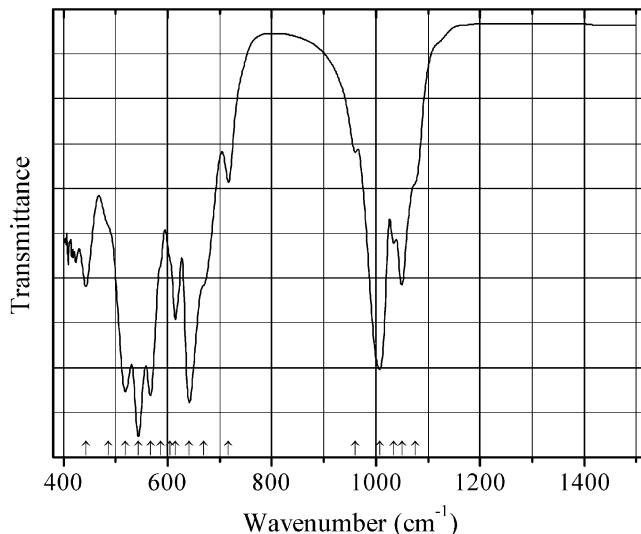
**Origin:** West Caradon Adit, Cornwall, GB.

**Description:** Blue collophorm crust from the association with fluorite. X-ray amorphous. The empirical formula is  $(\text{Cu}_{0.89}\text{Mg}_{0.03}\text{Zn}_{0.02}\text{Cu}_{0.02})\text{Al}_{5.03}[(\text{PO}_4)_{0.39}(\text{SiO}_3)_0.33(\text{AsO}_4)_{0.18}(\text{SO}_4)_{0.12}] (\text{OH})_{12.74}\text{F}_{1.00} \cdot n\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3500s, 3360s, 2090w, 1653, 1520w, 1455w, 1059s, 995sh, 870sh, 571s, (385sh).

**Note:** The spectrum was obtained by N.V. Chukanov.

**P819 Kuksite trigonal dimorph**  $\text{Pb}_3\text{Zn}_3\text{TeO}_6(\text{PO}_4)_2$ 

**Origin:** Synthetic.

**Description:** Synthesized by conventional solid-state methods from stoichiometric amounts of PbO, ZnO, H<sub>2</sub>TeO<sub>4</sub>·2H<sub>2</sub>O, and KH<sub>2</sub>PO<sub>4</sub> first at 400 °C for 20 h to decompose H<sub>2</sub>TeO<sub>4</sub>·2H<sub>2</sub>O and KH<sub>2</sub>PO<sub>4</sub>, and thereafter at 700 °C for 5 days, with intermediate grindings. Characterized by powder and single-crystal X-ray diffraction data. Trigonal, space group *P*321,  $a = 8.3831(3)$ ,  $c = 5.1930(4)$  Å,  $V = 316.05(3)$  Å<sup>3</sup>,  $Z = 1$ .  $D_{\text{calc}} = 6.469$  g/cm<sup>3</sup>.

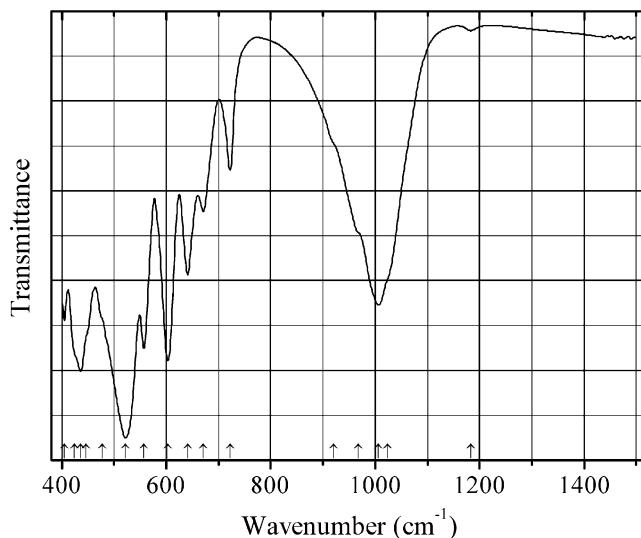
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Yu et al. (2016).

**Wavenumbers (cm<sup>-1</sup>):** 1075sh, 1050, 1034, 1007s, 961w, 717, 669sh, 642s, 615, 604sh, 587sh, 567s, 544s, 519s, 486sh, 443.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

#### P820 Kuksite trigonal Mg analogue Pb<sub>3</sub>Mg<sub>3</sub>TeO<sub>6</sub>(PO<sub>4</sub>)<sub>2</sub>



**Origin:** Synthetic.

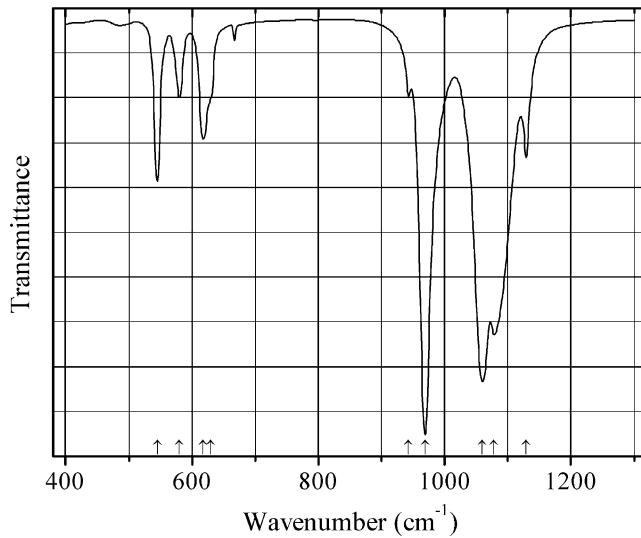
**Description:** Synthesized by conventional solid-state methods from stoichiometric amounts of PbO, MgO, H<sub>2</sub>TeO<sub>4</sub>·2H<sub>2</sub>O, and KH<sub>2</sub>PO<sub>4</sub> first at 400 °C for 20 h to decompose H<sub>2</sub>TeO<sub>4</sub>·2H<sub>2</sub>O and KH<sub>2</sub>PO<sub>4</sub>, and thereafter at 850 °C for 5 days, with intermediate grindings. Characterized by powder and single-crystal X-ray diffraction data. Trigonal, space group *P*321,  $a = 8.4072(4)$ ,  $c = 5.2158(5)$  Å,  $V = 319.27(4)$  Å<sup>3</sup>,  $Z = 1$ .  $D_{\text{calc}} = 5.763$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Yu et al. (2016).

**Wavenumbers (cm<sup>-1</sup>):** 1183w, 1024sh, 1006, 968sh, 920sh, 722, 671, 641, 603s, 557, 522s, 477sh, 447sh, 436s, 425sh, 405.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**P821 Natrophilite  $\text{NaMn}^{2+}(\text{PO}_4)$** 

**Origin:** Synthetic.

**Description:** Prepared hydrothermally from  $\text{KMnPO}_4 \cdot \text{H}_2\text{O}$  and  $\text{NaCH}_3\text{COO} \cdot 3\text{H}_2\text{O}$  at a ratio of 1:10 at 200 °C for 15 h. Characterized by powder X-ray diffraction data. Orthorhombic,  $a = 10.5177(3)$ ,  $b = 6.3144(2)$ ,  $c = 4.9873(2)$  Å,  $V = 331.227(22)$  Å<sup>3</sup>.

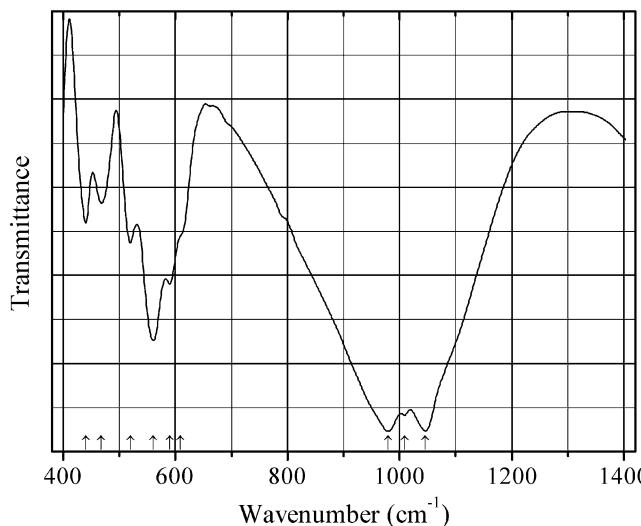
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Boyadzhieva et al. (2015).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1129, 1078s, 1060s, 969s, 943w, 630sh, 618, 580, 545.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1048w, 1006w, 946s, 650s, 577.

**P822 Paganoite phosphate analogue  $\text{NiBi}^{3+}\text{O}(\text{PO}_4)$** 

**Origin:** Synthetic.

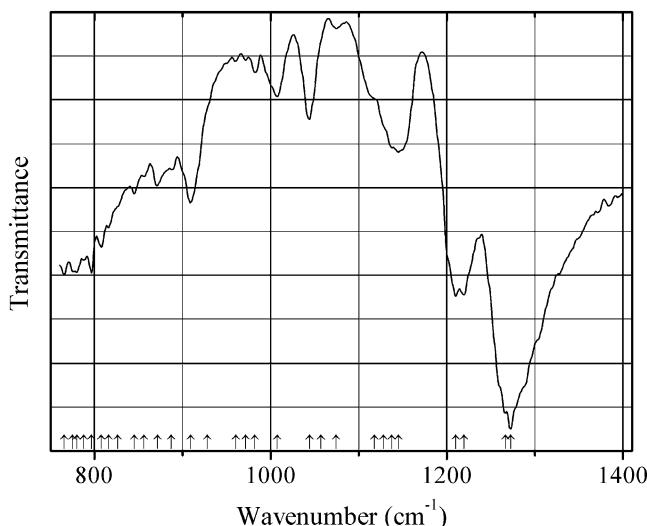
**Description:** Prepared by solid-state reaction from  $\text{Bi}_2\text{O}_3$ ,  $\text{CoO}$ , and  $(\text{NH}_4)_2(\text{HPO}_4)$ . The crystal structure is solved. Monoclinic, space group  $P2_1/n$ ,  $a = 7.2470(1)$ ,  $b = 11.2851(2)$ ,  $c = 5.2260(1)$  Å,  $\beta = 107.843(1)^\circ$ ,  $V = 406.91$  Å<sup>3</sup>,  $Z = 4$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 4.727 (44) (-101), 4.338 (69) (120), 3.372 (70) (111), 2.850 (100) (-221), 2.568 (43) (131), 2.516 (41) (230).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Ketani et al. (1999).

**Wavenumbers (cm<sup>-1</sup>):** 1046s, 1009s, 979s, 609sh, 590, 561s, 520, 468, 440.

## P823 Phosphorösslerite $Mg(HPO_4) \cdot 7H_2O$



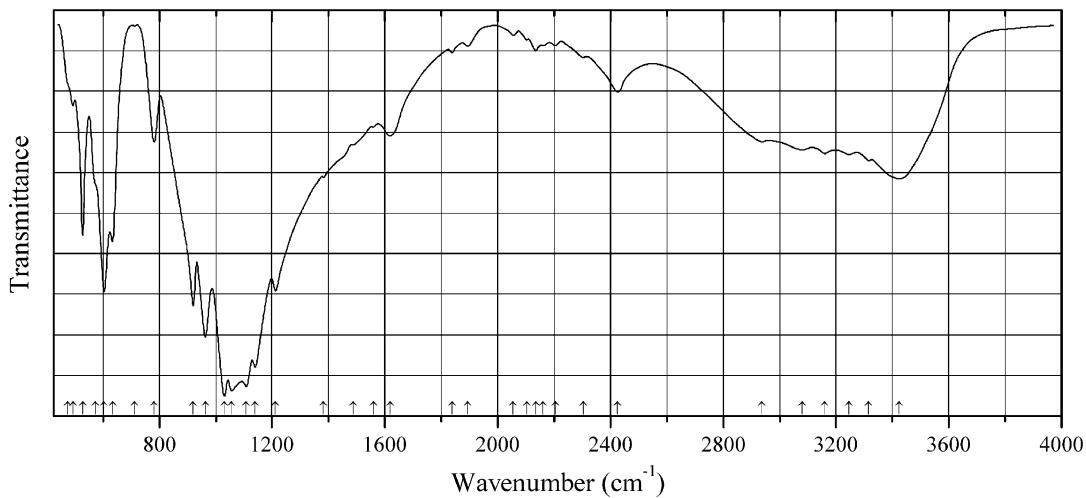
**Origin:** Synthetic.

**Description:** Commercial reactant (?).

**Kind of sample preparation and/or method of registration of the spectrum:** Absorption. Kind of sample preparation is not indicated.

Source: Pucka et al. (2000).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1272, 1219, 1210, 1145, 1137, 1118sh, 1074w, 1044, 1007, 982w, 909, 887, 871, (796).

**P824 Potassium zinc hydrogen phosphate**  $KZn_2(PO_4)(PO_3OH)$ 

**Origin:** Synthetic.

**Description:** The sample may contain  $KZn(PO_4)$  impurity.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Alibakhshi et al. (2012).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3424, 3316, 3247, 3160, 3081, 2938, 2426, 2304w, 2204w, 2161w, 2136w, 2103w, 2055w, 1894w, 1838w, 1618, 1559, 1488, 1383, 1212, 1140s, 1108s, 1056s, 1031s, 963s, 920s, 782, 712, 634, 604s, 574sh, 528, 493w, 474sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 3429s (broad), 3315, 3093, 2451, 2399, 2162w, 1979w, 1874w, 1813w, 1322w, 1240w, 1137, 1074, 1013s, 910s, 766w, 590, 490, 303s.

**P825 Raadeite**  $Mg_7(PO_4)_2(OH)_8$ 

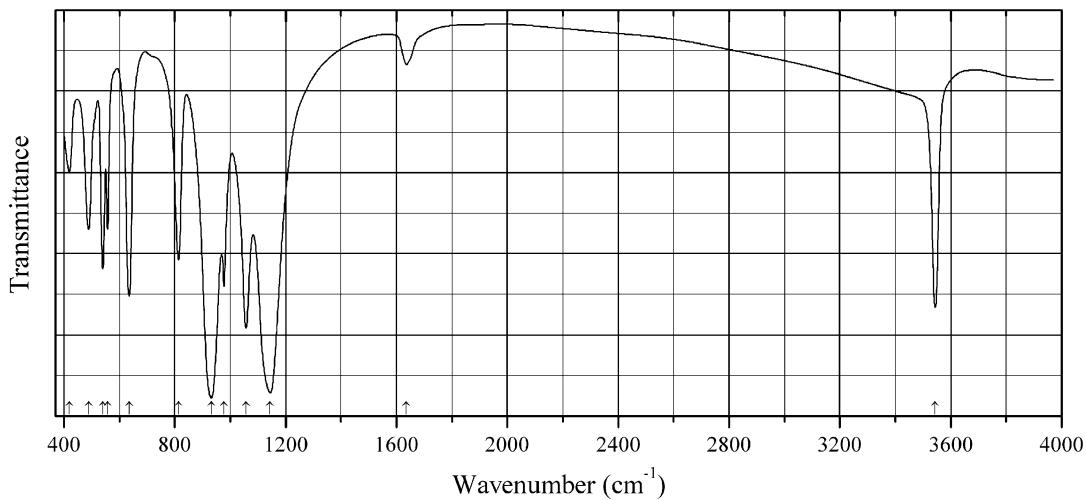
**Origin:** Tingelstadtfjern quarry, Modum, Buskerud, Norway (type locality).

**Description:** Anhedral inclusion in holtedahlite. Holotype sample. The crystal structure is solved. Monoclinic, space group  $P2_1/n$ ,  $a = 5.250(1)$ ,  $b = 11.647(2)$ ,  $c = 9.655(2)$  Å,  $\beta = 95.94(1)^\circ$ ,  $Z = 2$ . Optically biaxial (-),  $\alpha = 1.5945(5)$ ,  $\beta = 1.6069(5)$ ,  $\gamma = 1.6088(5)$ ,  $2V = 45.6(1)^\circ$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Reflection of a single-crystal grain.

**Source:** Chopin et al. (2001).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3580, 3540, 3475, 3375.

**P826 Vyacheslavite  $\text{U}^{4+}(\text{PO}_4)(\text{OH}) \cdot 2.5\text{H}_2\text{O}$** 

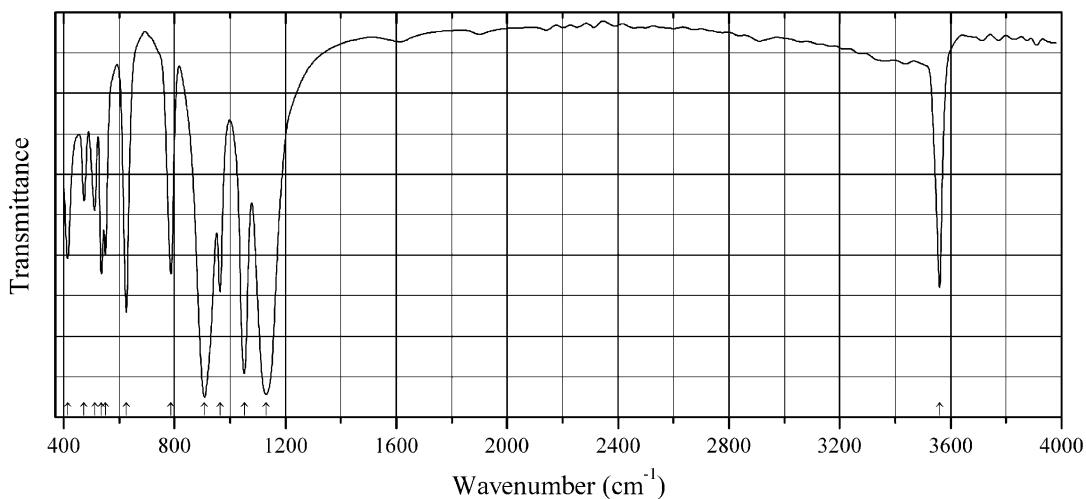
**Origin:** Synthetic.

**Description:** Prepared hydrothermally using hydrolyzed uranium bromide phosphate. Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Brandel et al. (2001).

**Wavenumbers (cm⁻¹):** 3544, 1636w, 1144s, 1058s, 978, 932s, 814, 636s, 558, 540, 490, 420.

**P827 Vyacheslavite anhydrous Th analogue  $\text{Th}^{4+}(\text{PO}_4)(\text{OH})$** 

**Origin:** Synthetic.

**Description:** Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group *Cmca*,  $a = 7.1393(2)$ ,  $b = 9.2641(2)$ ,  $c = 12.5262(4)$  Å,  $V = 828.46(4)$  Å<sup>3</sup>,  $Z = 8$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

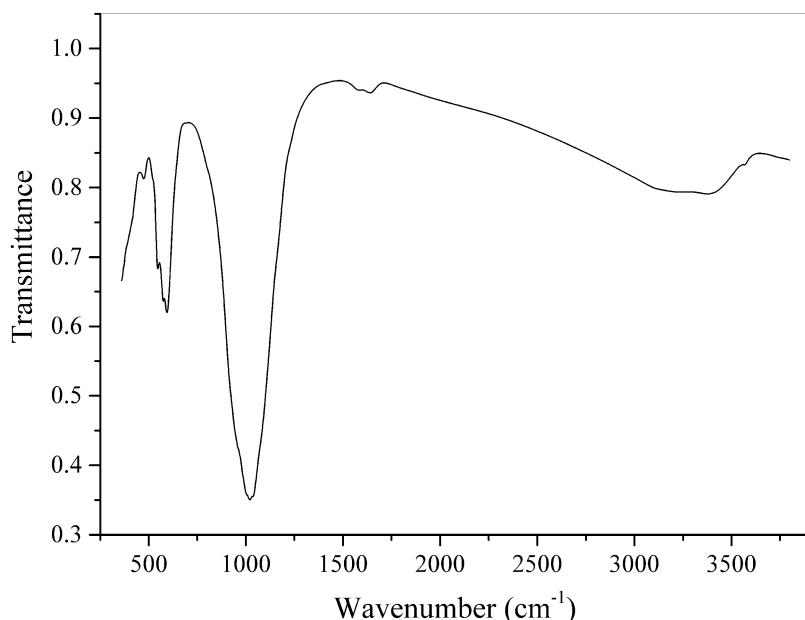
**Source:** Brandel et al. (2001), Dacheux et al. (2007).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3560, 1130s, 1052s, 964, 908s, 787, 626, 550, 536, 512, 474, 414.

**Note:** Raman spectrum is given by Dacheux et al. (2007).

**Wavenumbers (Raman, cm<sup>-1</sup>):** 3568s, 1195w, 1078s, 1060s, 989s, 799w, 789w, 618, 568, 556, 449, 416, 368, 282, 236.

#### P828 Fupingqiuite (Na,Mn<sup>2+</sup>,□)<sub>2</sub>Mn<sup>2+</sup><sub>2</sub>Fe<sup>3+</sup>(PO<sub>4</sub>)<sub>3</sub>



**Origin:** Nancy pegmatite, Chacabuco department, San Luis, Argentina (type locality).

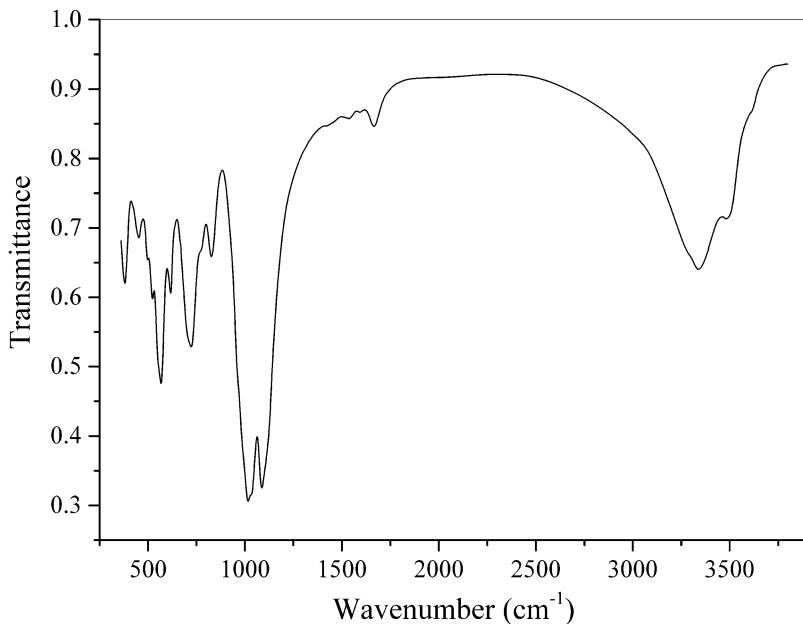
**Description:** Dark brownish-gray grains with perfect cleavage. Partly altered and contaminated by a hydrous phosphate.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** (3563w), (3384), (3250), 1636w, 1587w, 1040sh, 1023s, 1015sh, 965sh, 594s, 578, 549, 474w, 390sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P829 Guimarãesite**  $\text{Ca}_2\text{Be}_4\text{Zn}_5(\text{PO}_4)_6(\text{OH})_4 \cdot 6\text{H}_2\text{O}$



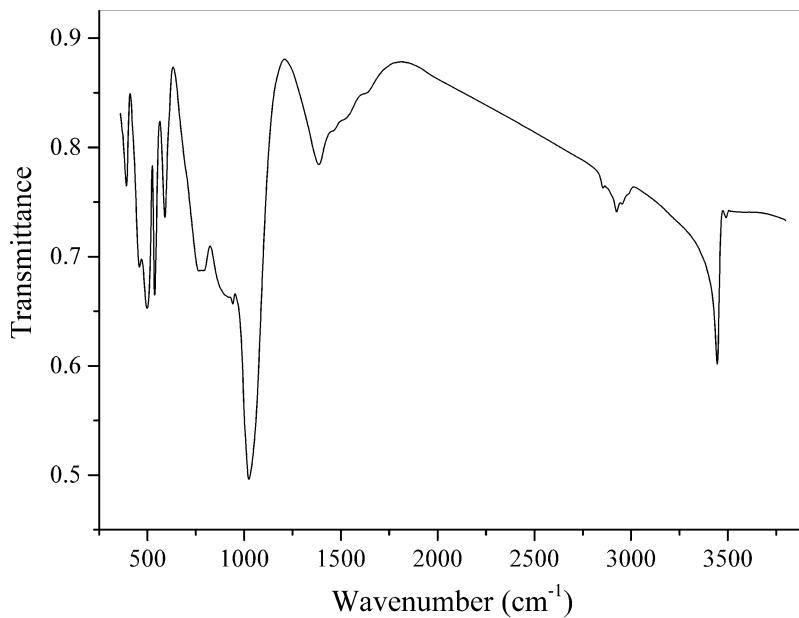
**Origin:** Piauí River, Itinga County, Minas Gerais, Brazil (type locality).

**Description:** Peripheral zones of zanazziite crystals from the association with albite, microcline, quartz, elbaite, lepidolite, schorl, eosphorite, moraesite, and saleelite. Monoclinic,  $a = 15.98$  (1) Å,  $b = 11.84(2)$  Å,  $c = 6.63(1)$  Å,  $\beta = 95.15(15)$ °,  $V = 1249.4(34)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 2.963$  g/cm<sup>3</sup>. Optically biaxial (−),  $\alpha = 1.562(2)$ ,  $\beta = 1.600(2)$ ,  $\gamma = 1.602(2)$ ,  $2V = 55\text{--}75$ °. The empirical formula is  $\text{Ca}_{1.93}(\text{Zn}_{2.61}\text{Mg}_{1.11}\text{Fe}^{2+}_{0.41}\text{Al}_{0.37}\text{Mn}_{0.34})\text{Be}_{4.00}(\text{PO}_4)_{6.00}(\text{OH})_{3.90} \cdot 6.41\text{H}_2\text{O}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 9.98 (90) (110), 5.98 (100) (020), 4.82 (80) (310), 3.152 (90) (−202), 3.052 (70) (−421), 2.961 (70) (040, 202), 2.841 (70) (−312), 2.708 (80) (041).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>−1</sup>):** 3610sh, 3485, 3336s, 3295sh, 1667, 1594w, 1537w, 1416w, 1110sh, 1087s, 1030sh, 1016s, 827, 770sh, 723s, 616, 567s, 523, 502, 452, 380.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P830 Drugmanite**  $\text{Pb}_2\text{Fe}^{3+}(\text{PO}_4)(\text{PO}_3\text{OH})(\text{OH})_2$ 

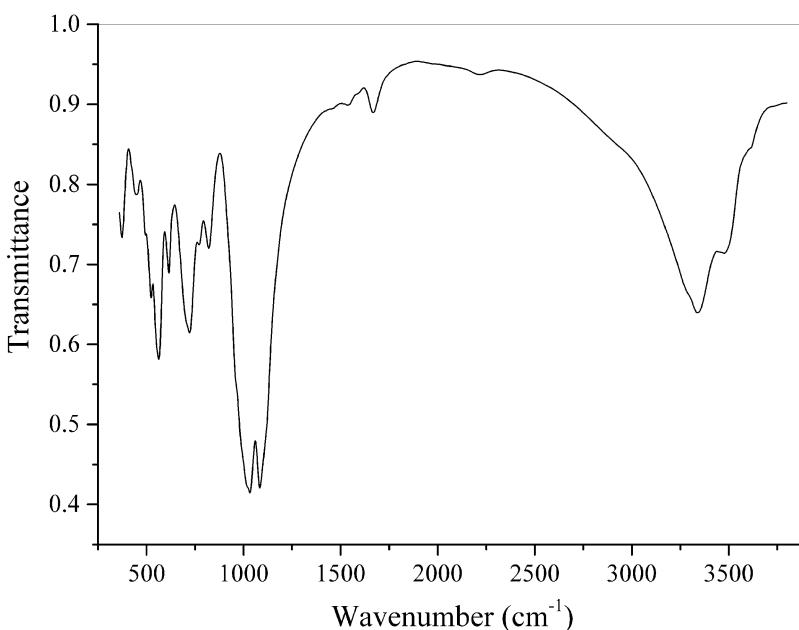
**Origin:** Bleialf, Prüm, Eifel, Germany.

**Description:** Spherulitic crust on galena. The empirical formula is (electron microprobe):  $\text{H}_x\text{Pb}_{2.18}(\text{Fe}_{0.99}\text{Al}_{0.01})(\text{PO}_4)_{2.00}(\text{OH})_2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3491w, 3445, 1387, 1025s, 942, 915sh, 790, 766, 590, 537, 498, 459, 392.

**Note:** The spectrum was obtained by N.V. Chukanov. The band at 1387 cm<sup>-1</sup> corresponds to isolated H<sup>+</sup> cation. Weak bands between 1400 and 3000 cm<sup>-1</sup> are due to an organic impurity.

**P831 Roscherite**  $\text{Ca}_2(\text{Mn},\text{Fe}^{2+},\text{Fe}^{3+},\text{Mg},\text{Al},\text{Zn})_5\text{Be}_4(\text{PO}_4)_6(\text{OH})_4 \cdot 6\text{H}_2\text{O}$ 

**Origin:** Taquaral, Itinga, Minas Gerais, Brazil.

**Description:** Olive-green spherulite from the association with eosphorite, feldspar, and metaautunite.

The empirical formula is (electron microprobe):  $\text{Ca}_{2.0}(\text{Mn}_{1.5}\text{Fe}_{1.3}\text{Zn}_{1.1}\text{Mg}_{0.5}\text{Al}_{0.1})\text{Be}_4(\text{PO}_4)_{6.0}(\text{OH})_4 \cdot 6\text{H}_2\text{O}$ .

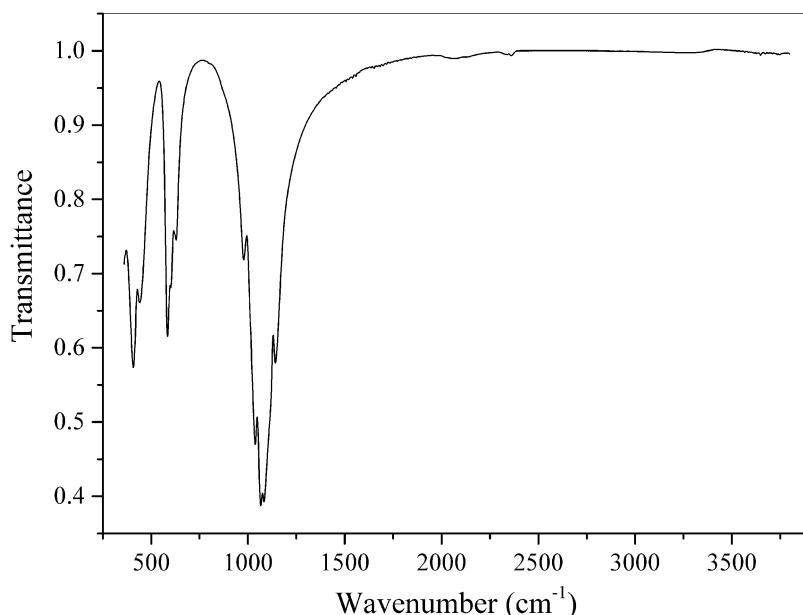
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3605sh, 3439, 3336s, 3290sh, 2950sh, 2217w, 1667, 1538w, 1450sh, 1084s,

1033s, 1020sh, 820, 771, 722s, 615, 563s, 523, 497, 451, 374.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P832 Thadeuite  $\text{Ca}(\text{Mg},\text{Fe}^{2+})_3(\text{PO}_4)_2(\text{OH},\text{F})_2$**



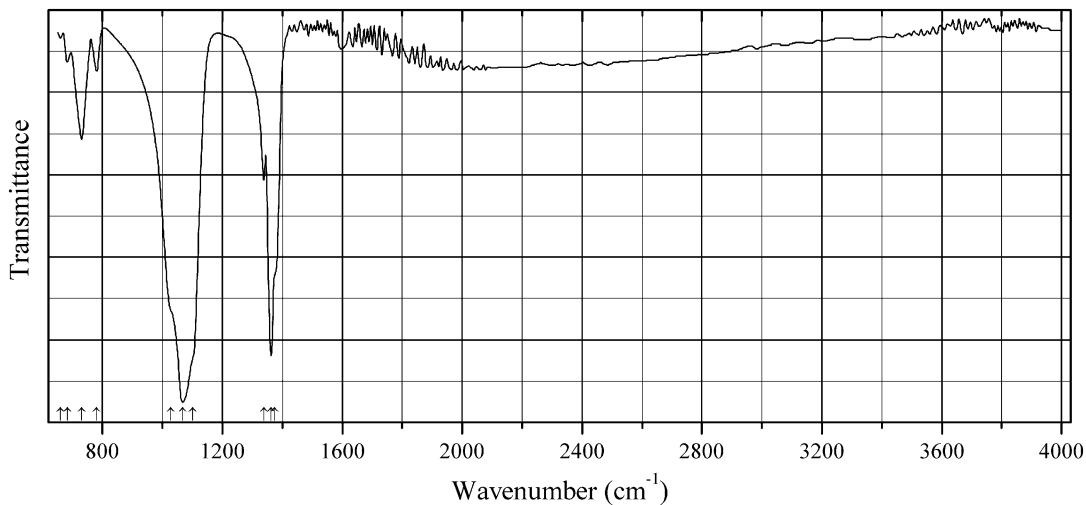
**Origin:** Panasqueira Mines, Covilhã, Castelo Branco district, Portugal (type locality).

**Description:** Yellow anhedral grains. Investigated by A.V. Kasatkin. Characterized by single-crystal X-ray diffraction data and qualitative electron microprobe analyses. Orthorhombic,  $a = 6.465(14)$ ,  $b = 13.525(7)$ ,  $c = 8.539(5)$  Å,  $V = 727(2)$  Å<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 2120sh, 2060w, 1141s, 1083s, 1066s, 1038s, 978, 629, 599, 584s, 440, 407s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**P833 Minjiangite  $\text{BaBe}_2(\text{PO}_4)_2$** 

**Origin:** Nanping No. 31 pegmatite, Fujian Province, southeastern China (type locality).

**Description:** White crystals from the association with montebrasite, quartz, muscovite, hydroxylapatite, and palermoite. Holotype sample. The crystal structure is solved. Hexagonal, space group  $P\bar{6}/mmm$ ,  $a = 5.029(1)$ ,  $c = 7.466(1)$  Å,  $V = 163.52(1)$  Å $^3$ ,  $Z = 1$ .  $D_{\text{calc}} = 3.49$  g/cm $^3$ . Optically biaxial (+),  $\omega = 1.587(3)$ ,  $\epsilon = 1.602(2)$ . The empirical formula is  $(\text{Ba}_{0.99}\text{Ca}_{0.01})\text{Be}_{1.98}(\text{P}_{1.99}\text{Si}_{0.01})\text{O}_8$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Reflection.

**Source:** Rao et al. (2015).

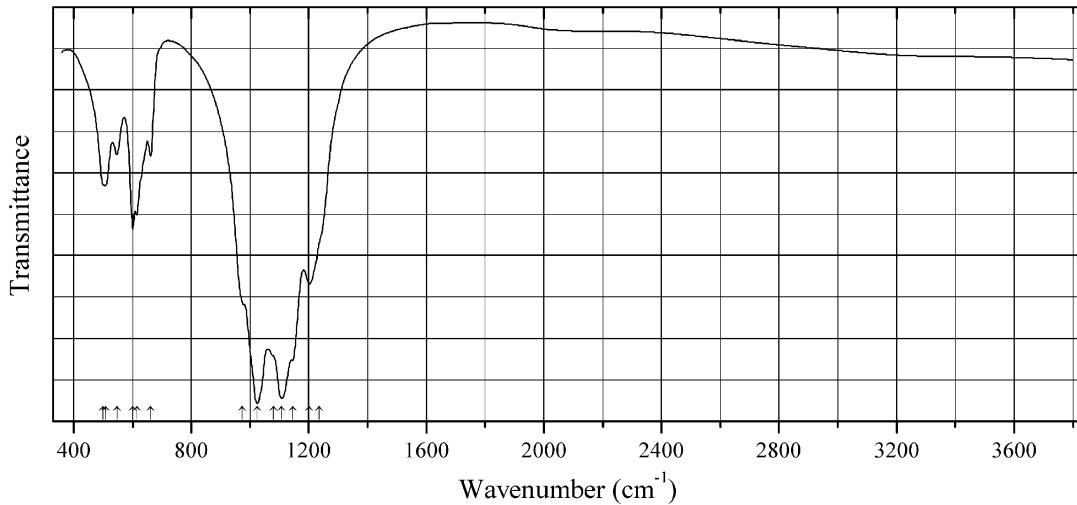
**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1375s, 1363s, 1339s, 1101sh, 1068s, 1027sh, 781, 730, 683w, 660w.

**Note:** Possibly, an erroneous spectrum. In particular, assignment of the strong bands at 1375, 1363, and 1339 cm $^{-1}$  to Be–O-stretching vibrations (Rao et al. 2015) is questionable. Dal Bo et al. (2014) give another IR spectrum for the synthetic analogue of minjiangite. The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1233s, 1050s, 491, 478, 328w, 189w.

## 2.9 Sulfides, Sulfites, Sulfates, Carbonato-Sulfates, Phosphato-Sulfates, and Tellurato-Sulfates

**S554 Eleomelanite** ( $K_2PbCu_4O_2(SO_4)_4$ )



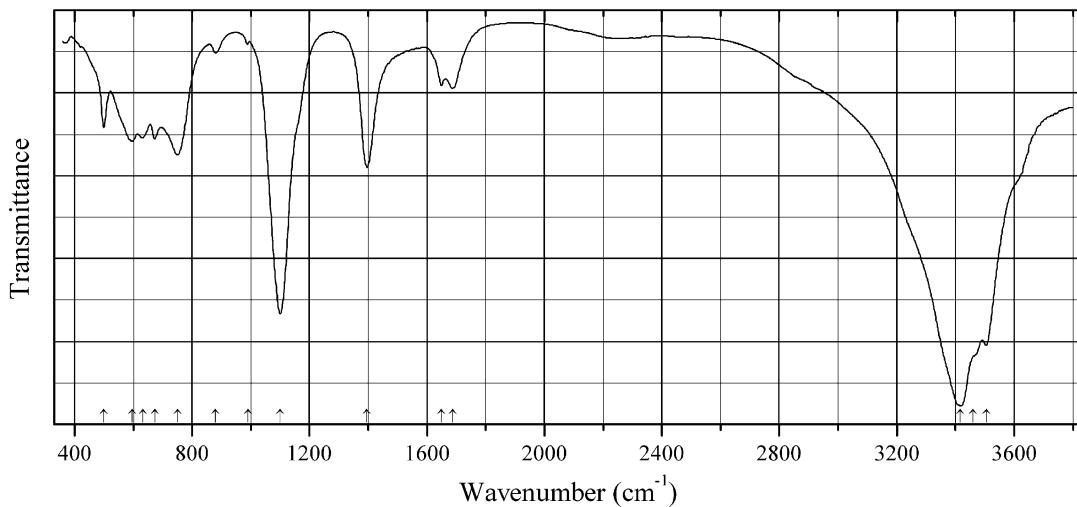
**Origin:** Arsenatnaya fumarole, Second scoria cone of the Northern Breakthrough of the Great Tolbachik Fissure Eruption, Tolbachik volcano, Kamchatka Peninsula, Far-Eastern Region, Russia (type locality).

**Description:** Dark green crystalline crust from the association with euhorline, wulffite, klyuchevskite, alumoklyuchevskite, fedotovite, anglesite, cryptochalcite, langbeinite, aphthalite, chalcocyanite, dolerophanite, piyrite, anhydrite, steklite, etc. Holotype sample. The crystal structure is solved. Monoclinic, space group  $P2_1/n$ ,  $a = 9.3986(3)$ ,  $b = 4.9811(1)$ ,  $c = 18.2293(5)$  Å,  $\beta = 104.409(3)^\circ$ ,  $V = 811.63(4)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{calc}} = 3.790$  g/cm $^3$ . Optically biaxial (−),  $\alpha = 1.646$  (3),  $\beta = 1.715(6)$ ,  $\gamma = 1.734(6)$ ,  $2V = 60(15)^\circ$ . The empirical formula is (electron microprobe):  $(K_{1.88}Pb_{0.79}Ca_{0.20}Rb_{0.05}Cs_{0.02})_{\Sigma 2.94}Cu_{4.07}S_{3.99}O_{18}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 9.07 (63) (−101), 7.38 (44) (101), 3.699 (78) (112, 202), 3.658 (100) (−204), 3.173 (40) (211, −213), 2.576 (51) (310, −116).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm $^{-1}$ ):** 1235sh, 1202s, 1145s, 1108s, 1080sh, 1025s, 975sh, 662, 615, 601s, 547, 508, 500sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**S555 Kottenheimite dimorph**  $\text{Ca}_3\text{Si}(\text{SO}_4)_2(\text{OH})_6 \cdot 12\text{H}_2\text{O}$ 

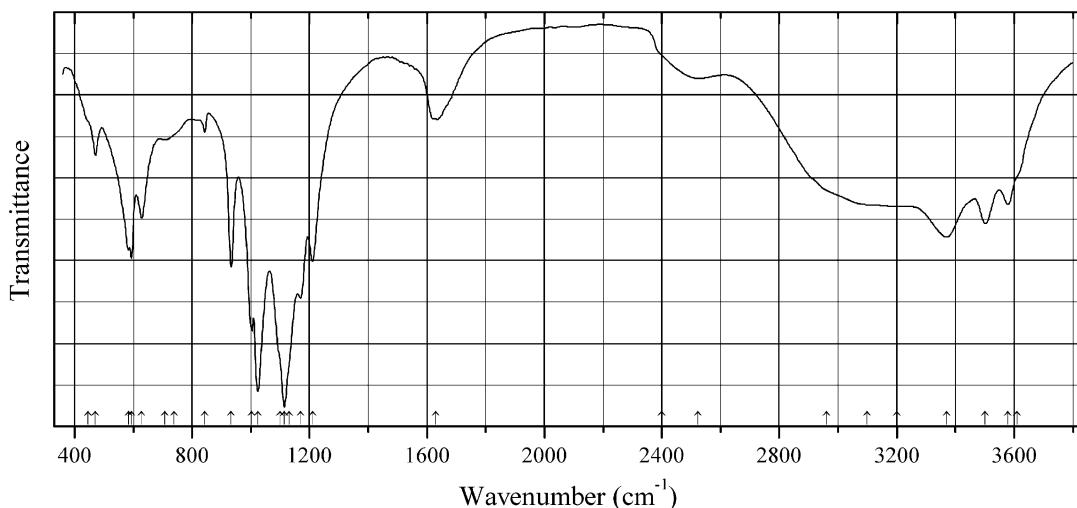
**Origin:** Bellerberg, near Mayen, Eifel, Rheinland-Pfalz (Rhineland-Palatinate), Germany.

**Description:** White random aggregate of acicular crystals. Isostructural with thaumasite. The empirical formula is (electron microprobe):  $\text{Ca}_{3.05}(\text{Si}_{0.9}\text{Al}_{0.1})(\text{SO}_4)[(\text{SO}_4)_{0.6}(\text{CO}_3)_{0.4}](\text{OH})_6 \cdot n\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3505s, 3460sh, 3417s, 1688, 1650, 1396s, 1100s, 990w, 880, 750s, 673, 632, 596, 499.

**Note:** The spectrum was obtained by N.V. Chukanov.

**S556 Bobcookite**  $\text{NaAl}(\text{UO}_2)_2(\text{SO}_4)_4 \cdot 18\text{H}_2\text{O}$ 

**Origin:** Blue Lizard Mine, Red Canyon, White Canyon District, San Juan Co., Utah, USA (type locality).

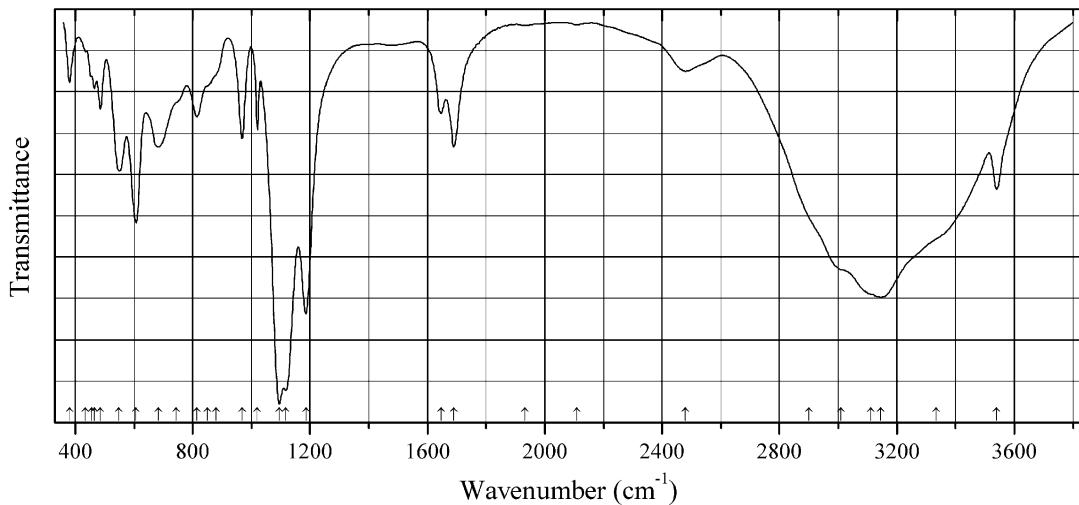
**Description:** Green-yellow crystals. Investigated by A.V. Kasatkin, the coauthor of bobcookeite first description.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3610sh, 3578, 3502, 3370, 3200sh, 3100sh, 2960sh, 2523w, 2400sh, 1630, 1210, 1169s, 1130sh, 1114s, 1100sh, 1024s, 1004s, 933, 843w, 740sh, 708w, 628, 594, 583, 471, 445sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

### S557 Riotintoite Al(SO<sub>4</sub>)(OH)·3H<sub>2</sub>O



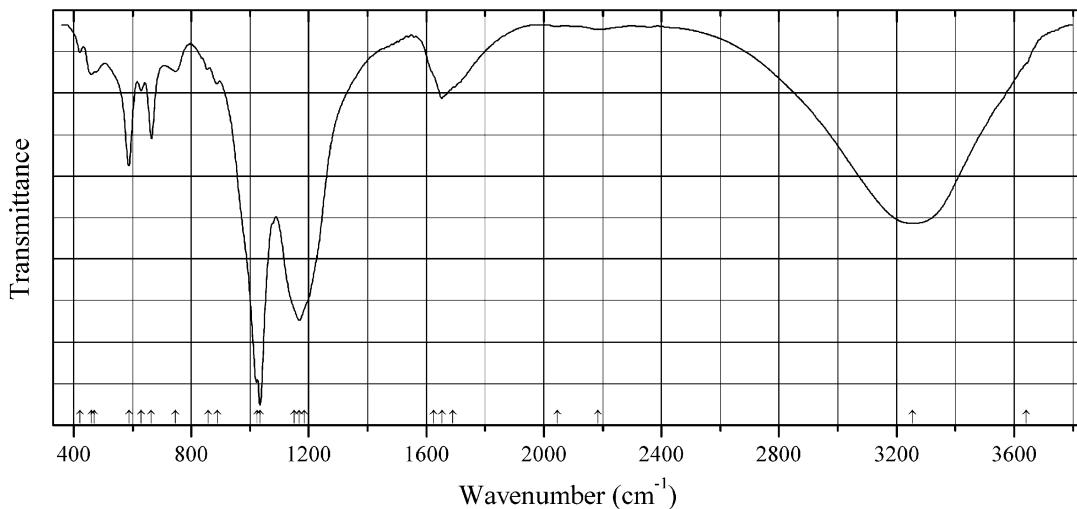
**Origin:** La Vendida copper mine (Mina La Vendida), about 5 km WNW of Sierra Gorda, Antofagasta Region, Atacama desert, Chile (type locality).

**Description:** Colorless platy crystals from cavities in massive aggregates of eriochalcite, Mg-rich aubertite, magnesioaubertite, belloite, and clay minerals. Holotype sample. Triclinic, space group  $P-1$ ,  $a = 5.6000$ ,  $b = 7.4496(8)$ ,  $c = 7.6709(9)$  Å,  $\alpha = 74.7847^\circ$ ,  $\beta = 86.0419^\circ$ ,  $\gamma = 75.8103^\circ$ ,  $V = 299.37$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{meas}} = 2.11(2)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 2.129$  g/cm<sup>3</sup>. Optically biaxial (-),  $\alpha = 1.513(2)$ ,  $\beta = 1.522(2)$ ,  $\gamma = 1.526(2)$ ,  $2V = 70(5)^\circ$ . The empirical formula is  $\text{Al}_{0.93}(\text{SO}_4)_{0.99}(\text{OH})_{0.81} \cdot 3.25\text{H}_2\text{O}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %)] are: 6.975 (100), 4.466 (18), 4.379 (19), 3.698 (18), 3.487 (20), 2.882 (17), 2.669 (54), 2.397 (40).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3540, 3335sh, 3145s, 3110sh, 3010sh, 2900sh, 2480, 2110w, 1933w, 1690, 1647, 1186s, 1117s, 1095s, 1021, 968, 880sh, 850sh, 814, 745sh, 683, 607s, 549, 485, 465, 455sh, 435sh, 382.

**Note:** The spectrum was obtained by N.V. Chukanov.

**S558 Rhomboclase**  $(\text{H}_5\text{O}_2)\text{Fe}^{3+}(\text{SO}_4)_2 \cdot 2\text{H}_2\text{O}$ 

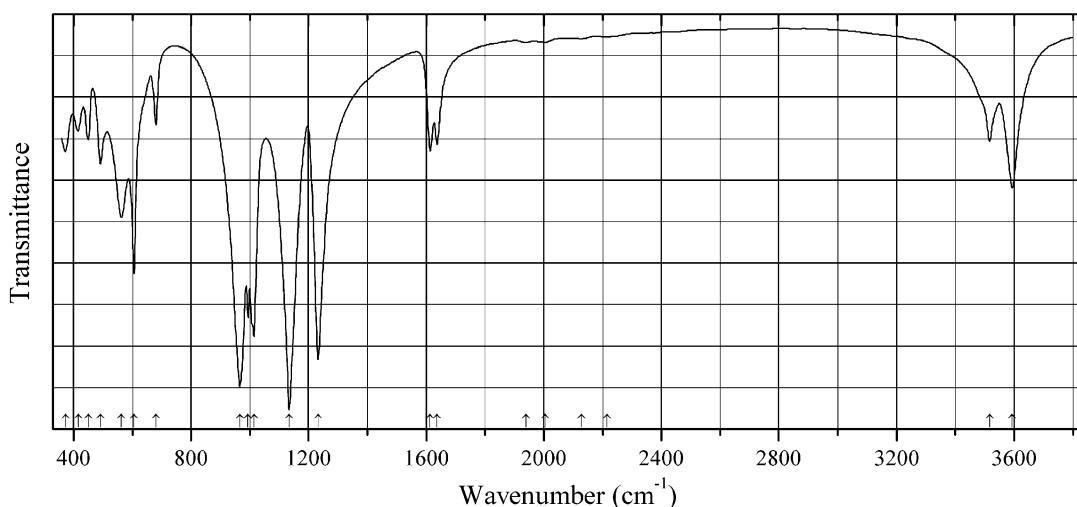
**Origin:** Alcaparrosa mine, Cerritos Bayos, Calama, El Loa Province, Antofagasta, Chile.

**Description:** Light gray grains. Investigated by I.V. Pekov. Characterized by single-crystal X-ray diffraction data. Orthorhombic,  $a = 5.426(3)$ ,  $b = 9.470(7)$ ,  $c = 18.333(17)$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3640sh, 3255s (broad), 2185w, 2045w, 1690sh, 1653, 1625sh, 1185sh, 1168s, 1150sh, 1034s, 1025s, 888w, 857w, 747w, 665, 630, 588, 471, 460, 421w.

**Note:** The sample has altered as a result of a reaction with KBr. The spectrum was obtained by N.V. Chukanov.

**S559 Ferrinatrite**  $\text{Na}_3\text{Fe}^{3+}(\text{SO}_4)_3 \cdot 3\text{H}_2\text{O}$ 

**Origin:** Coronel Manuel Rodríguez mine, Mejillones peninsula, Mejillones, Antofagasta Province, Antofagasta Region, Chile.

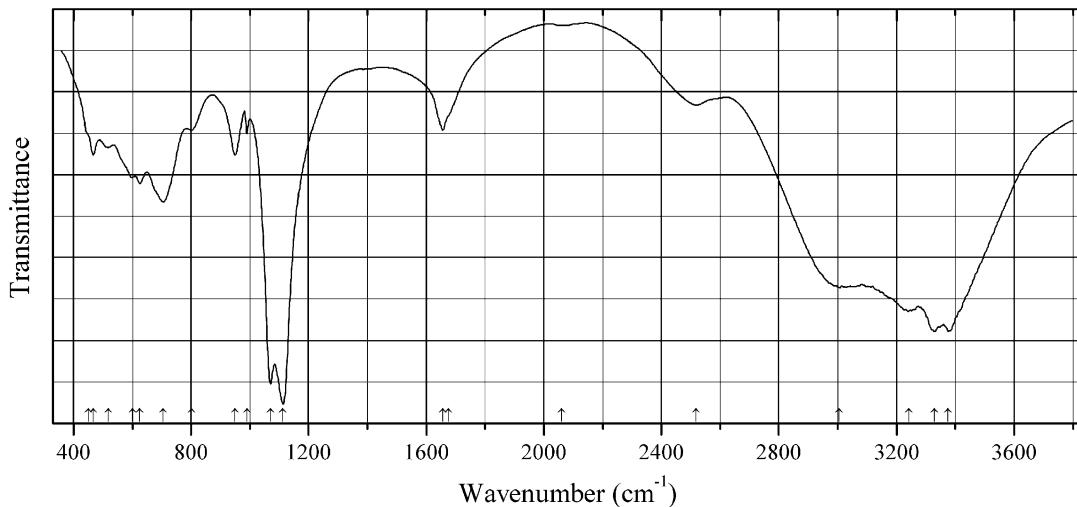
**Description:** White aggregate of acicular crystals. Investigated by I.V. Pekov. Characterized by powder X-ray diffraction data and electron microprobe analyses.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3594, 3517, 2215w, 2128w, 2005w, 1939w, 1637, 1614, 1232s, 1133s, 1014s, 994s, 966s, 680, 606, 563, 491, 450, 416, 373.

**Note:** The spectrum was obtained by N.V. Chukanov.

**S560 Magnesioaubertite** MgAl(SO<sub>4</sub>)<sub>2</sub>Cl·14H<sub>2</sub>O



**Origin:** La Vendida copper mine, about 5 km WNW of Sierra Gorda, Antofagasta Region, Atacama desert, Chile.

**Description:** Turquoise-blue granular aggregate from the association with vendidaite and eriochalcite.

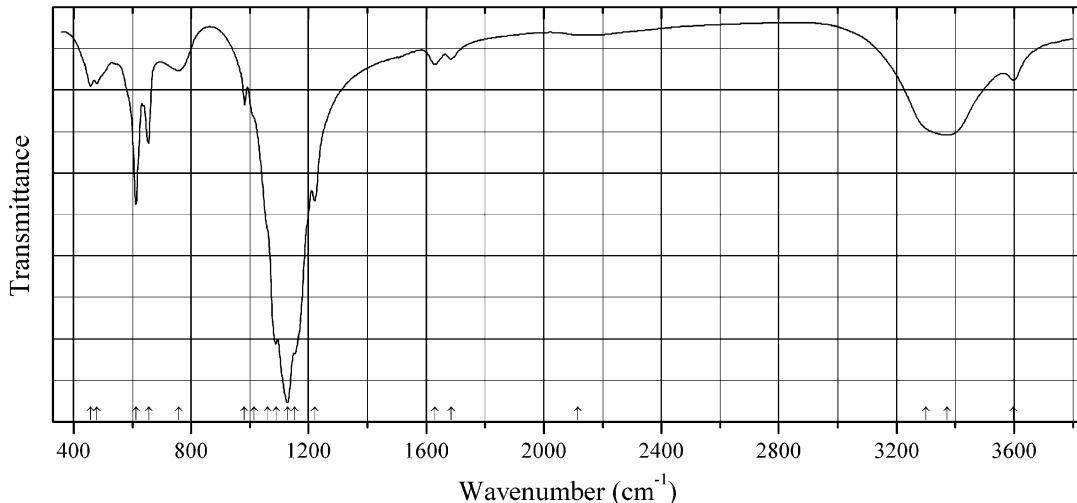
Investigated by I.V. Pekov. Characterized by powder X-ray diffraction data. The empirical formula is (electron microprobe): Mg<sub>0.56</sub>Cu<sub>0.39</sub>Al<sub>1.09</sub>(SO<sub>4</sub>)<sub>2.00</sub>Cl<sub>0.65</sub>(OH)<sub>x</sub>·nH<sub>2</sub>O.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3376s, 3330s, 3241s, 3005s, 2519, 2060w, 1675sh, 1656, 1112s, 1070s, 990, 950, 802, 706s, 626, 600, 518, 468, 450sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**S561 Antofagastaite** Na<sub>2</sub>Ca(SO<sub>4</sub>)<sub>2</sub>·1.5H<sub>2</sub>O



**Origin:** Coronel Manuel Rodríguez mine, Mejillones peninsula, Mejillones, Antofagasta region, Chile (type locality).

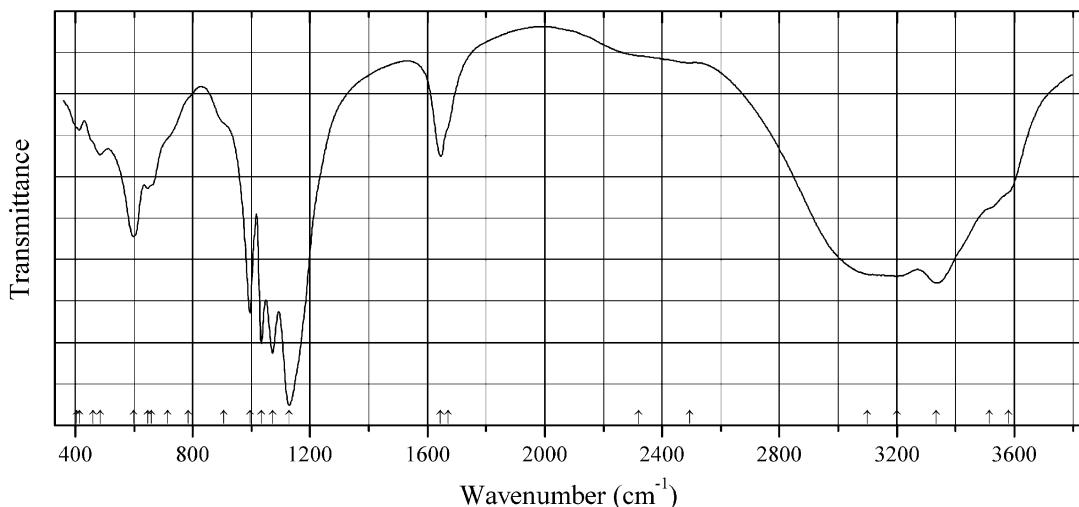
**Description:** Colorless prismatic crystals from the association with sideronatrite, metasideronatrite, aubertite, gypsum, ferrinatrite, glauberite, and amarillite. Holotype sample. The crystal structure is solved. Monoclinic, space group  $P2_1/m$ ,  $a = 6.4596(4)$ ,  $b = 6.8703(5)$ ,  $c = 9.4685(7)$  Å,  $\beta = 104.580(4)^\circ$ ,  $V = 406.67(5)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{meas}} = 2.42(1)$  g/cm $^3$ ,  $D_{\text{calc}} = 2.465$  g/cm $^3$ . Optically biaxial (−),  $\alpha = 1.489$  (2),  $\beta = 1.508$  (2),  $\gamma = 1.510$  (2),  $2V = 40(10)^\circ$ . The empirical formula is  $\text{Na}_{2.06}\text{Ca}_{0.95}\text{S}_{2.01}\text{O}_8 \cdot 1.35\text{H}_2\text{O}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 9.17 (100) (001), 5.501 (57) (011), 4.595 (32) (002), 3.437 (59) (020), 3.058 (43) (−103, 003), 2.918 (50) (−211), 2.795 (35) (−113, 013).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm $^{-1}$ ):** 3598, 3373, 3300sh, 1685w, 1629w, 1220, 1153s, 1128s, 1090s, 1060sh, 1015sh, 982, 758, 656, 613, 480, 458.

**Note:** The spectrum was obtained by N.V. Chukanov. Very weak absorptions in the range 2100–2250 cm $^{-1}$  correspond to overtones and combination modes.

### S562 Römerite $\text{Fe}^{2+}\text{Fe}^{3+}_2(\text{SO}_4)_4 \cdot 14\text{H}_2\text{O}$



**Origin:** Alcaparrosa mine, Cerritos Bayos, Calama, El Loa Province, Antofagasta, Chile.

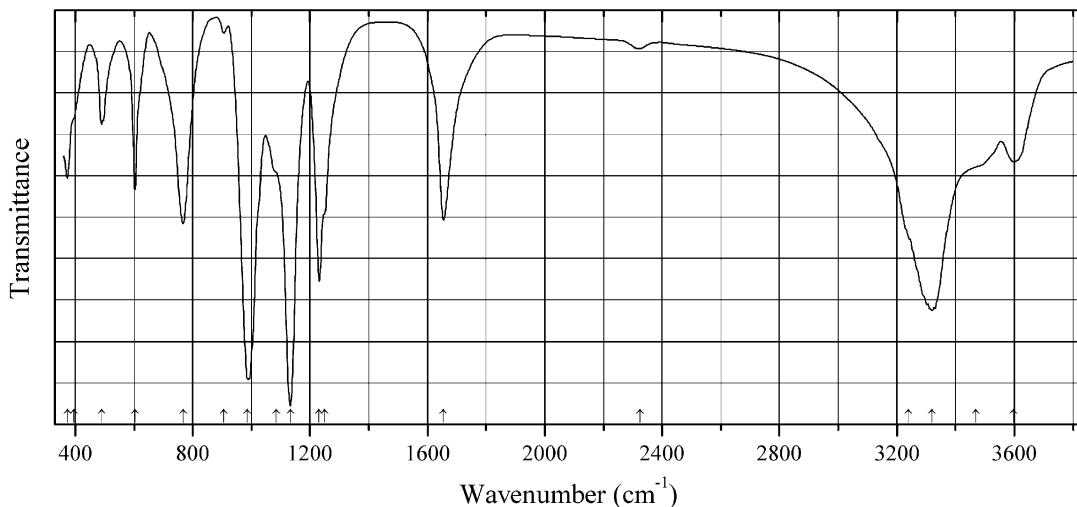
**Description:** Reddish-brown crystals from the association with coquimbite, metavoltine, and voltaite.

Investigated by I.V. Pekov. Characterized by single-crystal X-ray diffraction data. Triclinic,  $a = 6.317(4)$ ,  $b = 6.453(4)$ ,  $c = 15.318(10)$  Å,  $\alpha = 85.61(5)^\circ$ ,  $\beta = 89.78(5)^\circ$ ,  $\gamma = 79.06(5)^\circ$ ,  $V = 611.2(7)$  Å $^3$ . Only Fe and S have been found by means of electron microprobe analyses.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm $^{-1}$ ):** 3580sh, 3515sh, 3334s, 3200s, 3100sh, 2495w, 2320sh, 1670sh, 1645, 1129s, 1072s, 1034s, 995s, 905sh, 785sh, 715sh, 660sh, 646, 599s, 484, 460sh, 414, 405sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**S563 Calamaite**  $\text{Na}_2\text{TiO}(\text{SO}_4)_2 \cdot 2\text{H}_2\text{O}$ 

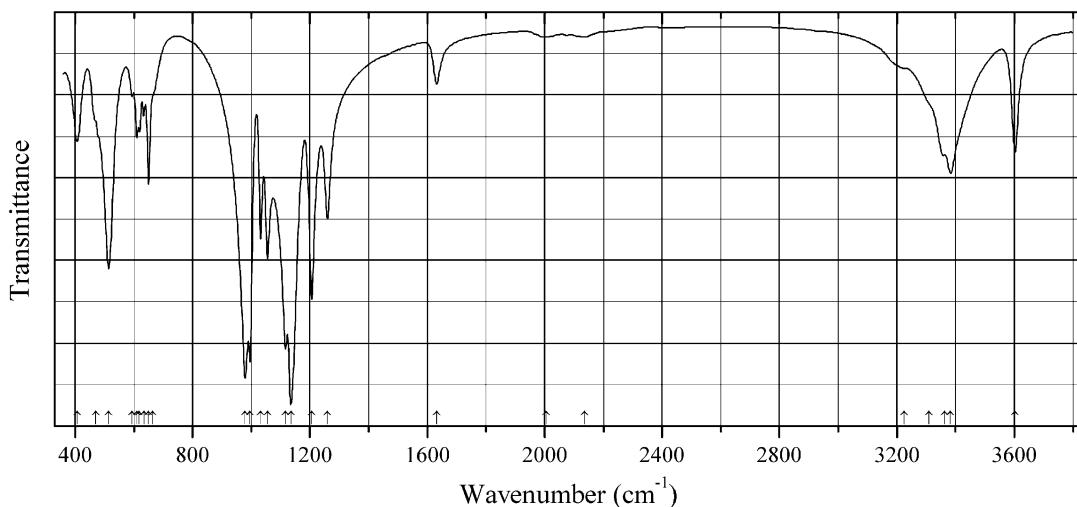
**Origin:** Alcaparrosa mine, Cerro Alcaparrosa, Calama commune, El Loa province, Antofagasta region, Chile (type locality).

**Description:** Colorless acicular crystals from the association with römerite, coquimbite, metavoltine, rhomboclase, tamarugite, halotrichite, and szomolnokite. Holotype sample. The crystal structure is solved. Orthorhombic, space group *Ibam*,  $a = 16.0989(11)$ ,  $b = 16.2399(9)$ ,  $c = 7.0135(4)$  Å,  $V = 1833.6(2)$  Å<sup>3</sup>,  $Z = 8$ .  $D_{\text{calc}} = 2.45$  g/cm<sup>3</sup>. Optically biaxial (+),  $\alpha = 1.557(2)$ ,  $\beta = 1.562(2)$ ,  $\gamma = 1.671(3)$ ,  $2V = 30(10)$ °. The empirical formula is (electron microprobe):  $\text{Na}_{1.97}\text{Ti}_{0.92}\text{Fe}^{3+}_{0.07}\text{S}_{0.99}\text{O}_{9.20}\text{H}_2\text{O}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 8.10 (100) (020, 200), 5.04 (55) (121, 211), 3.787 (26) (231), 3.619 (18) (240, 420), 3.417 (27) (141, 411), 2.943 (20) (341, 431), 2.895 (20) (132, 312).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3598, 3470sh, 3320s, 3240sh, 2324w, 1655s, 1250sh, 1231s, 1133s, 1085sh, 987s, 906w, 767s, 603, 489, 395sh, 373.

**Note:** The spectrum was obtained by N.V. Chukanov.

**S564 Metasideronatrite**  $\text{Na}_2\text{Fe}^{3+}(\text{SO}_4)_2(\text{OH}) \cdot \text{H}_2\text{O}$ 

**Origin:** Coronel Manuel Rodríguez mine, Mejillones peninsula, Mejillones, Antofagasta Province, Antofagasta Region, Chile.

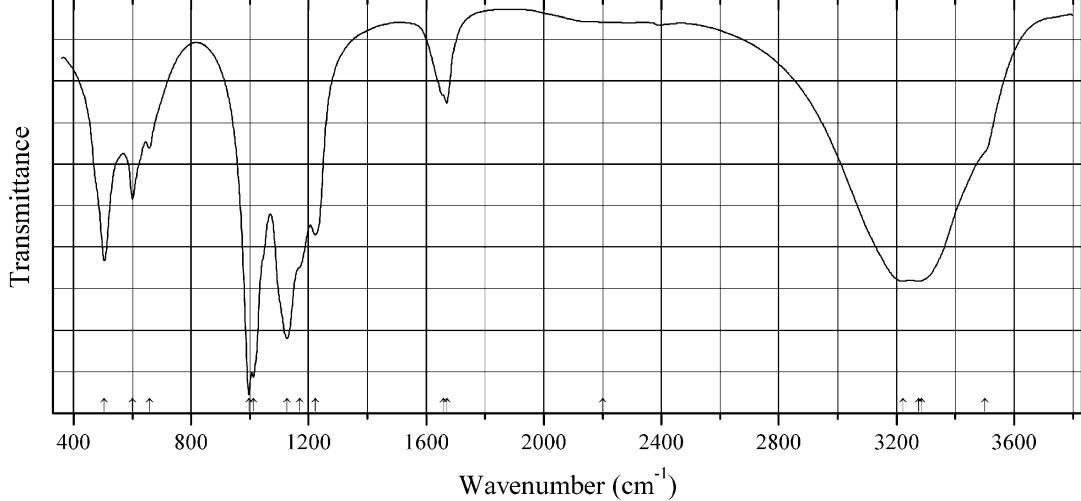
**Description:** Orange-beige pseudomorphs after prismatic sideronatite crystals. Investigated by I.V. Pekov. Characterized by powder X-ray diffraction data and electron microprobe analyses.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3603, 3383, 3362, 3310sh, 3225sh, 2135w, 2004w, 1632, 1260, 1206s,

**Note:** The spectrum was obtained by N.V. Chukanov.

### S565 Parabutlerite Fe<sup>3+</sup>(SO<sub>4</sub>)(OH)·2H<sub>2</sub>O



**Origin:** Coronel Manuel Rodríguez mine, Mejillones peninsula, Mejillones, Antofagasta Province, Antofagasta Region, Chile.

**Description:** Orange-brown crystals from the association with gypsum. Investigated by I.V. Pekov.

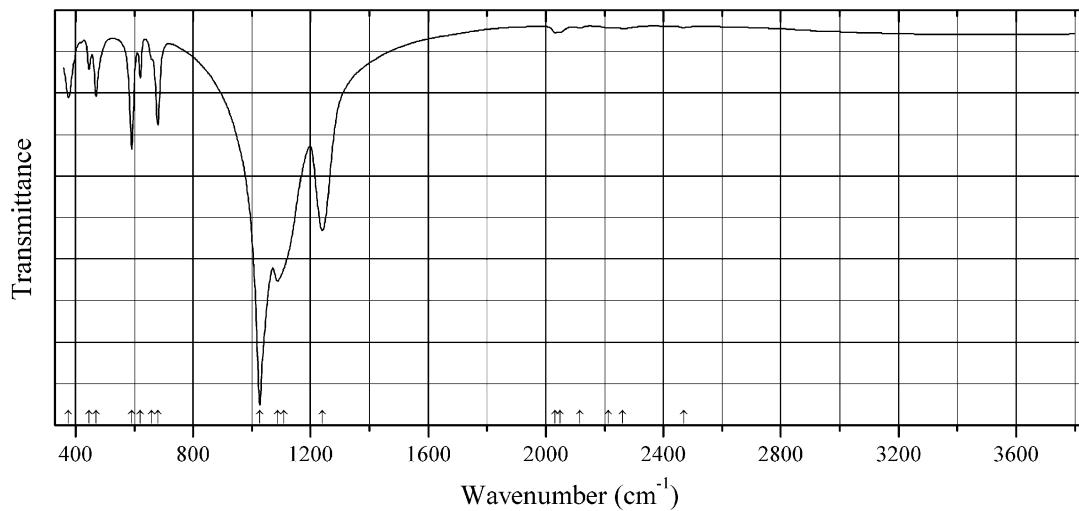
Characterized by single-crystal X-ray diffraction data. Orthorhombic,  $a = 7.386(3)$ ,  $b = 7.405(4)$ ,  $c = 20.091(10)$  Å,  $V = 1072(1)$  Å<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3500sh, 3276s, 3223s, 3285w, (2200sh), 1670, 1660sh, 1222s, 1170sh, 1126s, 1012s, 997s, 658, 601, 505s.

**Note:** The spectrum was obtained by N.V. Chukanov.

## S566 Yavapaiite $\text{KFe}^{3+}(\text{SO}_4)_2$



**Origin:** Alcaparrosa mine, Cerritos Bayos, Calama, El Loa Province, Antofagasta, Chile.

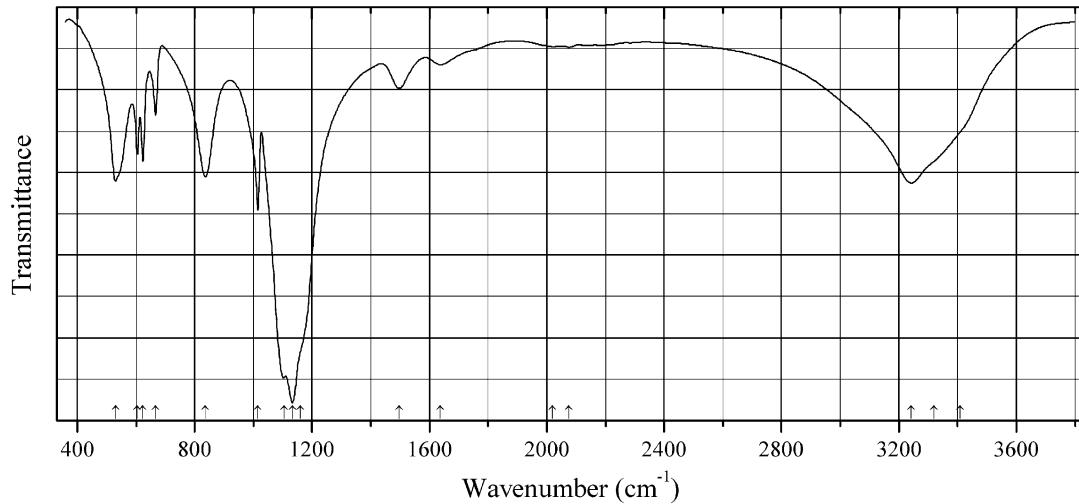
**Description:** Pink platy crystals from the association with coquimbite and rhomboclase. Investigated by I.V. Pekov. Characterized by single-crystal X-ray diffraction data. Monoclinic,  $a = 8.186(8)$ ,  $b = 5.156(6)$ ,  $c = 7.893(8)$  Å,  $\beta = 94.69(10)^\circ$ ,  $V = 332.0(6)$  Å $^3$ . The empirical formula is (electron microprobe): K<sub>0.98</sub>Fe<sub>1.01</sub>(SO<sub>4</sub>)<sub>2.00</sub>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 2470w, 2262w, 2212w, 2117w, 2049w, 2032w, 1240s, 1110sh, 1087s, 1027s, 680, 660sh, 621, 591, 470, 446, 377.

**Note:** The spectrum was obtained by N.V. Chukanov.

## S567 Szomolnokite $\text{Fe}(\text{SO}_4) \cdot \text{H}_2\text{O}$



**Origin:** Alcaparrosa mine, Cerritos Bayos, Calama, El Loa Province, Antofagasta, Chile.

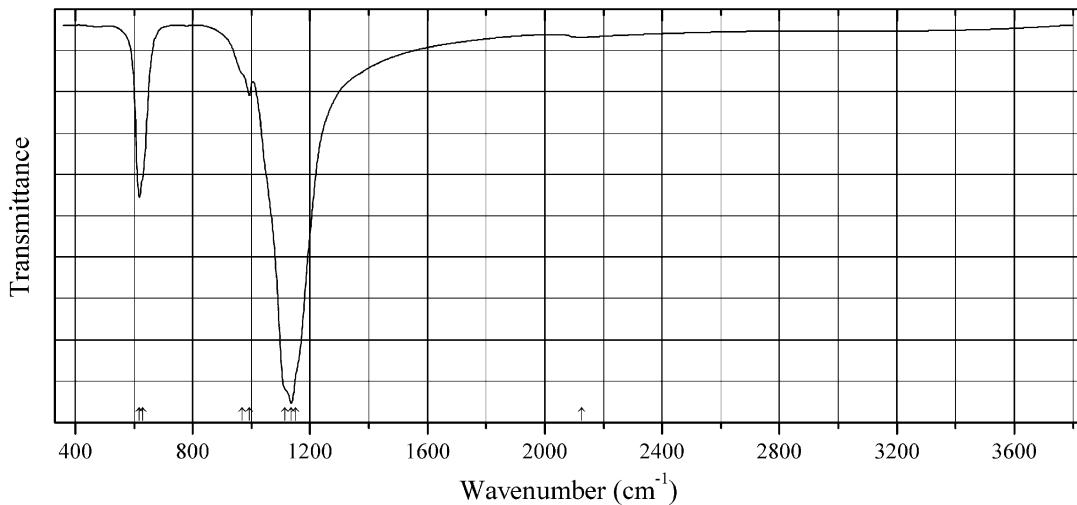
**Description:** Pale greenish-yellow crystals from the association with metavoltine, coquimbite, and römerite. Investigated by I.V. Pekov. Characterized by single-crystal X-ray diffraction data. Monoclinic,  $a = 7.66$ ,  $b = 7.53$ ,  $c = 7.09$  Å,  $\beta = 116.66^\circ$ ,  $V = 365.7$  Å $^3$ . The empirical formula is (electron microprobe):  $(\text{Fe}_{0.89}\text{Zn}_{0.05}\text{Mg}_{0.03})\text{S}_{1.01}\text{O}_4 \cdot \text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm $^{-1}$ ):** 3410sh, 3320sh, 3243s, 2076w, 2020w, 1637, 1497, 1160sh, 1133s, 1105s, 1016s, 837s, 667, 624, 604, 530s.

**Note:** The spectrum was obtained by N.V. Chukanov.

### S568 Metathénardite $\text{Na}_2(\text{SO}_4)$



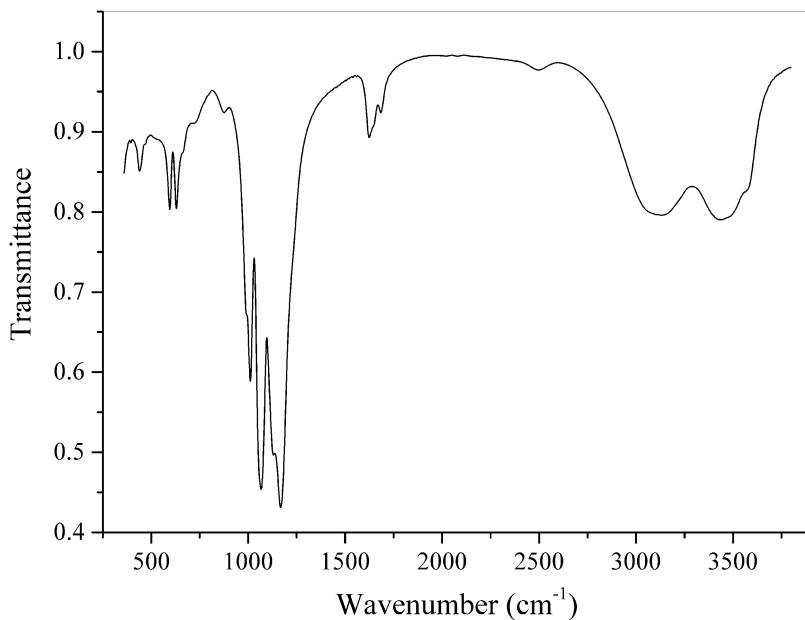
**Origin:** Yadovitaya (Poisonous) fumarole, Second scoria cone, Tolbachik volcano, Kamchatka peninsula, Far-Eastern Region, Russia.

**Description:** Pale blue crystals. Investigated by I.V. Pekov, the author of the first description of metathénardite.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm $^{-1}$ ):** 2125w, 1150sh, 1136s, 1115sh, 993, 970sh, 630sh, 618s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**S569 Magnesiovoltaitaite**  $K_2Mg_5Fe^{3+}_3Al(SO_4)_{12} \cdot 18H_2O$ 

**Origin:** Alcaparrosa mine, Cerro Alcaparrosa, El Loa province, Antofagasta region, Chile (type locality).

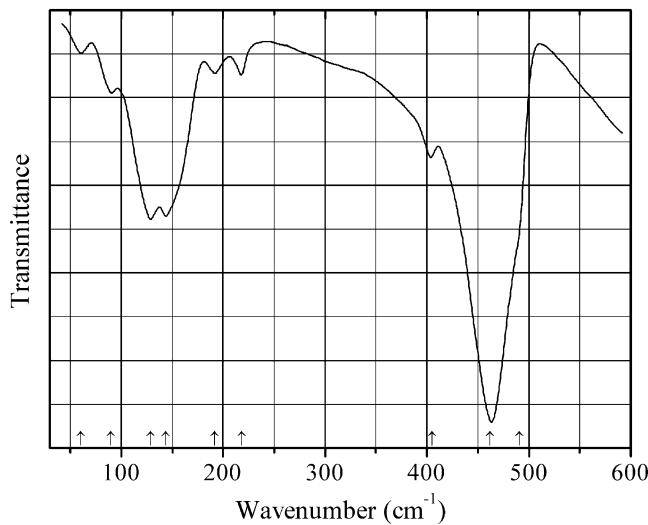
**Description:** Yellow crystals from the association with coquimbite, tamarugite, alum-(Na), rhomboclase, yavapaiite, voltaite, and opal. Holotype sample. The crystal structure is solved. Cubic, space group  $Fd\text{-}3c$ ,  $a = 27.161(1)$  Å,  $V = 20038(2)$  Å<sup>3</sup>,  $Z = 16$ .  $D_{\text{meas}} = 2.51(2)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 2.506$  g/cm<sup>3</sup>. Optically anomalously anisotropic, uniaxial with  $\epsilon = 1.584$  (2) and  $\omega = 1.588$  (2), or biaxial (−) with  $\alpha = 1.584$  (2),  $\beta = 1.587$  (2), and  $\gamma = 1.588$  (2). The empirical formula is  $(K_{1.85}Na_{0.08})(Mg_{4.25}Mn_{0.46}Zn_{0.14})Fe^{3+}_{3.14}Al_{0.91}(SO_4)_{11.91}(H_2O)_{18.325}O_{0.035}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 9.56 (29) (022), 6.77 (37) (004), 5.53 (61) (224), 3.532 (68) (137), 3.392 (100) (008), 3.034 (45) (048), 2.845 (30) (139).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3565sh, 3480sh, 3441, 3134, (3070sh), 2496w, 1684w, 1640sh, 1624, 1168s,

1133s, 1067s, 1011s, 995sh, 876w, 718sh, 660sh, 629, 596, 440.

**Note:** The spectrum was obtained by N.V. Chukanov.

**S570 Barium titanium sulfide  $\text{Ba}_2\text{TiS}_4$** 

**Origin:** Synthetic.

**Description:** Orthorhombic, space group  $Pnma$ . The crystal structure contains  $\text{TiS}_4$  tetrahedra.

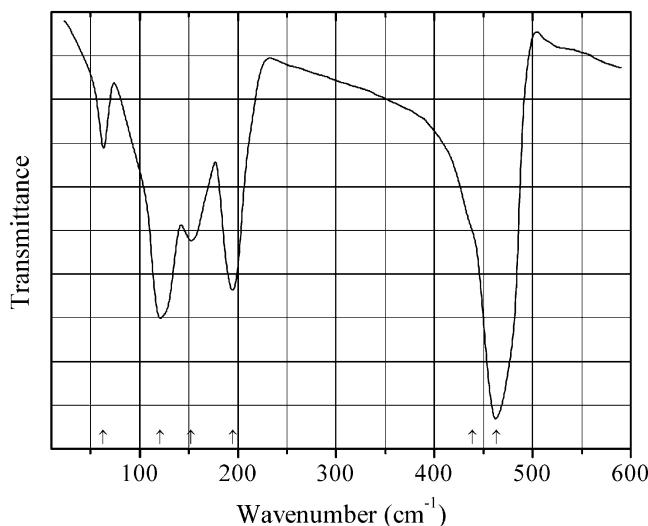
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission of a polycrystalline powder sample.

**Source:** Ishii and Saeki (1992).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 491sh, 462s, 405, 218w, 192w, 144, 129, 90, 60w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 477, 457w, 441w, 445sh, 403s.

**S571 Barium titanium sulfide  $\text{Ba}_3\text{TiS}_5$** 

**Origin:** Synthetic.

**Description:** Tetrahedral, space group  $I4/mcm$ . The crystal structure contains  $\text{TiS}_4$  tetrahedra.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission of a polycrystalline powder sample.

**Source:** Ishii and Saeki (1992).

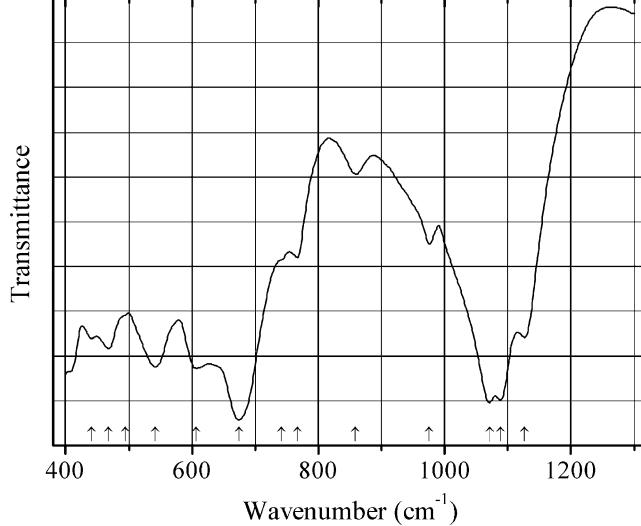
### Wavenumbers (IR, cm<sup>-1</sup>): 46

Note: The wavenumbers were partly determined by us based on the IR spectrum.

Note: The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 478, 462, 416s.

## **SS72 Bismuth copper sulfate tellurite BiCu<sub>2</sub>(TeO<sub>3</sub>)(SO<sub>4</sub>)(OH)<sub>3</sub>**



**Origin:** Synthetic.

**Description:** Synthesized hydrothermally from  $\text{Bi}_2\text{O}_3$ ,  $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ ,  $\text{TeO}_2$ , and  $\text{H}_2\text{SO}_4$  at 230 °C for 3 days. Monoclinic, space group  $P2_1/n$ ,  $a = 9.5513(15)$ ,  $b = 6.3022(10)$ ,  $c = 13.955(2)$  Å,  $\beta = 102.845(3)^\circ$ ,  $V = 819.0(2)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 5.318$  g/cm<sup>3</sup>.

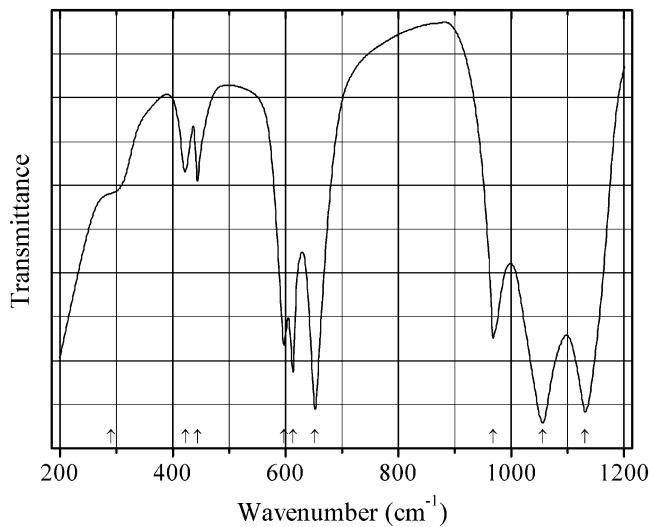
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Chen et al. (2015a).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1127, 1089s, 1071s, 976, 858w, 767, 742sh, 675s, 607, 542, 494sh, 468, 441.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1110w, 1092w, 1071w, 977, 760, 690w, 630, 563w, 438, 412, 354s, 273, 228, 211, 155, 134s, 120s

**S573 Bismuth sulfate  $\text{Bi}_2(\text{SO}_4)_3$** 

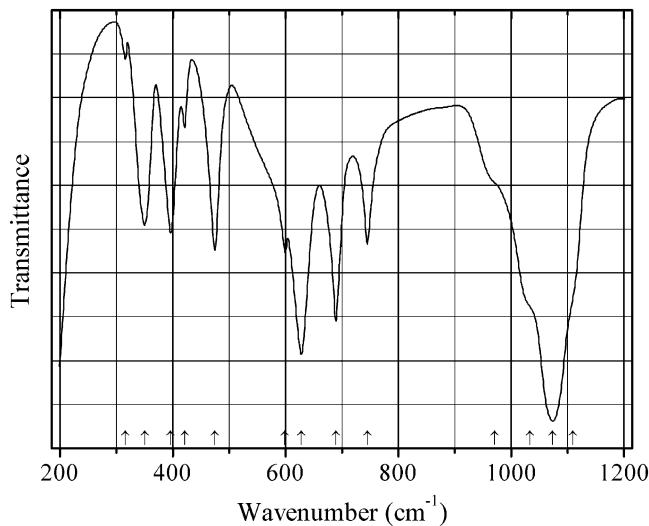
**Origin:** Synthetic.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Botto et al. (1995).

**Wavenumbers (cm⁻¹):** 1131s, 1056s, 968, 652s, 613, 597, 444w, 422w, 290sh.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**S574 Bismuthyl sulfate  $(\text{BiO})_2(\text{SO}_4)$** 

**Origin:** Synthetic.

**Description:** Product of heating of tetradyomite at 500 °C in air. The sample contains admixture of tellurium oxide.

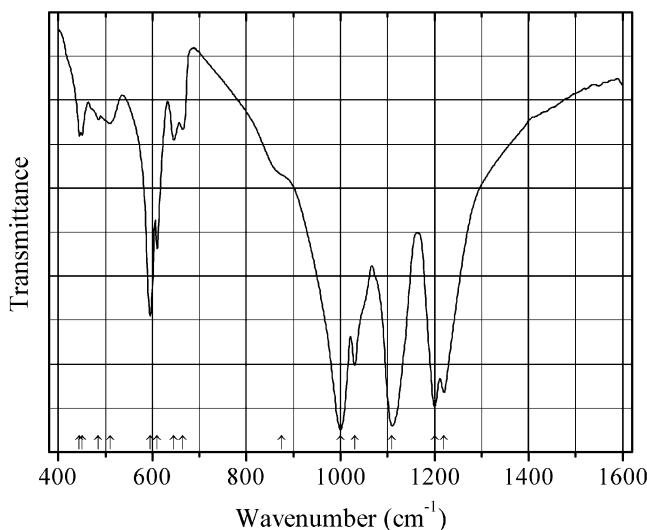
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Botto et al. (1995).

**Wavenumbers (cm<sup>-1</sup>):** 1110sh, 1074s, 1033sh, 971sh, 745, 689, 628s, 599, 475, 421w, 396, 350, 316w.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. The bands located at 745 and 689 cm<sup>-1</sup> can be tentatively assigned to a tellurium oxide.

### S575 Cesium iron sulfate Cs<sub>3</sub>Fe(SO<sub>4</sub>)<sub>3</sub>



**Origin:** Synthetic.

**Description:** Trigonal, space group *R*3c.

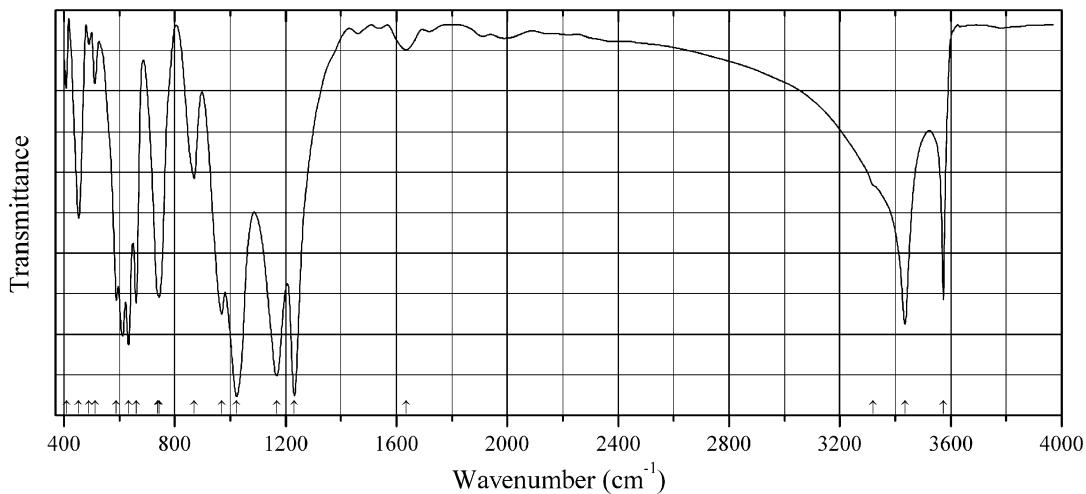
**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

**Source:** Bremard et al. (1986).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1220, 1200s, 1110s, 1030, 1000s, 875sh, 665w, 645w, 610, 595, 510w, 485w, 445w, 450w, 314, 264w, 244w, 200w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>, at 77 K):** 1237sh, 1225sh, 1205, 1115w, 1035sh, 1030w, 1010, 990s, 650w, 620, 615sh, 603, 597, 463, 447, 263, 258, 246sh, 204, 178sh, 168w, 155w, 138w, 57w, 37.5w.

**S576 Dysprosium copper hydroxysulfate  $\text{Dy}_2\text{Cu}(\text{SO}_4)_2(\text{OH})_4$**   $\text{Dy}_2\text{Cu}(\text{SO}_4)_2(\text{OH})_4$ 

**Origin:** Synthetic.

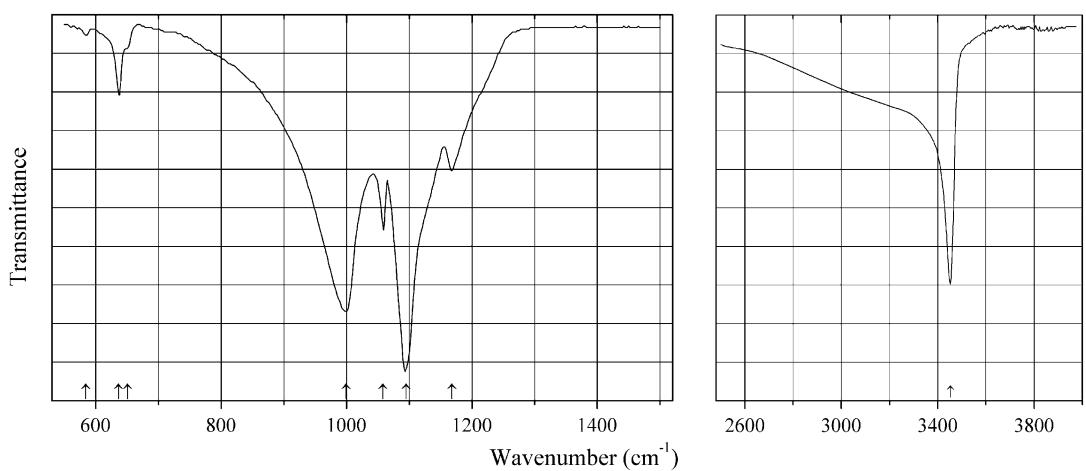
**Description:** Synthesized by a hydrothermal method. Monoclinic, space group  $P2_1/c$ ,  $a = 6.304(4)$ ,  $b = 6.663(4)$ ,  $c = 10.724(6)$  Å,  $\beta = 98.527(1)$ °,  $V = 445.5(5)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 4.806$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Tang et al. (2015).

**Wavenumbers (cm<sup>-1</sup>):** 3573, 3435, 3320sh, 1635w, 1232s, 1168s, 1023s, 970, 870, 744, 739sh, 661, 634s, 612s, 589, 512w, 491w, 454, 409w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**S577 Iron(III) basic sulfate  $\text{Fe}(\text{SO}_4)(\text{OH})$** 

**Origin:** Synthetic.

**Description:** Prepared hydrothermally from  $\text{Fe}_2(\text{SO}_4)_3 \cdot n\text{H}_2\text{O}$ . Monoclinic, space group  $P2_1/c$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of a powdered sample.

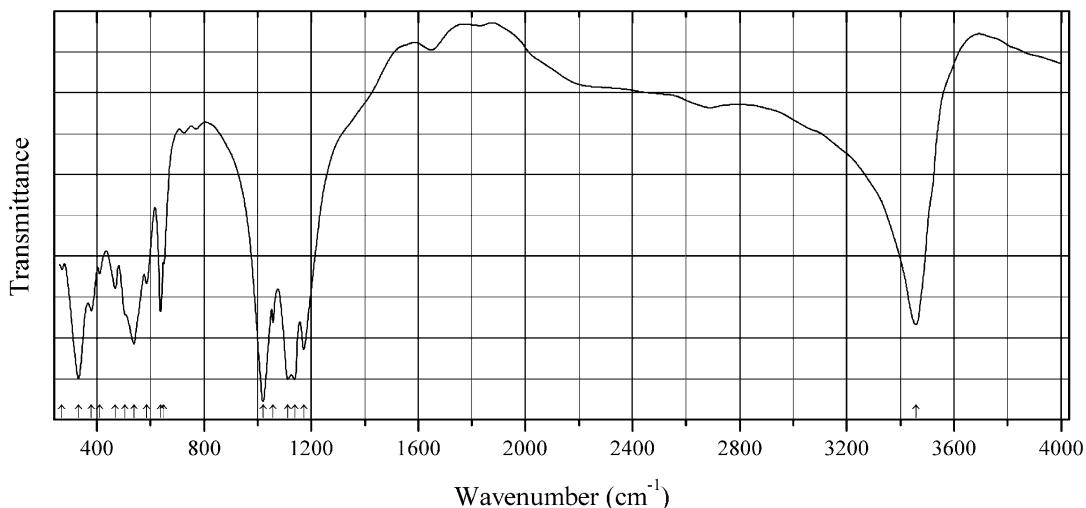
**Source:** Gomez et al. (2013).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3452, 1168, 1095s, 1058, 999s, 651sh, 636, 584w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 3077, 3453s, 3587w, 1183, 1122, 1100s, 1062, 1026, 914w, 645, 556, 480, 418w, 370, 231.

### S578 Iron(III) basic sulfate $\text{Fe}(\text{SO}_4)(\text{OH})$



**Origin:** Synthetic.

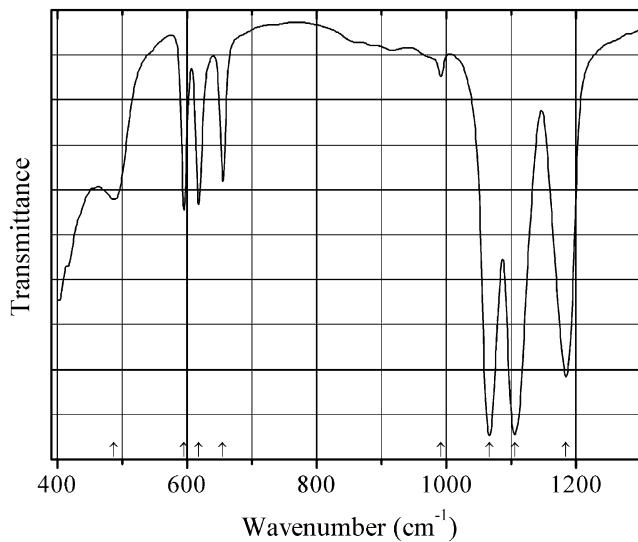
**Description:** Orthorhombic, space group  $Pnma$ ,  $a = 7.33$ ,  $b = 6.42$ ,  $c = 7.14$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr and TiBr discs. Transmission.

**Source:** Powers et al. (1975).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3458s, 1172s, 1138s, 1112s, 1058, 1020s, 650, 638, 585, 538, 505, 468, 410w, 380, 331s, 270w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**S579 Lanthanum oxosulfate**  $\text{La}(\text{SO}_4)\text{O}_2$ 

**Origin:** Synthetic.

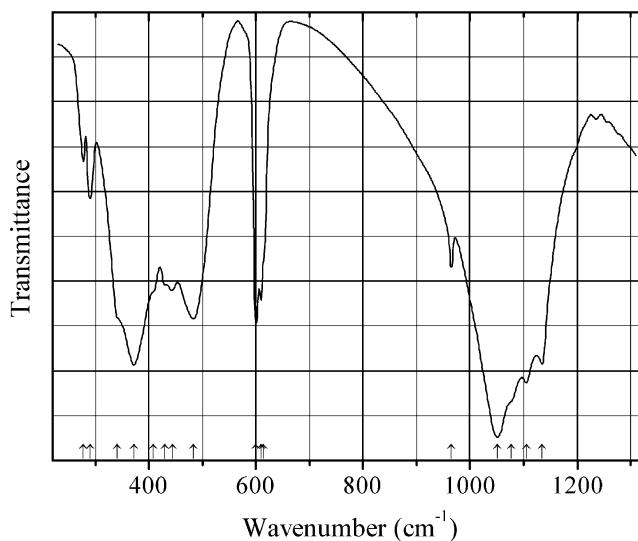
**Description:** Synthesized by a template-assisted route described elsewhere. Characterized by powder X-ray diffraction data. Monoclinic,  $a = 14.354(3)$ ,  $b = 4.2862(6)$ ,  $c = 8.388(2)$  Å,  $\beta = 107.16(2)$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Zhang et al. (2008).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1185s, 1106s, 1067s, 992w, 655, 618, 595, 487.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**S580 Lead(II) oxysulfate**  $\text{Pb}_5(\text{SO}_4)\text{O}_4$ 

**Origin:** Synthetic.

**Description:** Microcrystalline powder obtained by the reaction of PbO with diluted H<sub>2</sub>SO<sub>4</sub> at 80 °C during 4–6 h and subsequent heating of the product at 550 °C. Monoclinic, space group *P2<sub>1</sub>/c*, *Z* = 4.

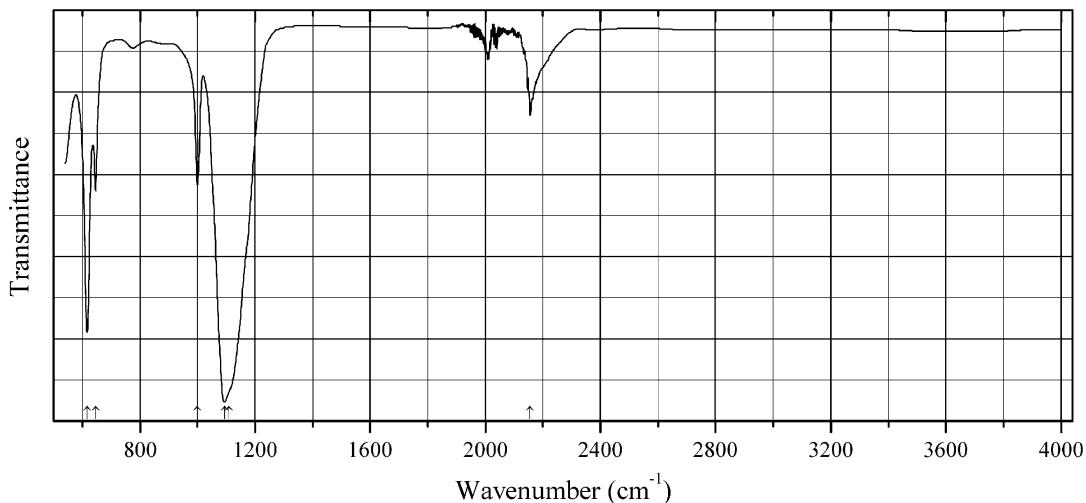
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Grasselli and Baran (1984).

**Wavenumbers (cm<sup>-1</sup>):** 1135s, 1105s, 1077sh, 1051s, 965, 614sh, 609, 600, 483, 445, 430sh, 408sh, 372s, 341sh, 290, 278w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### S581 Lithium iron(II) sulfate fluoride tavorite-type LiFe(SO<sub>4</sub>)F



**Origin:** Synthetic.

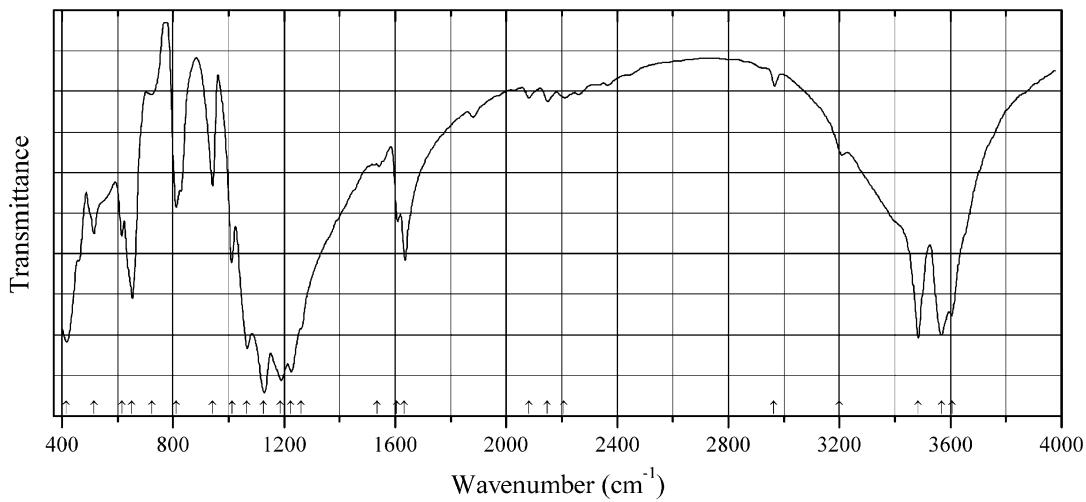
**Description:** Prepared from Fe(SO<sub>4</sub>)·H<sub>2</sub>O and LiF by a low-temperature solvothermal approach. Characterized by powder X-ray diffraction data. Triclinic, space group *P-1*, *a* = 5.1760(4), *b* = 5.4909(4), *c* = 7.2214(5) Å,  $\alpha$  = 106.511°,  $\beta$  = 107.187(3)°,  $\gamma$  = 97.847(2)°, *V* = 182.46 (2) Å<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of a powdered sample.

**Source:** Sobkowiak et al. (2013).

**Wavenumbers (cm<sup>-1</sup>):** 2156, 1110sh, 1094s, 1000, 646, 617s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**S582 Magnesium hydroxysulfate hydrate**  $Mg_3(SO_4)_2(OH)_2 \cdot 2H_2O$ 

**Origin:** Synthetic.

**Description:** Crystals grown hydrothermally from NaOH and MgSO<sub>4</sub> at 160 °C for 21 days. The crystal structure is solved. Orthorhombic, space group *Pbcm*, *a* = 7.177(1), *b* = 9.804(2), *c* = 12.775(2) Å, *V* = 898.9(2) Å<sup>3</sup>, *Z* = 4. *D*<sub>calc</sub> = 2.476 g/cm<sup>3</sup>.

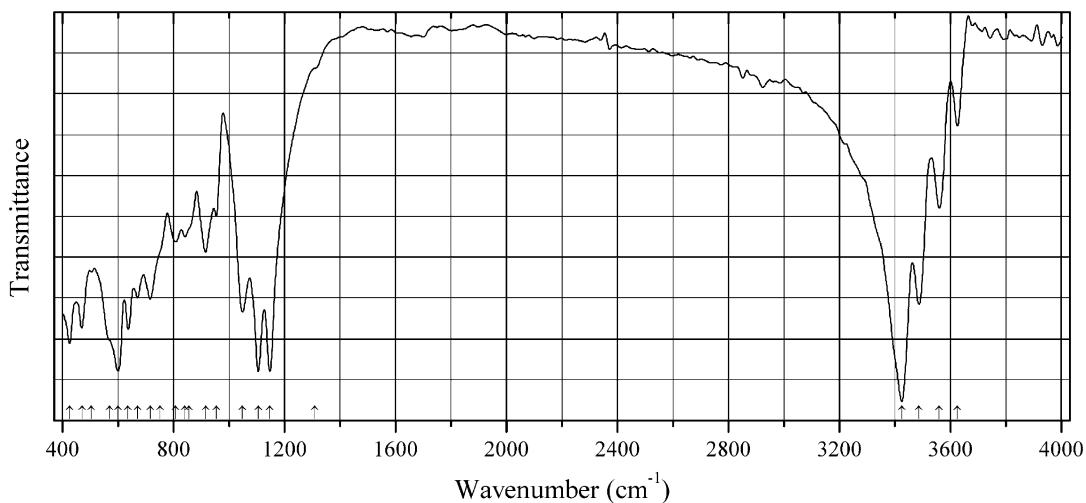
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Tao et al. (2002).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3607, 3567, 3483, 3200w, 2964w, 2207w, 2148w, 2081w, 1633, 1606, 1534w, 1261sh, 1224s, 1187s, 1126s, 1066s, 1012, 943, 813, 725w, 652, 616, 516, 416s.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 3604s, 3565s, 3484s, 1215, 1103, 1027s, 653, 634, 494, 459, 270.

**S583 Manganese hydroxysulfate**  $Mn_5(SO_4)(OH)_8$   $Mn_5(SO_4)(OH)_8$ 

**Origin:** Synthetic.

**Description:** Prepared under mild hydrothermal conditions. Characterized by powder X-ray diffraction data. The crystal structure is solved. Triclinic, space group  $P\bar{1}$ ,  $a = 7.5501(5)$ ,  $b = 8.5558(6)$ ,  $c = 8.6059(5)$  Å,  $\alpha = 98.122(4)^\circ$ ,  $\beta = 102.370(4)^\circ$ ,  $\gamma = 99.646(4)^\circ$ ,  $V = 526.19(6)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 3.199$  g/cm<sup>3</sup>. Mn atoms have five- and sixfold coordination.

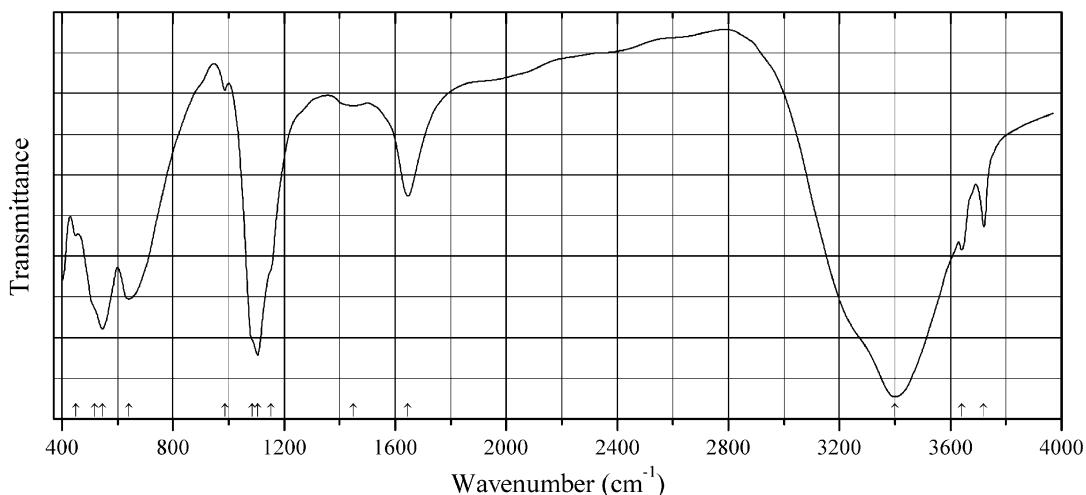
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Fan et al. (2005).

**Wavenumbers (cm<sup>-1</sup>):** 3626, 3560, 3487, 3424s, 1310sh, 1148s, 1106, 1049, 954, 916, 857sh, 841, 809, 753sh, 716, 670, 637, 601s, 569sh, 505, 470, 425.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

#### S584 Magnesium sulfate hydroxide Mg<sub>6</sub>(SO<sub>4</sub>)(OH)<sub>10</sub>·7H<sub>2</sub>O Mg<sub>6</sub>(SO<sub>4</sub>)(OH)<sub>10</sub>·7H<sub>2</sub>O



**Origin:** Synthetic.

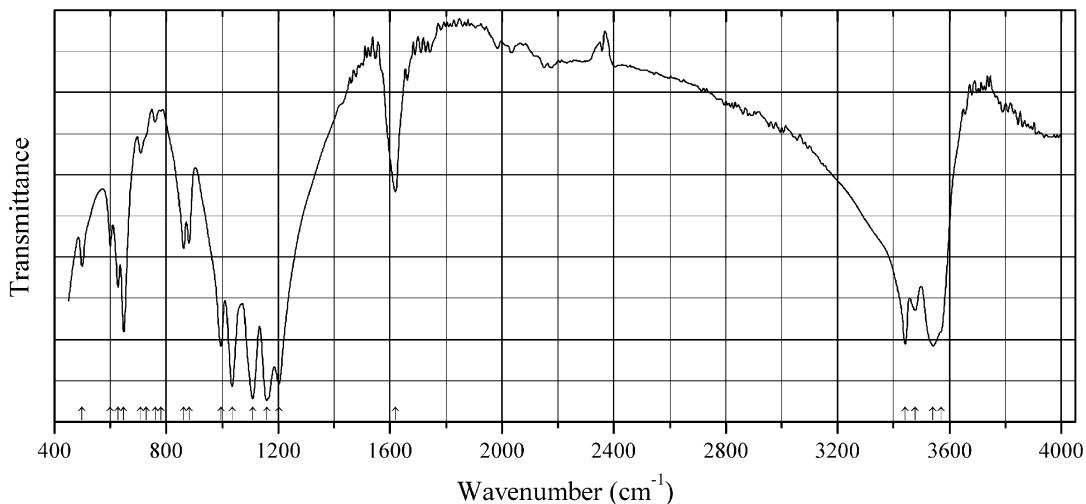
**Description:** Synthesized in the reaction between MgO and MgSO<sub>4</sub> aqueous solutions in the presence of citric acid, at 20 °C for 168 h. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $I121$ ,  $a = 10.260(3)$ ,  $b = 6.307(1)$ ,  $c = 15.138(3)$  Å,  $\beta = 103.98(2)^\circ$ ,  $V = 950.6(4)$  Å<sup>3</sup>,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Runčevski et al. (2013).

**Wavenumbers (cm<sup>-1</sup>):** 3720, 3640, 3400s, 1646, 1450, 1152sh, 1105s, 1086sh, 987w, 640, 546s, 517sh, 450w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**S585 Nickel hydroxysulfate hydrate  $\text{Ni}_3(\text{SO}_4)_2(\text{OH})_2 \cdot 2\text{H}_2\text{O}$   $\text{Ni}_3(\text{SO}_4)_2(\text{OH})_2 \cdot 2\text{H}_2\text{O}$** 

**Origin:** Synthetic.

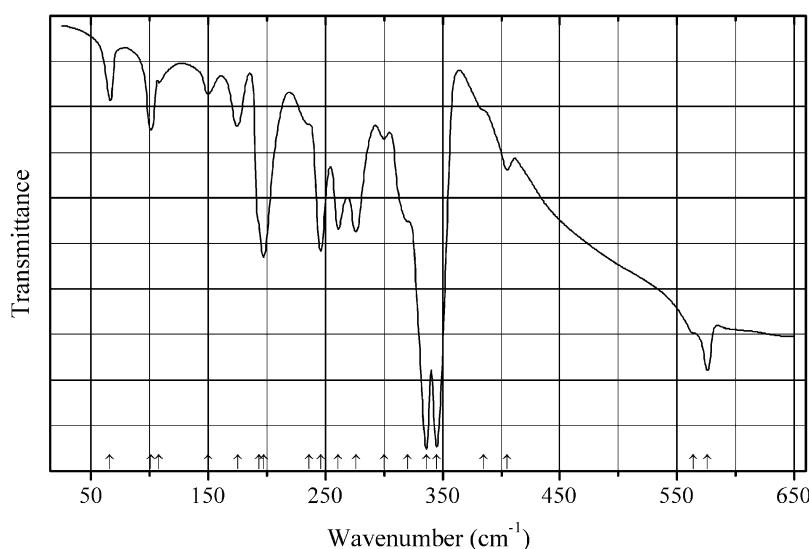
**Description:** Green crystals prepared hydrothermally from  $\text{Ni}(\text{SO}_4) \cdot 7\text{H}_2\text{O}$  and  $\text{NaOH}$  with the ratio  $\text{Ni:Na:H}_2\text{O} = 1:0.25:250$  at  $215\text{--}240\text{ }^\circ\text{C}$  for 1–4 days. Orthorhombic, space group  $Pbcm$ ,  $a = 7.1485(3)$ ,  $b = 9.6844(4)$ ,  $c = 12.6643(3)$  Å,  $V = 876.74(6)$  Å<sup>3</sup>,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Vilminot et al. (2003).

**Wavenumbers (cm<sup>-1</sup>):** 3570sh, 3541, 3477, 3442, 1619, 1202s, 1159s, 1109s, 1035s, 995, 881, 862, 780w, 760w, 727sh, 709w, 648, 627, 600, 499.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**S586 Niobium sulfide  $\text{NbS}_3$   $\text{NbS}_3$** 

**Origin:** Synthetic.

**Description:** Obtained by a chemical vapor transport method. Triclinic, space group  $P\bar{1}$ ,  $a = 4.963(2)$ ,  $b = 6.730(2)$ ,  $c = 9.144(4)$  Å,  $\alpha = 90^\circ$ ,  $\beta = 97.17(1)^\circ$ ,  $\gamma = 90^\circ$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

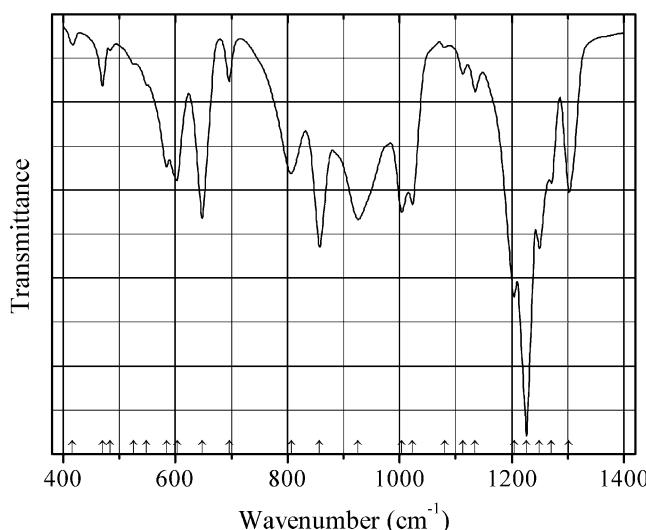
**Source:** Sourisseau et al. (1990).

**Wavenumbers (IR, cm<sup>-1</sup>):** 576, 564w, 405w, 385sh, 345s, 336s, 320sh, 300w, 276, 261, 246, 236sh, 197, 193sh, 175, 150w, 108w, 101, 66.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 602w, 573, 559w, 522w, 462w, 400sh, 392, 388sh, 380, 352, 341, 323, 303, 300, 288w, 281, 263, 257, 241w, 203sh, 195s, 172sh, 160, 152s, 133w, 108, 94, 85, 68.

### S587 Potassium borosulfate K<sub>5</sub>[B(SO<sub>4</sub>)<sub>4</sub>] K<sub>5</sub>[B(SO<sub>4</sub>)<sub>4</sub>]



**Origin:** Synthetic.

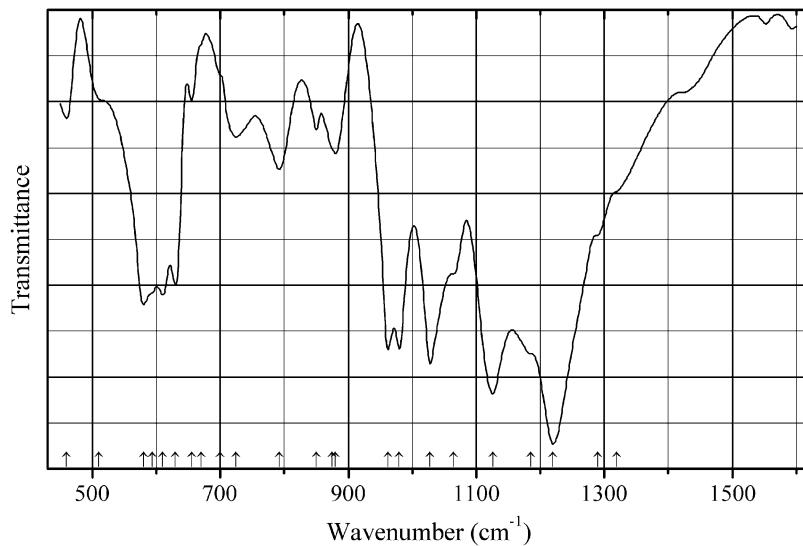
**Description:** Single crystals obtained by thermal decomposition of K<sub>3</sub>[B(SO<sub>4</sub>)<sub>3</sub>] at 673 K for 12 h. The crystal structure is solved. Tetragonal, space group  $P4_1$ ,  $a = 9.9044(14)$ ,  $c = 16.215(3)$  Å,  $Z = 4$ .  $D_{\text{calc}} = 2.466$  g/cm<sup>3</sup>. The structure contains isolated [B(SO<sub>4</sub>)<sub>4</sub>]<sup>5-</sup> anions.

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection.

**Source:** Daub et al. (2013).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1302, 1271, 1249, 1226s, 1204s, 1135w, 1113w, 1080w, 1023, 1004, 926, 857, 807, 696, 648, 603, 585, 549, 526, 484, 470, 417w.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. In the cited paper, a figure of the Raman spectrum is given.

**S588 Potassium sodium vanadyl sulfate  $K_6Na_2(VO)_2(SO_4)_7$** 

**Origin:** Synthetic.

**Description:** Prepared from the mixture of  $\text{Na}_2\text{S}_2\text{O}_7$ ,  $\text{K}_2\text{S}_2\text{O}_7$ , and  $\text{V}_2\text{O}_5$  at  $325^\circ\text{C}$ . The crystal structure is solved. Tetragonal, space group  $P4_32_12$ ,  $a = 9.540(3)$ ,  $c = 29.551(5)$  Å,  $V = 2689.5$  (13) Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 2.684$  g/cm $^3$ . The shortest V–O bond length is equal to 1.552(6) Å.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Karydis et al. (2002).

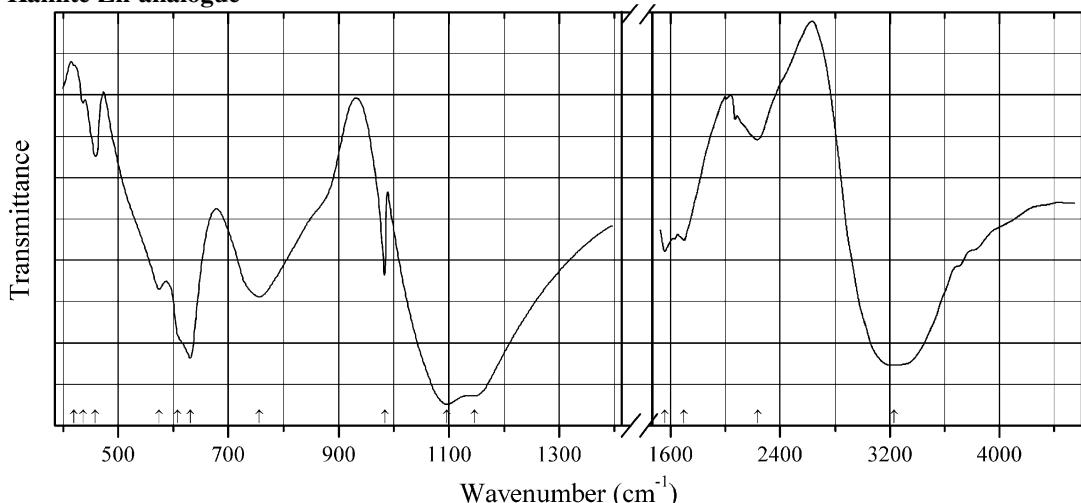
**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1320sh, 1290sh, 1220s, 1185sh, 1126s, 1065sh, 1028s, 980s, 962s, 880, 875sh, 850, 792, 725, 700sh, 670w, 655, 630, 610, 594sh, 580, 510sh, 460w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1310w, 1230w, 1165w, 1028, 1005, 968, 895w, 860w, 790, 685w, 630s, 605s, 570w, 490w, 445w, 396s, 302, 260w, 174s, 140s.

**S589 Potassium zinc sulfate chloride trihydrate  $\text{KZn}(\text{SO}_4)\text{Cl}\cdot3\text{H}_2\text{O}$** 

**Kainite Zn-analogue**



**Origin:** Synthetic.

**Description:** Single crystals doped by Cu<sup>2+</sup> ions. Monoclinic, space group *C2/m*.

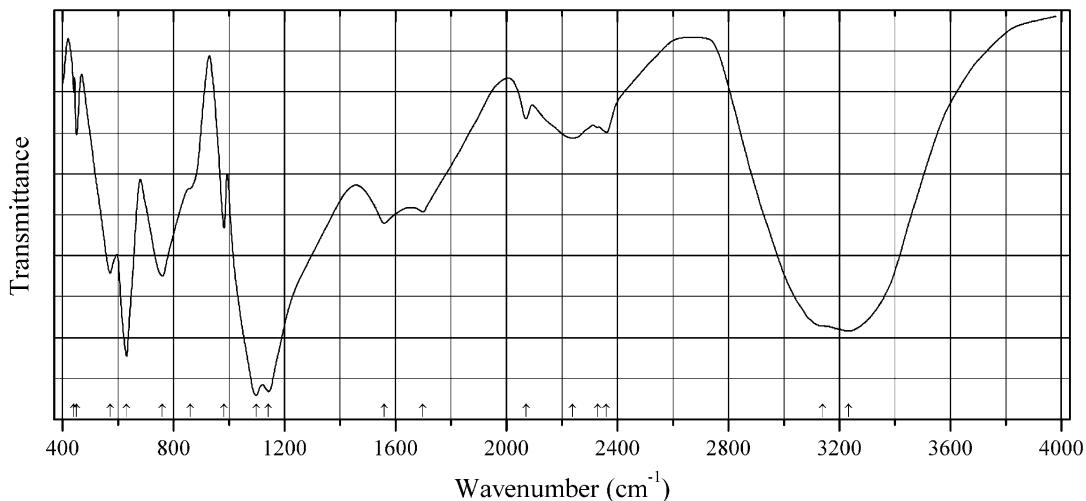
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Narasimhulu et al. (2000).

**Wavenumbers (cm<sup>-1</sup>):** 3230s, 2236, 1700, 1559, 1146s, 1096s, 984, 756, 631s, 608sh, 575, 459, 436w, 420sh.

### S590 Potassium zinc sulfate hexahydrate K<sub>2</sub>Zn(SO<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O

#### Picromerite Zn-analogue



**Origin:** Synthetic.

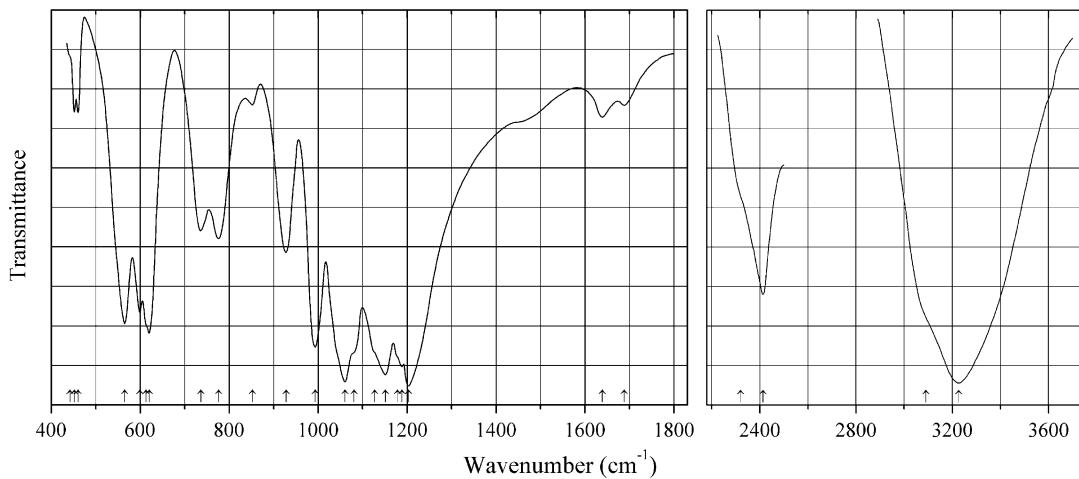
**Description:** Crystals grown from aqueous solution by slow evaporation. Characterized by powder X-ray diffraction data. Monoclinic, space group *P2<sub>1</sub>/c*. Isostructural with picromerite.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Manonmoni et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 3233s, 3140sh, 2360, 2328w, 2238, 2070w, 1699, 1559, 1142s, 1098s, 983, 862sh, 760, 631s, 572, 451, 441.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**S591 Rubidium beryllium sulfate hydrate  $\text{Rb}_2\text{Be}(\text{SO}_4)_2 \cdot 2\text{H}_2\text{O}$** 

**Origin:** Synthetic.

**Description:** Obtained from the three-component system  $\text{Rb}_2\text{SO}_4-\text{BeSO}_4-\text{H}_2\text{O}$  by the method of isothermal decrease of supersaturation. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 11.371(2)$ ,  $b = 11.858(2)$ ,  $c = 7.431(1)$  Å,  $\beta = 96.33(1)^\circ$ ,  $V = 996.0$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 2.722$  g/cm $^3$ . In the structure, the  $[\text{Be}(\text{SO}_4)_2(\text{H}_2\text{O})_2]^{2-}$  units are arranged to form double layers.

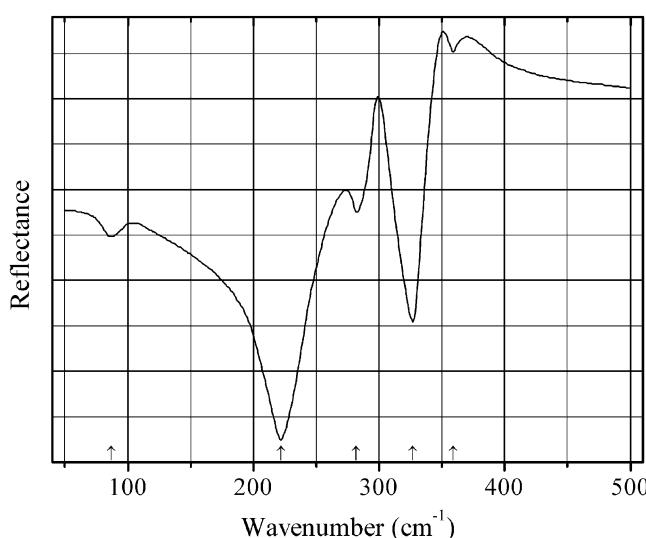
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Georgiev et al. (2007).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3226s, 3090sh, 2413, 2320sh, 1688w, 1639, 1203s, 1188s, 1178sh, 1151s, 1127sh, 1081sh, 1060s, 993s, 928, 852w, 776, 736, 620s, 613sh, 599, 565s, 460, 452, 442sh.

**Note:** The bands indicated by Georgiev et al. (2007) at 3054 and 2294  $\text{cm}^{-1}$  are observed as shoulders at 3090 and 2320  $\text{cm}^{-1}$ . In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1212, 1185, 1156, 1120w, 1078s, 1007s, 993sh, 924w, 757, 633, 606, 589, 557w, 497, 461, 436, 387, 311w, 266.

**S592 Silver indium sulfide  $\text{AgIn}_5\text{S}_8$   $\text{AgIn}_5\text{S}_8$** 

**Origin:** Synthetic.

**Description:** A compound with cubic spinel-type structure. Space group  $Fd\bar{3}m$ ,  $Z = 2$ . One indium atom has tetrahedral coordination, and four indium atoms have octahedral coordination.

**Kind of sample preparation and/or method of registration of the spectrum:** Reflection of a single crystal.

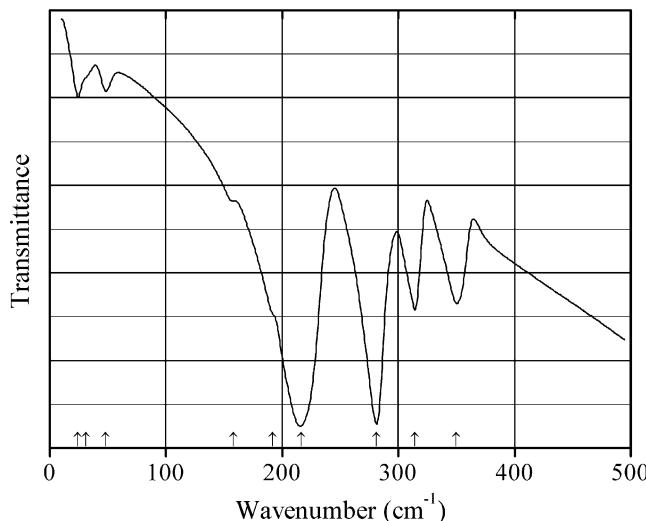
**Source:** Gasanly et al. (1993).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 359w, 327s, 282, 222s, 87.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 354, 328s, 292, 181, 69.

### S593 Silver tantalum sulfide $\text{AgTaS}_3$



**Origin:** Synthetic.

**Description:** Prepared by heating a mixture of Ta, S, and  $\text{Ag}_2\text{S}$  powders at 500 °C for 4 days. Orthorhombic, with a layered structure;  $a = 3.3755(2)$ ,  $b = 14.0608(11)$ ,  $c = 7.7486(7)$  Å,  $Z = 4$ .  $D_{\text{meas}} = 6.82(3)$  g/cm<sup>3</sup>.

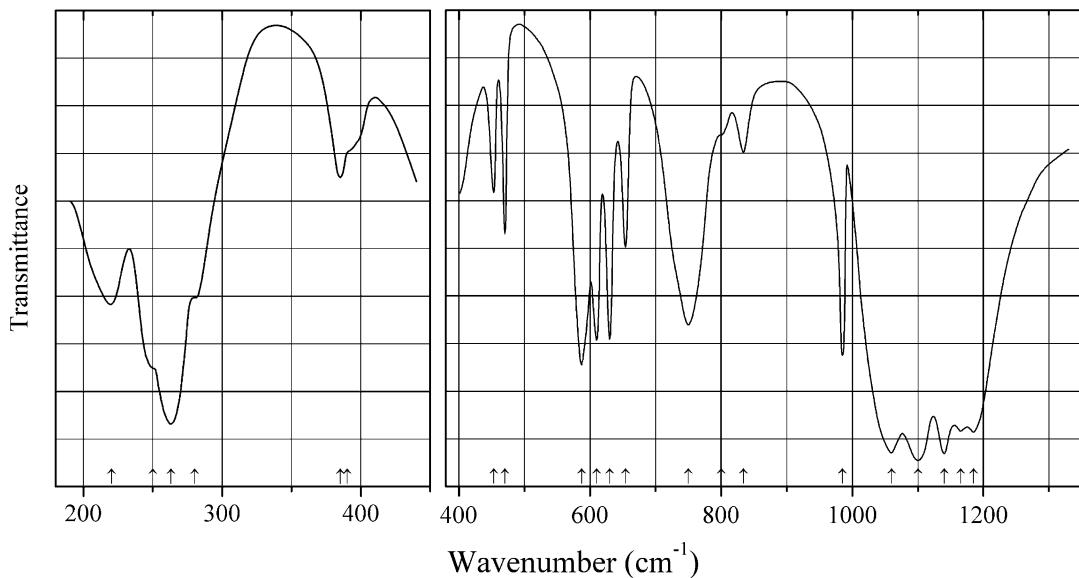
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Ishii and Wada (2000).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 350, 314, 281s, 216s, 192sh, 158sh, 48w, 31sh, 24w.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 384s, 355, 322, 307, 260, 209, 166, 124s, 111s, 30.

**S594 Sodium cadmium sulfate hydrate**  $\text{NaCd}(\text{SO}_4)_2 \cdot 2\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Monoclinic, space group  $P2_1/c$ .

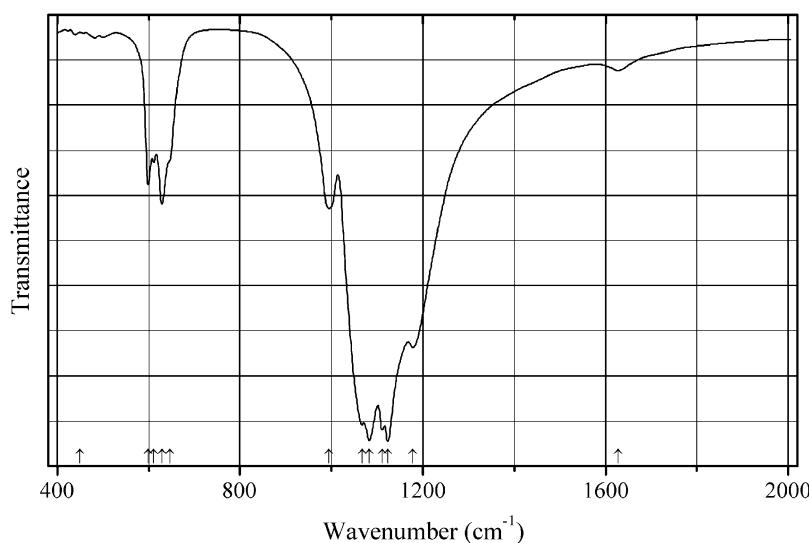
**Kind of sample preparation and/or method of registration of the spectrum:** CsI and/or KBr disc. Transmission.

**Source:** Peytavin et al. (1972a).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1185s, 1165s, 1140s, 1100s, 1060s, 985, 834w, 800sh, 750, 654, 630, 610, 587, 470, 453, 390sh, 385w, 280sh, 263s, 250sh, 220.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1174, 1165sh, 1132s, 1120sh, 1047s, 991s, 800w, 750w, 652, 633, 619, 590, 467s, 446s, 358w, 310sh, 270, 260, 220sh,  $\sim 150$ sh.

**S595 Sodium manganese(II) sulfate alluaudite-type**  $\text{Na}_{2+x}\text{Mn}_{2-x/2}(\text{SO}_4)_3$ 

**Origin:** Synthetic.

**Description:** Prepared by dehydratation of the compound  $\text{Na}_2\text{Mn}(\text{SO}_4)_3 \cdot 2\text{H}_2\text{O}$  with a kröhnkite-type structure. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 11.541(1)$ ,  $b = 12.944(1)$ ,  $c = 6.5875(6)$  Å,  $\beta = 95.149(3)^\circ$ ,  $V = 980.13(26)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 3.078$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

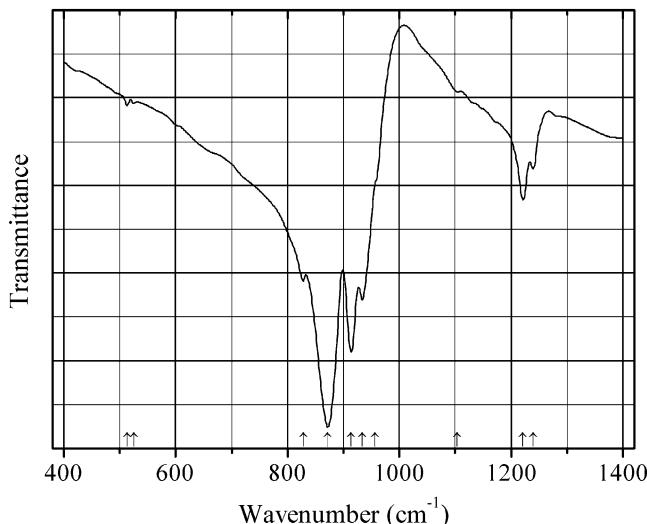
**Source:** Marinova et al. (2015).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1627w, 1178, 1123s, 1111s, 1083s, 1067s, 999, 991, 647sh, 629, 611, 599, ~450w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The weak band at 1627 cm<sup>-1</sup> corresponds to the admixture of H<sub>2</sub>O. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1220w, 1117w, 1051w, 1012s, 993sh, 664, 635, 616, 602, 466.

### S596 Sodium thioborate Na<sub>3</sub>B<sub>3</sub>S<sub>6</sub> Na<sub>3</sub>B<sub>3</sub>S<sub>6</sub>



**Origin:** Synthetic.

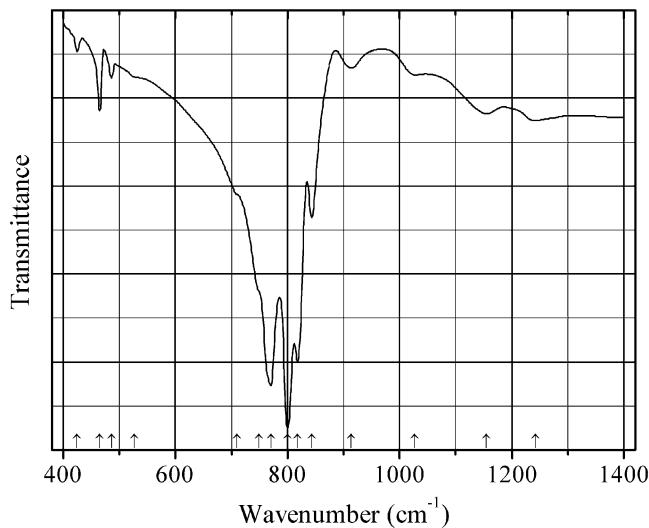
**Description:** Obtained from melt prepared from Na<sub>2</sub>S and B<sub>2</sub>S<sub>3</sub>. Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Martin and Bloyer (1991).

**Wavenumbers (cm<sup>-1</sup>):** 1239w, 1221, 1104w, 957sh, 934, 914s, 872s, 828, 525w, 513w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The bands above 1100 cm<sup>-1</sup> may correspond to the admixture of a borate.

**S597 Sodium thioborate  $\text{Na}_3\text{BS}_3$   $\text{Na}_3\text{BS}_3$** 

**Origin:** Synthetic.

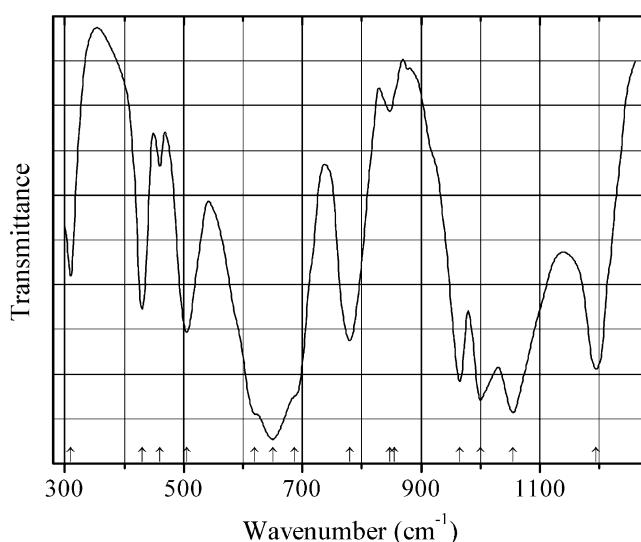
**Description:** Obtained from melt prepared from  $\text{Na}_2\text{S}$  and  $\text{B}_2\text{S}_3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Martin and Bloyer (1991).

**Wavenumbers (cm⁻¹):** 1242, 1155, 1027w, 914w, 843, 818s, 800s, 770s, 749sh, 710sh, 527sh, 486w, 465, 425w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The bands above  $1100 \text{ cm}^{-1}$  may correspond to the admixture of a borate.

**S598 Tellurium(IV) oxosulfate  $\text{Te}_2(\text{SO}_4)\text{O}_3$** 

**Origin:** Synthetic.

**Description:** Orthorhombic, space group  $P2_1mn$ ,  $a = 4.676(2)$ ,  $b = 8.911(3)$ ,  $c = 6.879(4)$  Å,  $V = 286.63$  Å $^3$ ,  $Z = 2$ .  $D_{\text{calc}} = 4.61$  g/cm $^3$ .

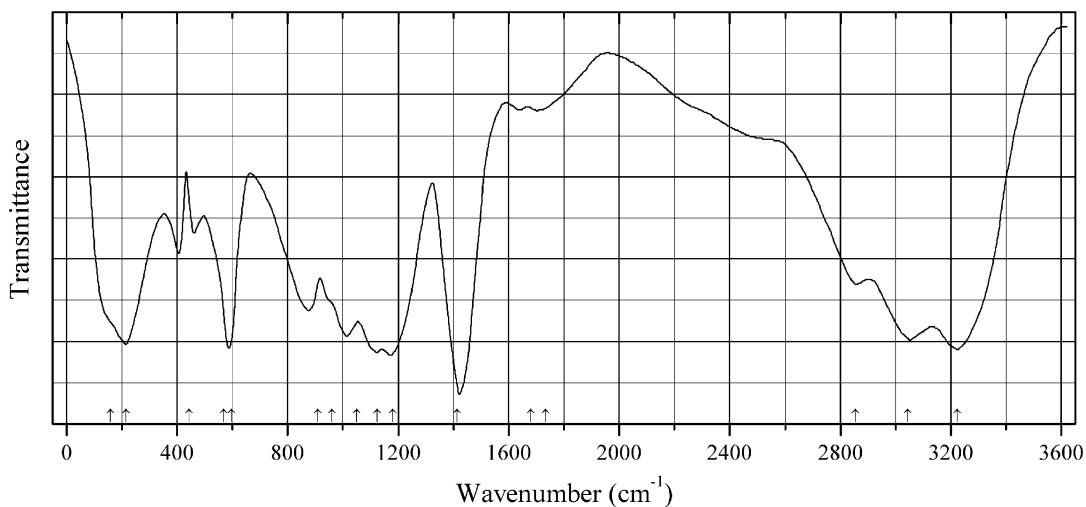
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Gaitán et al. (1985).

**Wavenumbers (cm $^{-1}$ ):** 1195, 1055s, 1000s, 965, 855sh, 848w, 780, 687sh, 650s, 620, 505, 460w, 430, 310.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### S599 Triammonium hydrogen disulfate $(\text{NH}_4)_3\text{H}(\text{SO}_4)_2$



**Origin:** Synthetic.

**Description:** Monoclinic, space group  $C2/c$ ,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Nujol and Fluorolube mulls. Transmission.

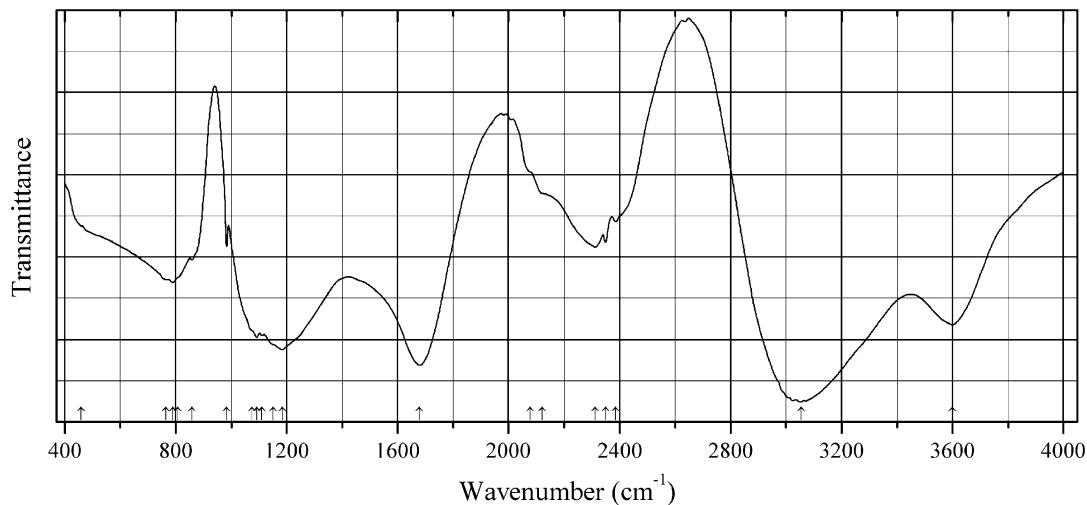
**Source:** Kamoun et al. (1988).

**Wavenumbers (IR, cm $^{-1}$ ):** 3223s, 3043s, 2855, 1733w, 1680w, 1414s, 1180s, 1125s, 1080, 960sh, 910, 597s, (570), 444.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 3145, 2870sh, 1674w, 1415w, 1078s, 966s, 619, 606, 590, 467, 442.

## S600 Alpersite ( $Mg, Cu$ ) $(SO_4)$ $\cdot 7H_2O$



**Origin:** Malanjkhand porphyry copper mine, near Balaghet, Madhya Pradesh, India.

**Description:** Light blue crusts associated with epsomite, hexahydrite, and gypsum. Characterized by powder X-ray diffraction data and semiquantitative electron microprobe analysis.

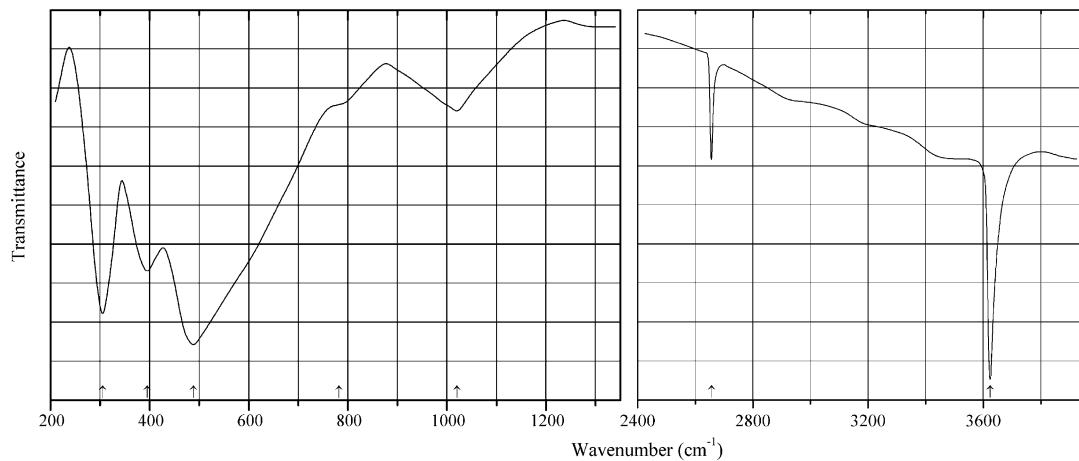
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Equeenuddin (2015).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3600, 3054s, 2312, 2121sh, 2077sh, 1679s, 1184s, (1152sh), (1111), (1092), (1074sh), 984w, 859, (809sh), 790, (765sh), 460sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The bands of H<sub>2</sub>O (at 3054 and 1679 cm<sup>-1</sup>) are anomalously strong and may be due to adsorbed water.

**S601 Aluminocopiapite**  $(\text{Al},\text{Mg})\text{Fe}^{3+}_4(\text{SO}_4)_6(\text{OH},\text{O})_2 \cdot 20\text{H}_2\text{O}$



**Origin:** Synthetic.

**Description:** Prepared from  $\text{Fe}_2(\text{SO}_4)_3 \cdot 6\text{H}_2\text{O}$  and  $\text{Al}_2(\text{SO}_4)_3 \cdot 17\text{H}_2\text{O}$  at  $25^\circ$ , in the presence of excess of water. Characterized by powder X-ray diffraction data. Triclinic,  $a = 7.3853(7)$ ,  $b = 18.249(2)$ ,  $c = 7.3280(6)$  Å,  $\alpha = 93.873(7)^\circ$ ,  $\beta = 102.221(6)^\circ$ ,  $\gamma = 99.163(6)^\circ$ ,  $V = 947.7(2)$  Å<sup>3</sup>.

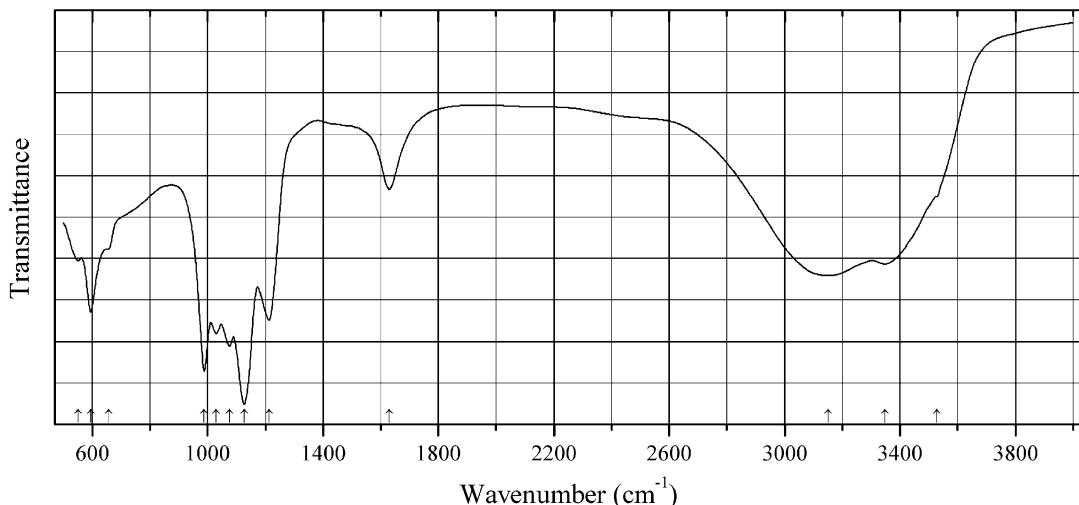
**Kind of sample preparation and/or method of registration of the spectrum:** KCl disc. Absorption.

**Source:** Majzlan and Michallik (2007).

**Wavenumbers (cm<sup>-1</sup>):** 3528sh, 3348, 3150 (broad), 1630, 1127s, 1075, 1030, 988s, 657sh, 595, 551.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

### S602 Amarillite $\text{NaFe}^{3+}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$



**Origin:** Xitieshan Pb-Zn deposit, Qaidam basin, Qinghai province, China.

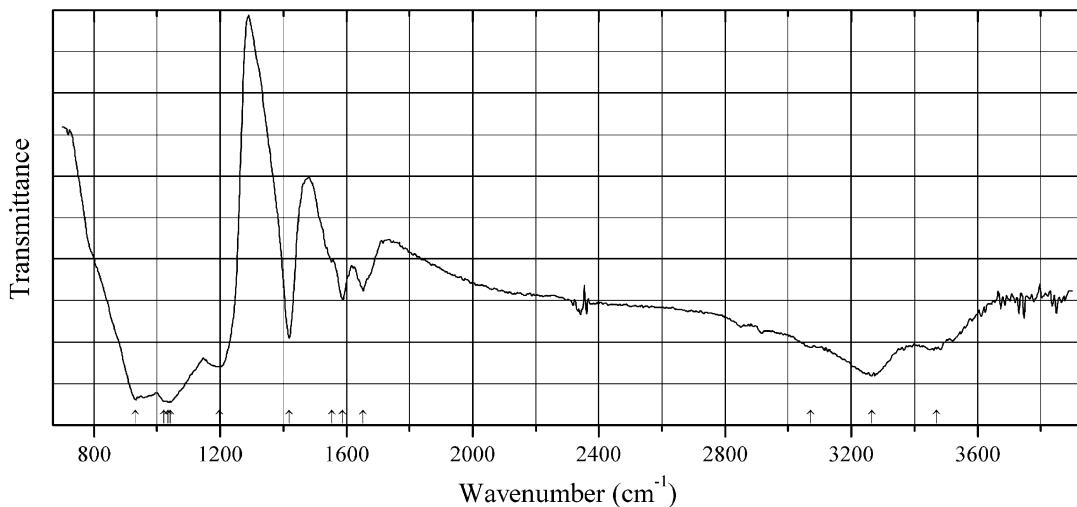
**Description:** Pale yellow or white, fibrous and tabular aggregates, from the association with copiapite, römerite, coquimbite, and melanterite. The crystal structure is solved. Monoclinic, space group  $P12/c1$ ,  $a = 8.4219(17)$ ,  $b = 10.844(2)$ ,  $c = 12.461(3)$  Å,  $\beta = 95.59(3)^\circ$ ,  $V = 1132.6(4)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 2.223$  g/cm<sup>3</sup>. The empirical formula is  $(\text{Na}_{0.97}\text{Ca}_{0.01}\text{Pb}_{0.01})\text{Fe}_{1.04}\text{Al}_{0.07}(\text{SO}_4)_{1.05}(\text{OH})_{0.42} \cdot 5.78\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Yang and Giester (2016).

**Wavenumbers (cm<sup>-1</sup>):** 3522sh, 3478, 3350sh, 3110, 1631, 1213w, 1092s, 989s, 708, 675, 634, 595, 549s, 446.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The band position denoted by Yang and Giester (2016) as 3442 cm<sup>-1</sup> was determined by us at 3478 cm<sup>-1</sup>.

**S603 Campostriniite** ( $\text{Bi}_{2.5}\text{Na}_{0.5}(\text{NH}_4)_2\text{Na}_2(\text{SO}_4)_6 \cdot \text{H}_2\text{O}$ )

**Origin:** La Fossa crater, Vulcano island, Lipari, Eolie (Aeolian) islands, Messina province, Sicily, Italy (type locality).

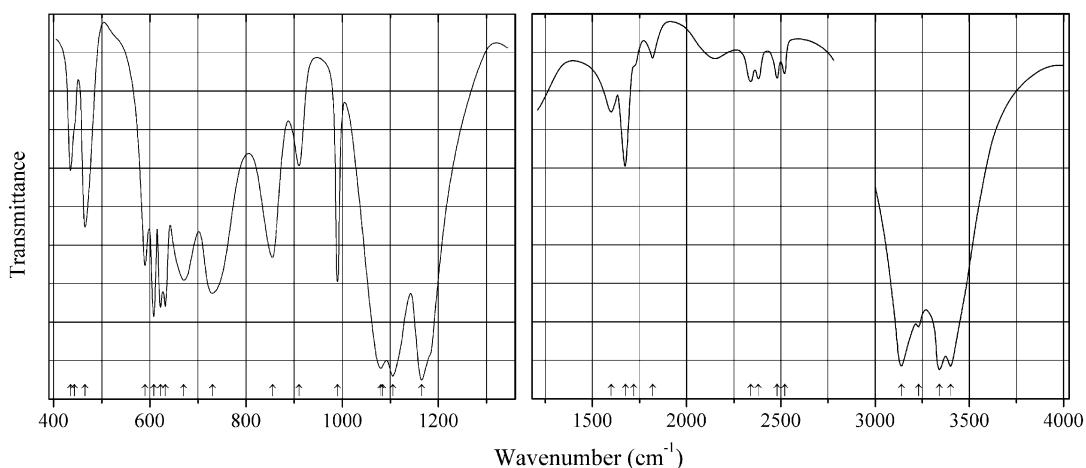
**Description:** White prismatic crystals from the association with adranosite, demicheleite-(Br), demicheleite-(I), argesite, and sassolite. Holotype sample. The crystal structure is solved. Monoclinic, space group  $C2/c$ ,  $a = 17.748(3)$ ,  $b = 6.982(1)$ ,  $c = 18.221(3)$  Å,  $\beta = 113.97(1)^\circ$ ,  $V = 2063(1)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 3.87$  g/cm<sup>3</sup>. The empirical formula is  $\text{Bi}_{2.43}\text{N}_{1.52}\text{Na}_{2.41}\text{K}_{0.48}\text{S}_{6.07}\text{H}_{8.08}\text{O}_{25}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 6.396 (100) (110), 7.507 (75) (-202), 2.766 (60) (-316), 3.380 (57) (312), 5.677 (55) (111), 3.166 (50) (402).

**Kind of sample preparation and/or method of registration of the spectrum:** No data.

**Source:** Demartin et al. (2015).

**Wavenumbers (cm<sup>-1</sup>):** 3470, 3265s, 3071, 1654, 1588, 1553sh, 1418s, 1198s, 1043s, 1036s, 1021sh, 932s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. Weak bands in the range from 2800 to 3000 cm<sup>-1</sup> correspond to the admixture of an organic substance. Weak bands in the range from 2300 to 2400 cm<sup>-1</sup> correspond to atmospheric CO<sub>2</sub>.

**S604 Changoite (slightly deuterated)**  $\text{Na}_2\text{Zn}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Prepared by crystallization from aqueous solurion. Monoclinic, space group  $P2_1/a$ ,  $a = 5.536$ ,  $b = 8.249$ ,  $c = 11.078$  Å,  $\beta = 100.25^\circ$ .

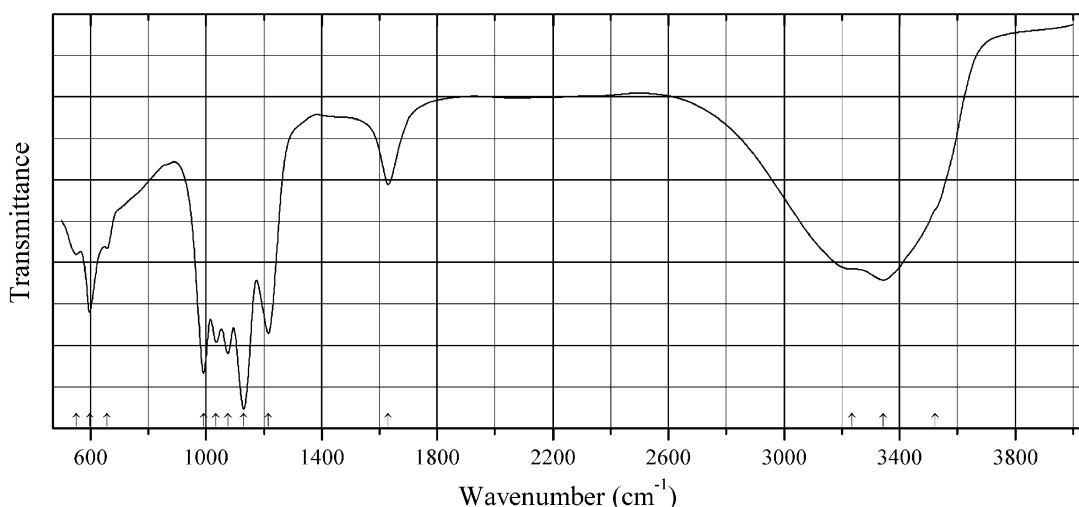
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission.

**Source:** Peytavin et al. (1972b).

**Wavenumbers (cm<sup>-1</sup>):** 3400s, 3340s, 3230, 3140s, 2520w, 2480w, 2380w, 2340w, 1820w, 1720sh, 1675, 1600, 1165s, 1105s, 1084sh, 1080s, 990, 910, 855, 730, 670, 632, 622, 608, 590, 465, 443sh, 435.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The weak bands in the range from 2000 to 2600 cm<sup>-1</sup> correspond to D–O-stretching vibrations.

### S605 Copiapite $\text{Fe}^{2+}\text{Fe}^{3+}_4(\text{SO}_4)_6(\text{OH})_2 \cdot 20\text{H}_2\text{O}$



**Origin:** Synthetic.

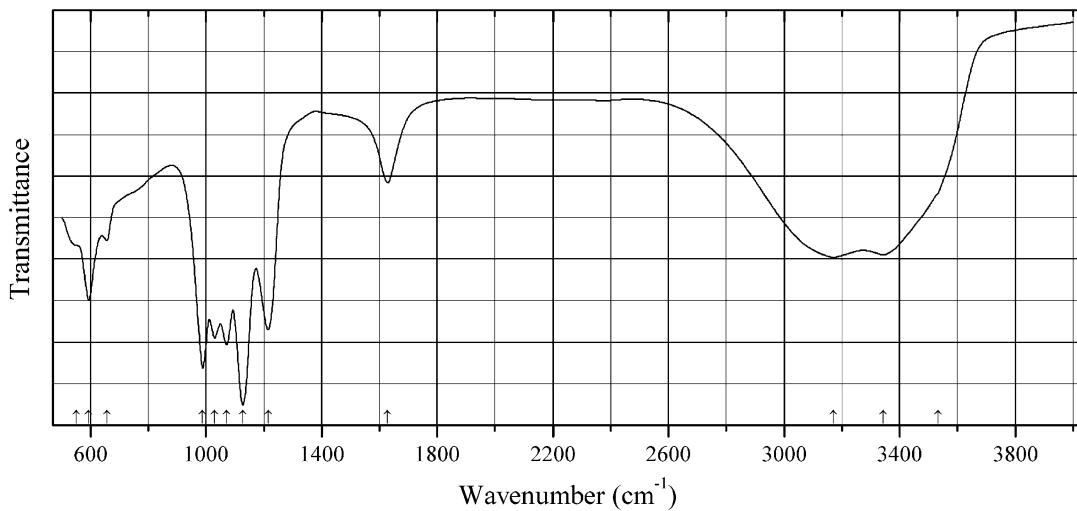
**Description:** Prepared from  $\text{Fe}_2(\text{SO}_4)_3 \cdot 6.25\text{H}_2\text{O}$  and  $\text{Fe}(\text{SO}_4) \cdot 7\text{H}_2\text{O}$  at 25°, in the presence of excess of water. Characterized by powder X-ray diffraction data. Triclinic,  $a = 7.3858(9)$ ,  $b = 18.592(3)$ ,  $c = 7.3543(8)$  Å,  $\alpha = 92.273(9)^\circ$ ,  $\beta = 102.274(8)^\circ$ ,  $\gamma = 98.290(9)^\circ$ ,  $V = 973.9(2)$  Å<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KCl disc. Absorption.

**Source:** Majzlan and Michalik (2007).

**Wavenumbers (cm<sup>-1</sup>):** 3523sh, 3344, 3234sh, 1630, 1216s, 1130s, 1075s, 1035s, 991s, 657, 597, 551.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**S606 Ferricopiaite**  $\text{Fe}^{3+}_{0.67}\text{Fe}^{3+}_4(\text{SO}_4)_6(\text{OH})_2 \cdot 20\text{H}_2\text{O}$ 

**Origin:** Synthetic.

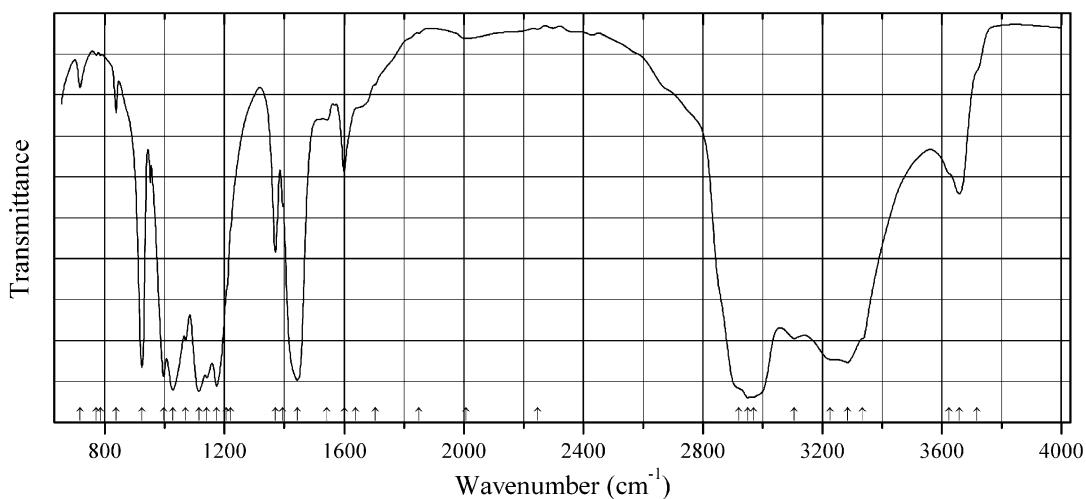
**Description:** Prepared from  $\text{Fe}_2(\text{SO}_4)_3 \cdot 6.25\text{H}_2\text{O}$  in the presence of excess of water at 25 °C. Characterized by powder X-ray diffraction data. Triclinic,  $a = 7.3871(5)$ ,  $b = 18.362(1)$ ,  $c = 7.3286(4)$  Å,  $\alpha = 93.938(5)^\circ$ ,  $\beta = 102.208(4)^\circ$ ,  $\gamma = 98.920(4)^\circ$ ,  $V = 954.5(1)$  Å<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KCl disc. Absorption.

**Source:** Majzlan and Michallik (2007).

**Wavenumbers (cm<sup>-1</sup>):** 3532sh, 3343, 3170, 1628, 1215s, 1127s, 1071s, 1030s, 988s, 656w, 551sh.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**S607 Geschieberite (?)**  $\text{K}_2(\text{UO}_2)(\text{SO}_4)_2 \cdot 2\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Prepared by cooling a hot saturated solution of potassium sulfate and uranyl sulfate mixed in equimolar proportions. Characterized by chemical analyses.

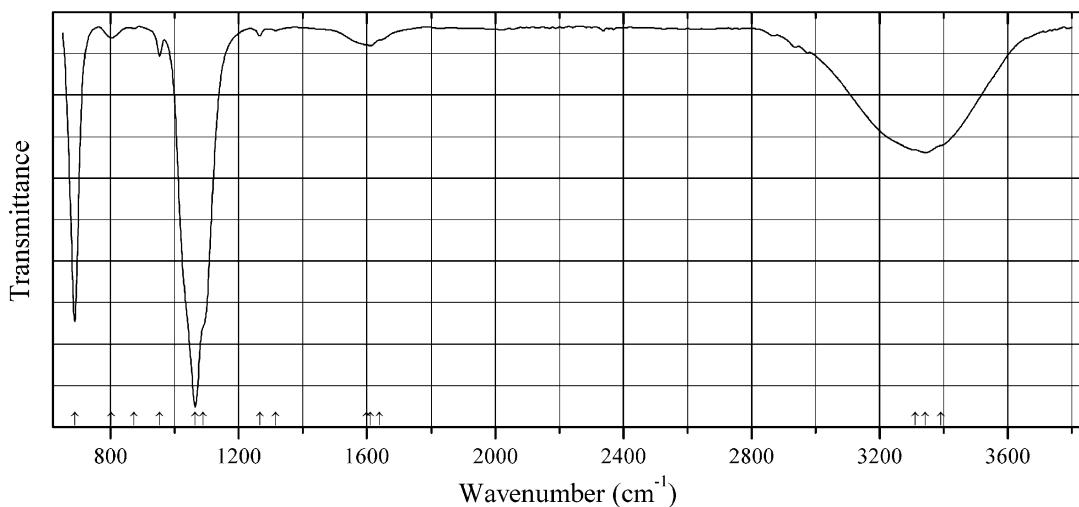
**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull. Transmission.

**Source:** Narasimham and Girija (1967).

**Wavenumbers (cm<sup>-1</sup>):** 3717sh, 3658, 3623sh, 3334sh, 3284s, 3226sh, 3106, 2970sh, 2950s, 2920sh, 2247w, 2008w, 1850w, 1704sh, 1638sh, 1600, 1543w, 1444s, 1395, 1370, 1220sh, 1207sh, 1173s, 1141s, 1114s, 1070, 1027s, 996s, 924s, 837w, 785w, 771w, 717w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### S608 Gianellaite ( $\text{Hg}_2\text{N}_2(\text{SO}_4)_2 \cdot n\text{H}_2\text{O}$ )



**Origin:** Perry Pit of the Mariposa mine, Terlingua District, Brewster Co., Texas, USA (type locality).

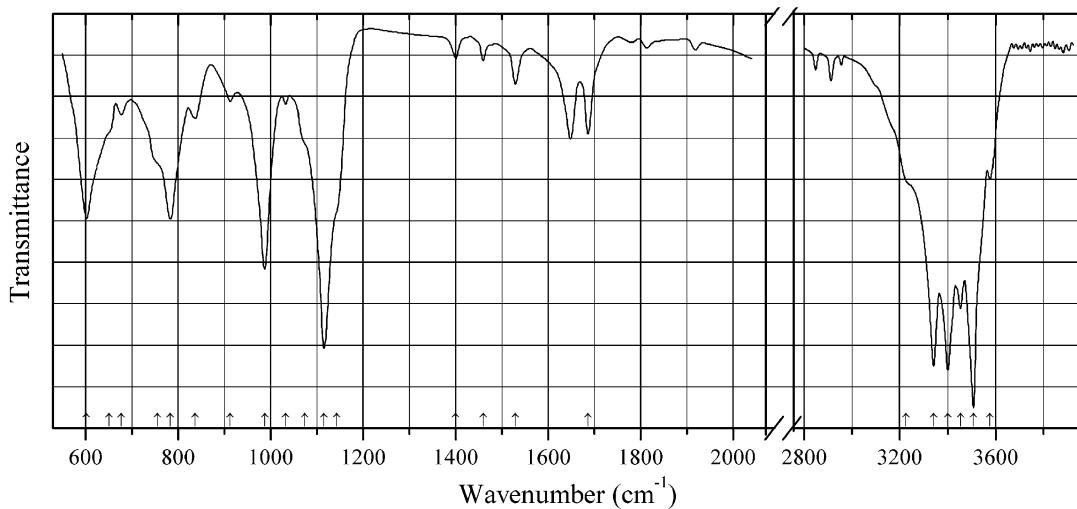
**Description:** Type material deposited in the Natural History Museum of Los Angeles Co., Museum No. 44159. The crystal structure is solved. Cubic, space group  $F-43m$ ,  $a = 863.1(16)$  Å,  $Z = 4$ . The  $(\text{NHg}_4)$  tetrahedra sharing corners form a framework of the cuprite-type structure.

**Kind of sample preparation and/or method of registration of the spectrum:** Thin film, prepared by a diamond micro-compression cell. Absorption.

**Source:** Cooper et al. (2016a).

**Wavenumbers (cm<sup>-1</sup>):** 3390sh, 3342, 3310, 1640sh, 1610, 1600sh, 1315w, 1265w, 1088sh, 1064s, 953, 872w, 803, 688s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**S609 Gordaite**  $\text{NaZn}_4(\text{SO}_4)(\text{OH})_6\text{Cl}\cdot 6\text{H}_2\text{O}$ 

**Origin:** Juan de Fuca Ridge, northeastern Pacific Ocean ( $130^{\circ} 22' 34'' \text{ W}$ ,  $44^{\circ} 38' 53'' \text{ N}$ ).

**Description:** Tabular crystals from the association with sphalerite, baryte, with minor pyrite, pyrrhotite, sulfur, and Fe-hydroxides. Characterized by electron microprobe analysis. Trigonal,  $a = 8.353$  (2),  $c = 13.087(8)$  Å. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 13.19 (100) (001), 3.737 (24) (103), 2.967 (30) (104), 2.737 (24) (120), 2.675 (34) (121), 2.523 (30) (122), 2.098 (24) (124).

**Kind of sample preparation and/or method of registration of the spectrum:** Thin-tabular chip. Transmission.

**Source:** Nasdala et al. (1998).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3577w, 3508s, 3454, 3401s, 3342s, 3235sh, 1687, 1649, 1530, 1460w, 1400w, 1144sh, 1116s, 1074sh, 1033w, 988s, 913w, 837, 784s, 756sh, 678w, 651sh, 603s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 3508, 3422, 1099, 973s, 598, 394.

**S610 Ivsite**  $\text{Na}_3\text{H}(\text{SO}_4)_2$ 

**Origin:** Synthetic.

**Description:** Monoclinic, space group  $P2_1/c$ ,  $Z = 4$ .

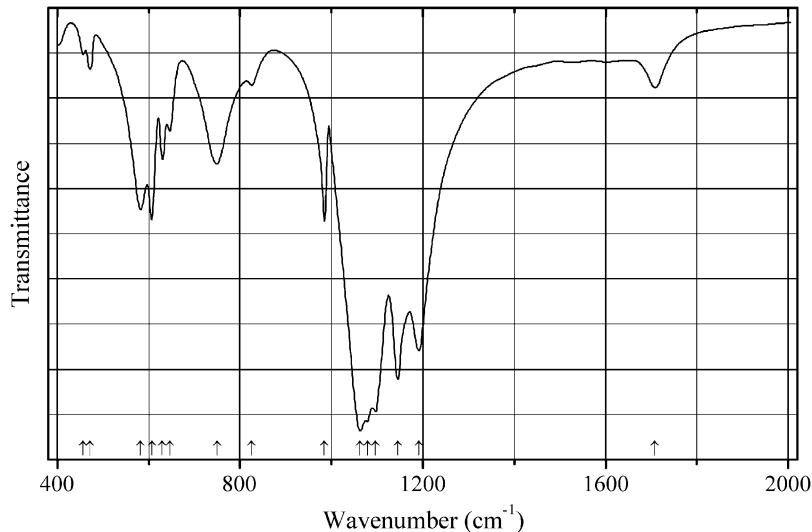
**Kind of sample preparation and/or method of registration of the spectrum:** Nujol and Fluorolube mulls at 20 K. Transmission.

**Source:** Filliaux et al. (1991).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1635, 1535, 1400, 1236, 1197, 1170, 1095, 972, 940, 850sh, 772, 658, 610, 580, 530, 500, 458, 438, 310.

**Note:** These wavenumbers given by Filliaux et al. (1991) in a table don't conform to the figure from this paper. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1242, 1198, 1162, 1154, 1115, 973, 639, 613, 604, 522, 479, 445, 437, 308, 182, 155, 126, 95, 76, 51.

**S611 Joegoldsteinite** MnCr<sub>2</sub>S<sub>4</sub>**Origin:** Synthetic.**Description:** Characterized by powder X-ray diffraction data. Cubic, space group *Fd3m*.**Kind of sample preparation and/or method of registration of the spectrum:** Reflection.**Source:** Lutz et al. (1983).**Wavenumbers (cm<sup>-1</sup>):** 385s, 321s, 257w, 118w.**S612 Kalininite** ZnCr<sub>2</sub>S<sub>4</sub>**Origin:** Synthetic.**Description:** Characterized by powder X-ray diffraction data. Cubic, space group *Fd3m*.**Kind of sample preparation and/or method of registration of the spectrum:** Reflection.**Source:** Lutz et al. (1983).**Wavenumbers (cm<sup>-1</sup>):** 390s, 342s, 245w, 112w.**S613 KröhnkiteMn analogue** Na<sub>2</sub>Mn(SO<sub>4</sub>)<sub>2</sub>·2H<sub>2</sub>O**Origin:** Synthetic.**Description:** Prepared by crystallization from the Na<sub>2</sub>SO<sub>4</sub>–MnSO<sub>4</sub>–H<sub>2</sub>O system at 25 °C using the method of isothermal decrease in super-saturation. Characterized by DTA, TG, and powder X-ray diffraction data. Monoclinic, space group *P2<sub>1</sub>/c*, *a* = 5.8206(2), *b* = 12.9958(21), *c* = 5.4920 (18) Å,  $\beta$  = 106.10(4)°, *V* = 399.1 Å<sup>3</sup>, *Z* = 4.**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.**Source:** Marinova et al. (2015).**Wavenumbers (IR, cm<sup>-1</sup>):** 1708w, 1192s, 1146s, 1097s, 1079s, 1063s, 985, 825w, 750, 646, 630, 607, 582, 472w, 456w.**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.**Wavenumbers (Raman, cm<sup>-1</sup>):** 1170w, 1128, 1045, 1020, 988s, 646w, 632w, 619, 463, 446w.

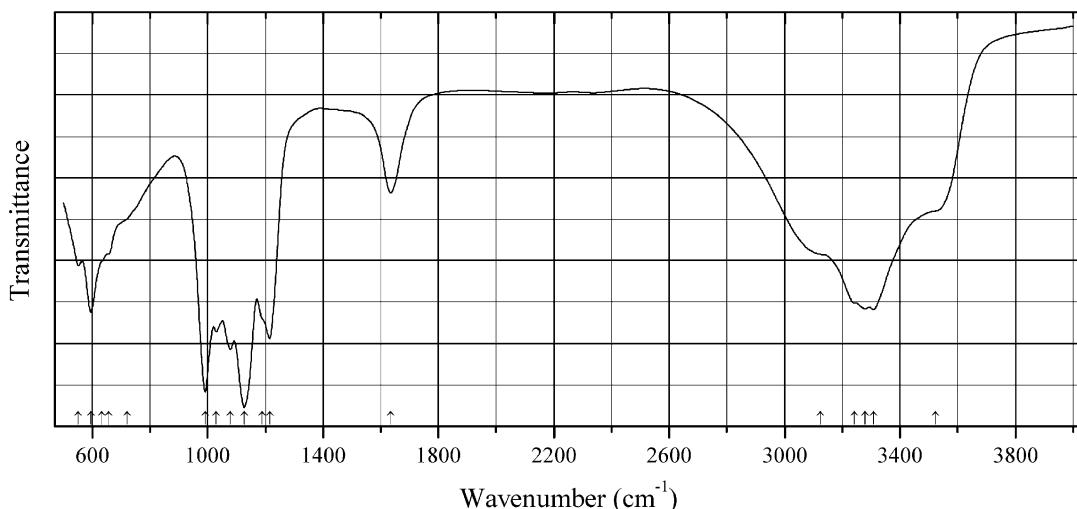
**S614 Lishizhenite**  $\text{ZnFe}^{3+}_2(\text{SO}_4)_4 \cdot 14\text{H}_2\text{O}$ 

**Origin:** Xitieshan, Qinghai Province, China (type locality).

**Description:** Pale violet tabular crystals from the association with römerite, copiapite, sulfur, gypsum, pyrite, and quartz. Holotype sample. Triclinic, space group  $P$ ,  $a = 6.477(1)$ ,  $b = 15.298(3)$ ,  $c = 6.309(1)$ ,  $\alpha = 90.20(1)^\circ$ ,  $\beta = 101.11(1)^\circ$ ,  $\gamma = 93.97(1)^\circ$ ,  $V = 611.9(1) \text{ \AA}^3$ ,  $Z = 1$ .  $D_{\text{meas}} = 2.206(4) \text{ g/cm}^3$ ,  $D_{\text{calc}} = 2.201 \text{ g/cm}^3$ . Optically biaxial (-),  $\alpha = 1.522(2)$ ,  $\beta = 1.568(1)$ ,  $\gamma = 1.578(4)$ ,  $2V = 70(5)^\circ$ .

**Source:** Li and Chen (1990).

**Wavenumbers ( $\text{cm}^{-1}$ , for absorption intervals):** 3351–3035s, 1658–1651, 1131–997s, 667–537, 481.

**S615 Magnesiocopiaite**  $\text{MgFe}^{3+}_4(\text{SO}_4)_6(\text{OH})_2 \cdot 20\text{H}_2\text{O}$ 

**Origin:** Synthetic.

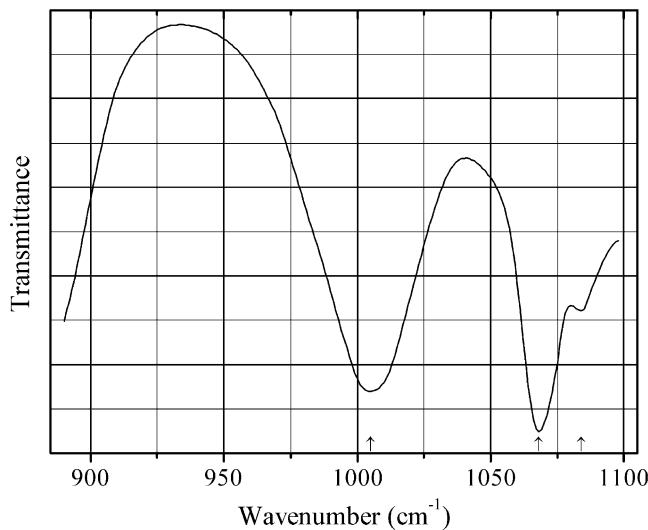
**Description:** Prepared from  $\text{Fe}_2(\text{SO}_4)_3 \cdot 6.25\text{H}_2\text{O}$  and  $\text{Mg}(\text{SO}_4) \cdot 7\text{H}_2\text{O}$  at  $25^\circ$ , in the presence of excess of water. Characterized by powder X-ray diffraction data. Triclinic,  $a = 7.3451(4)$ ,  $b = 18.794(1)$ ,  $c = 7.3891(4) \text{ \AA}$ ,  $\alpha = 91.369(5)^\circ$ ,  $\beta = 102.169(4)^\circ$ ,  $\gamma = 98.831(4)^\circ$ ,  $V = 983.6(1) \text{ \AA}^3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KCl disc. Absorption.

**Source:** Majzlan and Michalik (2007).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3523sh, 3308s, 3278s, 3242sh, 3125sh, 1634, 1215s, 1188sh, 1127s, 1078, 1030, 991s, 721sh, 657sh, 633sh, 595s, 552.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**S616 Mercallite KHSO<sub>4</sub>**

**Origin:** Synthetic.

**Description:** Crystals grown from aqueous solution of H<sub>2</sub>SO<sub>4</sub> and K<sub>2</sub>SO<sub>4</sub> by slow evaporation.

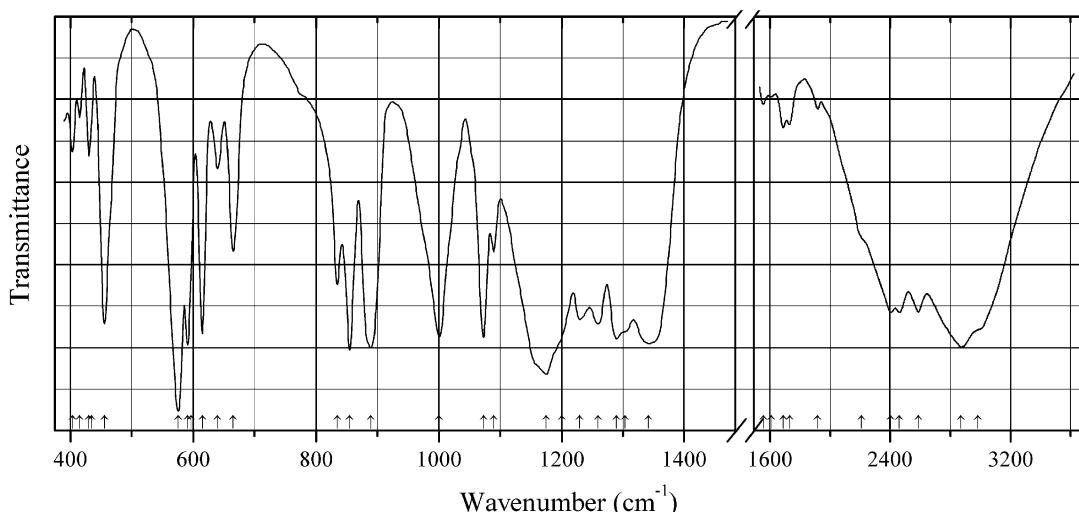
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc and Nujol mull. Transmission.

**Source:** Dey et al. (1982).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3100s, 2930, 2510, 1328s, 1295sh, 1284s, 1255s, 1228s, 1170s, 1084sh, 1068s, 1005s, 884s, 872s, 849s, 660, 632, 616s, 589s, 576s, 454, 435, 405w, 265, 220, 183, 160, 153, 141sh, 132sh, 112, 103, 94, 80, 54, 36.

**Note:** The intensities of the IR bands are indicated in accordance with authors' tabular data. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 2700, 1337, 1265, 1242, 1170, 1026, 1001, 872, 855, 598, 589, 581, 572, 452, 445, 182, 139, 126, 102, 82, 50, 46.

**S617 Mercallite KHSO<sub>4</sub>**

**Origin:** Synthetic.

**Description:** Pyramidal crystals grown from aqueous solution of  $\text{H}_2\text{SO}_4$  and  $\text{K}_2\text{SO}_4$ . Orthorhombic, space group *Pbca*.

**Kind of sample preparation and/or method of registration of the spectrum:** Absorption of a polycrystalline sample at 90 K. Kind of sample preparation is not indicated.

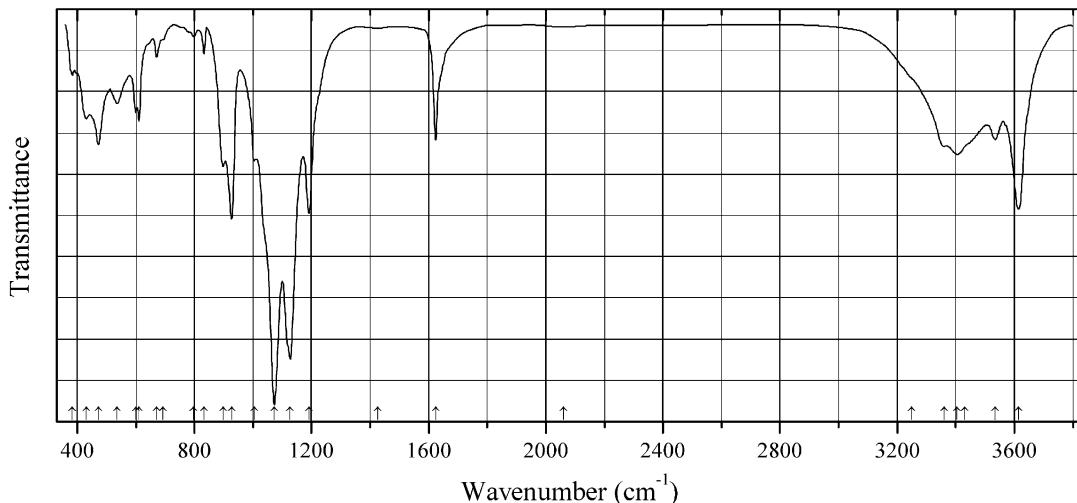
**Source:** Goypiron et al. (1980).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 2984sh, 2873, 2587, 2460, 2405, 2210sh, 1916w, 1730w, 1687w, 1608w, 1555w, 1342s, 1303sh, 1290s, 1259, 1230, 1200sh, 1175s, 1089, 1073s, 1000s, 889s, 855s, 835, 665, 640, 615s, 597s, 591sh, 576s, 456s, 435, 431sh, 416w, 404

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, for a polycrystalline sample at 300 K,  $\text{cm}^{-1}$ ):** 2860w, 1257sh, 1244w, 1219w, 1171w, 1026s, 1001s, 883w, 870w, 855, 837w, 625w, 600sh, 596, 589, 581, 573sh, 455sh, 444, 419sh, 411, 192, 182, 139, 128, 126, 124, 116, 108, 102, 96, 84, 83, 82, 76, 75, 60, 50, 47, 45, 37.

### S618 Plášilite $\text{Na}(\text{UO}_2)(\text{SO}_4)(\text{OH}) \cdot 2\text{H}_2\text{O}$



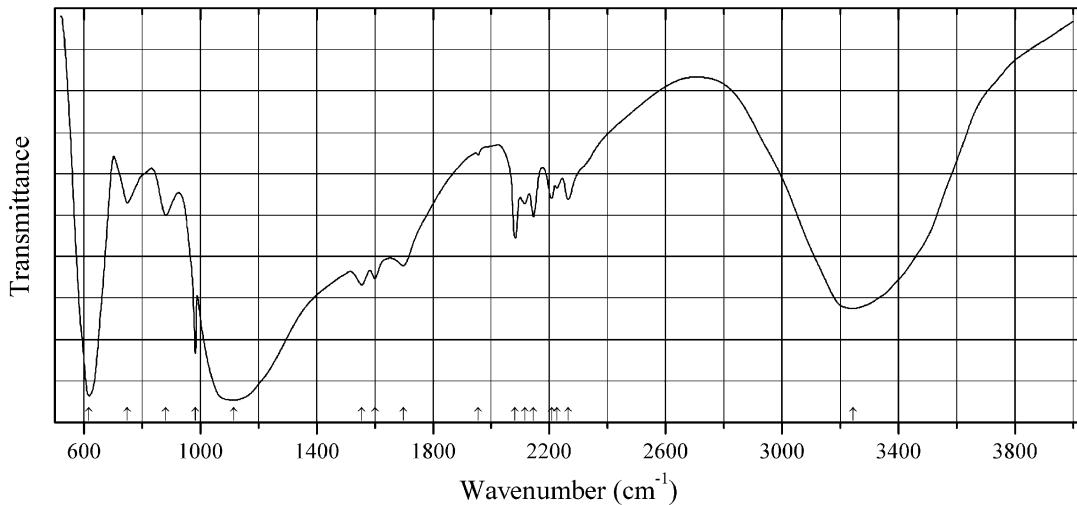
**Origin:** Blue Lizard mine, White Canyon District, San Juan County, Utah, USA (type locality).

**Description:** Yellow platelets. Investigated by A.V. Kasatkin. Characterized by single-crystal X-ray diffraction data. Monoclinic,  $a = 8.702$ ,  $b = 13.822$ ,  $c = 7.042$  Å,  $\beta = 112.08^\circ$ ,  $V = 384.9$  Å<sup>3</sup>. The empirical formula is (electron microprobe):  $\text{Na}_{0.88}(\text{UO}_2)_{1.06}(\text{SO}_4)_{1.06}(\text{OH})_x \cdot n\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3614s, 3535, 3430sh, 3405, 3360, 3250sh, 2060w, 1624, 1426w, 1191s, 1127s, 1073s, 1006, 927s, 898, 833, 797w, 693w, 671, 611, 601, 536, 472, 431, 384.

**Note:** The spectrum was obtained by N.V. Chukanov.

**S619 Picromerite dimorph (?)  $K_2Mg(SO_4)_2 \cdot 6H_2O$** 

**Origin:** Synthetic.

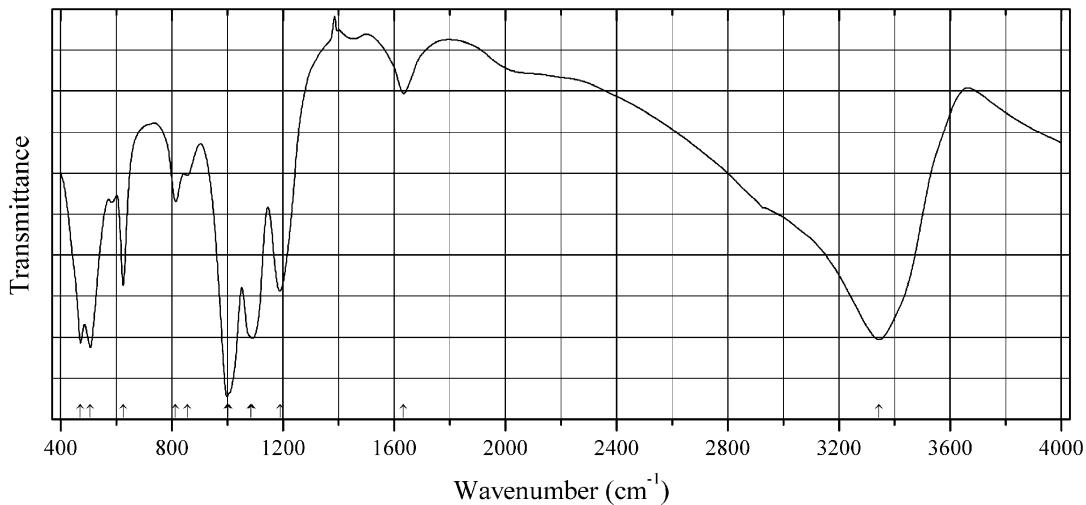
**Description:** Crystals obtained from saturated aqueous solution by slow evaporation at room temperature. Characterized by thermoanalytical data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Dhandapani et al. (2006).

**Wavenumbers (cm⁻¹):** 3243s, 2265, 2226, 2208, 2146, 2115, 2083, 1955, 1698, 1600, 1555, 1115s, 983s, 882, 749, 618s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The bands at 2265, 2226, 2208, 2146, 2115, 2083, and 1955 cm⁻¹ may correspond to acid groups.

**S620 Hydronium jarosite Pb,As-bearing  $(H_3O,Pb)Fe^{3+}_3(SO_4,AsO_4)_2(OH,H_2O)_6$** 

**Origin:** Synthetic.

**Description:** Prepared from an aqueous solution containing  $\text{Pb}(\text{NO}_3)_2$ ,  $\text{Fe}_2(\text{SO}_4)_3 \cdot 5\text{H}_2\text{O}$ , and  $\text{H}_3\text{AsO}_4$  at  $95^\circ\text{C}$ . Characterized by elemental analysis and powder X-ray diffraction data. Trigonal,  $a = 7.3417(8)$ ,  $c = 16.9213(6)$  Å. The empirical formula is  $(\text{H}_3\text{O})_{0.68}\text{Pb}_{0.32}\text{Fe}_{2.86}(\text{SO}_4)_{1.69}(\text{AsO}_4)_{0.31}(\text{OH})_{5.59}(\text{H}_2\text{O})_{0.41}$ .

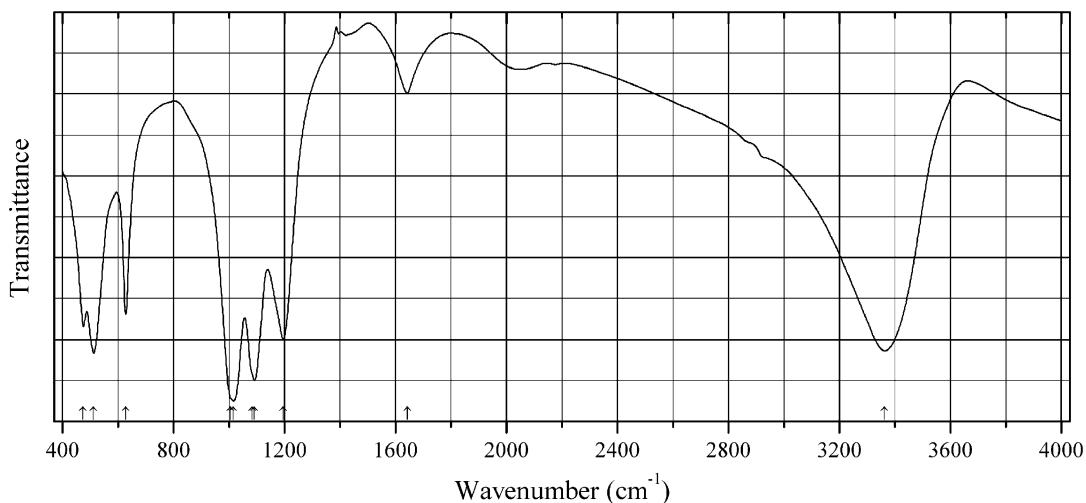
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Forray et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 3343s, 2930sh, 1634, 1189, 1090s, 1083sh, 1005sh, 999s, 855, 814, 625, 507s, 472s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### S621 Hydronium jarosite Pb,Cu-bearing ( $\text{H}_3\text{O},\text{Pb})(\text{Fe}^{3+},\text{Cu}^{2+})_3(\text{SO}_4)_2(\text{OH})_6$ )



**Origin:** Synthetic.

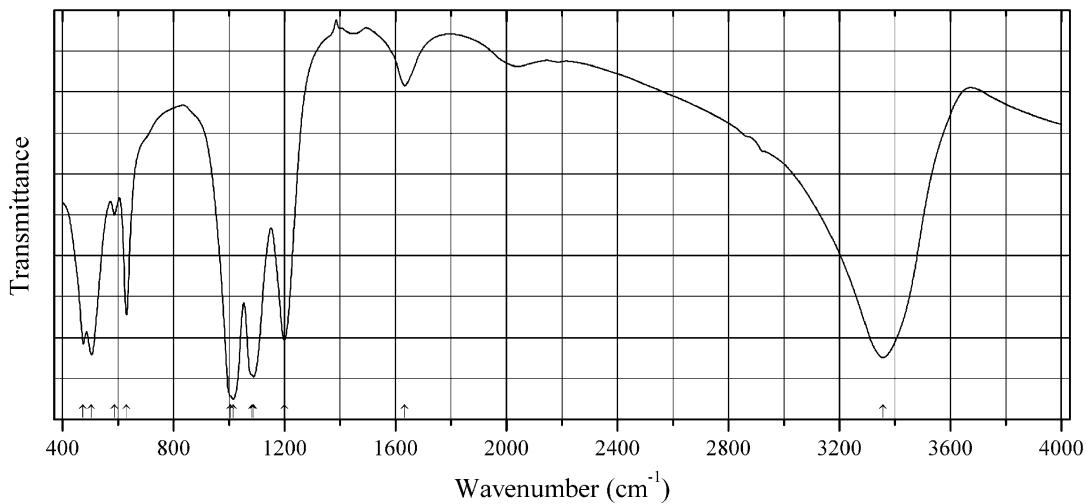
**Description:** Prepared from an aqueous solution containing  $\text{Pb}(\text{NO}_3)_2$ ,  $\text{Fe}_2(\text{SO}_4)_3 \cdot 5\text{H}_2\text{O}$ , and  $\text{H}_2\text{SO}_4$ , and  $\text{Cu}(\text{SO}_4) \cdot 5\text{H}_2\text{O}$  at  $95^\circ\text{C}$ . Characterized by elemental analysis and powder X-ray diffraction data. Trigonal,  $a = 7.3208(8)$ ,  $c = 17.0336(7)$  Å. The empirical formula is  $(\text{H}_3\text{O})_{0.67}\text{Pb}_{0.33}\text{Fe}_{2.71}\text{Cu}_{0.25}(\text{SO}_4)_{2.00}(\text{OH})_{5.96}(\text{H}_2\text{O})_{0.04}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Forray et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 3362s, 1642, 1195, 1092s, 1083sh, 1016s, 1005sh, 628, 513s, 475.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**S622 Hydronium jarosite Pb,Zn-bearing** ( $\text{H}_3\text{O},\text{Pb})(\text{Fe}^{3+},\text{Zn})_3(\text{SO}_4)_2(\text{OH})_6$ 

**Origin:** Synthetic.

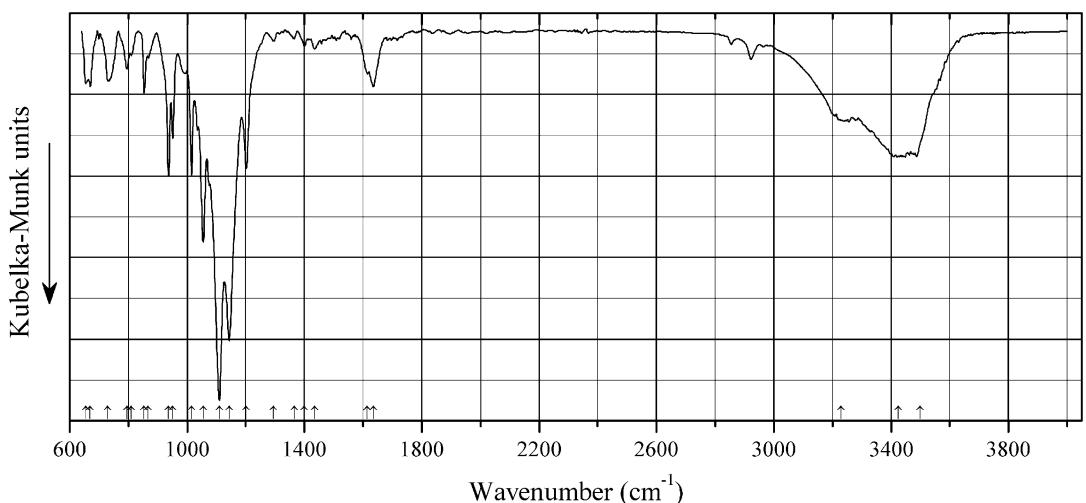
**Description:** Prepared from an aqueous solution containing  $\text{Pb}(\text{NO}_3)_2$ ,  $\text{Fe}_2(\text{SO}_4)_3 \cdot 5\text{H}_2\text{O}$ , and  $\text{H}_2\text{SO}_4$ , and  $\text{Zn}(\text{SO}_4) \cdot 7\text{H}_2\text{O}$  at 95 °C. Characterized by elemental analysis and powder X-ray diffraction data. Trigonal,  $a = 7.3208(8)$ ,  $c = 17.0336(7)$  Å. The empirical formula is  $(\text{H}_3\text{O})_{0.57}\text{Pb}_{0.43}\text{Fe}_{2.70}\text{Zn}_{0.21}(\text{SO}_4)_{2.00}(\text{OH})_{5.95}(\text{H}_2\text{O})_{0.05}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Forray et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 3357s, 1634, 1199, 1089s, 1083sh, 1015s, 1005sh, 631, 587, 505s, 475.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**S623 Shumwayite** ( $\text{UO}_2)_2(\text{SO}_4)_2 \cdot 5\text{H}_2\text{O}$ 

**Origin:** White Canyon district, San Juan Co., Utah, USA (type locality).

**Description:** Greenish-yellow prisms from the association with other secondary sulfates. Holotype sample. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 6.74747(15)$ ,  $b = 12.5026(3)$ ,  $c = 16.9032(12)$  Å,  $\beta = 90.919(6)^\circ$ ,  $V = 1425.79(11)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 3.831$  g/cm $^3$ . Optically biaxial (+/−),  $\alpha = 1.581(1)$ ,  $\beta = 1.588(1)$ ,  $\gamma = 1.595(1)$ ,  $2V = 89.8(8)^\circ$ . The empirical formula is (electron microprobe):  $\text{U}_{2.01}\text{S}_{1.99}\text{O}_{12.00} \cdot 5\text{H}_2\text{O}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 5.58 (48) (−111, 111), 5.11 (100) (013), 4.86 (44) (−112, 112), 4.04 (47) (031), 3.459 (42) (−131, −114, 114), 3.373 (50) (200, 033, −132).

**Kind of sample preparation and/or method of registration of the spectrum:** Reflection of powdered mineral mixed with KBr.

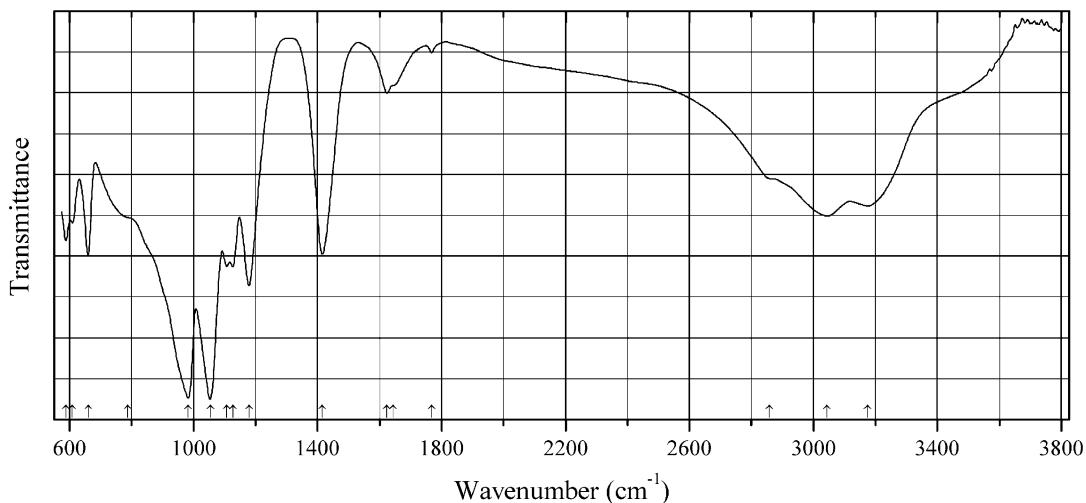
**Source:** Kampf et al. (2016f).

**Wavenumbers (IR, cm $^{-1}$ ):** 3500, 3425, 3230sh, 1635, 1615w, 1435w, 1400w, 1365w, 1295w, 1202, 1143s, 1110s, 1055s, 1015, 951, 937, 868, 854, 810, 795, 730, 670, 655.

**Note:** The band position denoted by Kampf et al. (2016f) as 927 cm $^{-1}$  was determined by us at 937 cm $^{-1}$ . In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 1185, 1155, 1100, 1073s, 1050, 1035, 1015, 930, 865s, 850s, 645, 615, 470, 430, 273sh, 255, 210, 200s, 160, 150.

#### S624 Carlsonite $(\text{NH}_4)_5\text{Fe}^{3+} \cdot 3(\text{SO}_4)_6\text{O} \cdot 7\text{H}_2\text{O}$



**Origin:** Near Huron River, 6.1 km WSW of Milan, USA (type locality).

**Description:** Yellow to orange-brown crystals from the association with anhydrite, boussingaultite, gypsum, and lonecreekite. Holotype sample. The crystal structure is solved. Triclinic, space group  $P-1$ ,  $a = 9.5927(2)$ ,  $b = 9.7679(3)$ ,  $c = 18.3995(13)$  Å,  $\alpha = 93.250(7)^\circ$ ,  $\beta = 95.258(7)^\circ$ ,  $\gamma = 117.993(8)^\circ$ ,  $V = 1506.15(16)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{calc}} = 2.167$  g/cm $^3$ . Optically biaxial (−),  $\alpha = 1.576(1)$ ,  $\beta = 1.585(1)$ ,  $\gamma = 1.591(1)$ ,  $2V = 80(1)^\circ$ . The empirical formula is  $[(\text{NH}_4)_{4.64}\text{Na}_{0.24}\text{K}_{0.12}]\text{Fe}^{3+} \cdot 3.05\text{O}(\text{SO}_4)_6 \cdot 6.93\text{H}_2\text{O}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 9.23 (100) (002), 8.26 (40) (100, 011), 7.57 (43) (−111, 1−11, 011), 4.93 (23) (−1−11, −120), and 3.144 (41) (multiple).

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of powdered mineral.

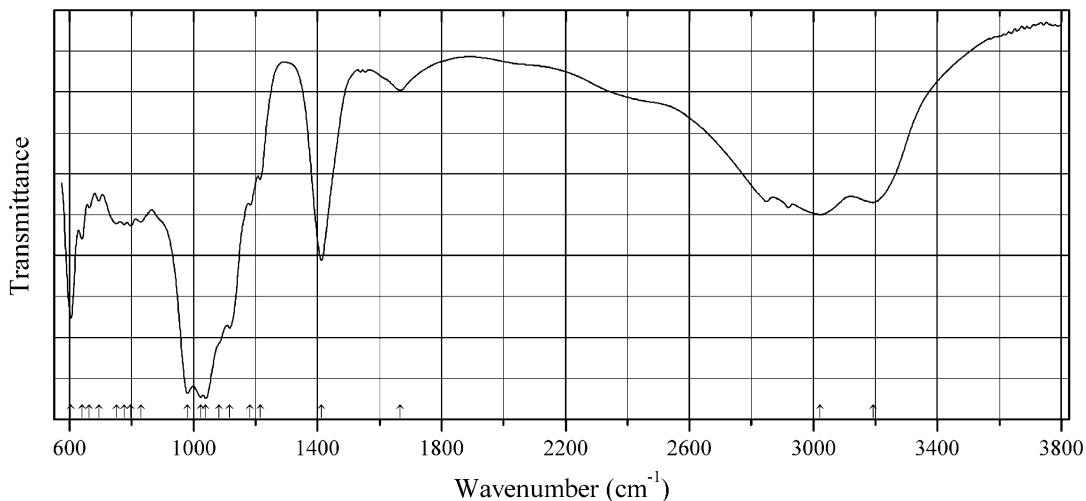
**Source:** Kampf et al. (2016h).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3176, 3044, 2858, 1768w, 1644sh, 1624, 1416, 1179s, 1127, 1107, 1054s, 983s, 788sh, 660, 610, 588.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1219, 1188, 1160, 1140, 1104, 1066, 1015s, 670w, 629w, 617w, 576, 552, 514, 487, 436, 275s, 245s.

### S625 Huizingite-(Al) $(\text{NH}_4)_9(\text{Al},\text{Fe}^{3+})_3(\text{SO}_4)_8(\text{OH})_2 \cdot 4\text{H}_2\text{O}$



**Origin:** Near Huron River, 6.1 km WSW of Milan, USA (type locality).

**Description:** Yellow drusy aggregates from the association with adranosite-(Al), anhydrite, boussingaultite, mascagnite, and salammoniac. Holotype sample. The crystal structure is solved. Triclinic, space group  $P-1$ ,  $a = 9.7093(3)$ ,  $b = 10.4341(3)$ ,  $c = 10.7027(8)$  Å,  $\alpha = 77.231(5)^\circ$ ,  $\beta = 74.860(5)^\circ$ ,  $\gamma = 66.104(5)^\circ$ ,  $V = 948.73(9)$  Å<sup>3</sup>,  $Z = 1$ .  $D_{\text{calc}} = 2.026$  g/cm<sup>3</sup>. Optically biaxial (+),  $\alpha = 1.543(1)$ ,  $\beta = 1.545(1)$ ,  $\gamma = 1.563(1)$ ,  $2V = 40(3)^\circ$ . The empirical formula is  $[(\text{NH}_4)_{8.76}\text{Na}_{0.22}\text{K}_{0.02}](\text{Al}_{1.65}\text{Fe}^{3+}_{3.05})(\text{SO}_4)_{8.00} \cdot 4.02\text{H}_2\text{O}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are:

8.82 (60) (100), 5.04 (69) (121), 3.427 (100) (-2-21), 3.204 (68) (-211), 3.043 (94) (2-12, 312).

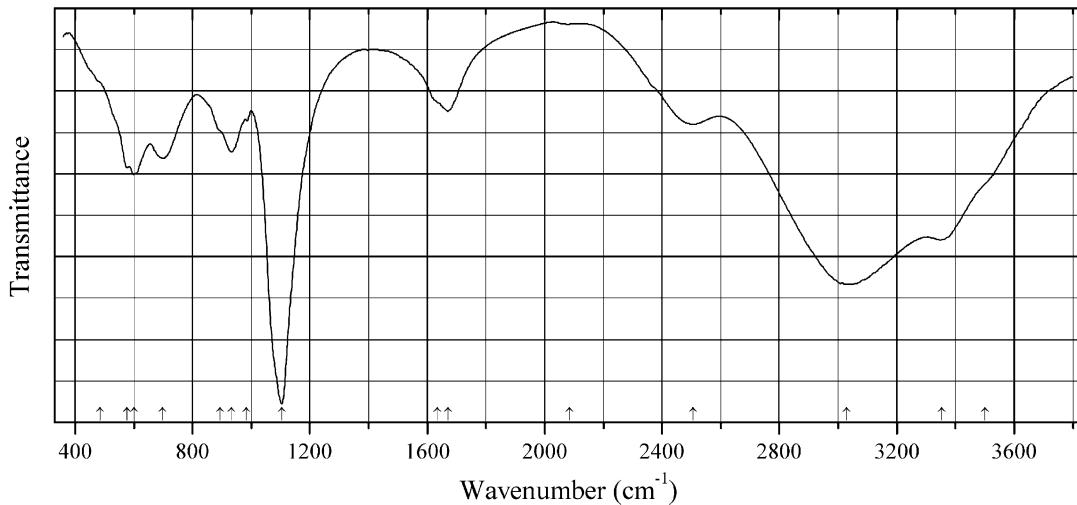
**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of powdered mineral.

**Source:** Kampf et al. (2016h).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3192, 3022, 1667w, 1413, 1215w, 1183w, 1117, 1083sh, 1040s, 1023s, 980s, 831w, 798w, 776w, 751w, 694w, 664w, 640, 605.

**Note:** Bands in the range from 2800 to 3000  $\text{cm}^{-1}$  correspond to the admixture of an organic substance. The IR bands at 1083, 798, 776, and 694  $\text{cm}^{-1}$  are close to those of quartz. The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1205, 1151, 1123, 1064, 1027s, 1010s, 1003s, 980s, 673, 641, 618, 478, 468, 448, 263, 223.

**S626 Alunogen**  $\text{Al}_2(\text{SO}_4)_3(\text{H}_2\text{O})_{12} \cdot 5\text{H}_2\text{O}$ 

**Origin:** Kalamos fumarole field, Milos Island, Greece.

**Description:** White sugar-like aggregate. Characterized by powder X-ray diffraction data. The empirical formula is (electron microprobe):  $(\text{Al}_{1.97}\text{Fe}_{0.03})(\text{SO}_4)_3 \cdot n\text{H}_2\text{O}$ .

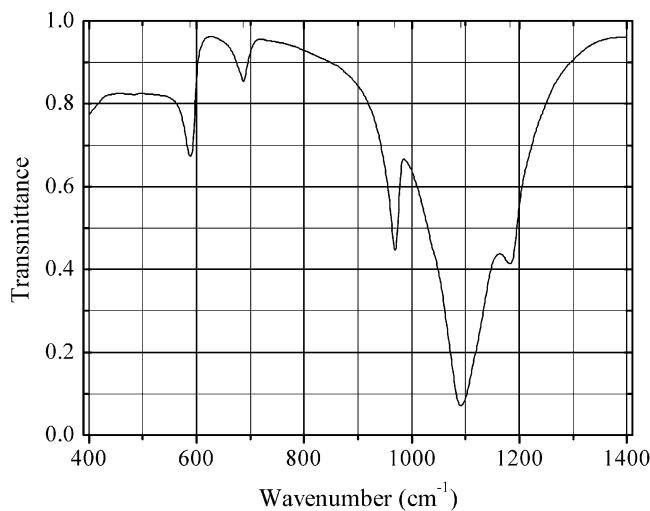
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3500sh, 3353s, 3030s, 2505, 2085w, 1670, 1635sh, 1104s, 983, 933, 895sh, 699, 600, 578, 485sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

**S627 Vanadyl sulfate (VO)(SO<sub>4</sub>)**

**Pauflerite tetragonal dimorph**



**Origin:** Synthetic.

**Description:** Obtained by heating commercial  $\text{VSO}_5 \cdot x\text{H}_2\text{O}$  first at 165 °C for 12 h, then at 260 °C for 4 h, and finally at 330 °C for 1 h. Tetragonal, space group  $P4/n$ .

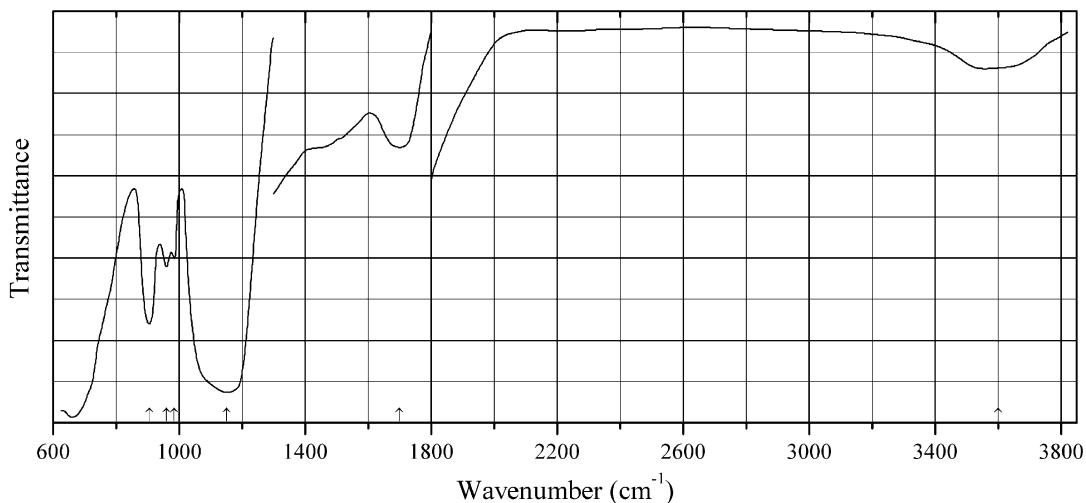
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Stranford and Condrate Sr (1984a).

**Wavenumbers (cm<sup>-1</sup>):** 1183, 1091s, 969, 687w, 588.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. In the cited paper, a figure of the Raman spectrum is given.

### S628 Zaherite $\text{Al}_{12}(\text{SO}_4)_5(\text{OH})_{26} \cdot 20\text{H}_2\text{O}$



**Origin:** Pofadder, Bushmanland, South Africa.

**Description:** White to light bluish-green cryptocrystalline aggregate in narrow veins, in close association with natro-alunite and hotsonite. Triclinic,  $a = 5.55$ ,  $b = 9.74$ ,  $c = 18.43$  Å,  $\alpha = 99.71^\circ$ ,  $\beta = 89.13^\circ$ ,  $\gamma = 94.97^\circ$ .

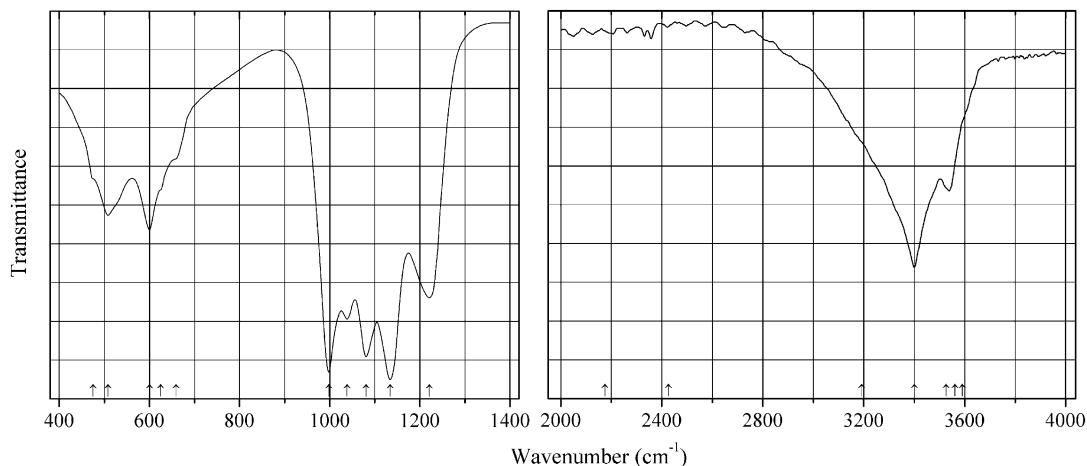
Characterized by chemical analyses and thermal data. The ratio Al:S is close to 12:5. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 18.12 (100) (001), 9.56 (5) (010), 9.08 (4) (002), 4.82 (6) (0-21), 4.61 (8) (110), 4.56 (4) (0-22), 4.44 (4) (021), 3.61 (4) (1-2-1), 3.33 (8) (015).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Beukes et al. (1984).

**Wavenumbers (cm<sup>-1</sup>):** 3600, 1700, 1150s, 985, 960, 905.

**Note:** The intensity of the band of O–H-stretching vibrations (at 3600 cm<sup>-1</sup>) is anomalously low.

**S629 Fibroferrite**  $\text{Fe}^{3+}(\text{SO}_4)(\text{OH}) \cdot 5\text{H}_2\text{O}$ 

**Origin:** Ancient Pb-Zn mine of Saint Felix de Paillères, Anduze, Gard, Languedoc-Roussillon, France.

**Description:** Hand-picked crystals. The crystal structure is solved. Trigonal, space group  $R\bar{3}$ ,  $a = 24.199(3)$ ,  $c = 7.6476(9)$  Å,  $V = 3878.4(8)$  Å<sup>3</sup>.

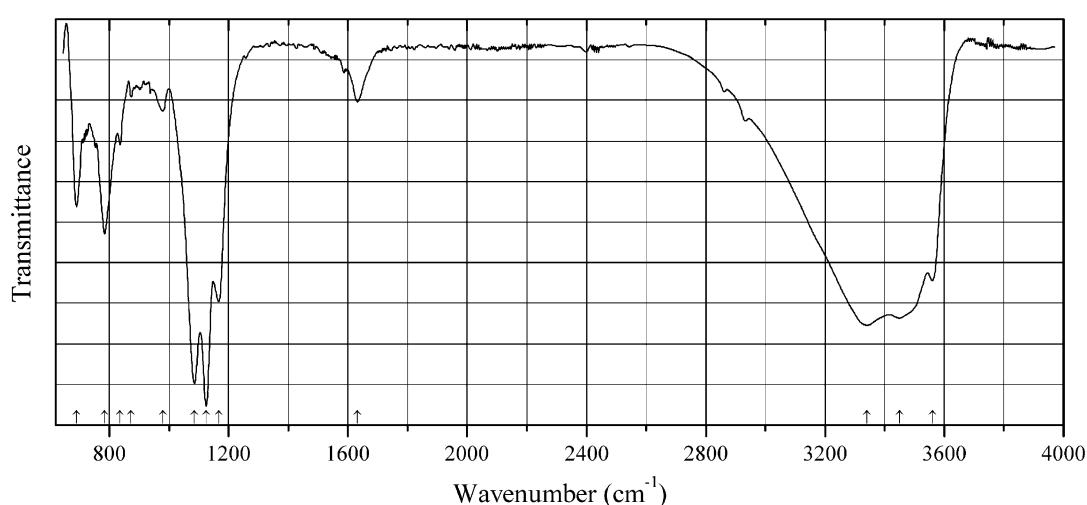
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Ventruti et al. (2016).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 5180w, 4487w, 4234w, 3590sh, 3561sh, 3526, 3400s, 3192sh, 2427w, 2175w, 1662, 1612, 1426w, 1221s, 1134s, 1081s, 1038s, 998s, 659sh, 625sh, 600, 508, 475sh.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 3590, 3522, 3140, 3411, 1175, 1135, 1097, 1073, 1031, 998s, 613, 590, 523, 488, 427, 390, 297, 287, 272, 256, 219, 187, 173, 133, 114.

**S630 Pauladamsite**  $\text{Cu}_4(\text{SeO}_3)(\text{SO}_4)(\text{OH})_4 \cdot 2\text{H}_2\text{O}$ 

**Origin:** Santa Rosa mine, Darwin district, Inyo Co., California, USA (type locality).

**Description:** Green crystals from the association with brochantite, chalcanthite, gypsum, ktenasite, mimetite, schulenbergite, and smithsonite. Holotype sample. The crystal structure is solved. Triclinic, space group  $P\bar{1}$ ,  $a = 6.0742(7)$ ,  $b = 8.4147(11)$ ,  $c = 10.7798(15)$  Å,  $\alpha = 103.665(7)^\circ$ ,  $\beta = 95.224(7)^\circ$ ,  $\gamma = 90.004(6)^\circ$ ,  $V = 533.03(12)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{calc}} = 3.535$  g/cm $^3$ . Optically biaxial (-),  $\alpha = 1.667$  (calc.),  $\beta = 1.723(2)$ ,  $\gamma = 1.743(2)$ ,  $2V = 60(2)^\circ$ . The empirical formula is (electron microprobe, H<sub>2</sub>O calculated): H<sub>8.50</sub>Cu<sub>3.55</sub>Zn<sub>0.25</sub>Se<sub>0.98</sub>S<sub>1.00</sub>O<sub>13</sub>. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 10.5 (46) (011), 3.245 (100) (001), 5.81 (50) (011), 2.743 (49) (112), 3.994 (67) (012), 3.431 (23) (-112, -1-21, -120), 2.692 (57) (0-32, -122, -2-12), 2.485 (39) (2-12, -1-32, 0-24).

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission, with a micro diamond compression cell.

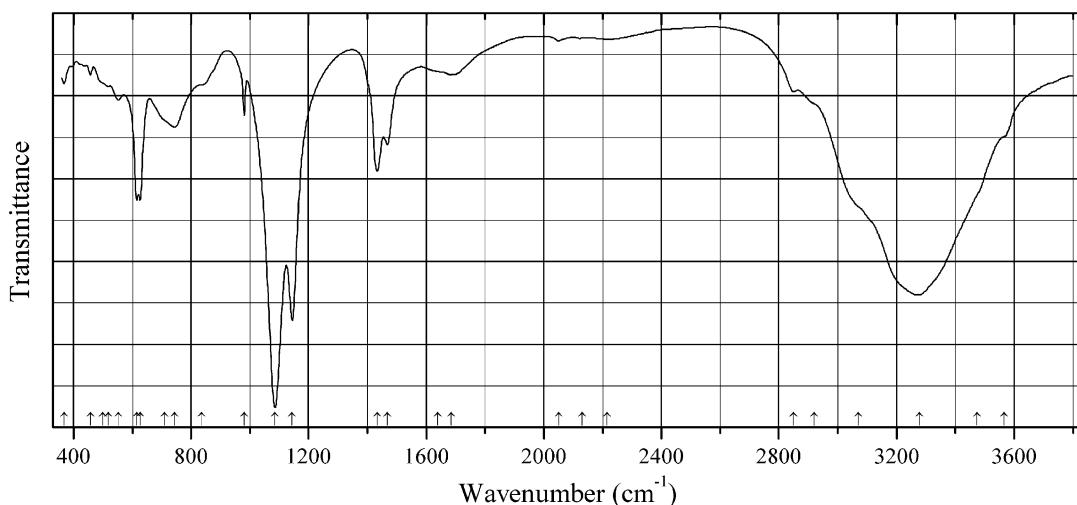
**Source:** Kampf et al. (2016d).

**Wavenumbers (IR, cm $^{-1}$ ):** 3560, 3450s, 3341s, 1633, 1167, 1125s, 1086s, 980w, 873w, 836, 784, 690.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 1166, 1076, 989s, 839s, 745, 679, 638w, 610w, 487, 412, 396, 299, 270, 222, 166, 153.

### S631 Katerinopoulosite (NH<sub>4</sub>)<sub>2</sub>Zn(SO<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O



**Origin:** Esperanza mine, Lavrion District, Attikí Prefecture, Greece (type locality).

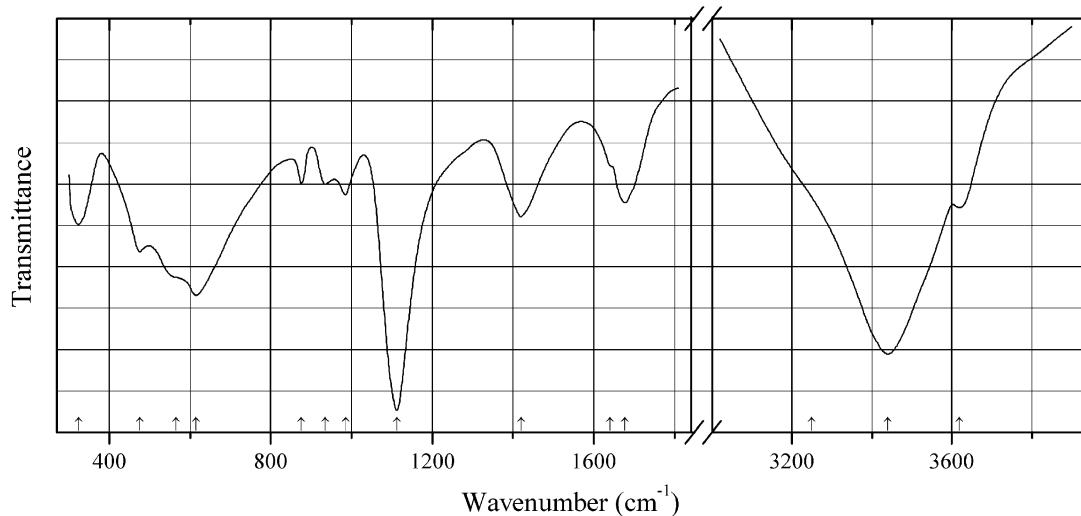
**Description:** Greenish antholite crust from the association with chalcanthite, nickelboussingaultite, ammoniojarosite, aurichalcite, and goethite. Holotype sample. Monoclinic, space group:  $P2_1/a$ ,  $a = 9.230(6)$ ,  $b = 12.476(4)$ ,  $c = 6.249(4)$  Å,  $\beta = 106.79(5)^\circ$ ,  $V = 688.9(9)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{meas}} = 1.97(2)$  g/cm $^3$ ,  $D_{\text{calc}} = 1.986$  g/cm $^3$ . Optically biaxial (+),  $\alpha = 1.492(2)$ ,  $\beta = 1.496(2)$ ,  $\gamma = 1.502(2)$ ,  $2V = 80(5)^\circ$ . The empirical formula is (H<sub>3</sub>O)<sub>0.13</sub>(NH<sub>4</sub>)<sub>1.91</sub>(Zn<sub>0.86</sub>Ni<sub>0.10</sub>Cu<sub>0.02</sub>)(SO<sub>4</sub>)<sub>2.00</sub>·6.62H<sub>2</sub>O. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 5.400 (37) (011), 4.411 (19) (200), 4.314 (19) (021), 4.229 (24) (12-1), 4.161 (100) (20-1, 210, 111), 3.749 (53) (130), 3.034 (29) (211, 11-2).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3565sh, 3475sh, 3278s, 3070sh, 2920sh, 2850, 2215w, 2130w, 2050w, 1685, 1640sh, 1468, 1433, 1144s, 1086s, 981, 835sh, 743, 710sh, 627, 615, 552w, 519w, 500sh, 459w, 368w.

**Note:** The spectrum was obtained by N.V. Chukanov.

**S632 Charlesite**  $\text{Ca}_6\text{Al}_2(\text{SO}_4)_2\text{B}(\text{OH})_4(\text{OH},\text{O})_{12}\cdot 26\text{H}_2\text{O}$



**Origin:** Wessels mine, Hotazel, Kalahari manganese fields, Northern Cape province, South Africa.

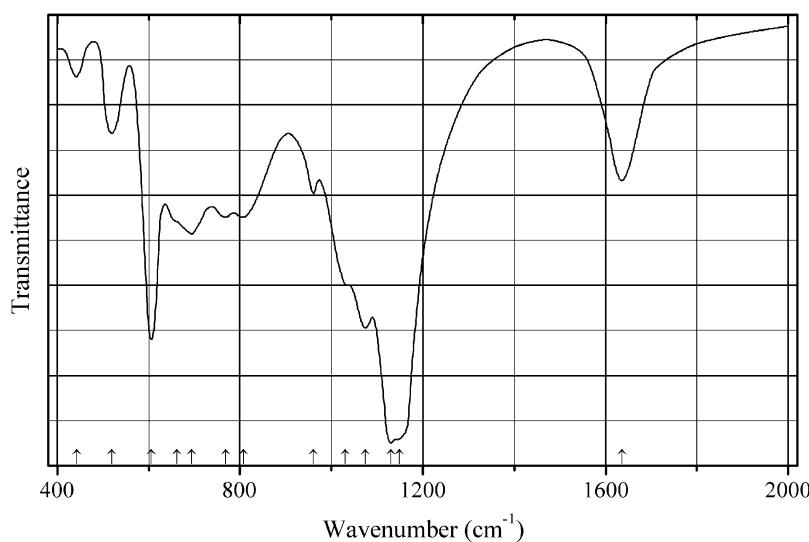
**Description:** Yellow. Intermediate zone of a mixed ettringite-charlesite-sturmanite crystal. The empirical formula is (electron microprobe):  $\text{Ca}_{6.00}(\text{Al}_{0.7}\text{Fe}_{0.6}\text{Si}_{0.5}\text{Mn}_{0.2})(\text{SO}_4)_{2.27}(\text{CO}_3)_x[\text{B}(\text{OH})_4]_{~1}(\text{OH},\text{O})_{12}\cdot n\text{H}_2\text{O}$  ( $x \ll 1$ ).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3620, 3440s, 3250sh, 1678, 1641sh, 1420, 1112s, 986, 935, 876, 615s, 565sh, 475, 324.

**Note:** The spectrum was obtained by N.V. Chukanov.

**S633 Osakaite**  $\text{Zn}_4(\text{SO}_4)_6(\text{OH})_6\cdot 5\text{H}_2\text{O}$



**Origin:** Synthetic.

**Description:** Obtained by mixing of 1 g ZnO powder with 30 ml 0.5 M solution of ZnSO<sub>4</sub> for 72 h.  
Characterized by thermal and powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Stanimirova et al. (2016).

**Wavenumbers (cm<sup>-1</sup>):** 1636, 1149s, 1130s, 1074, 1031, 961, 807, 768, 694, 661sh, 606s, 519, 442w.

#### S634 Stephanite Ag<sub>5</sub>SbS<sub>4</sub>

**Origin:** Proano mine, Fresnillo, Zacatecas, Mexico.

**Description:** Black pseudohexagonal crystals. Orthorhombic,  $a = 7.8396(7)$ ,  $b = 12.4684(9)$ ,  $c = 8.536(1)$  Å.

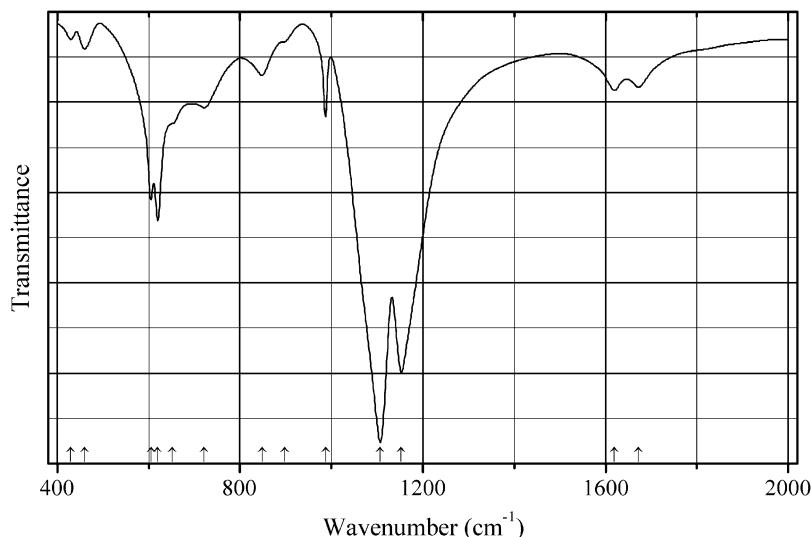
**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of powdered mineral.

**Source:** RRUFF (2007).

**Wavenumbers (cm<sup>-1</sup>):** 343s, 322s, 262, 235.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

#### S635 Changoite Na<sub>2</sub>Zn(SO<sub>4</sub>)<sub>2</sub>·4H<sub>2</sub>O



**Origin:** Synthetic.

**Description:** Obtained by crystallization from aqueous solution.

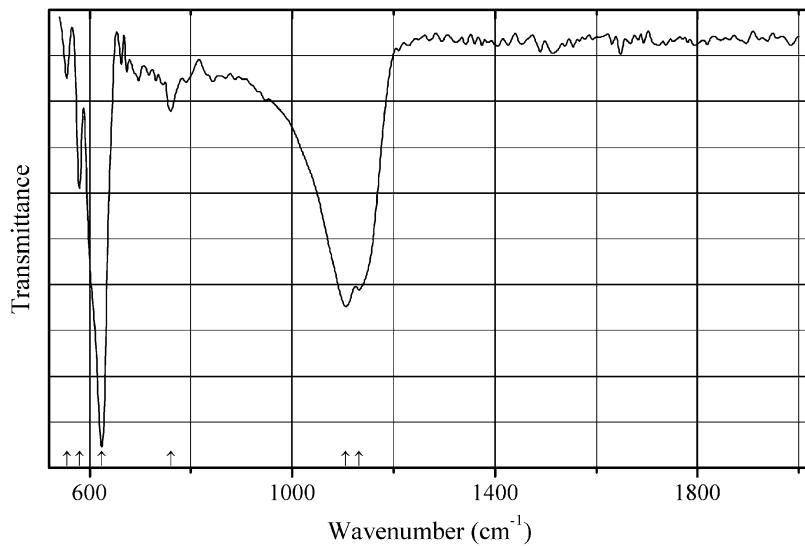
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Georgiev et al. (2016).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1672w, 1620w, 1153s, 1107s, 987, 898sh, 848w, 721, 652sh, 620s, 605s, 460, 430.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1190, 1160w, 1101w, 1067, 989s, 615, 473, 451.

**S636 Galeite**  $\text{Na}_{15}(\text{SO}_4)_5\text{ClF}_4$ 

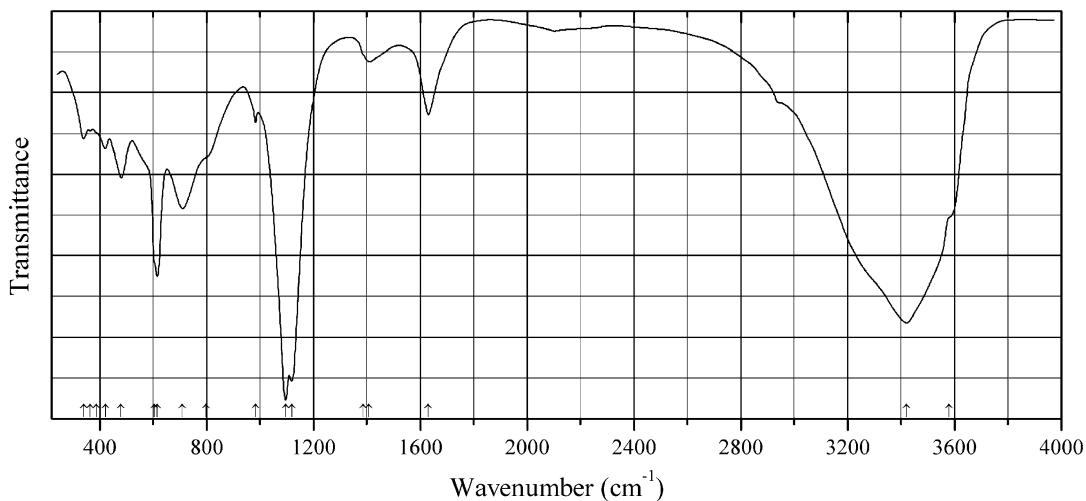
**Origin:** Synthetic.

**Description:** Ce<sup>3+</sup>-doped sample prepared using a wet chemical method. Characterized by powder X-ray diffraction data. The crystal structure is solved. Trigonal, space group  $P31m$ ,  $a = 12.19$ ,  $c = 13.95$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Bhake et al. (2016).

**Wavenumbers (cm<sup>-1</sup>):** 1132, 1106s, 760w, 624s, 580, 555.

**S637 Ktenasite**  $(\text{Cu},\text{Zn})_5(\text{SO}_4)_2(\text{OH})_6 \cdot 6\text{H}_2\text{O}$ 

**Origin:** Hirao mine, Minoo, Osaka, Japan.

**Description:** Aggregates of flattened prismatic crystals from the association with primary sulfides, gypsum, smithsonite, hydrozincite, aurichalcite, schulenbergite, brianyoungite, serpierite, brochantite, etc. Characterized by powder X-ray diffraction data. Monoclinic,  $a = 5.590(1)$ ,  $b = 6.161(1)$ ,  $c = 23.741(3)$  Å,  $\beta = 95.628(3)^\circ$ .  $D_{\text{meas}} = 2.93$  g/cm<sup>3</sup>. The empirical formula is  $(\text{Cu}_{3.446}\text{Zn}_{1.451}\text{Co}_{0.080}\text{Pb}_{0.018}\text{Ni}_{0.007})(\text{SO}_4)_{2.003}(\text{OH})_{5.998}\cdot 5.99\text{H}_2\text{O}$ .

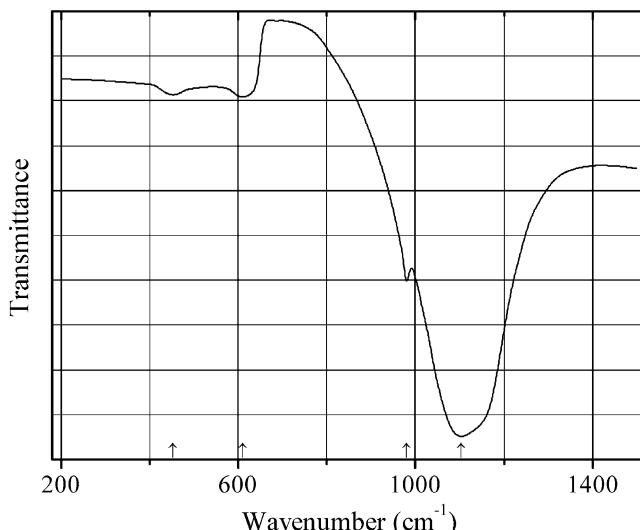
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Ohnishi et al. (2002).

**Wavenumbers (cm<sup>-1</sup>):** 3580sh, 3420s, 1630, 1408w, 1118s, 1095s, 983w, 798sh, 710, 615s, 605sh, 480, 420, 387sh, 364w, 340w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### S638 Lazaridisite $\text{Cd}_3(\text{SO}_4)_3\cdot 8\text{H}_2\text{O}$



**Origin:** Synthetic.

**Description:** Crystals grown from aqueous solution by slow evaporation. Monoclinic, space group  $C2/c$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Murthy et al. (1992).

**Wavenumbers (cm<sup>-1</sup>):** 1103s, 980, 610, 453.

## S639 Pyracmonite $(\text{NH}_4)_3\text{Fe}(\text{SO}_4)_3$

**Origin:** La Fossa crater, Vulcano Island, Lipari, Eolie (Aeolian) islands, Messina province, Sicily, Italy (type locality).

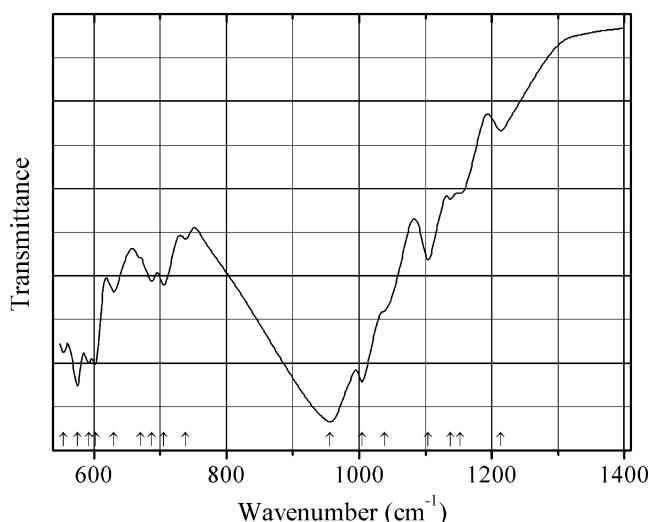
**Description:** Holotype sample. Trigonal, space group  $R\bar{3}c$ ,  $a = 15.2171(14)$ ,  $c = 8.9323(8)$  Å,  $V = 1791.3(3)$  Å<sup>3</sup>,  $Z = 6$ . The empirical formula is  $[(\text{NH}_4)_{2.74}\text{K}_{0.23}](\text{Fe}_{0.94}\text{Al}_{0.04})\text{S}_{3.02}\text{O}_{12}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 7.596 (100) (110), 3.320 (30) (122), 3.371 (26) (131), 4.358 (23) (12-1), 2.829 (14) (312), 2.863 (8) (321).

**Kind of sample preparation and/or method of registration of the spectrum:** No data.

**Source:** Demartin et al. (2010).

**Wavenumbers (cm<sup>-1</sup>):** 3203s, 3064s, 1430s.

**S640 Rhodium sulfate**  $\text{Rh}_2(\text{SO}_4)_3$



**Origin:** Synthetic.

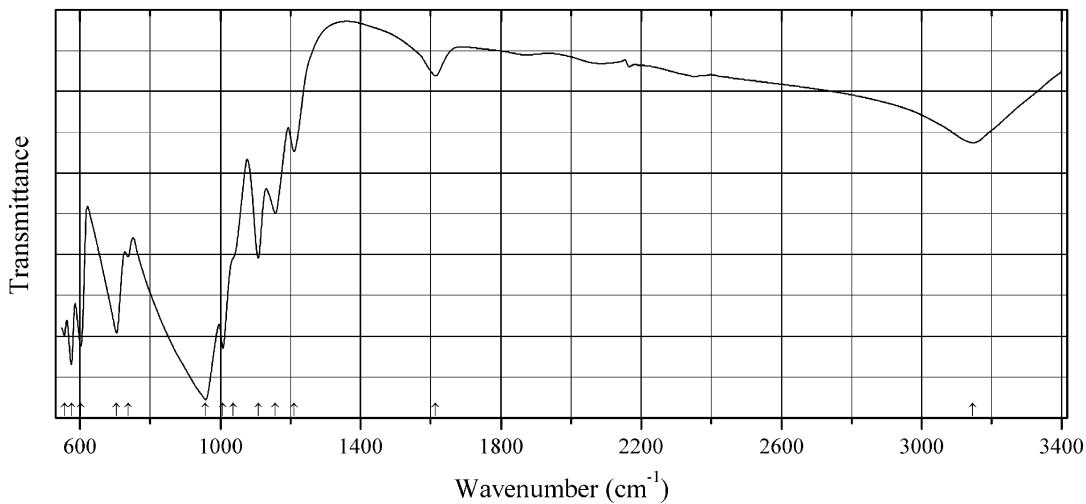
**Description:** The crystal structure is solved. Trigonal, space group  $R\bar{3}$ ,  $a = 8.068(1)$ ,  $c = 22.048(4)$  Å,  $V = 1242.8(4)$  Å<sup>3</sup> (at 153 K),  $Z = 6$ .

**Kind of sample preparation and/or method of registration of the spectrum:** No data.

**Source:** Wickleder et al. (2016).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1214w, 1138w, 1152sh, 1104, 1038sh, 1004s, 956s, 738w, 705, 687, 670sh, 630, 602, 592, 575s, 554

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**S641 Rhodium sulfate hydrate  $\text{Rh}_2(\text{SO}_4)_3 \cdot 2\text{H}_2\text{O}$** 

**Origin:** Synthetic.

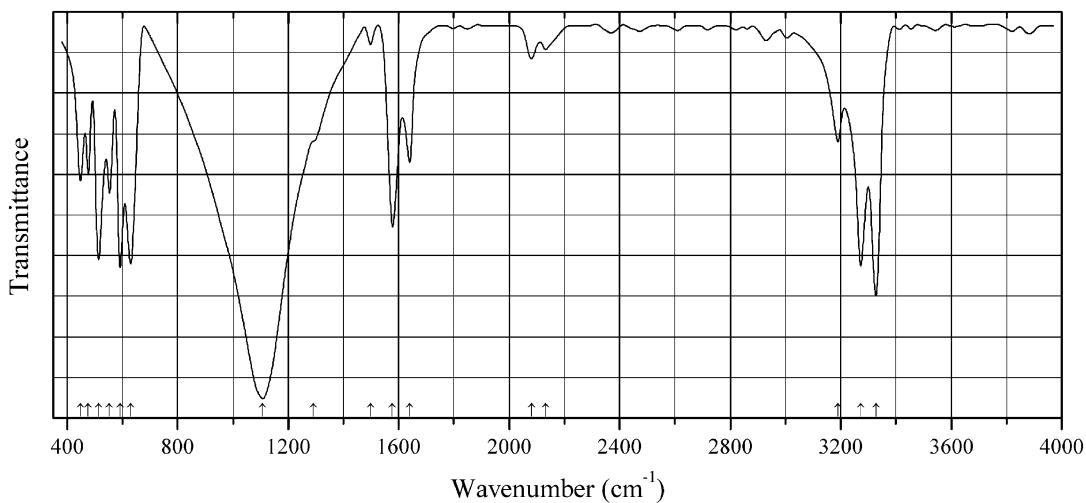
**Description:** The crystal structure is solved. Orthorhombic, space group  $Pnma$ ,  $a = 9.2046(2)$ ,  $b = 12.4447(3)$ ,  $c = 8.3337(2)$  Å,  $V = 954.61(4)$  Å $^3$  (at 153 K),  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** No data.

**Source:** Wickleder et al. (2016).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3146, 1614w, 1211, 1157, 1108, 1037sh, 1007s, 957s, 737, 704s, 602s, 575s, 555.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**S642 Sanderite  $\text{Fe}^{2+}$  analogue  $\text{Fe}^{2+}(\text{SO}_4) \cdot 2\text{H}_2\text{O}$** 

**Origin:** Synthetic.

**Description:** Synthesized by the hydro/solvothermal method. The crystal structure is solved. Orthorhombic, space group  $Pccn$ ,  $a = 6.3160$ ,  $b = 7.7550$ ,  $c = 8.9880 \text{ \AA}$ ,  $V = 440.2 \text{ \AA}^3$ ,  $Z = 4$ .

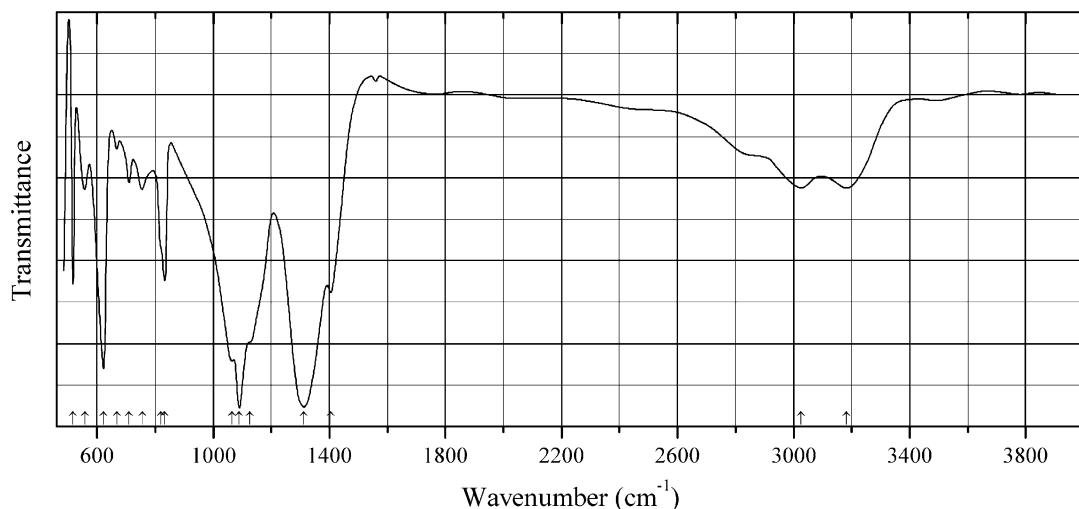
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Zhao et al. (2015).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3328s, 3273s, 3190, 2132w, 2081w, 1640, 1578s, 1498w, 1292sh, 1108s, 630s, 592s, 553, 514s, 477, 448.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### S643 Schairerite $\text{Na}_{21}(\text{SO}_4)_7\text{ClF}_6$



**Origin:** Synthetic.

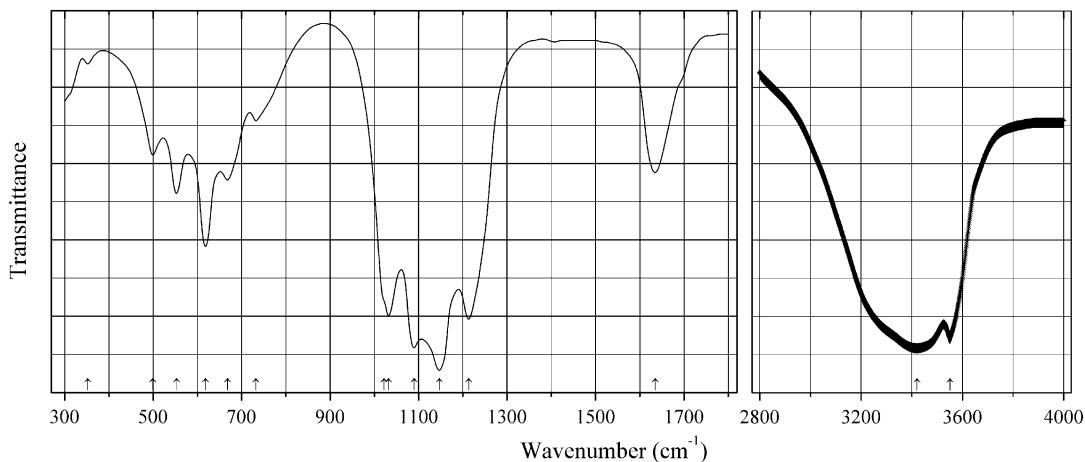
**Description:** Ce-doped sample synthesized by a wet method. Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Shinde and Dhoble (2015), Shinde et al. (2015).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3183, 3026, 1405, 1313s, 1125sh, 1090s, 1064, 833, 820sh, 755, 710, 667w, 622s, 557, 517.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The bands in the range from 2800 to 3200  $\text{cm}^{-1}$  indicate the presence of covalent O–H-bonds. The band at 833  $\text{cm}^{-1}$  may correspond to Na···O–H bending vibrations. The band at 1313  $\text{cm}^{-1}$  may be due to an impurity.

**S644 Zincobotryogen  $\text{ZnFe}^{3+}(\text{SO}_4)_2(\text{OH})\cdot 7\text{H}_2\text{O}$** 

**Origin:** Xitieshan Pb-Zn deposit, Qinghai, China (type locality).

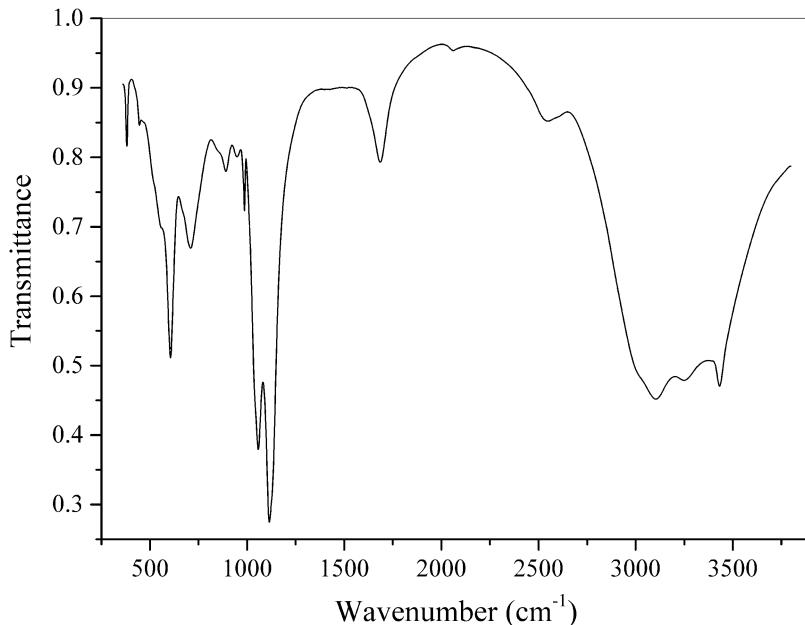
**Description:** Orange-red prismatic crystals from the association with jarosite, copiapite, zincocopiaite, and quartz. Holotype sample. The crystal structure is solved. Monoclinic, space group P12<sub>1</sub>/n,  $a = 10.504(2)$ ,  $b = 17.801(4)$ ,  $c = 7.1263(14)$  Å,  $\beta = 100.08(3)^\circ$ ,  $V = 1311.9$  (5) Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{meas}} = 2.20(1)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 2.266$  g/cm<sup>3</sup>. Optically biaxial (+),  $\alpha = 1.542(5)$ ,  $\beta = 1.551(5)$ ,  $\gamma = 1.587(5)$ . The empirical formula is (electron microprobe): (Zn<sub>0.73</sub>Mg<sub>0.16</sub>Mn<sub>0.08</sub>Fe<sub>0.99</sub>(SO<sub>4</sub>)<sub>2.04</sub>(OH)<sub>0.82</sub>·7H<sub>2</sub>O. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 8.92 (100) (100), 6.32 (77) (-101), 5.56 (23) (021), 4.08 (22) (-221), 3.21 (31) (231), 3.03 (34) (032), 2.77 (22) (042).

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Yang et al. (2016b).

**Wavenumbers (cm<sup>-1</sup>):** 3550s, 3420s, 1635, 1213s, 1147s, 1090s, 1032s, 1022sh, 732, 668, 618s, 553, 499, 352w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**S645 Jurbanite**  $\text{Al}(\text{SO}_4)(\text{OH}) \cdot 5\text{H}_2\text{O}$ 

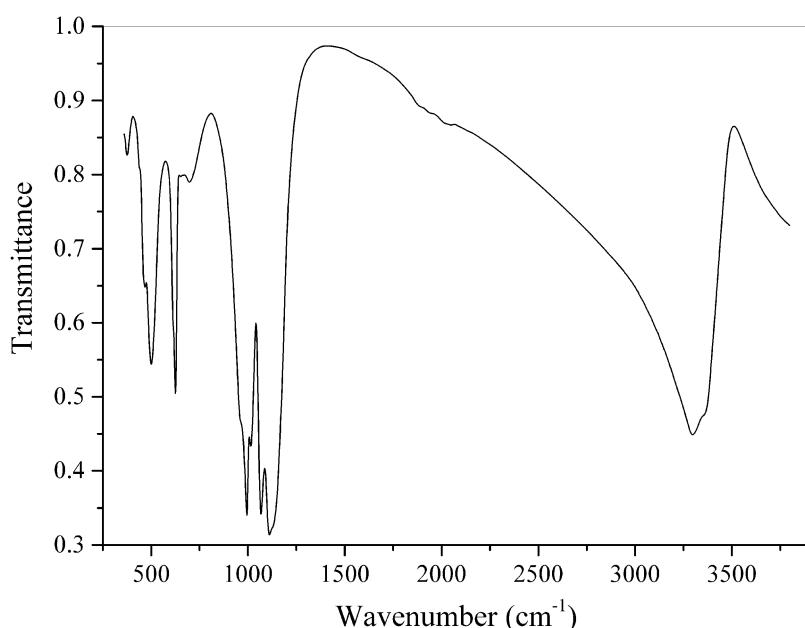
**Origin:** Le Cetine di Cotorniano mine, Chiusdino, Siena province, Tuscany, Italy.

**Description:** White aggregate. Investigated by A.V. Kasatkin. Characterized by powder X-ray diffraction data and electron microprobe analyses.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3432s, 3252s, 3104s, 3025sh, 2519, 2061w, 1685, 1114s, 1057s, 987, 949w, 891, 885sh, 709, 605s, 560sh, 447w, 381.

**Note:** The spectrum was obtained by N.V. Chukanov.

**S646 Beaverite-(Zn)**  $\text{Pb}(\text{Fe}^{3+}, \text{Zn})(\text{SO}_4)_2(\text{OH})_6$ 

**Origin:** San Francisco mine, Sierra Gorda, Chile.

**Description:** Brown crystalline crusts from the association with atacamite and paratacamite.

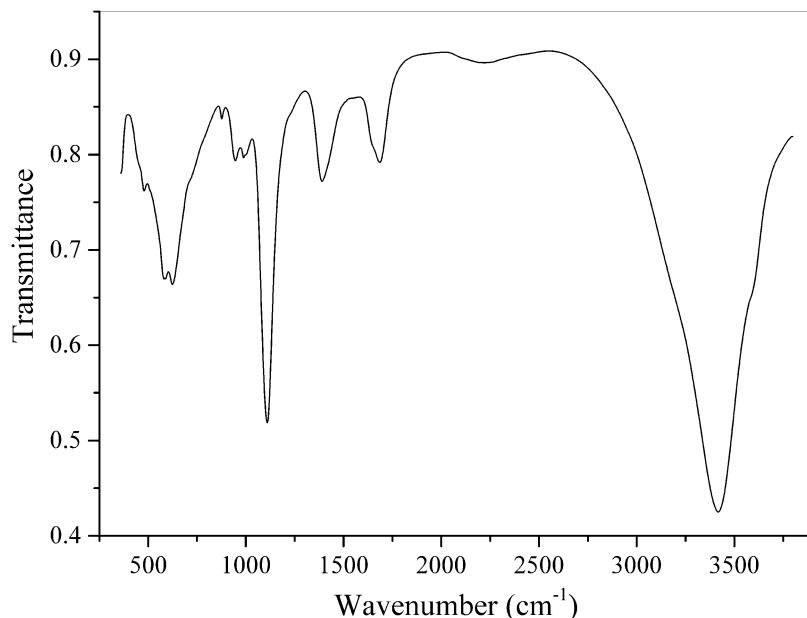
Characterized by powder X-ray diffraction data and qualitative electron microprobe analyses.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3350sh, 3296s, 2032w, 1947w, 1888w, 1130sh, 1111s, 1067s, 1015, 995s, 965sh, 697w, 655w, 625, 500, 468, 440sh, 346w.

**Note:** The spectrum was obtained by N.V. Chukanov.

**S647 Jouravskite**  $\text{Ca}_3\text{Mn}^{4+}(\text{SO}_4)(\text{CO}_3)(\text{OH})_6 \cdot 12\text{H}_2\text{O}$



**Origin:** N'Chwaning 3 mine, Kuruman, Kalahari manganese field, Northern Cape province, South Africa.

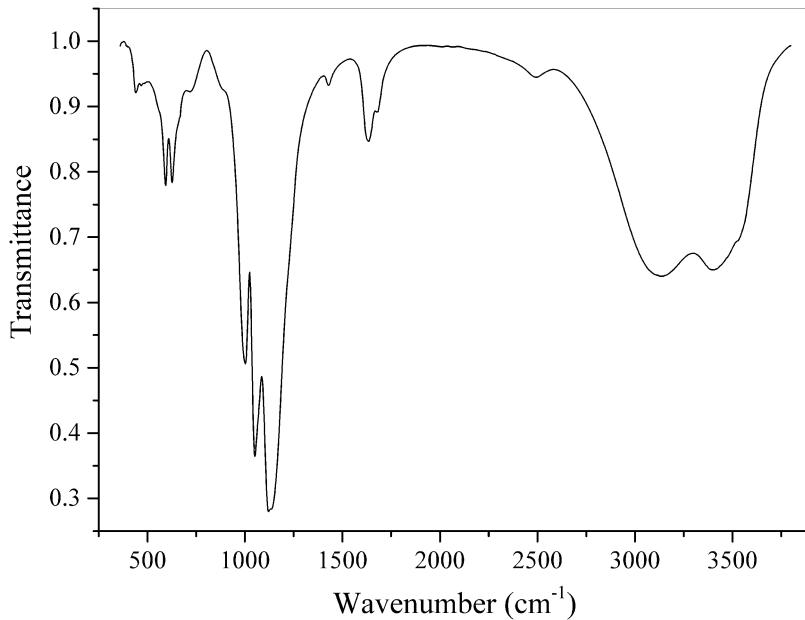
**Description:** Yellow crystals. A boron-bearing variety. The empirical formula is (electron microprobe):  $\text{Ca}_{3.0}(\text{Mn}_{0.95}\text{Fe}_{0.04})(\text{SO}_4)_{1.00}[\text{CO}_3,\text{B}(\text{OH})_4](\text{OH},\text{O})_6 \cdot n\text{H}_2\text{O}$ . The content of  $\text{B}_2\text{O}_3$  determined by ICP-OES is 0.39 wt%.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3485sh, 3421s, 3385sh, 3245sh, 3085sh, 2880sh, 2455w, 2257w, 1696, 1645, 1392s, 1104s, 1004w, 962, 887, 719, 639, 600sh, 578s, 550sh, 485sh, 460sh, 374.

**Note:** The spectrum was obtained by N.V. Chukanov.

**S648 Zincovoltaite**  $K_2Zn_5Fe^{3+}_3Al(SO_4)_{12} \cdot 18H_2O$



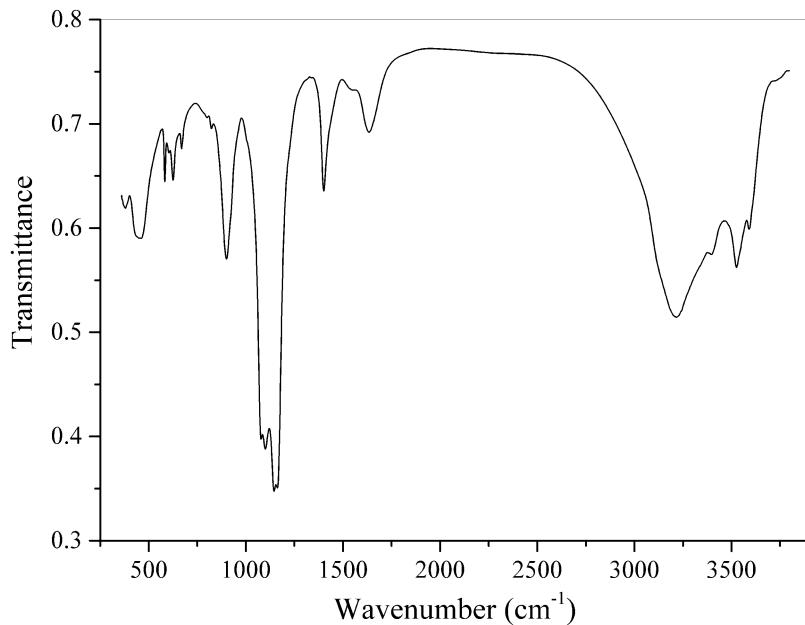
**Origin:** Muzhievskoe deposit, Transcarpathian Region, Ukraine.

**Description:** Black crystals from the association with zincocopiaite, bianschite, and boyleite. A NH<sub>4</sub>-bearing variety. Investigated by A.V. Kasatkin. Characterized by single-crystal X-ray diffraction data and electron microprobe analyses. Cubic,  $a = 27.2450(14)$  Å. The empirical formula is  $K_{1.57}(NH_4)_x(Zn_{3.54}Mg_{0.49}Cu_{0.44}Fe^{2+}_{0.36}Mn_{0.08})Fe^{3+}_{2.82}Al_{1.30}S_{11.97}O_{48} \cdot 18H_2O$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3520sh, 3406 (broad), 3134 (broad), 2493w, 1677, 1635, 1429w, 1134s, 1121s, 1051s, 1003, 890sh, 718w, 655sh, 626, 593, 468w, 441w.

**Note:** The spectrum was obtained by N.V. Chukanov. The band at 1429 cm<sup>-1</sup> corresponds to NH<sub>4</sub><sup>+</sup> cations.

**S649 Ammoniozippelite**  $(\text{NH}_4)_2[(\text{UO}_2)_2(\text{SO}_4)\text{O}_2] \cdot \text{H}_2\text{O}$ 

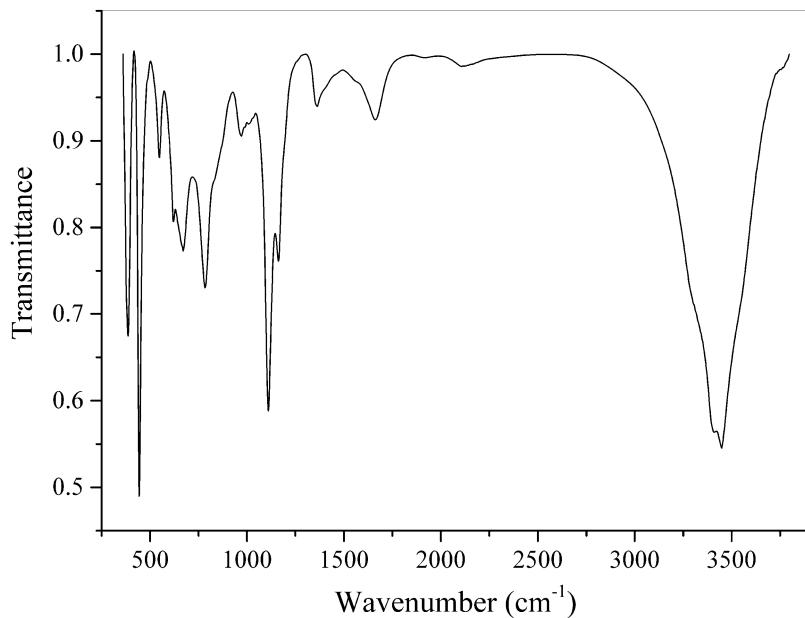
**Origin:** Blue Lizard Mine, Red Canyon, White Canyon District, San Juan Co., Utah, USA (cotype locality).

**Description:** Yellow acicular crystals. Investigated by A.V. Kasatkin. Characterized by powder X-ray diffraction data and electron microprobe analyses. The empirical formula is:  $(\text{NH}_4)_x[(\text{UO}_2)_{2.06}(\text{SO}_4)_{0.94}\text{O}_2] \cdot n\text{H}_2\text{O}$ . The observed lines of the powder X-ray diffraction pattern ( $d$ , Å) are: 8.42, 8.10s, 5.46w, 4.24, 3.65, 3.48s, 3.12s, 2.85, 2.65w, 2.37w, 2.20w, 2.11w, 2.04w, 1.96w, 1.87w, 1.74w, 1.70w.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3592, 3526, 3397, 3217s, 1635, 1551w, 1402, 1162s, 1145s, 1100s, 1081s, 901, 825w, 801w, 668, 625, 605w, 583, 462, 440sh, 380.

**Note:** The spectrum was obtained by N.V. Chukanov. The bands at 1402 cm<sup>-1</sup> correspond to NH<sub>4</sub><sup>+</sup>.

**S650 Motukoreaite-related mineral**  $[(\text{Mg},\text{Al})_9(\text{OH})_{18}][\text{Na}_x(\text{SO}_4,\text{CO}_3)_2(\text{H}_2\text{O})_{12}]$  (?)

**Origin:** Verkhnekamskoe salt deposit, western Urals, Russia.

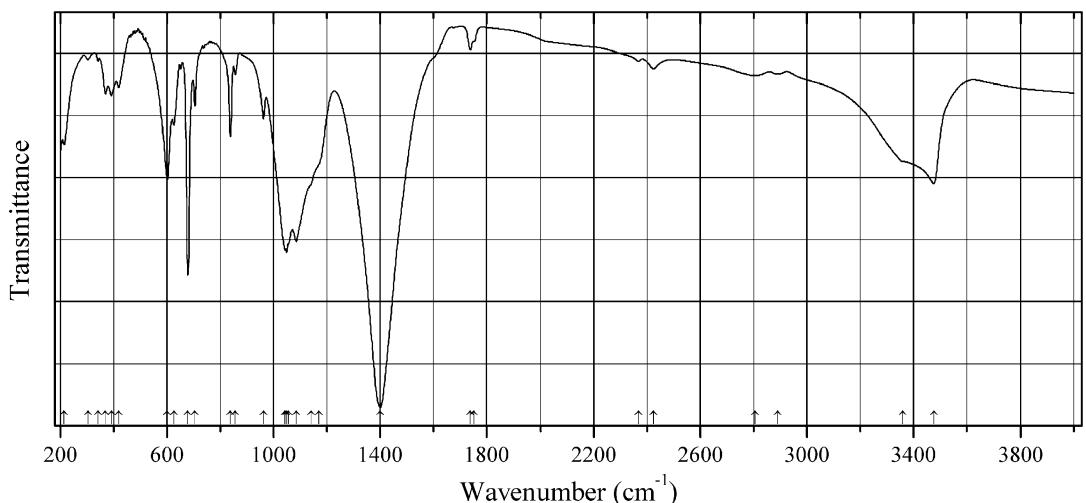
**Description:** Colorless grains from the association with halite. Investigated by I.V. Pekov.

Characterized by X-ray diffraction.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3520sh, 3449s, 3412s, 3320sh, 2104w, 1918w, 1662, 1565sh, 1363, 1162, 1110s, 1010w, 972, 830sh, 784, 670, 620, 548, 444s, 387s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**SC18 Leadhillite**  $\text{Pb}_4(\text{SO}_4)(\text{CO}_3)_2(\text{OH})_2$ 

**Origin:** Leadhills, South Lanarkshire, Strathclyde, Scotland, UK (type locality).

**Description:** Characterized by chemical analyses and powder X-ray diffraction data. The chemical composition is very close to that calculated from the ideal formula.

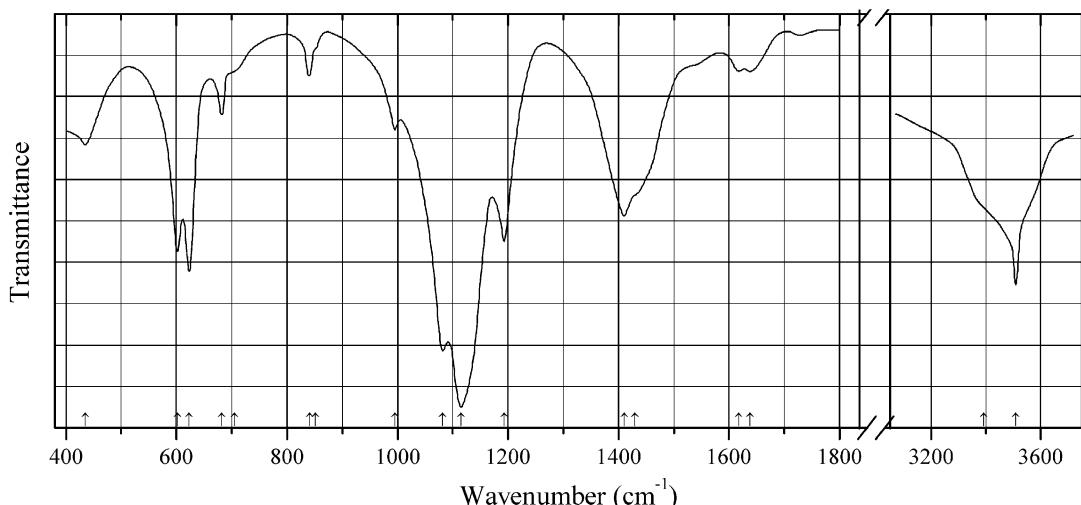
**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc. Transmission.

**Source:** Russell et al. (1983).

**Wavenumbers (cm<sup>-1</sup>):** 3475, 3360sh, 2890w, 2805w, 2425w, 2368w, 1751sh, 1738w, 1399s, 1170sh, 1140sh, 1085s, 1055s, 1049s, 1043sh, 962, 857, 838, 705, 679s, 626, 602, 419, 392, 370, 342w, 304w, 215.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### SC19 Leadhillite Pb<sub>4</sub>(SO<sub>4</sub>)(CO<sub>3</sub>)<sub>2</sub>(OH)<sub>2</sub>



**Origin:** Leadhills, South Lanarkshire, Strathclyde, Scotland, UK (type locality).

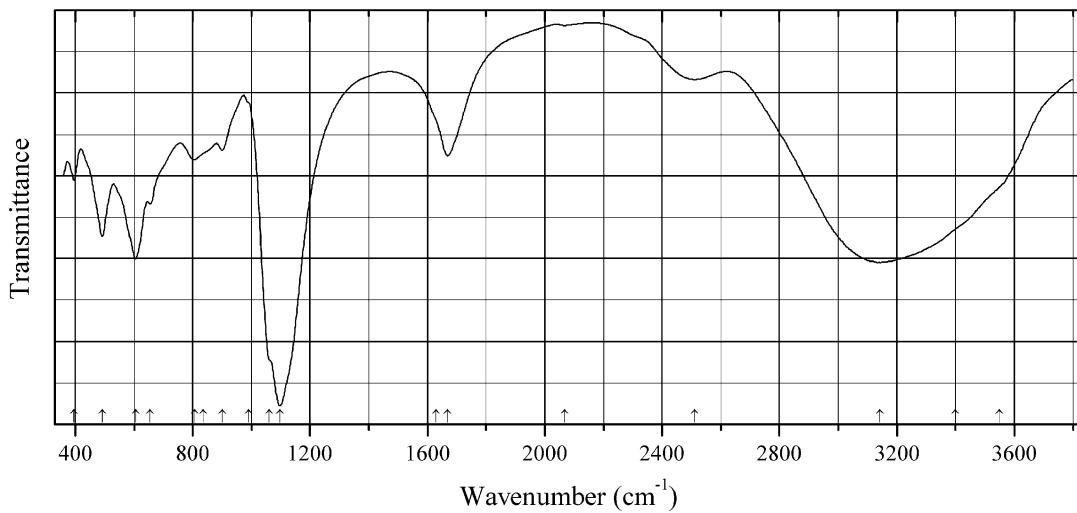
**Description:** Monoclinic, space group  $P2_1/a$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Moenke (1962). The spectrum was reproduced by Russell et al. (1983).

**Wavenumbers (cm<sup>-1</sup>):** 3508, 3392sh, 1638w, 1618w, 1430sh, 1410, 1193, 1115s, 1082s, 995, 852sh, 841, 705sh, 682, 623s, 602, 435.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**SP25 Arangasite**  $\text{Al}_2(\text{SO}_4)(\text{PO}_4)\text{F} \cdot 9\text{H}_2\text{O}$ 

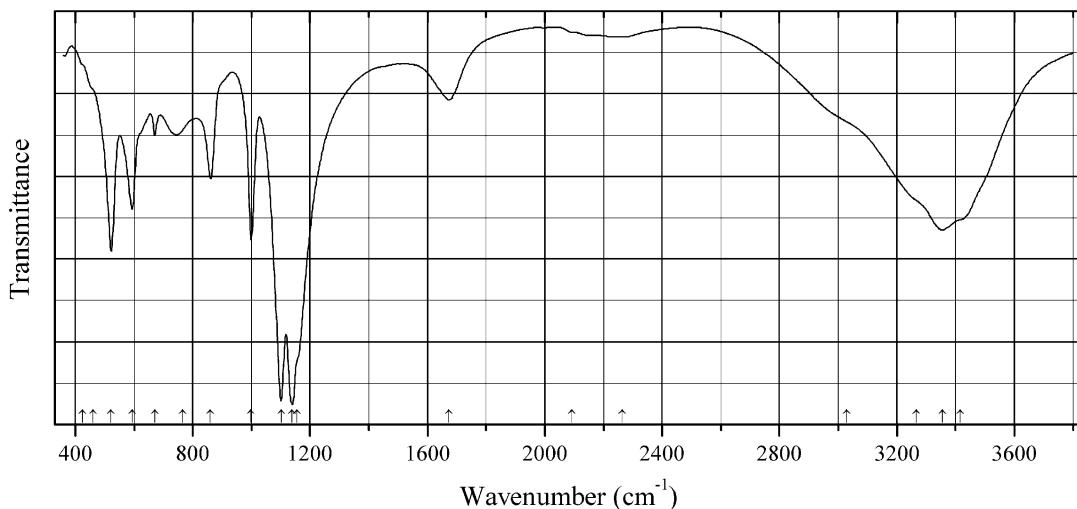
**Origin:** Alyaskitovoye Sn-W deposit, Ust'-Nera, Indigirka River Basin, Sakha Republic (Yakutia), Russia (type locality).

**Description:** White granular aggregate. Investigated by I.V. Pekov. The empirical formula is (electron microprobe):  $\text{Al}_{2.09}(\text{SO}_4)_{1.00}(\text{PO}_4)_{0.89}(\text{AsO}_4)_{0.105}(\text{SiO}_4)_{0.005}\text{F}_{1.41} \cdot n\text{H}_2\text{O}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %)] are: 10.68 (55), 9.66 (100), 5.33 (26), 4.21 (41), 3.491 (22), 3.145 (22).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm⁻¹):** 3550sh, 3400sh, 3143s (broad), 2511, 2068w, 1669, 1630sh, 1098s, 1060sh, 990sh, 901, 835sh, 806, 655, 605s, 491, 396.

**Note:** The spectrum was obtained by N.V. Chukanov.

**SP26 Ardealite**  $\text{Ca}_2(\text{PO}_3\text{OH})(\text{SO}_4) \cdot 4\text{H}_2\text{O}$ 

**Origin:** Cerro Mejillones, Mejillones Peninsula, Mejillones, Antofagasta, II Region, Chile.

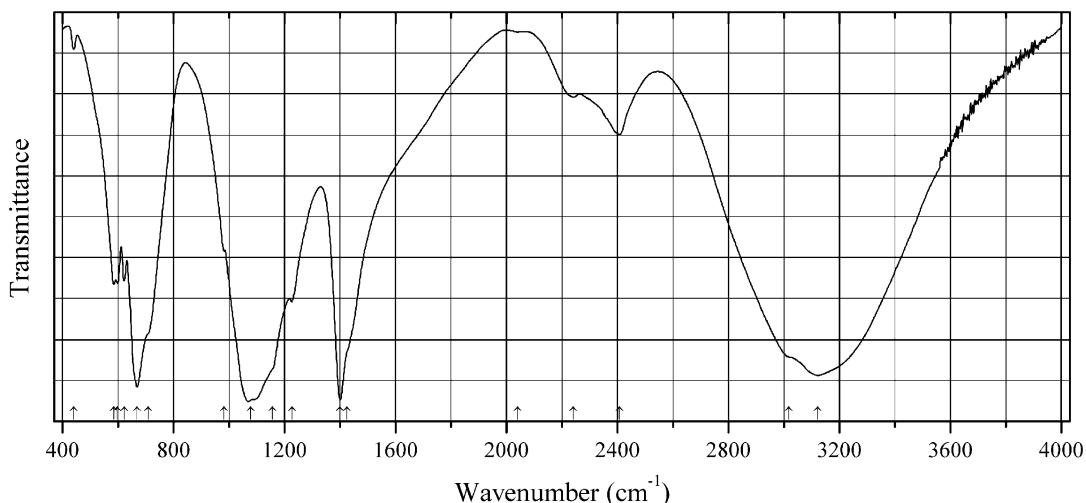
**Description:** White soft fine-granular aggregate. Investigated by I.V. Pekov. Characterized by qualitative electron microprobe analyses. Confirmed by the IR spectrum.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3415sh, 3355s, 3265sh, 3030sh, 2265w, 2092w, 1673, 1155sh, 1139s, 1101s, 999s, 861, 765, 671, 593, 522s, 460sh, 425sh.

**Note:** The spectrum was obtained by N.V. Chukanov.

### STe1 Ammonium sulfate tellurate $(\text{NH}_4)_2(\text{SO}_4)\cdot\text{Te}(\text{OH})_6$



**Origin:** Synthetic.

**Description:** As-doped sample produced from an aqueous stoichiometric solution of telluric acid, ammonium sulfate, ammonium carbonate, and arsenic acid. The empirical formula  $(\text{NH}_4)_2(\text{SO}_4)_{0.92}\text{H}(\text{AsO}_4)_{0.08}\text{Te}(\text{OH})_6$  given in the original paper isn't charge-balanced. The correct formula should be  $(\text{NH}_4)_2[(\text{SO}_4)_{0.92}(\text{HAsO}_4)_{0.08}]\cdot\text{Te}(\text{OH})_6$ . The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 11.382(5)$ ,  $b = 6.615(5)$ ,  $c = 13.707(5)$  Å,  $\beta = 106.731(5)$ °,  $V = 988.3(9)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 2.41$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Ghorbel et al. (2015).

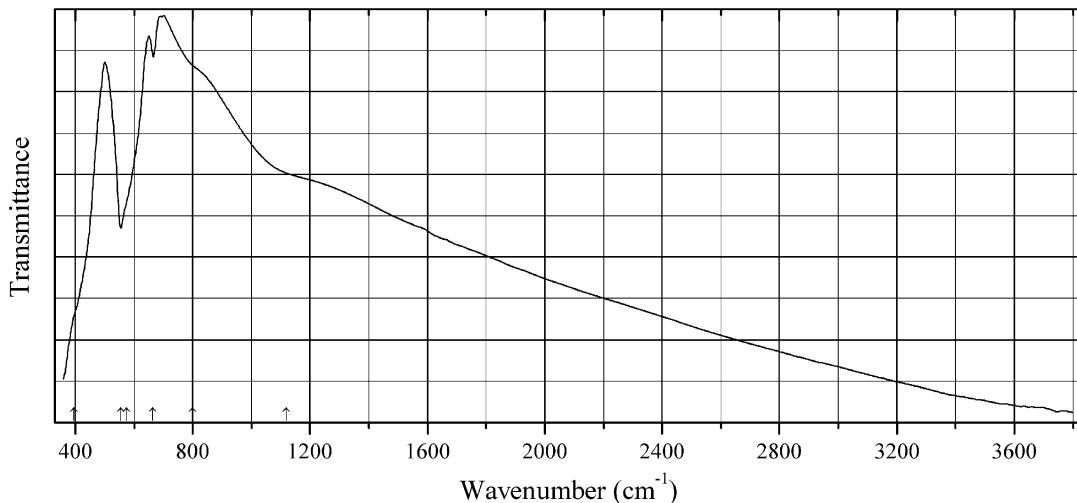
**Wavenumbers (IR, cm<sup>-1</sup>):** 3122s, 3017sh, 2407, 2241, 2041w, 1426sh, 1401s, 1227, 1156sh, 1079s, 1070s, 983sh, 708sh, 669s, 622, 599, 585, 441w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 3156, 1687, 1428, 1175, 1086, 977, 652, 622, 600, 475, 443, 363, 339, 323, 135, 96.

## 2.10 Chlorides and Hydroxychlorides

**Cl71 Schwartzembergite**  $\text{Pb}_5\text{H}_2(\text{IO}_2)\text{O}_4\text{Cl}_3$



**Origin:** San Francisco (Beatrix) mine, Caracoles, Sierra Gorda district, Antofagasta Region, Chile.

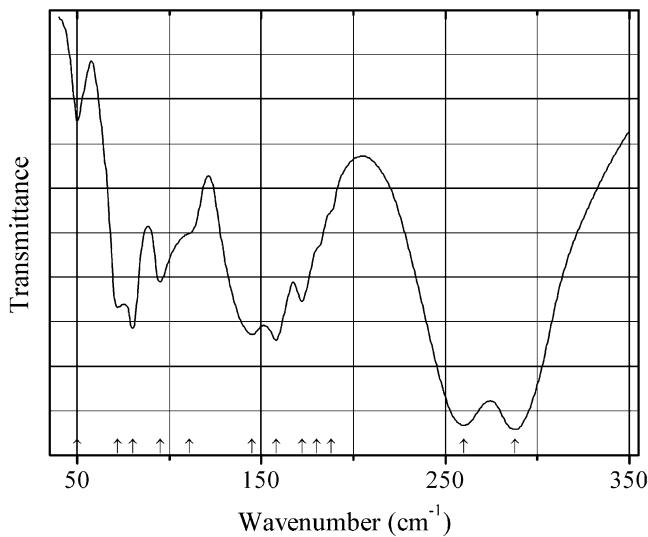
**Description:** Orange lenticular crystals from the association with paralaurionite. Investigated by I.V. Pekov. Characterized by powder X-ray diffraction data and electron microprobe analyses.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1120sh, 800sh, 665, 575sh, 555, 395sh.

**Note:** The spectrum was obtained by N.V. Chukanov. No bands corresponding to covalent O–H bonds are observed. The shoulder at  $1120 \text{ cm}^{-1}$  may correspond to the essentially ionic bond  $\text{Cl}^- \cdots \text{H}^+$ .

**Cl72 Cesium copper chloride**  $\text{CsCuCl}_3$



**Origin:** Synthetic.

**Description:** Crystallized by slow evaporation from hot concentrated aqueous solutions of CsCl and CuCl<sub>2</sub> in a 1:1 mole ratio. Hexagonal, space group  $P6_122$ ,  $a = 7.2157$  Å,  $c = 18.1777$  Å,  $Z = 6$ .

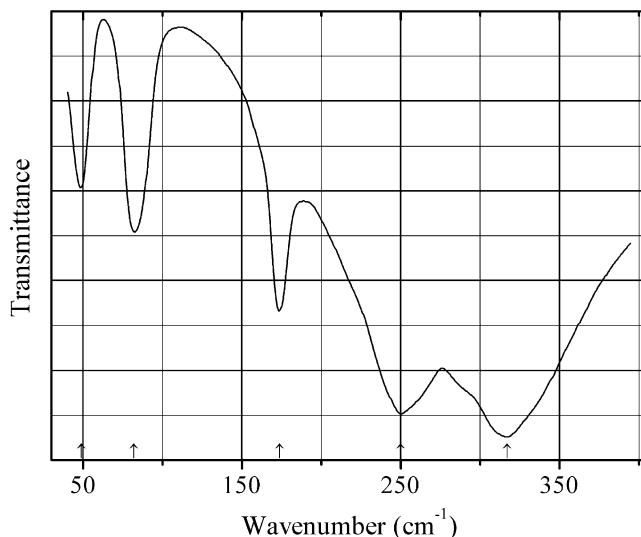
**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull between polyethylene plates. Transmission.

**Source:** McPherson and Chang (1973).

**Wavenumbers (cm<sup>-1</sup>):** 288s, 260s, 188sh, 180sh, 172, 158, 145, 111sh, 95, 80, 72, 50w.

**Note:** In the cited paper, IR spectra of other compounds CsMCl<sub>3</sub> ( $M = \text{Mg, V, Cr, Mn, Fe, Co, Ni}$ ) are given.

### CI73 Cesium magnesium chloride CsMgCl<sub>3</sub>



**Origin:** Synthetic.

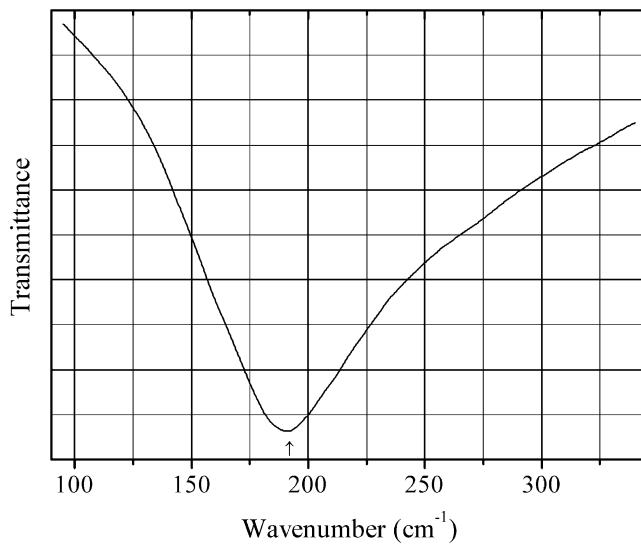
**Description:** Prepared by fusing equimolar mixture of CsCl and MgCl<sub>2</sub> in evacuated quartz ampoule. Hexagonal,  $a = 7.269$ ,  $c = 6.187$  Å,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull between polyethylene plates. Transmission.

**Source:** McPherson and Chang (1973).

**Wavenumbers (cm<sup>-1</sup>):** 317s, 250s, 174, 82, 49.

**Note:** In the cited paper, IR spectra of other compounds CsMCl<sub>3</sub> ( $M = \text{Cu, V, Cr, Mn, Fe, Co, Ni}$ ) are given.

**Cl74 Cesium sodium stibiochloride**  $\text{Cs}_2\text{NaSbCl}_6$ 

**Origin:** Synthetic.

**Description:** Prepared by heating a mixture of stoichiometric quantities of  $\text{SbCl}_3$ ,  $\text{CsCl}$ , and  $\text{NaCl}$  at 800 °C. Characterized by powder X-ray diffraction data. Cubic,  $a = 10.770$ .

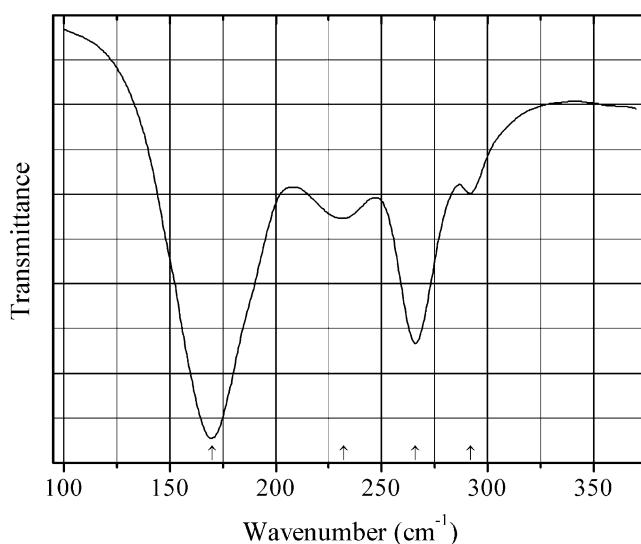
**Kind of sample preparation and/or method of registration of the spectrum:** Polyethylene disc. Absorption.

**Source:** Smit et al. (1990).

**Wavenumbers (IR, cm<sup>-1</sup>):** 192.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 314, 284, 228, 117, 68, 47, 34.

**Cl75 Cesium antimony chloride**  $\text{Cs}_3\text{Sb}_2\text{Cl}_9$ 

**Origin:** Synthetic.

**Description:** Trigonal  $\alpha$ -modification prepared by evaporating to dryness a hot aqueous HCl solution containing appropriate cations.

**Kind of sample preparation and/or method of registration of the spectrum:** Polyethylene disc. Transmission.

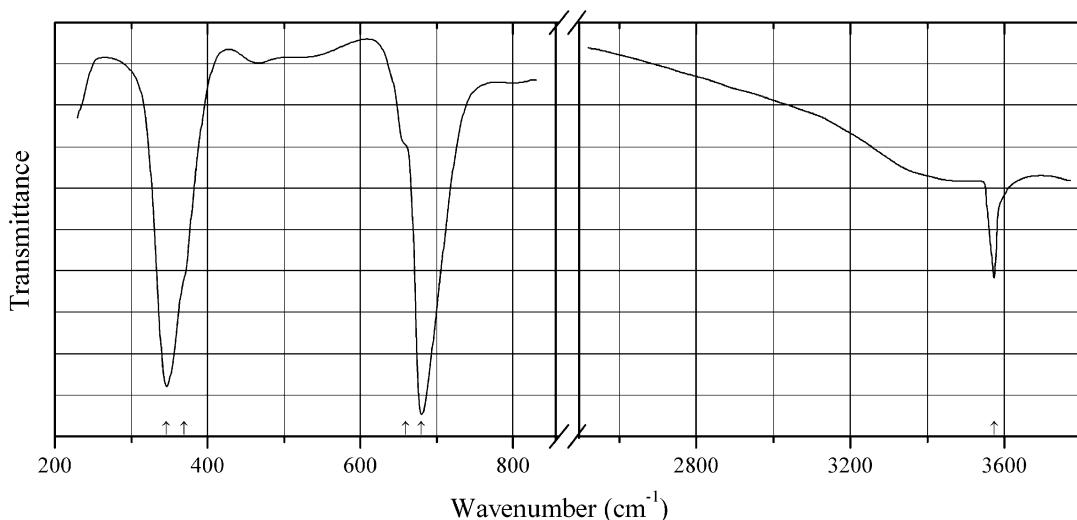
**Source:** Smit et al. (1990).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 292, 266s, 232, 170s.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 305s, 257s, 127, 102, 88, 55, 48, 42.

### Cl76 Calcium hydroxychloride $\text{Ca(OH)Cl}$



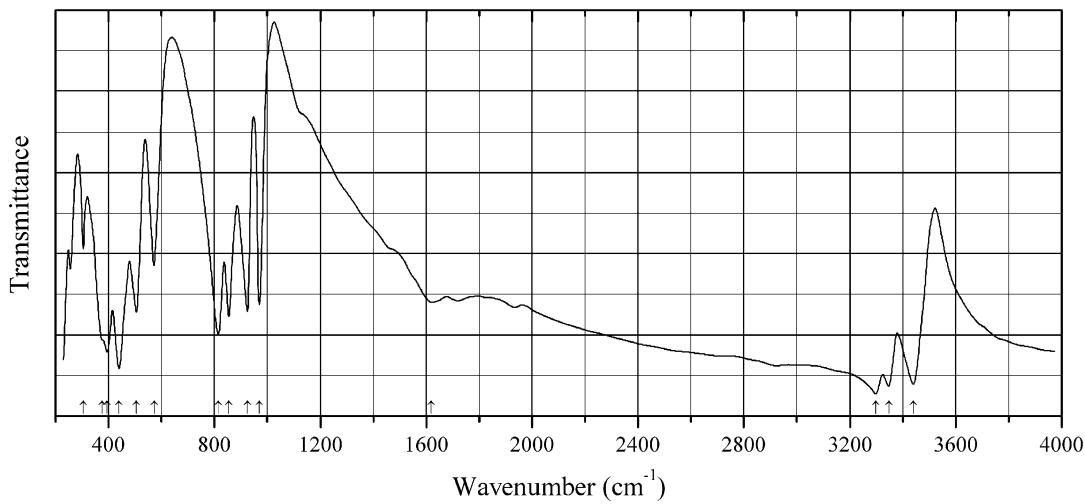
**Origin:** Synthetic.

**Description:** Prepared by heating stoichiometric amounts of anhydrous  $\text{CaCl}_2$  and  $\text{Ca(OH)}_2$  in a carbon glass crucible at 610 K for 3 weeks. Hexagonal, space group  $P6_3mc$ ,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc and Nujol mull. Transmission.

**Source:** Lutz et al. (1993).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3573, 680s, 659sh, 369sh, 346s.

**Cl77 Copper oxychloride hydrate**  $\text{Cu}_2\text{OCl}_2 \cdot 2\text{H}_2\text{O}$ .

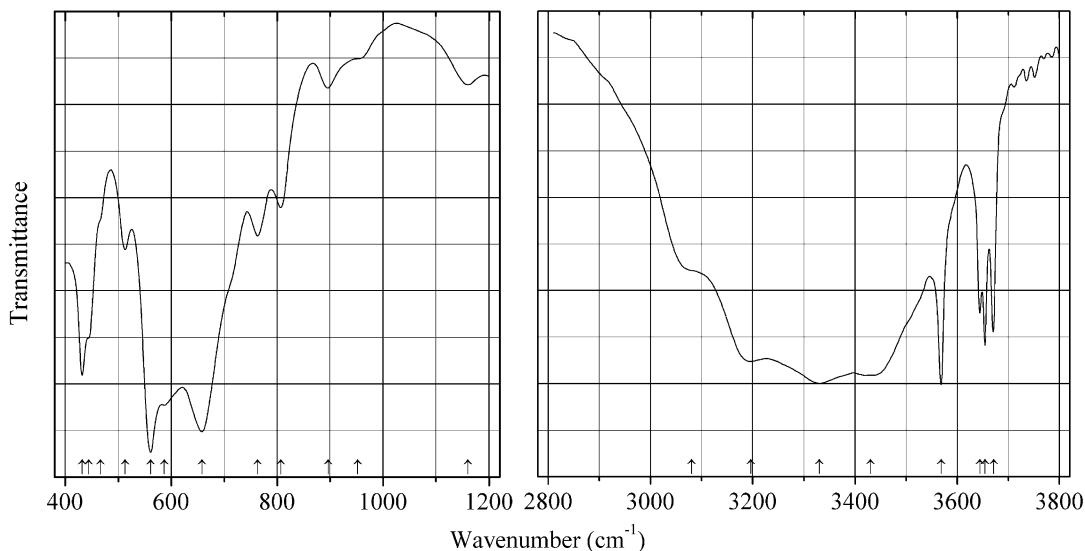
**Origin:** Synthetic.

**Description:** Precipitate prepared by mixing equal volumes of aqueous solutions of 0.1 M  $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$  and 0.5 M of urea. The mixture was heated to ~75 °C for 4–6 h. Characterized by the elemental analysis.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** El-Metwally and Al Thani (1989).

**Wavenumbers (cm<sup>-1</sup>):** 3440s, 3347s, 3298s, 1620, 970, 925, 855s, 815s, 572, 505, 440s, 395sh, 375, 305.

**Cl78 Magnesium oxychloride hydrate**  $\text{Mg}_3\text{Cl}_2(\text{OH})_4 \cdot 4\text{H}_2\text{O}$   $\text{Mg}_3\text{Cl}_2(\text{OH})_4 \cdot 4\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Monoclinic, space group  $C2/m$ ,  $a = 15.1263(3)$ ,  $b = 3.1707(1)$ ,  $c = 10.5236(2)$  Å,  $\beta = 101.546(2)$ . The crystal structure contains strongly distorted  $MgO_6$  octahedra.

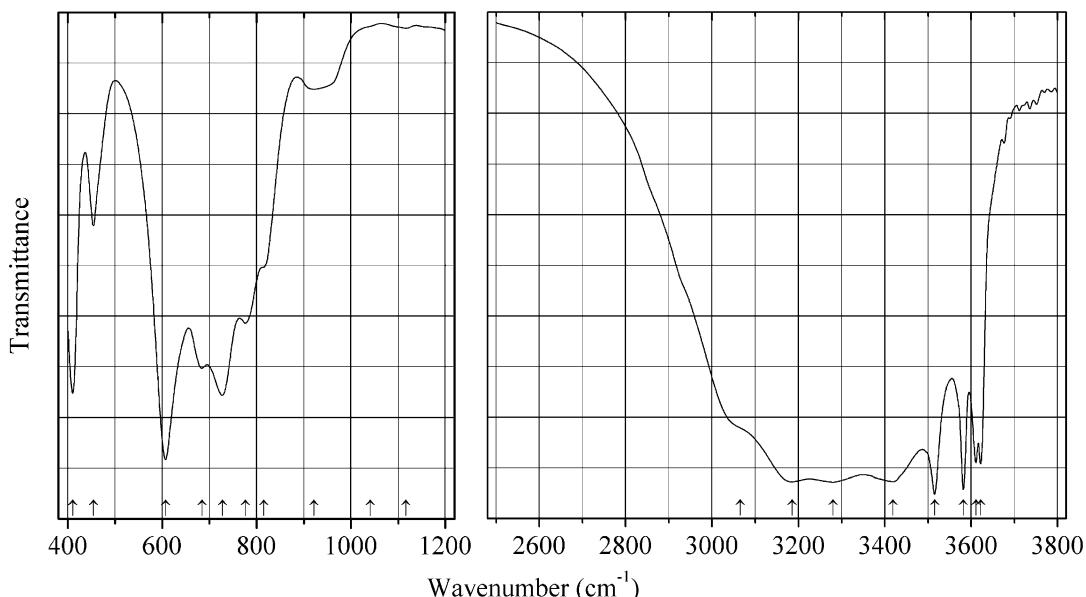
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Bette et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 3671, 3654, 3644, 3568s, 3430s, 3330s, 3196, 3080sh, 1160w, 952sh, 896w, 807, 763, 658s, 587, 561s, 513, 466sh, 444sh, 432.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### Cl79 Nickel oxychloride hydrate $Ni_3Cl_{2.1}(OH)_{3.9} \cdot 4H_2O$ $Ni_3Cl_{2.1}(OH)_{3.9} \cdot 4H_2O$



**Origin:** Synthetic.

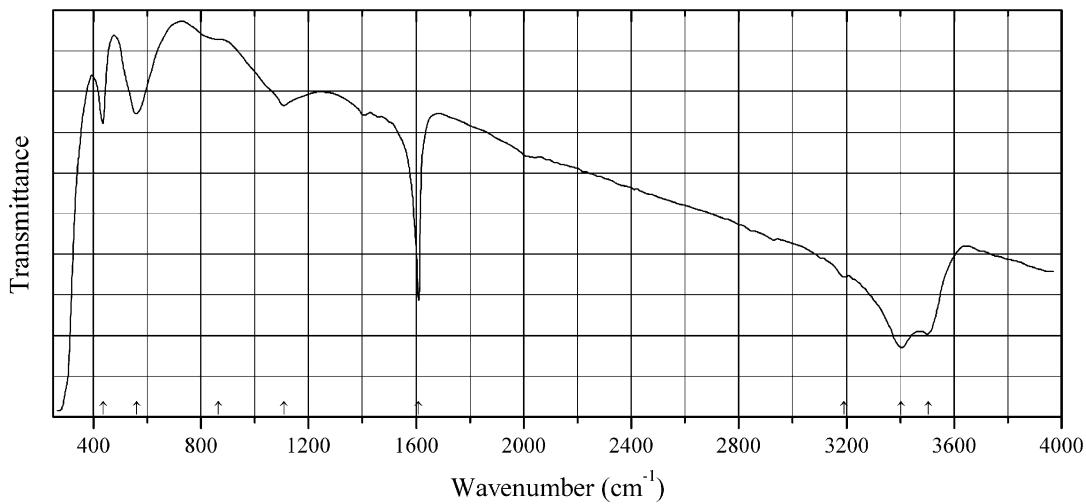
**Description:** Obtained in the reaction between NaOH and nickel chloride solution at 40 °C for 3 months. Characterized by powder X-ray diffraction data and chemical analyses. The crystal structure is solved. Monoclinic, space group  $C2/m$ ,  $a = 14.9575(4)$ ,  $b = 3.1413(1)$ ,  $c = 10.4818(5)$  Å,  $\beta = 101.482(1)$ °,  $V = 482.49(3)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 2.67$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Bette et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 3622, 3611, 3582s, 3515s, 3419s, 3280s, 3185s, 3065sh, 1116w, 1041sh, 921w, 815sh, 776, 727, 684, 607s, 454, 410.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Cl80 Potassium mercury chloride hydrate  $K_2HgCl_4 \cdot H_2O$** 

**Origin:** Synthetic.

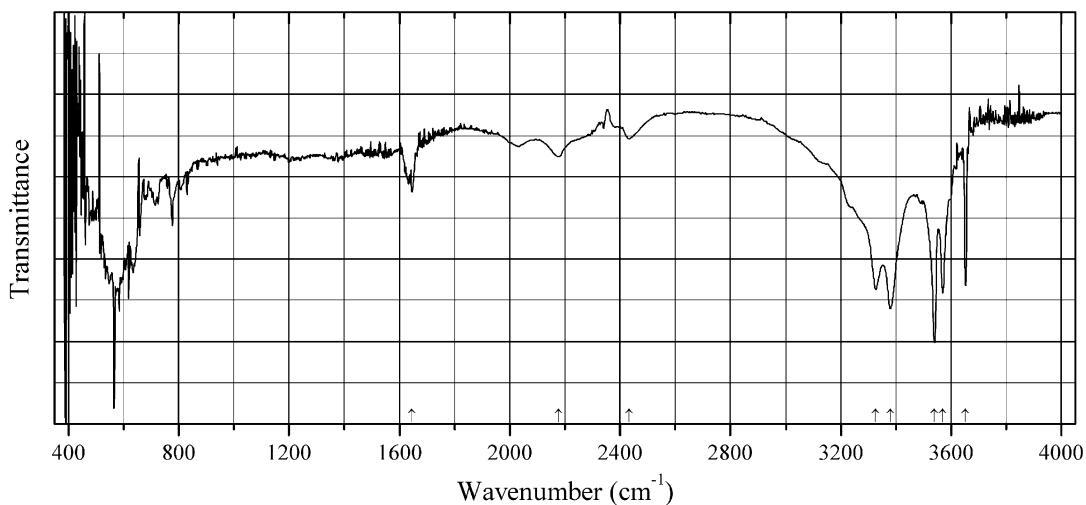
**Description:** Characterized by powder X-ray diffraction data. Orthorhombic, space group *Pbam*,  $a = 5.258$ ,  $b = 11.662$ ,  $c = 8.925$  Å,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KCl disc. Transmission.

**Source:** Falk and Knop (1977).

**Wavenumbers (cm<sup>-1</sup>):** 3505, 3404s, 3191w, 1610s, 1108, 865sh, 560, 436.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Cl81 Yttrium hydroxychloride hydrate  $Y_2(OH)_5Cl \cdot 1.5H_2O$** 

**Origin:** Synthetic.

**Description:** Prepared hydrothermally from  $\text{YCl}_3$  in the presence of  $\text{NaOH}$  and  $\text{NaCl}$  at  $150\text{ }^\circ\text{C}$  for 12 h. Characterized by powder X-ray diffraction data. Orthorhombic. Space group  $Pca2_1$  (?).

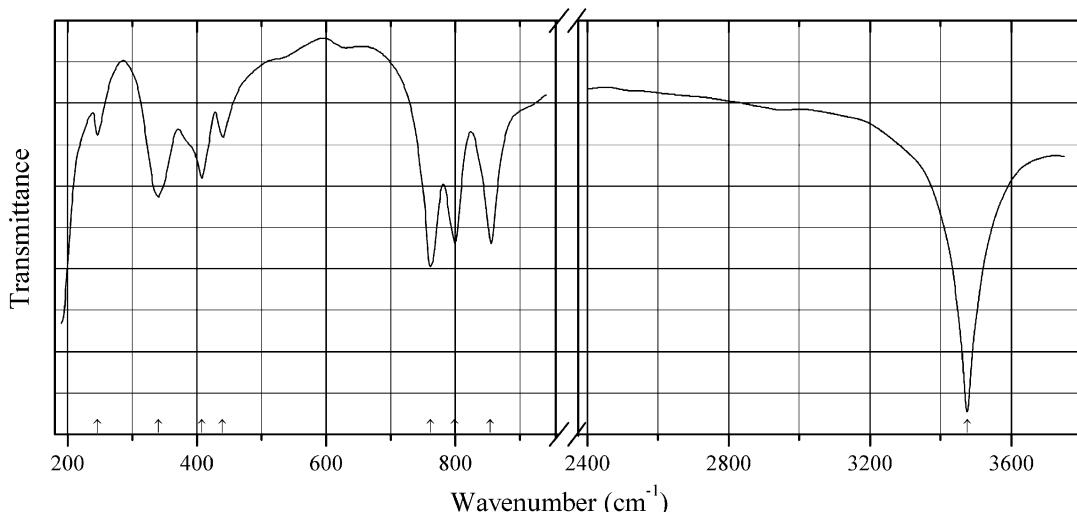
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Poudret et al. (2008).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3652s, 3570s, 3539s, 3380s, 3327s, 2433, 2177, 1644.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### Cl82 Zinc hydroxychloride $\text{Zn(OH)Cl}$



**Origin:** Synthetic.

**Description:** Prepared by heating of an aqueous solution of  $\text{ZnCl}_2$  at  $80\text{ }^\circ\text{C}$ , in the presence of  $\text{ZnO}$ . Orthorhombic, space group  $Pcab$ ,  $a \approx 5.86$ ,  $b \approx 6.58$ ,  $c \approx 11.33\text{ \AA}$ ,  $Z = 8$ .

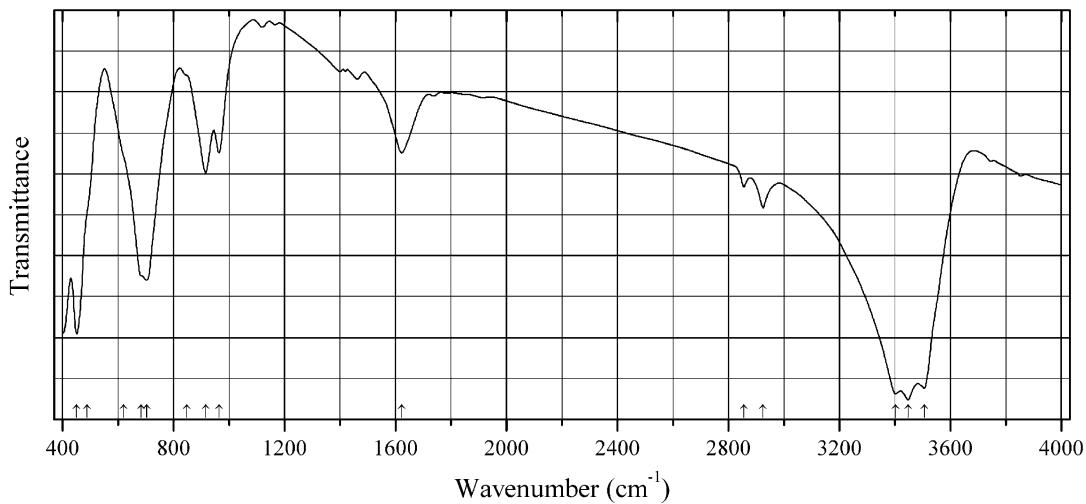
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc and Nujol mull. Transmission.

**Source:** Lutz et al. (1993).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3476s, 853s, 798s, 761s, 439, 407, 340, 246.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 3456s, 850w, 837w, 789w, 756w, 455w, 386, 349w, 293w, 216, 188s, 171, 114, 87, 57.

**Cl83 Centennialite**  $\text{CaCu}_3\text{Cl}_2(\text{OH})_6 \cdot n\text{H}_2\text{O}$  ( $n \sim 0.7$ )

**Origin:** Synthetic.

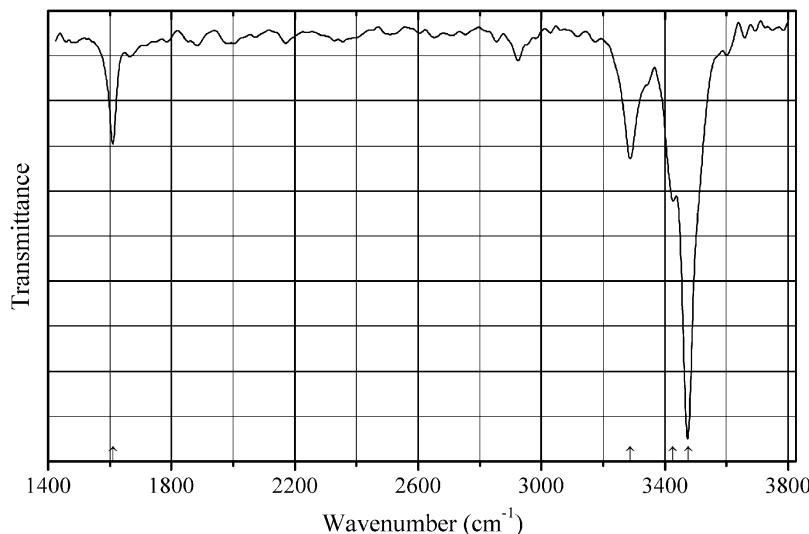
**Description:** Synthesized from  $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ ,  $\text{CaCl}_2$ ,  $\text{LiCl} \cdot \text{H}_2\text{O}$ , and  $\text{LiOH} \cdot \text{H}_2\text{O}$  through a solid-state reaction method. Characterized by electron microprobe analyses. The crystal structure is solved. Trigonal, space group  $P-3m1$ ,  $a = 6.6475(9)$ ,  $c = 5.7600(12)$  Å,  $V = 220.43(8)$   $\text{\AA}^3$ ,  $Z = 1$ .  $D_{\text{calc}} = 3.108$  g/cm $^3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Sun et al. (2015).

**Wavenumbers (cm $^{-1}$ ):** 3505s, 3447s, 3402s, (2925), (2855), 1623, 964, 916, 848sh, 703s, 685sh, 621sh, 490sh, 452s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. Weak bands in the range from 2800 to 3000  $\text{cm}^{-1}$  correspond to the admixture of an organic substance.

**Cl84 Comancheite**  $\text{Hg}^{2+}_{55}\text{N}^{3-}_{24}(\text{Cl},\text{Br})_{34}(\text{OH},\text{NH}_2)_4$ 

**Origin:** Mariposa mine, Terlingua district, Brewster Co., Texas, USA (type locality).

**Description:** Orange aggregate on calcite. Specimen No. 26686 from the collections of the Natural History Museum of Los Angeles Co. Characterized by electron microprobe analyses. The crystal structure is solved. Orthorhombic, space group  $Pnnm$ ,  $a = 18.414(5)$ ,  $b = 21.328(6)$ ,  $c = 6.6976$  (19) Å,  $V = 2630(2)$  Å<sup>3</sup>,  $Z = 1$ .  $D_{\text{calc}} = 8.25$  g/cm<sup>3</sup>. The crystal-chemical formula is  $\text{Hg}_{55}(\text{Cl}_{24.5}\text{Br}_{9.5})\text{N}_{24}(\text{OH},\text{O},\text{NH}_2)_4$ . The N<sup>3-</sup> anion shows a strong preference for tetrahedral coordination by Hg<sup>2+</sup>, which results in a strongly bonded three-dimensional Hg-N framework.

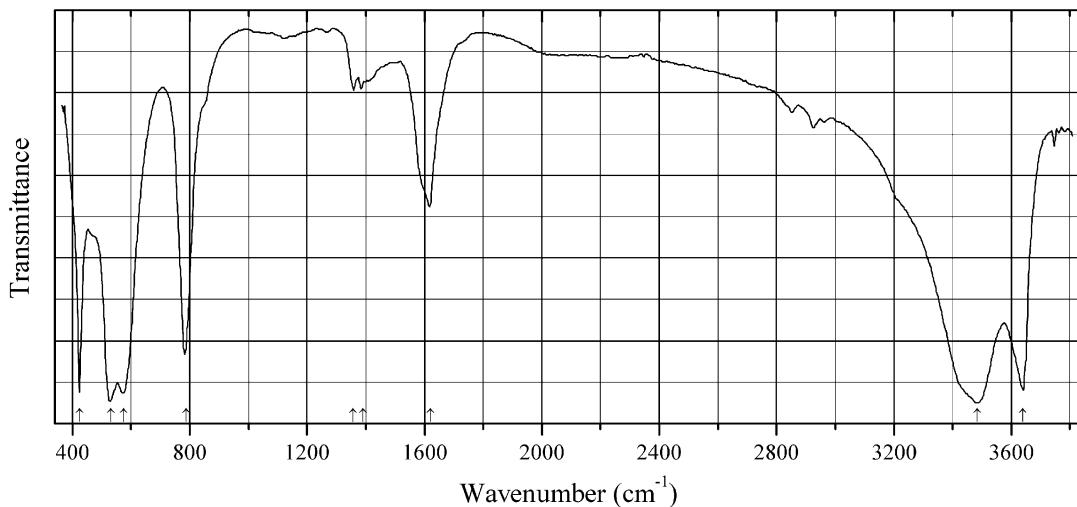
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission of a single crystal.

**Source:** Cooper et al. (2013a).

**Wavenumbers (cm<sup>-1</sup>):** 3475s, 3426, 3288, 1610.

**Note:** N was not determined chemically. Despite NH<sub>2</sub> group is considered as a subordinate component, the intensity of the band of H–N–H bending vibrations at 1610 cm<sup>-1</sup> is rather high. This band could be assigned to H–O–H bending vibrations. In the cited paper, Raman spectrum is given.

### CI85 Hydrocalumite $\text{Ca}_2\text{Al}(\text{OH})_6(\text{Cl},\text{CO}_3,\text{OH})_{1-x}\cdot 2\text{H}_2\text{O}$



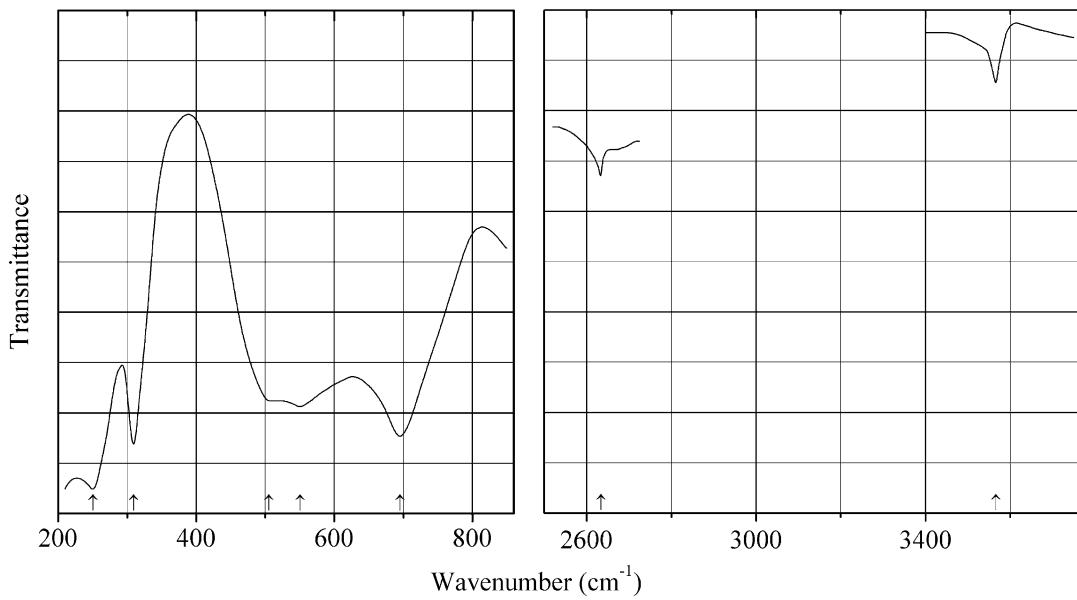
**Origin:** Synthetic.

**Description:** Obtained by adding tricalcium aluminate to an aqueous solution of CaCl<sub>2</sub> and keeping the mixture at 320 K for 3 days. Characterized by powder X-ray diffraction data, as well as chemical, TG, and DSC analyses. The formula of the sample obtained is  $\text{Ca}_2\text{Al}(\text{OH})_6\text{Cl}_{0.90}(\text{CO}_3)_{0.05}\cdot 2\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Grishchenko et al. (2013).

**Wavenumbers (cm<sup>-1</sup>):** 3639s, 3484s, 1620, 1390w, 1356w, 787, 575s, 532s, 424s.

**Cl86 Laurionite Ba-analogue**  $\text{Ba}(\text{OH})\text{Cl}$ 

**Origin:** Synthetic.

**Description:** Characterized by powder X-ray diffraction data and thermoanalytical methods. Isostructural with laurionite.

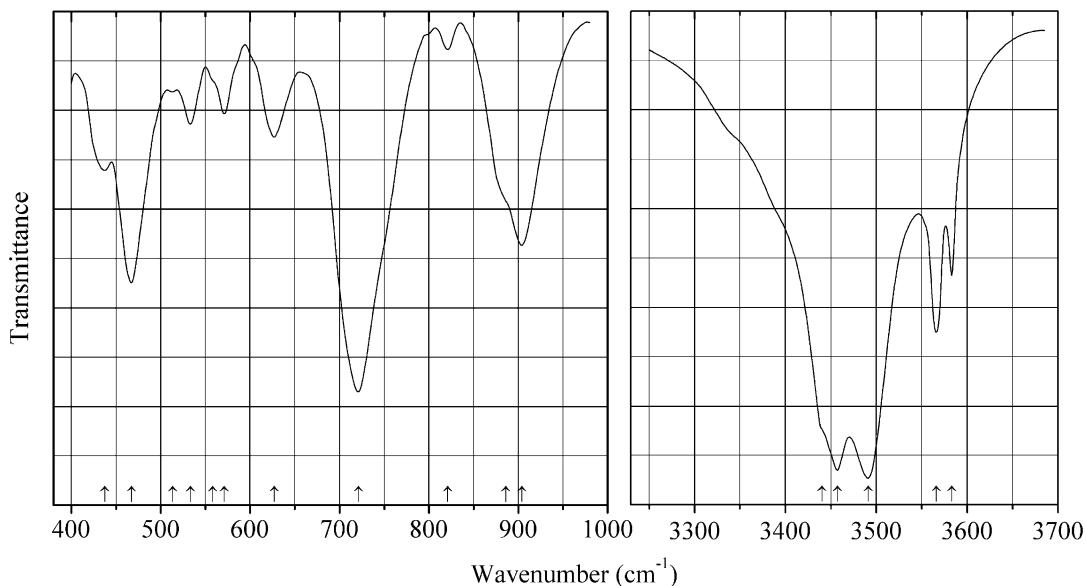
**Kind of sample preparation and/or method of registration of the spectrum:** KBr or CsI disc, and Nujol or poly(chlortrifluorethen) mull. Transmission.

**Source:** Lutz et al. (1995).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3566, 695s, 550, 505sh, 309s, 250s.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 3594s, 480s, 265s, 249, 195, 142, 130sh, 93w, 78, 64.

**Cl87 Simonkolleite**  $\text{Zn}_5(\text{OH})_8\text{Cl}_2 \cdot \text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Prepared by precipitation method at about 80–90 °C. Characterized by DTA and powder X-ray diffraction data.

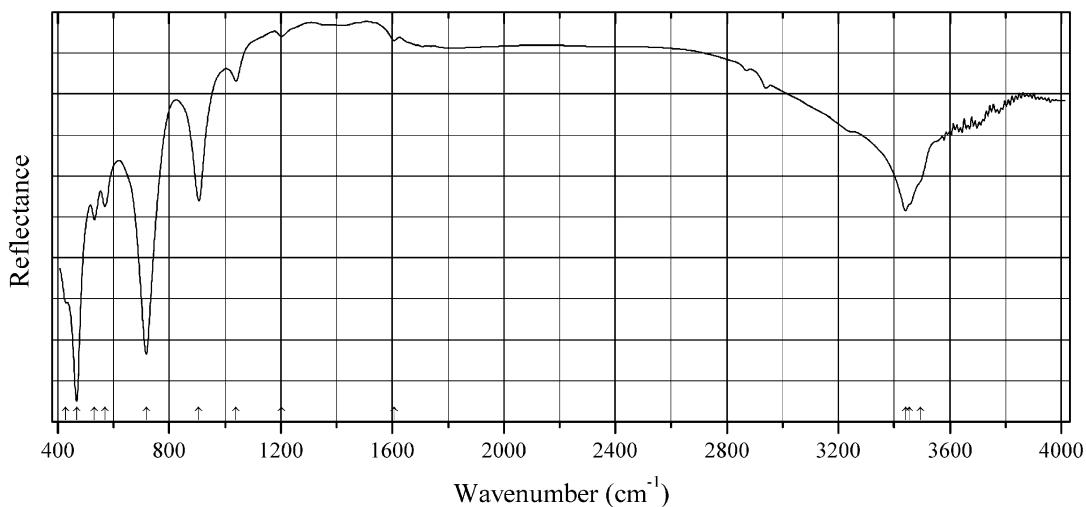
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Stoilova and Vassileva (2002).

**Wavenumbers (cm<sup>-1</sup>):** 3583, 3566, 3491s, 3457s, 3440sh, 904, 886sh, 821w, 721s, 627, 571, 558sh, 533, 513w, 467, 437.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### Cl88 Simonkolleite Zn<sub>5</sub>(OH)<sub>8</sub>Cl<sub>2</sub>·H<sub>2</sub>O



**Origin:** Synthetic.

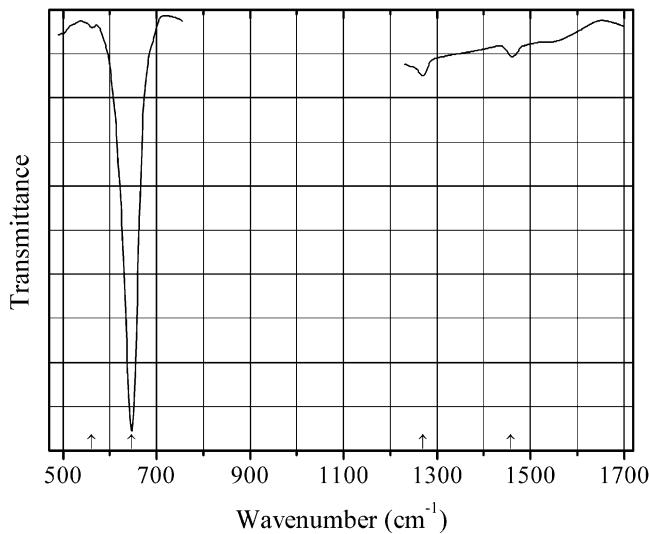
**Description:** Micro-platelets prepared hydrothermally from Zn(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O and NaCl in the presence of hexamethylenetetramine, at 85 °C. Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection.

**Source:** Sithole et al. (2012).

**Wavenumbers (cm<sup>-1</sup>):** 3495sh, 3455sh, 3441, 1607w, 1202w, 1040w, 906, 717s, 569, 532, 468s, 427sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Cl89 Terlinguacreekite  $\text{Hg}_3\text{O}_2\text{Cl}_2$** 

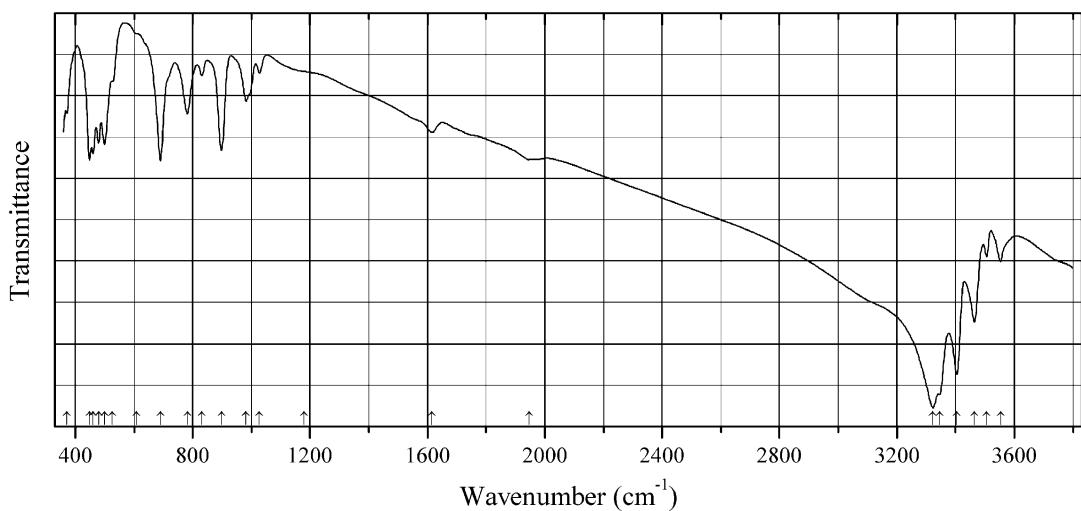
**Origin:** McDermitt mine, Opalite district, Humboldt Co., Nevada, USA.

**Description:** Orange powdery from the association with quartz and kleinite. Investigated by A.V. Kasatkin. The empirical formula is (electron microprobe):  $\text{Hg}_{3.00}\text{O}_{2.2}\text{Cl}_{1.6}$ . The observed lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %)] are: 12.8 (2), 6.42 (8), 5.41 (5), 5.27 (6), 4.64 (3), 4.26 (16), 4.06 (6), 3.75 (5), 3.45 (10), 3.34 (63), 3.25 (14), 3.21 (100), 3.02 (12), 2.97 (10).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 647, 561w.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Cl90 Cumengeite  $\text{Pb}_{21}\text{Cu}_{20}\text{Cl}_{42}(\text{OH})_{40} \cdot 6\text{H}_2\text{O}$** 

**Origin:** Boleo district, Santa Rosalía, Baja California, Mexico (type locality).

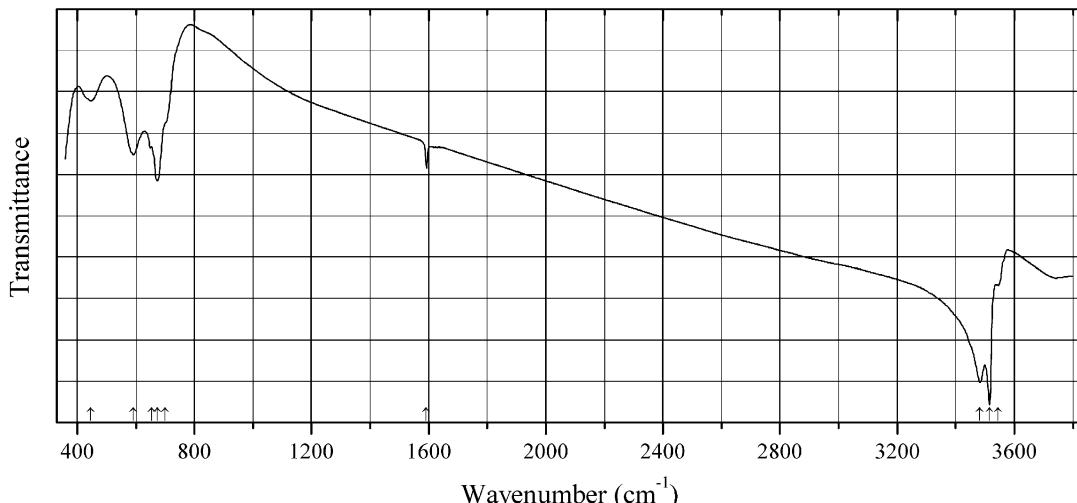
**Description:** Blue crystals.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3553, 3506w, 3464, 3405s, 3445s, 3322s, 1948w, 1616w, 1028w, 982, 898s, 831w, 782, 690s, 609w, 527, 499, 479, 461s, 448s, (372).

**Note:** The spectrum was obtained by N.V. Chukanov.

### Cl91 Fiedlerite-1A Pb<sub>3</sub>Cl<sub>4</sub>F(OH)·H<sub>2</sub>O



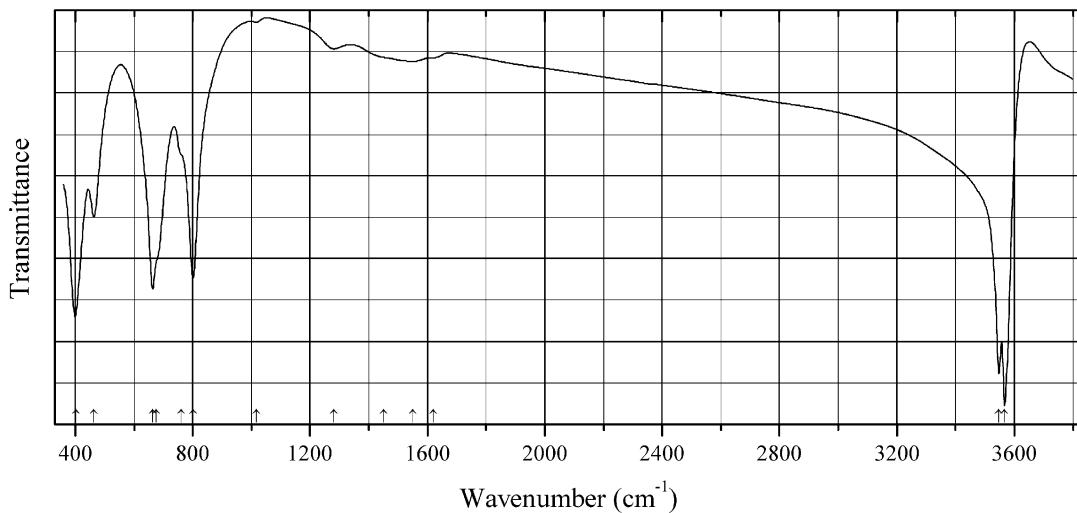
**Origin:** Pacha Limani (Passa Limani), Lavrion mining district, Attiki Prefecture, Greece.

**Description:** Colorless platy crystals from the association with phosgenite in ancient metallurgical slag. The crystal structure is solved. Triclinic, space group *P*-1, *a* = 8.5741(7), *b* = 8.0480(5), *c* = 7.2695(4) Å,  $\alpha$  = 90.087(5),  $\beta$  = 102.126(6),  $\gamma$  = 103.424(6) $^\circ$ , *V* = 476.37(6) Å<sup>3</sup>, *Z* = 2. The empirical formula is (electron microprobe): Pb<sub>3.00</sub>Cl<sub>3.98</sub>F<sub>0.96</sub>(OH)<sub>1.06</sub>·H<sub>2</sub>O.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3545w, 3515s, 3482, 1592, 700sh, 673s, 654, 592, 447.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Cl92 Kuliginite  $\text{Fe}_3\text{Mg}(\text{OH})_6\text{Cl}_2$** 

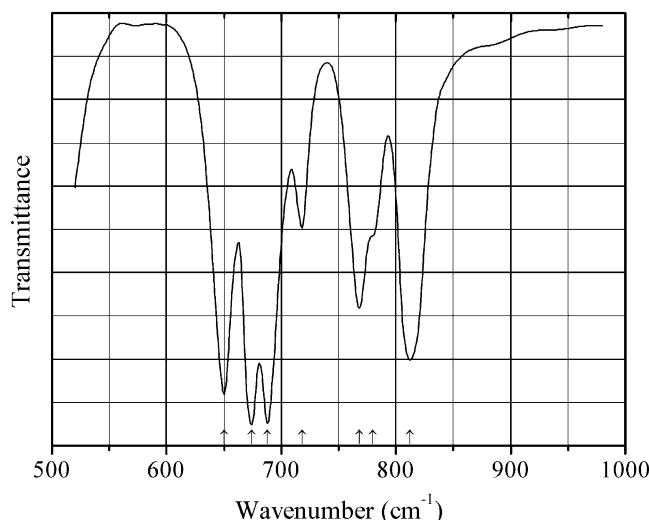
**Origin:** Udachnaya kimberlite pipe, Yakutia, Russia (type locality).

**Description:** Green crystals from the association with iowaite, gypsum, calcite, halite, baryte, celestine, etc. Holotype sample. The crystal structure is solved. Trigonal, space group  $R\bar{3}$ ,  $a = 6.9512(1)$ ,  $c = 14.5713(3)$  Å,  $V = 609.74(2)$  Å $^3$ ,  $Z = 3$ .  $D_{\text{meas}} = 3.1(1)$  g/cm $^3$ ,  $D_{\text{calc}} = 3.01$  g/cm $^3$ . Optically biaxial (+),  $\alpha = 1.709(3)$ ,  $\beta = 1.709(3)$ ,  $\gamma = 1.718$ ,  $2V = 10(5)^\circ$ . The empirical formula is  $(\text{Fe}_{2.99}\text{Mn}_{0.01})(\text{Mg}_{0.90}\text{Mn}_{0.10})(\text{OH}_{5.94}\text{F}_{0.03}\text{Cl}_{0.03})\text{Cl}_2$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 5.569 (54) (01–1), 2.949 (16) (021), 2.831 (35) (113), 2.324 (100) (024), 2.098 (18) (02–5), 1.856 (13) (033), 1.739 (36) (220).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm $^{-1}$ ):** 3567s, 3548s, 1620w, 1550 (broad), 1450sh, 1278w, 1018w, 801s, 760sh, 675sh, 663s, 464, 402s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Cl93 Magnesium hydroxychlorite atacamite-type  $\text{Mg}_2(\text{OH})_3\text{Cl}$** 

**Origin:** Synthetic.

**Description:** Prepared hydrothermally. Characterized by thermal and powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

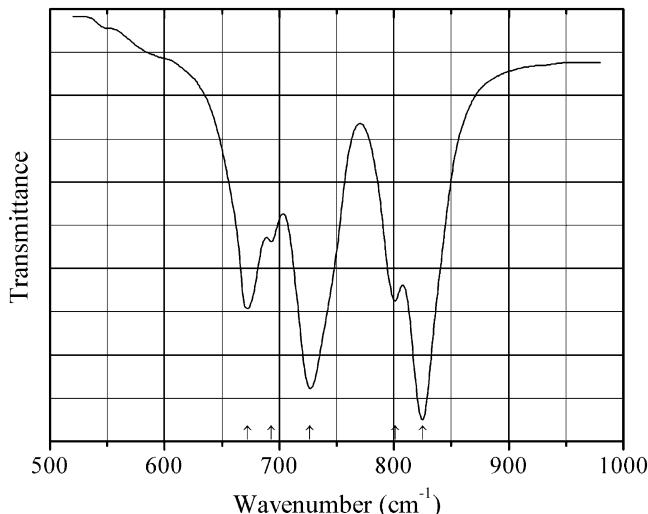
**Source:** Bette et al. (2015).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 812s, 780sh, 768, 718, 688s, 674s, 650s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 804, 786, 750s, 712, 635.

#### Cl94 Nickel hydroxychlorite atacamite-type $\text{Ni}_2(\text{OH})_3\text{Cl}$



**Origin:** Synthetic.

**Description:** Prepared hydrothermally. Characterized by thermal and powder X-ray diffraction data.

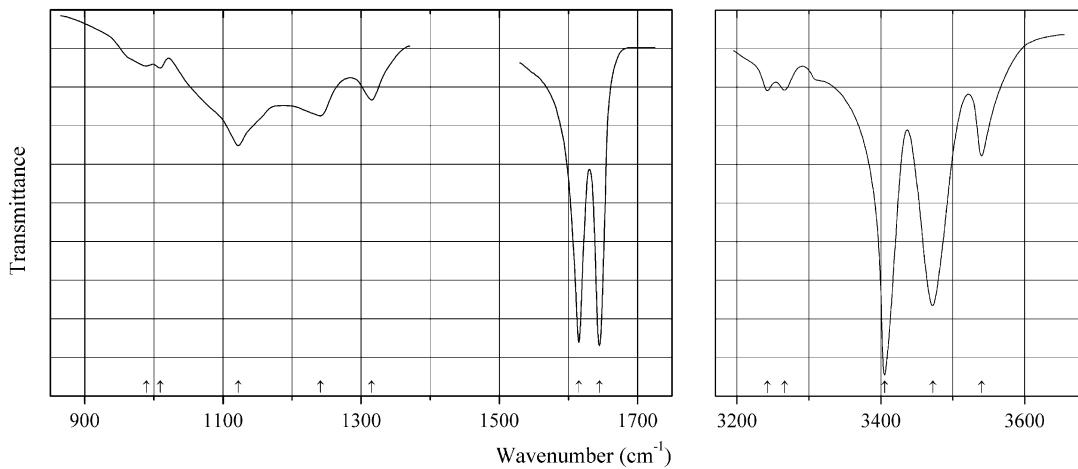
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Bette et al. (2015).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 825s, 801, 727s, 693, 672.

**Note:** The band positions denoted by Bette et al. (2015) as  $627 \text{ cm}^{-1}$  were determined by us at  $672 \text{ cm}^{-1}$ . In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 823, 799, 757s, 694, 675, 624.

**Cl95 Hydrohalite  $\text{NaCl} \cdot 2\text{H}_2\text{O}$** 

**Origin:** Synthetic.

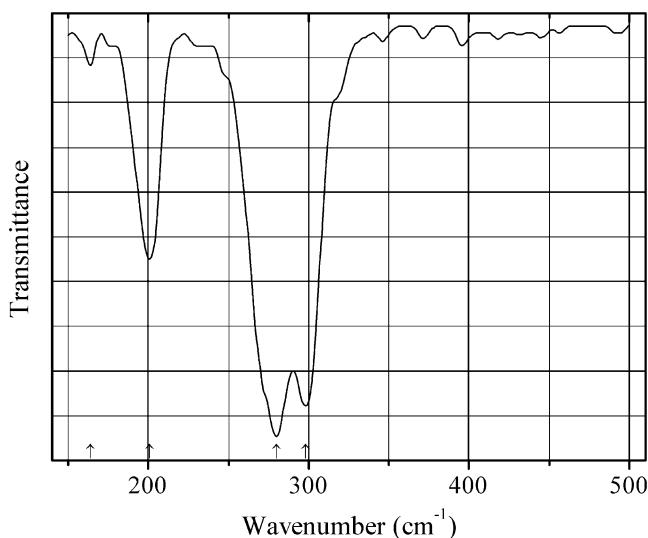
**Description:** A film obtained by slow condensation of  $\text{H}_2\text{O}$  vapor is on a cold  $\text{NaCl}$  plate with subsequent heating up to  $-20^\circ\text{C}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission of a thin film.

**Source:** Schiffer and Hornig (1961).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3540, 3472s, 3405s, 3266w, 3242w, 1615s, 1645s, 1315, 1241, 1122, 1009w, 989w.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**Cl96 Sanguite  $\text{KCuCl}_3$** 

**Origin:** Synthetic.

**Kind of sample preparation and/or method of registration of the spectrum:** Polyethylene disc.  
Absorption.

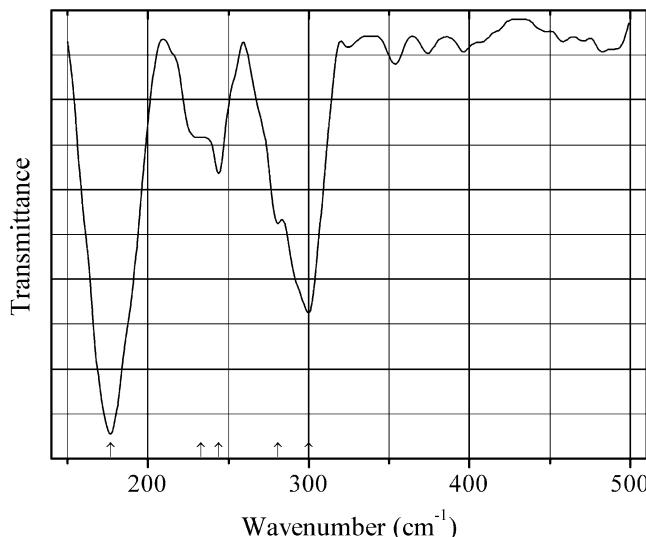
**Source:** Stepakova et al. (2008).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 284s, 208, 205sh, 129w, 94w [indicated by Stepakova et al. (2008)];  
298s, 280s, 201s, 164w (determined by us based on spectral curve analysis of the published spectrum).

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 274s, 236sh, 146w, 130w, 97w [indicated by Stepakova et al. (2008)]; 310sh, 274s, 205w (determined by us based on spectral curve analysis of the published spectrum).

#### Cl97 Tolbachite $\text{CuCl}_2$



**Origin:** Synthetic.

**Description:** Obtained by heating copper chloride hydrate to 150 °C.

**Kind of sample preparation and/or method of registration of the spectrum:** Polyethylene disc.  
Absorption.

**Source:** Stepakova et al. (2008).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 284s, 189s, 100w, 92w [indicated by Stepakova et al. (2008)]; 300s,  
281, 244, 233sh, 177s (determined by us based on spectral curve analysis of the published spectrum).

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 287s, 276sh, 166s, 119w, 107w [indicated by Stepakova et al. (2008)]; 287s, 276sh (?), 171s (determined by us based on spectral curve analysis of the published spectrum).

**Cl98 Telluroperite**  $\text{Pb}(\text{Te}_{0.5}\text{Pb}_{0.5})\text{O}_2\text{Cl}$ 

**Origin:** Synthetic.

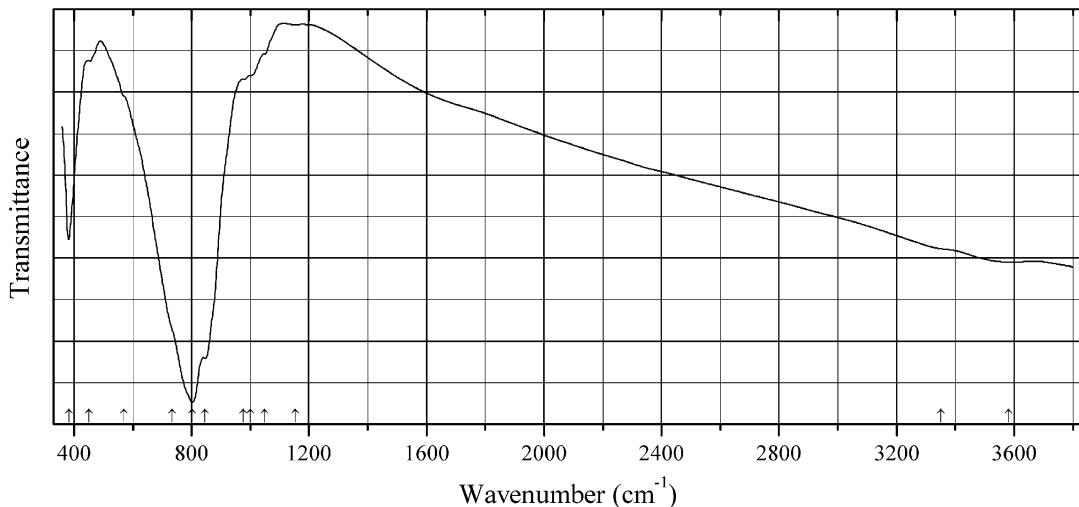
**Description:** Crystals grown by heating a mixture of  $\text{Pb}_3\text{O}_2\text{Cl}_2$  and  $\text{TeO}_2$  at 550 °C for 1 day. The crystal structure is solved. Orthorhombic, space group  $Bmm$ ,  $a = 5.576(1)$ ,  $b = 5.559(1)$ ,  $c = 12.4929(6)$  Å,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Porter and Halasyamani (2003).

**Wavenumbers (cm<sup>-1</sup>):** 661, 628, 509, 439.

## 2.11 Vanadates and Vanadium Oxides

**V116 Schäferite**  $(\text{NaCa}_2)\text{Mg}_2(\text{VO}_4)_3$ 

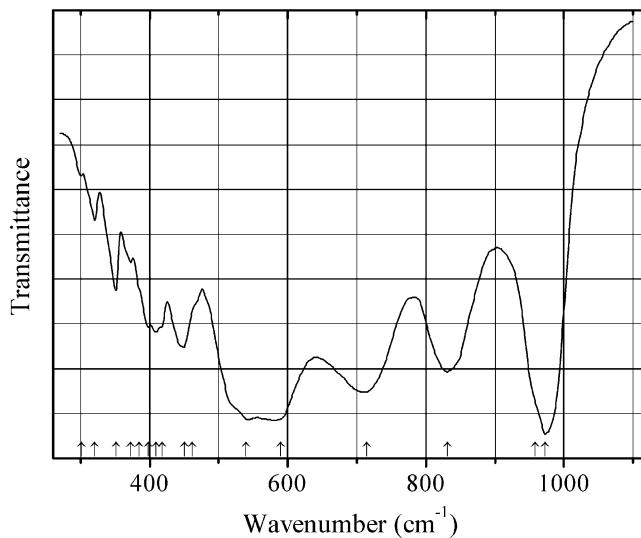
**Origin:** Slag dump near the Kamariza mine, Lavrion, mining district, Attikí (Attika, Attica) Prefecture, Greece.

**Description:** Brown crystals from the association with minerals of the forsterite–liebenbergite series, trevorite, albite, nosean, haüyne, bannermanite, a Ni-Mg-analogue of lyonsite, etc. The crystal structure is solved. Cubic, space group  $Ia3d$ ,  $a = 12.388(3)$  Å,  $V = 1901.1(14)$  Å<sup>3</sup>,  $Z = 8$ . The crystal-chemical formula is  $(\text{Na}_{1.5}\text{Ca}_{1.5})(\text{Mg}_{1.1}\text{Fe}_{0.5}\text{Ni}_{0.4})(\text{V}_{2.8}\text{P}_{0.2})(\text{O},\text{OH})_{12}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3580w, 3350w, 1152w, 1049w, 1000w, 977w, 846s, 803s, 735sh, 570sh, 451w, 383s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**V117 Aluminium decavanadate hydrate**  $\text{Al}_2\text{V}_{10}\text{O}_{28} \cdot 22\text{H}_2\text{O}$ 

**Origin:** Synthetic.

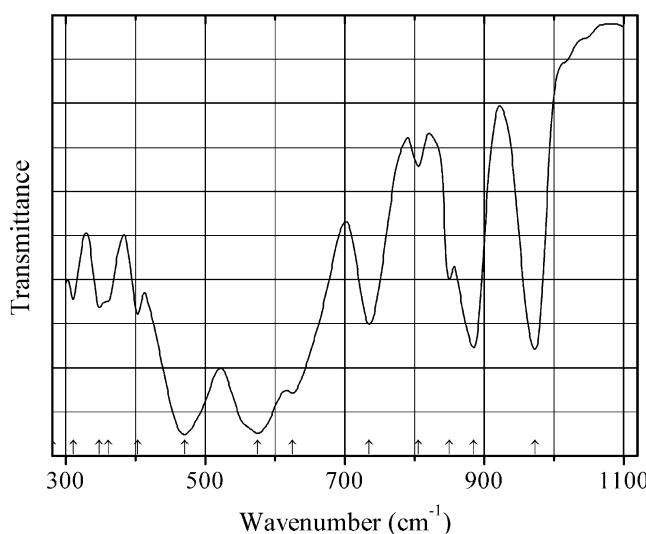
**Description:** Synthesized in the reaction between decavanadic acid and basic aluminium acetate.

Confirmed by chemical analysis, TG, and powder X-ray diffraction data. Orthorhombic, space group  $\text{Acmm}$ ,  $a = 10.618(5)$ ,  $b = 18.296(8)$ ,  $c = 21.560(10)$  Å,  $Z = 2$ .  $D_{\text{meas}} = 2.35$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 2.23$  g/cm<sup>3</sup>. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 10.83 (52) (002), 10.62 (100) (100), 6.94 (52) (120), 5.81 (42) (122), 2.914 (35) (244).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Rigotti et al. (1983).

**Wavenumbers (cm<sup>-1</sup>):** 3440, 2930, 1630, 973s, 958sh, 831s, 715s, 590s, 540s, 462sh, 450, 418sh, 409, 398, 385sh, 373w, 351, 320w, 301w.

**V118 Ammonium uranyl vanadate hydrate**  $(\text{NH}_4)(\text{UO}_2)(\text{VO}_4) \cdot 2.5\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Synthesized from  $(\text{NH}_4)(\text{VO}_3)$  and  $(\text{UO}_2)(\text{NO}_3)_2$  with subsequent heating of the precipitate at  $60^\circ\text{C}$  for 3 h. Orthorhombic,  $a = 13.29(1)$ ,  $b = 16.21(2)$ ,  $c = 12.05(1)$  Å. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %)] are: 6.78 (90), 4.23 (40), 3.51 (40), 3.15 (100), 2.15 (20).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

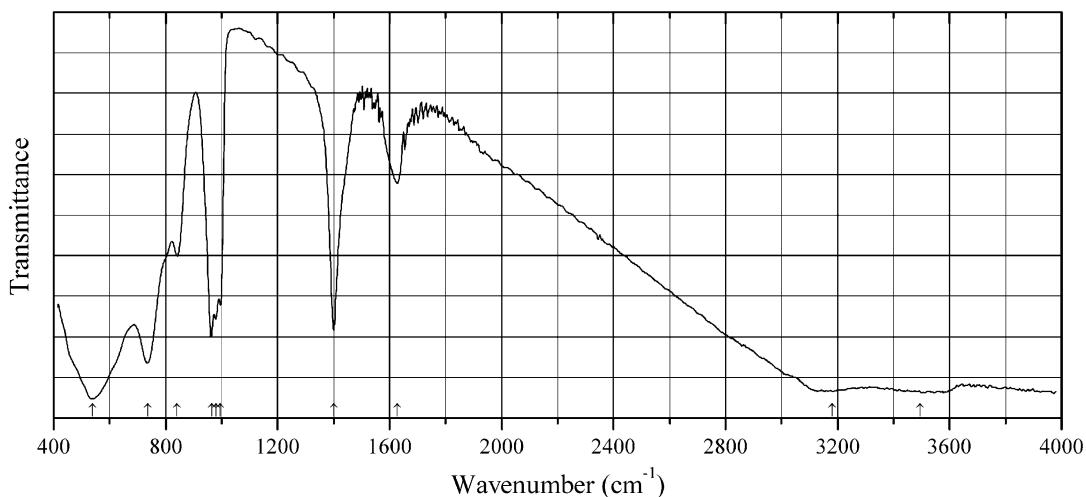
**Source:** Botto and Baran (1976).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 973, 885, 850, 805w, 735, 625s, 575s, 470s, 403, 360sh, 348, 310, 280.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 975, 822, 738, 645, 580, 540, 482, 410, 375, 360sh, 255, 230.

### V119 Ammonium vanadyl compound $(\text{NH}_4)_{0.5}\text{V}_2\text{O}_5 \cdot n\text{H}_2\text{O}$ $(\text{NH}_4)_{0.5}\text{V}_2\text{O}_5 \cdot n\text{H}_2\text{O}$



**Origin:** Synthetic.

**Description:** Synthesized using a surfactant-free hydrothermal method. Characterized by powder X-ray diffraction, TG, and EDX spectroscopy.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Chandrappa et al. (2011).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3495, 3180, 1628, 1400, 996, 981, 965, 841, 736, 539s.

**Note:** The formula is questionable and is to be checked.

**V120 Barium lanthanum thorium orthovanadate** BaLaTh(VO<sub>4</sub>)<sub>3</sub>

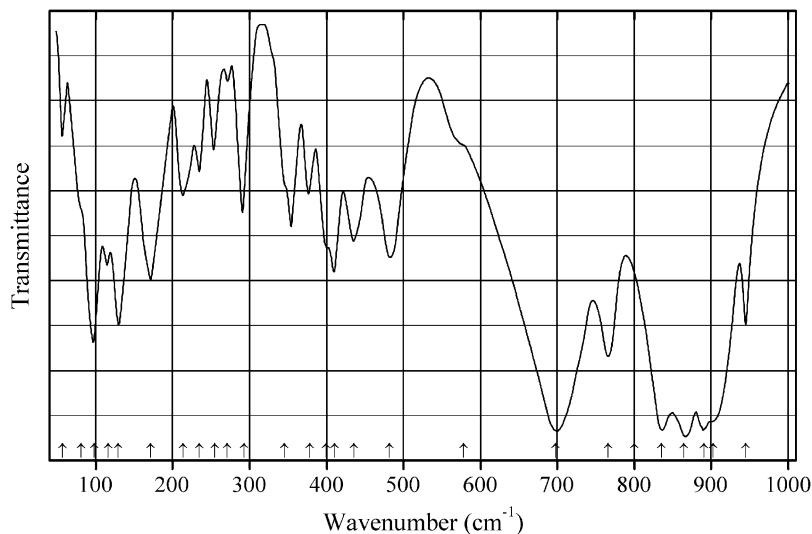
**Origin:** Synthetic.

**Description:** Obtained by treating stoichiometric mixture of corresponding metal nitrates with ammonium metavanadate in aqueous medium for 1 h followed by evaporation and calcination. Isostructural with monazite. Monoclinic,  $a = 7.070(5)$ ,  $b = 7.323(8)$ ,  $c = 6.810(6)$  Å,  $\beta = 104.96(7)^\circ$ ,  $V = 340.8$  Å<sup>3</sup>.  $D_{\text{meas}} = 5.52$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 5.54$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of a powdered sample. KBr disc. Transmission.

**Source:** Nabar and Mhatre (2001).

**Wavenumbers (cm<sup>-1</sup>):** 839sh, 810s, 780sh, 770sh, 750sh, 735sh, 478sh, 421, 412sh, 382w, 372sh, 350sh.

**V121 Barium vanadyl vanadate** Ba<sub>2</sub>(VO)(V<sub>2</sub>O<sub>8</sub>)

**Origin:** Synthetic.

**Description:** Prepared by the solid-state reaction of an intimate 4:1:1 mixture of Ba<sub>2</sub>V<sub>2</sub>O<sub>7</sub>, V<sub>2</sub>O<sub>3</sub>, and V<sub>2</sub>O<sub>5</sub> at 950 °C. Monoclinic, space group  $P2_1$ ,  $Z = 2$ . The crystal structure is built up of infinite chains of strongly distorted edge-sharing V<sup>IV</sup>O<sub>6</sub> octahedra, connected with V<sup>V</sup>O<sub>4</sub> tetrahedra.

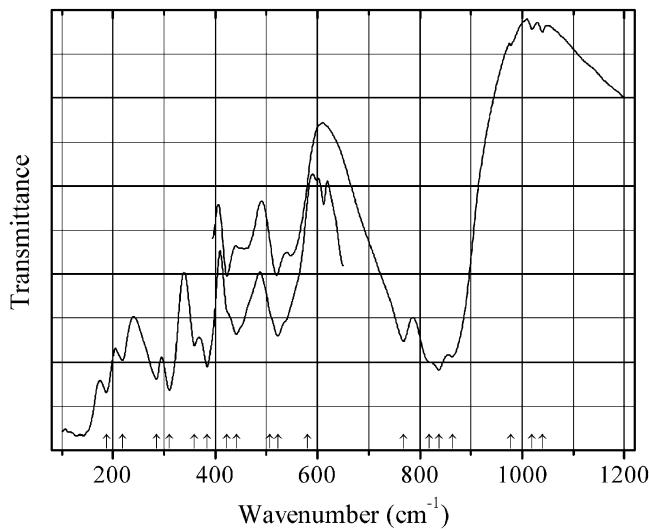
**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

**Source:** Baran (1997).

**Wavenumbers (IR, cm<sup>-1</sup>):** 945, 903sh, 891s, 864s, 835s, (800sh), 766s, 698s, 578sh, 482, 436, 411, 399, 378, 345sh, 293, 271w, 255, 235, 214, 172s, 129s, 116, 98s, 81sh, 57w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 902s, 872, 860sh, 830w, 802s, 762w, 737w, 696w, 676sh, 563w, 499w, 453w, 435sh, 397sh, 371, 345, 294, 268, 243, 212w, 163, 121, 85s.

**V122 Bismuth(III) magnesium oxovanadate  $\text{BiMg}(\text{VO}_4)\text{O}$   $\text{BiMg}(\text{VO}_4)\text{O}$** 

**Origin:** Synthetic.

**Description:** Prepared by solid-state reaction from a stoichiometric mixture of  $\text{Bi}_2\text{O}_3$ ,  $\text{MgO}$ , and  $\text{NH}_4\text{VO}_3$  gradually heated at 200, 500, and finally 850 °C for 18 h with intermediate grindings. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2_1/n$ ,  $a = 7.542(6)$ ,  $b = 11.615(5)$ ,  $c = 5.305(3)$  Å,  $\beta = 107.38(5)$ °,  $V = 443.5(5)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 5.455$  g/cm<sup>3</sup>.

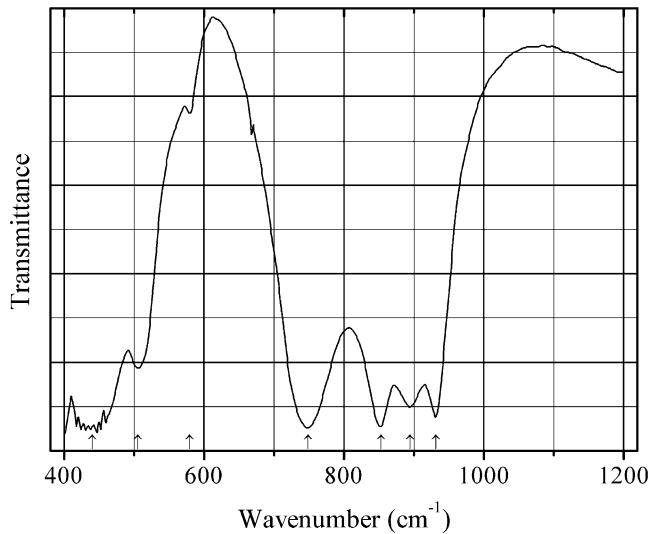
**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

**Source:** Benmokhtar et al. (2004).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1040w, 1019w, 978w, 864s, 837s, 819s, 768s, 581, 523, 507, 442, 423, 384, 359, 311, 285, 219, 188.

**Note:** Weak bands in the range from 900 to 1100 cm<sup>-1</sup> may correspond to the admixture of  $\text{PO}_4^{3-}$  groups. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 852s, 805s, 748sh, 570, 389w, 340, 303, 250w, 179, 133, 108.

**V123 Bismuth(III) magnesium oxovanadate  $\text{BiMg}_2(\text{VO}_4)\text{O}_2$** 

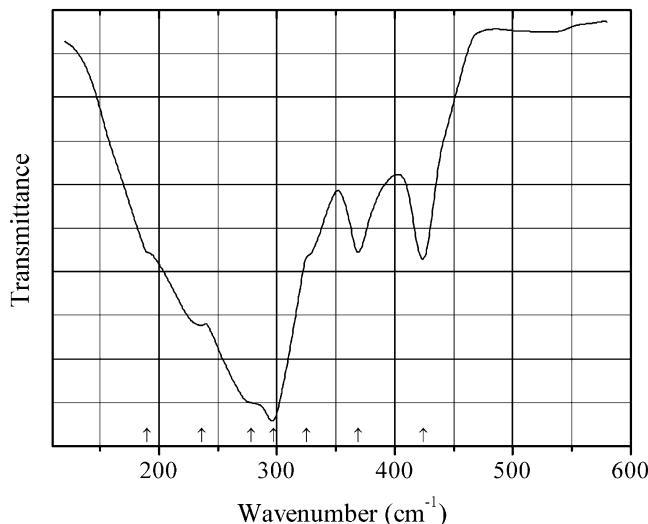
**Origin:** Synthetic.

**Description:** Synthesized by heating a mixture of  $\text{Bi}_2\text{O}_3$ ,  $\text{MgO}$ , and  $\text{NH}_4\text{VO}_3$  in the molar ratio  $\text{Bi:Mg:V} = 2:2:1$  first at  $700^\circ\text{C}$  for 12 h, then at  $800^\circ\text{C}$  for 6 h, and finally at  $1000^\circ\text{C}$  for 5 min. The product was structurally characterized from single crystal X-ray diffraction data. Orthorhombic, space group  $Cnmc$ ,  $a = 7.9136(6)$ ,  $b = 12.246(2)$ ,  $c = 5.444(2)$  Å,  $V = 527.6(2)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 5.093$  g/cm $^3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Huang and Sleight (1992).

**Wavenumbers (cm $^{-1}$ ):** 932s, 895s, 853s, 749s, 579w, 505, 440s.

**V124 Calcium orthovanadate trigonal polymorph  $\text{Ca}_3(\text{VO}_4)_2$** 

**Origin:** Synthetic.

**Description:** Prepared in a solid-state reaction, from the mixture of  $\text{CaCO}_3$  and  $\text{As}_2\text{O}_5$  at  $700\text{ }^\circ\text{C}$  for 4 h. Trigonal, space group  $R\bar{3}c$ ,  $Z = 7$ .

**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc. Transmission.

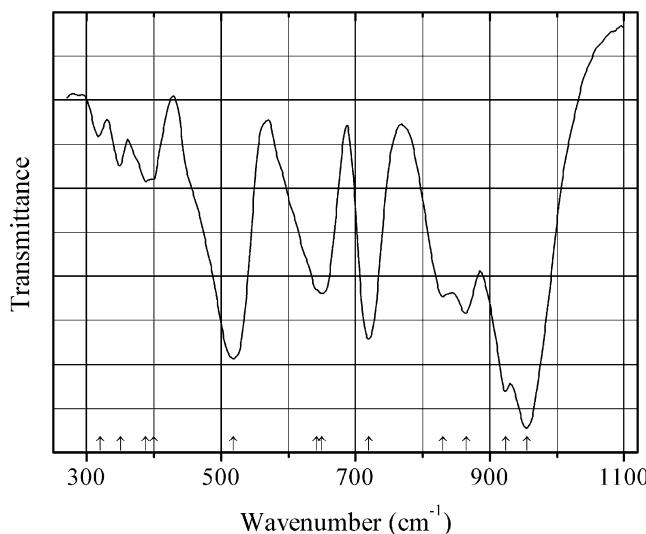
**Source:** Baran (1976).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 872, 910sh, 841sh, 810, 760sh, 424, 369, 325sh, 297s, 278sh, 236, 190sh.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 930, 912w, 865s, 850s, 825, 790sh, 770, 410w, 360s, 337s, 285, 225, 195, 163sh, 150.

### V125 Chromium iron(III) orthovanadate $\text{CrFe}(\text{VO}_4)_2$



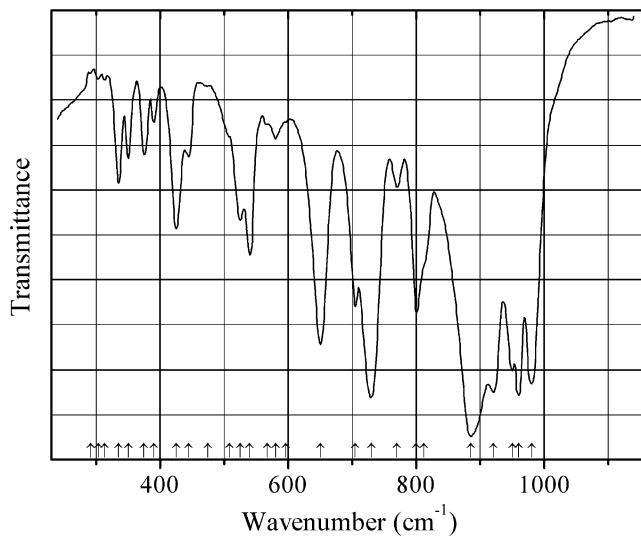
**Origin:** Synthetic.

**Description:** Prepared by a solid-state reaction. Characterized by powder X-ray diffraction data. Monoclinic, space group  $C2/m$ . Isostructural with  $\alpha\text{-MnMoO}_4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Lavat et al. (1989).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 956s, 924s, 865, 830, 720s, 650, 642sh, 518s, 400sh, 388, 350w, 320w.

**V126 Chromium vanadate  $\text{Cr}_2\text{V}_4\text{O}_{13}$   $\text{Cr}_2\text{V}_4\text{O}_{13}$** 

**Origin:** Synthetic.

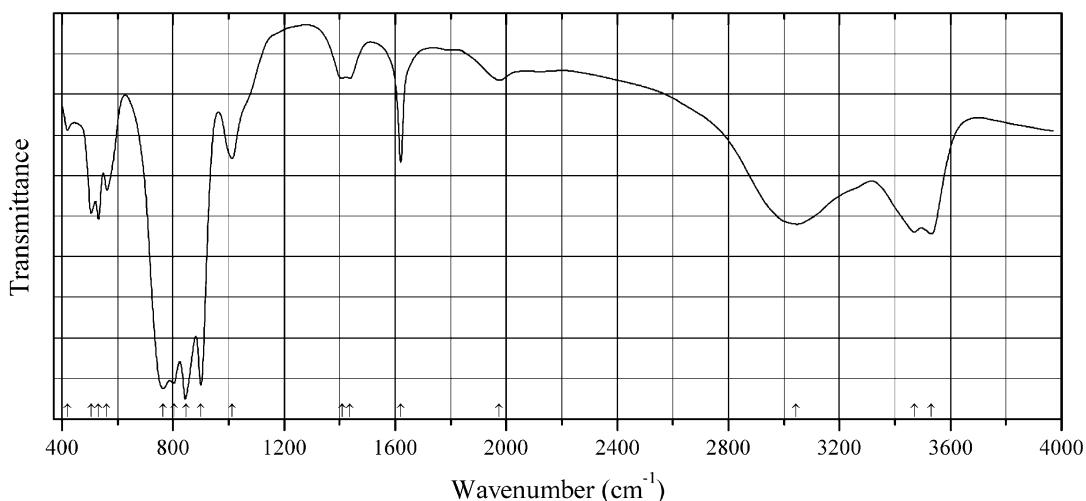
**Description:** Monoclinic, with a *P*-cell,  $a = 8.2663(17)$ ,  $b = 9.3033(26)$ ,  $c = 7.5373(16)$  Å,  $\beta = 109.638(37)^\circ$ ,  $V = 545.932$  Å<sup>3</sup>. Confirmed by chemical analyses. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 7.0928 (100) (001), 3.8938 (60) (200), 3.7026 (30) (-211), 3.5920 (50) (210), 3.3151 (75) (012), 2.8210 (30) (022).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Filipek et al. (1998).

**Wavenumbers (cm<sup>-1</sup>):** 980s, 960s, 950s, 920s, 885s, 812sh, 800, 770, 730s, 705, 650, 596w, 580w, 567sh, 540, 525, 508sh, 475w, 445, 425, 390w, 375, 350, 335, 313w, 303w, 291w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, the wavenumber 650 cm<sup>-1</sup> is erroneously indicated as 605 cm<sup>-1</sup>.

**V127 Copper divanadate hydroxide hydrate  $\text{Cu}_3(\text{V}_2\text{O}_7)(\text{OH})_2 \cdot n\text{H}_2\text{O}$** 

**Origin:** Synthetic.

**Description:** Nanoparticles obtained by heating (at 140 °C for 24 h) of a precipitate formed in the reaction between V<sub>2</sub>O<sub>5</sub> and CuSO<sub>4</sub>·7H<sub>2</sub>O in the presence of hexamethylenetetramine, Na<sub>2</sub>SO<sub>4</sub>, and H<sub>2</sub>O. Characterized by EDS analysis and powder X-ray diffraction data. Monoclinic,  $a = 10.61$ ,  $b = 5.86$ ,  $c = 7.205$  Å,  $\beta = 94.86^\circ$  (see JCPDS, No. 46-1443).

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

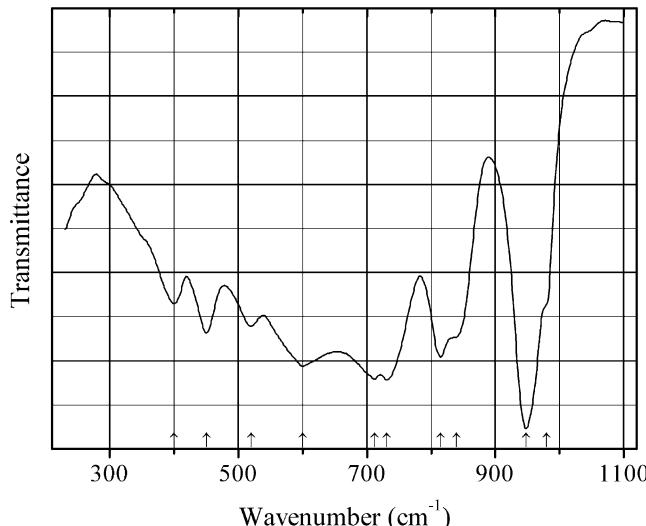
**Source:** Ni et al. (2010a).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3531, 3470, 3044, 1974w, 1620, 1437w, 1409w, 1012, 900s, 847s, 804s, 763s, 562, 531, 505, 419w.

**Note:** The wavenumber 1620 cm<sup>-1</sup> is erroneously indicated by Ni et al. (2010a) as 1920 cm<sup>-1</sup>. The weak bands at 1437 and 1409 cm<sup>-1</sup> may correspond to the admixture of a carbonate. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 894s, 820s, 758, 476, 438, 342, 236, 164w.

### V128 Dysprosium decavanadate hydrate Dy<sub>2</sub>V<sub>10</sub>O<sub>28</sub>·24H<sub>2</sub>O



**Origin:** Synthetic.

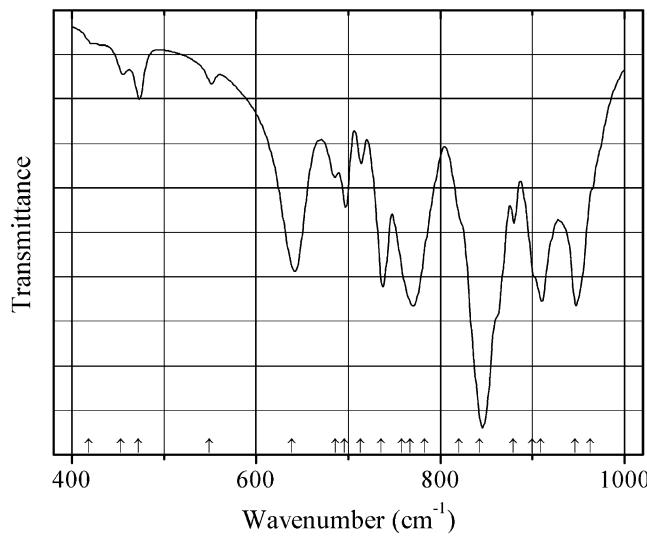
**Description:** Obtained by slow evaporation of an aqueous solution containing decavanadic acid and dysprosium acetate. Triclinic, space group P-1,  $a = 9.22(2)$ ,  $b = 9.99(7)$ ,  $c = 13.98(6)$  Å,  $\alpha = 108.2$  (7)°,  $\beta = 62.3(5)$ °,  $\gamma = 89.1(3)$ °,  $V = 1063$  Å<sup>3</sup>,  $Z = 1$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Rigotti et al. (1981).

**Wavenumbers (IR, cm<sup>-1</sup>):** 980sh, 948s, 840sh, 815, 731s, 712s, 600, 520, 450, 400.

**Note:** The band at 725 cm<sup>-1</sup> indicated by Rigotti et al. (1981) is a doublet (731+712 cm<sup>-1</sup>). In the cited paper, Raman spectrum is given as a figure, without indication of positions of the bands.

**V129 Lanthanum uranyl orthovanadate divanadate**  $\text{La}(\text{UO}_2)_2(\text{VO}_4)(\text{V}_2\text{O}_7)$ 

**Origin:** Synthetic.

**Description:** Prepared by conventional solid-state reaction, using  $\text{LaCl}_3 \cdot 7\text{H}_2\text{O}$ ,  $\text{U}_3\text{O}_8$ , and  $\text{V}_2\text{O}_5$  as initial materials. Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group  $P2_12_12_1$ ,  $a = 6.9470(2)$ ,  $b = 7.0934(2)$ ,  $c = 25.7464(6)$  Å,  $V = 1268.73(5)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 5.276$  g/cm<sup>3</sup>.

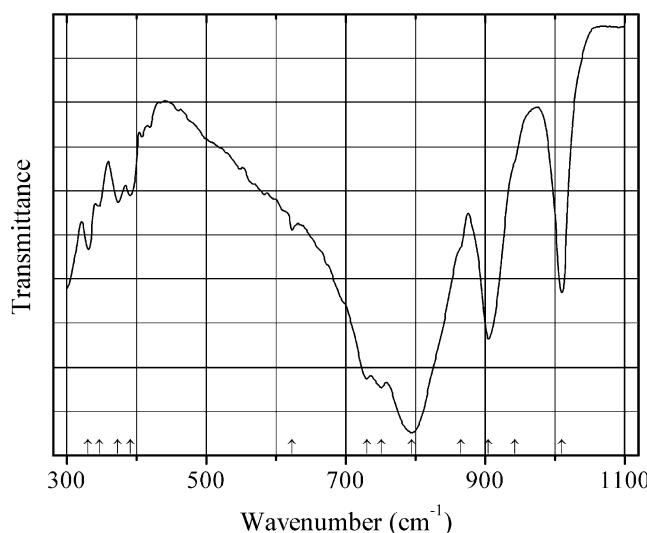
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Mer et al. (2012).

**Wavenumbers (IR, cm<sup>-1</sup>):** 963sh, 946s, 909s, 900sh, 879, 843s, 820, 783, 767s, 758sh, 736s, 713w, 696, 686, 639s, 549w, 472w, 453w, 418w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 951s, 943, 918, 909s, 898, 868, 860, 787s, 766s, 753, 739s, 711w, 592w, 562w, 516w, 450sh, 431, 413, 360, 345, 334, 328.

**V130 Lead iron(III) trivanadate**  $\text{Pb}_2\text{FeV}_3\text{O}_{11}$ 

**Origin:** Synthetic.

**Description:** Yellow solid formed in the solid-state reaction between  $\text{FeVO}_4$  and  $\text{Pb}_2\text{V}_2\text{O}_7$ . Monoclinic,  $a = 11.385(13)$ ,  $b = 5.6414(7)$ ,  $c = 7.4970(9)$  Å,  $\beta = 81.72(1)^\circ$ .  $D_{\text{meas}} = 5.52(5)$  g/cm<sup>3</sup>. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 11.277 (27) (100), 3.372 (27) (-211), 3.126 (100) (310), 3.086 (52) (112), 2.821 (38) (020), 2.767 (26) (401).

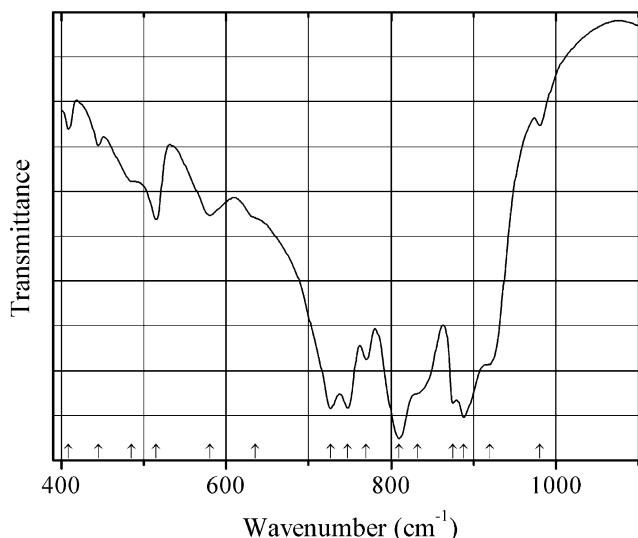
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Blonska-Tabero (2009).

**Wavenumbers (cm<sup>-1</sup>):** 1010, 943sh, 905s, 865sh, 795s, 751s, 730s, 623w, 391w, 373w, 346w, 330.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### V131 Lead uranyl divanadate $\text{Pb}(\text{UO}_2)(\text{V}_2\text{O}_7)$



**Origin:** Synthetic.

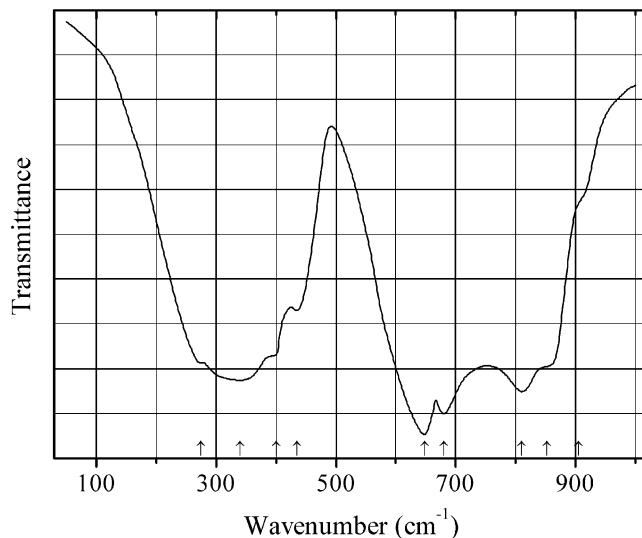
**Description:** Synthesized by solid-state reaction of  $\text{PbO}$ ,  $\text{V}_2\text{O}_5$ , and  $\text{U}_3\text{O}_8$  in the metallic ratio  $\text{Pb:V:U} = 1:6:2$  in air, at 680 °C, for 2 h. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2_1/n$ ,  $a = 6.9212(9)$ ,  $b = 9.6523(13)$ ,  $c = 11.7881(16)$  Å,  $\beta = 91.74(1)^\circ$ ,  $V = 787.2(2)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{meas}} = 5.82(3)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 5.81(1)$  g/cm<sup>3</sup>. The structure is based on a three-dimensional framework composed by edge- and corner-sharing U- and V-centered polyhedra forming elliptic tunnels occupied by  $\text{Pb}^{2+}$  ions.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Obbade et al. (2004).

**Wavenumbers (cm<sup>-1</sup>):** 980w, 920sh, 888s, 875, 832sh, 810s, 770, 747s, 727s, 635sh, 580w, 515, 485sh, 445w, 409w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**V132 Lithium nickel vanadate** LiNi(VO<sub>4</sub>)

**Origin:** Synthetic.

**Description:** Synthesized by a solid-state reaction technique. Characterized by powder X-ray diffraction data. Cubic, space group *Fd-3m*,  $a = 8.221(1)$ , which corresponds to the inverse spinel structure.

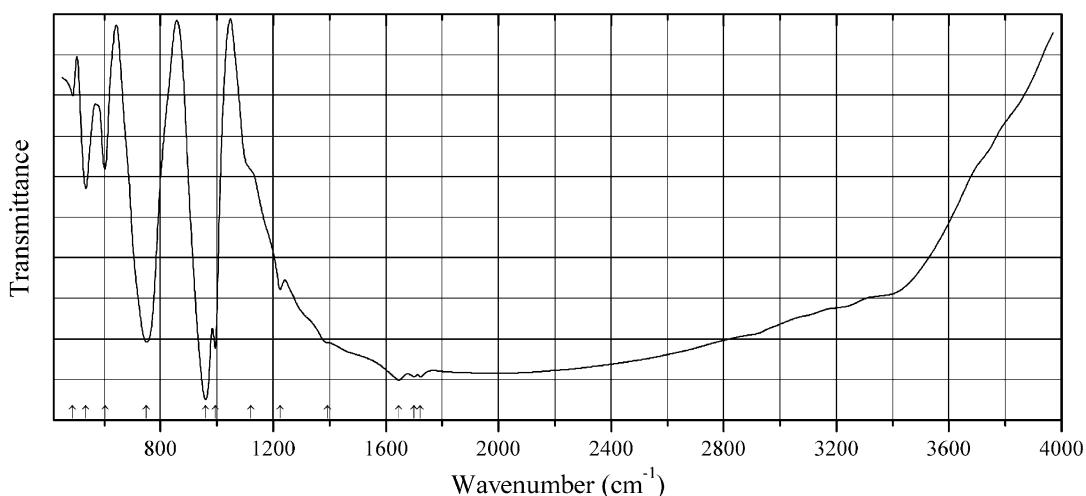
**Kind of sample preparation and/or method of registration of the spectrum:** Fine powder painted onto polyethylene slab. Absorption.

**Source:** Chitra et al. (2000).

**Wavenumbers (IR, cm<sup>-1</sup>):** 905sh, 852, 810s, 680s, 648s, 435, 400sh, 340s, 275sh.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 902sh, 823s, 790s, 660, 481, 420, 337, 190w.

**V133 Lithium trivanadate** LiV<sub>3</sub>O<sub>8</sub>

**Origin:** Synthetic.

**Description:** Prepared by stepwise heating a mixture of  $\text{Li}_2\text{CO}_3$  and  $\text{V}_2\text{O}_5$  powders up to 700 °C.

Characterized by powder X-ray diffraction data. Monoclinic, space group  $P2_1/m$ ,  $a = 6.68$ ,  $b = 3.60$ ,  $c = 12.03 \text{ \AA}$ ,  $\beta = 107^\circ$ , which corresponds to the JCPDS card No. 72-1193.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Ramaraghavulu et al. (2012).

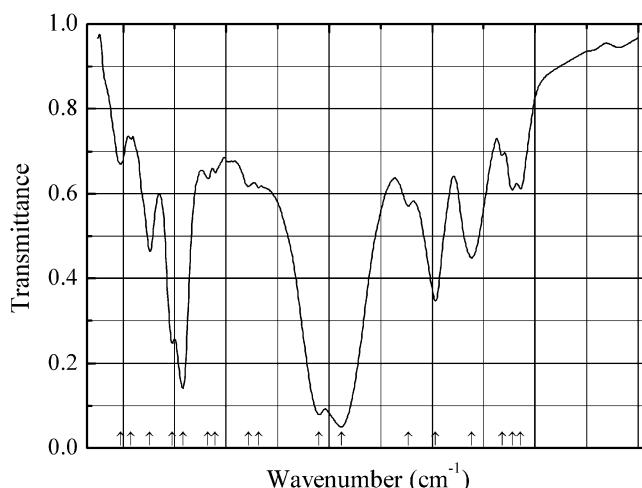
**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1723w, 1700w, 1646w, 1392sh, 1224w, 1120sh, 994s, 960s, 750s, 602, 535, 488w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 999w, 782s, 555, 491, 395w, 295.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

#### V134 Lithium tungstate vanadate brannerite-type $\text{LiWVO}_6$



**Origin:** Synthetic.

**Description:** Synthesized by heating to 400 °C of a precursor formed in the reaction between  $\text{Li}(\text{NO}_3)_2$ ,  $(\text{NH}_4)(\text{VO}_3)_2$ , and tungstic acid in aqueous solution, in the presence of glycine, with subsequent calcination of the product at 550 °C. Characterized by powder X-ray diffraction data. Monoclinic, space group  $C2$ ,  $a = 9.347$ ,  $b = 3.670$ ,  $c = 6.593 \text{ \AA}$ ,  $\beta = 111.83^\circ$ .

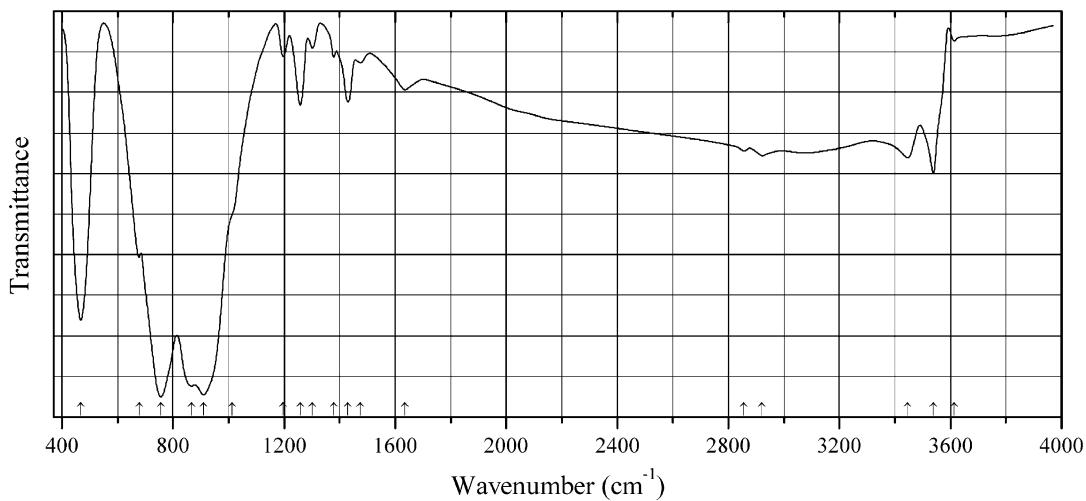
**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc. Absorption.

**Source:** Amdouni et al. (2003).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 972, 956, 936w, 877, 807, 754, 624s, 581s, (463), 443w, 379w, 365w, 316s, 295, 252, (215), 195.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 970s, 860sh, 826, 743, 524w, 449, 324, 268, 238, 207, 146s, 117.

**V135 Magnesium vanadate  $Mg_7V_4O_{16}(OH)_2 \cdot H_2O$   $Mg_7V_4O_{16}(OH)_2 \cdot H_2O$** 


**Origin:** Synthetic.

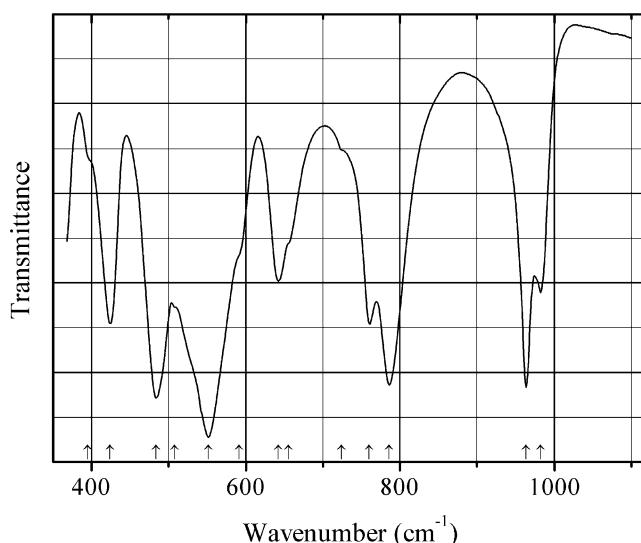
**Description:** Prepared hydrothermally from  $V_2O_5$  and  $Mg(BO_2)_2 \cdot H_2O$  at 200 °C for 5 days. A compound with non-centrosymmetric tunnel structure. See supplementary data at doi: <https://doi.org/10.1016/j.inoche.2008.05.019>.

**Kind of sample preparation and/or method of registration of the spectrum:** No data in the cited paper.

**Source:** Hu et al. (2008).

**Wavenumbers (cm⁻¹):** 3614, 3538, 3445, (2920w), (2856w), 1635w, 1475w, 1430, 1379w, 1302w, 1258, 1197w, 1013sh, 910s, 867s, 756s, 678, 468.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. Weak bands in the range from 2800 to 3000 cm⁻¹ correspond to the admixture of an organic substance.

**V136 Potassium chromium divanadate  $KCrV_2O_7$** 


**Origin:** Synthetic.

**Description:** Prepared by solid-state reaction in air, by stepwise heating a stoichiometric mixture of  $K_2Cr_2O_7$  and  $V_2O_5$  up to 600 °C with intermediate regrindings. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2/c$ ,  $a = 7.9526(1)$ ,  $b = 4.87543(5)$ ,  $c = 6.8910(1)$  Å,  $\beta = 101.162(1)^\circ$ ,  $V = 262.1(1)$  Å<sup>3</sup>,  $Z = 2$ . Vanadium has sixfold coordination with one long and two short V–O bonds.

**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull. Transmission.

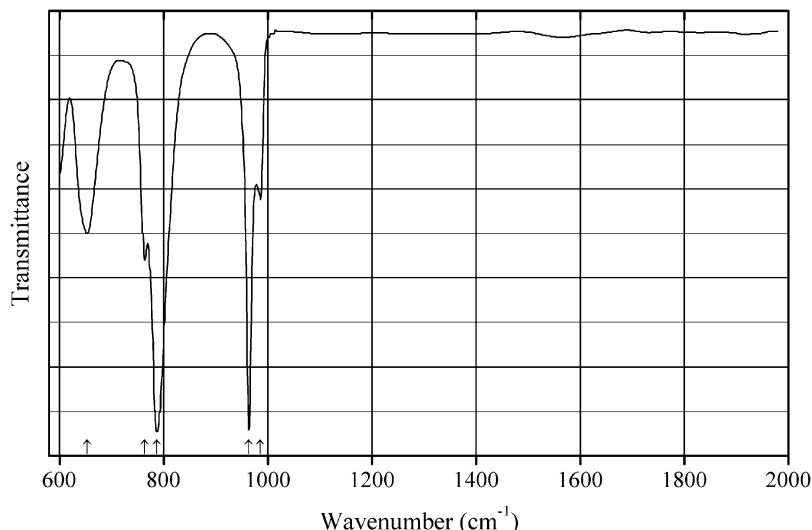
**Source:** Tyutyunnik et al. (2006).

**Wavenumbers (IR, cm<sup>-1</sup>):** 982, 963s, 786s, 760, 724sh, 655sh, 642, 591sh, 551s, 508sh, 484s, 424, 395sh.

**Note:** For another treatment of the crystal structure see Wang et al. (2012). In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 985s, 960w, 890, 868, 836, 768s, 712, 685, 663, 567w, 562, 542s, 483, 397, 342, 316, 283, 257, 218, 201, 173, 142.

### V137 Potassium chromium divanadate $KCrV_2O_7$



**Origin:** Synthetic.

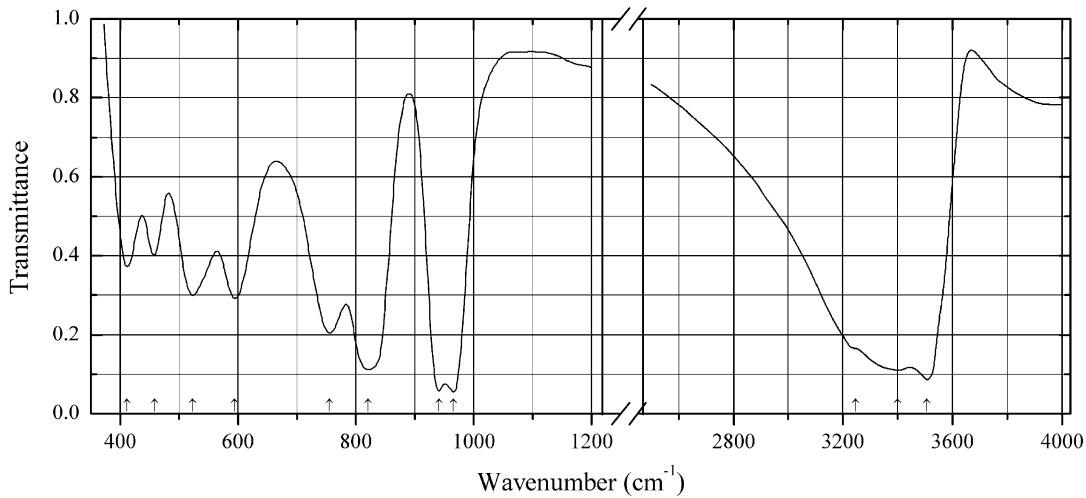
**Description:** Prepared by a solid-state reaction. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2/c$ ,  $a = 7.9529(6)$ ,  $b = 4.87548(5)$ ,  $c = 6.8917(2)$  Å,  $\beta = 101.15(4)^\circ$ ,  $V = 262.14$  Å<sup>3</sup>,  $Z = 2$ . Vanadium has fivefold coordination with two short V–O bonds.

**Kind of sample preparation and/or method of registration of the spectrum:** Absorption. Kind of sample preparation is not indicated.

**Source:** Wang et al. (2012).

**Wavenumbers (cm<sup>-1</sup>):** 986, 964s, 787s, 764, 654.

**Note:** For another treatment of the crystal structure see Tyutyunnik et al. (2006). The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**V138 Potassium decavanadate decahydrate**  $K_6(V_{10}O_{28}) \cdot 10H_2O$ 

**Origin:** Synthetic.

**Description:** Brown-orange crystals obtained in the reaction of  $V_2O_5$  with potassium malate solution.

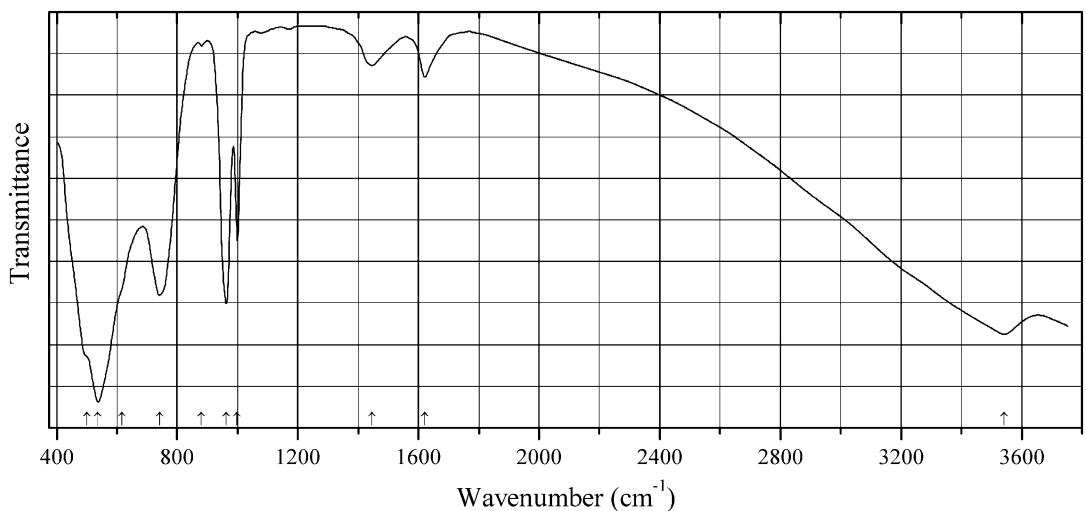
The crystal structure is solved. Triclinic, space group  $P-1$ ,  $a = 10.5334(4)$ ,  $b = 10.6600(4)$ ,  $c = 17.7351(5)$  Å,  $\alpha = 76.940(2)^\circ$ ,  $\beta = 75.836(2)^\circ$ ,  $\gamma = 64.776(2)^\circ$ ,  $V = 1729.86(10)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 2.634$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Guilherme et al. (2010).

**Wavenumbers (cm<sup>-1</sup>):** 3507s, 3400s, 3245sh, 966s, 942s, 821s, 755, 594, 523, 458, 411.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**V139 Potassium hexavanadate hydrate**  $K_2(V_6O_{16}) \cdot 1.5H_2O$ 

**Origin:** Synthetic.

**Description:** Nanobelts prepared by a low-temperature hydrothermal method. Monoclinic, space group  $P2_1/c$ ,  $a = 12.29 \text{ \AA}$ ,  $b = 3.60 \text{ \AA}$ ,  $c = 16.01 \text{ \AA}$ ,  $\beta = 93.89^\circ$ . Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

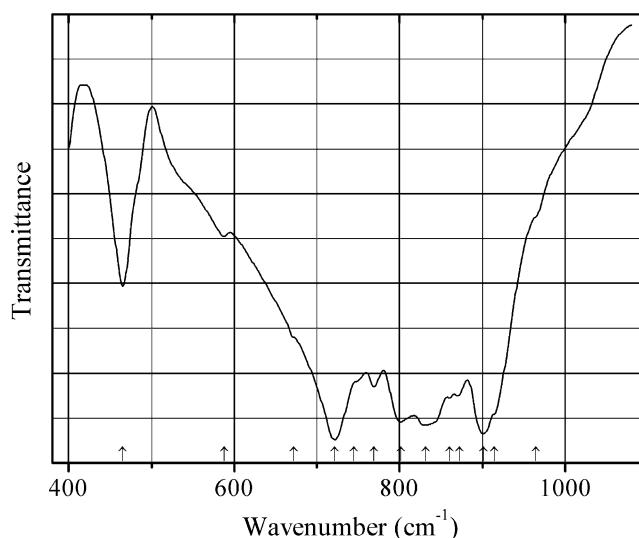
**Source:** Bai et al. (2013).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3542, 1620, 1445, 999, 962s, 880w, 741s, 617sh, 537s, 500sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1011w, 774, 686, 507, 270, 154s.

**V140 Strontium vanadyl vanadate**  $\text{Sr}_2(\text{VO})(\text{VO}_4)_2$



**Origin:** Synthetic.

**Description:** Prepared from a mixture of SrCO<sub>3</sub>, V<sub>2</sub>O<sub>5</sub>, and VO<sub>2</sub> pressed into pellet and heated with a CO<sub>2</sub> laser in a nitrogen atmosphere. Monoclinic, space group *I2/a*,  $a = 6.929$ ,  $b = 16.246$ ,  $c = 7.260$  Å,  $\beta = 115.82^\circ$ ,  $Z = 4$ .

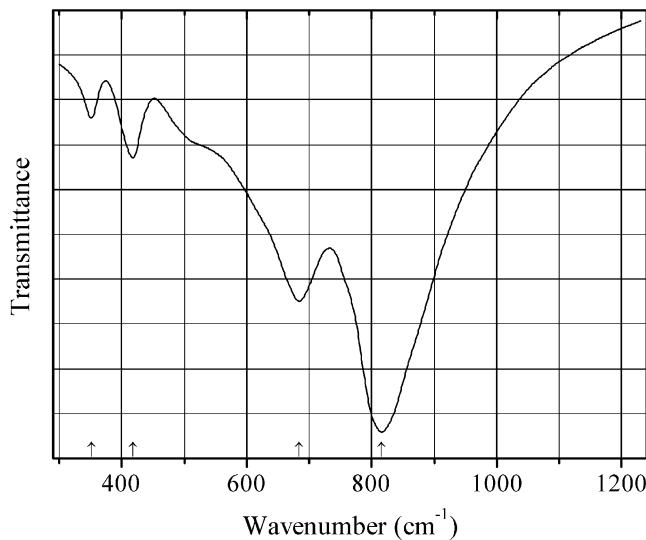
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Baran (1996).

**Wavenumbers (IR, cm<sup>-1</sup>):** 965sh, 914sh, 901s, 872, 860, 831s, 802s, 769, 745sh, 721s, 672sh, 588w, 465.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 912, 893, 870sh, 860s, 831s, 791w, 772, 720w, 468w, 430s, 400w, 370sh, 358w.

**V141 Tantalum oxyvanadate**  $Ta(VO_4)O$ 

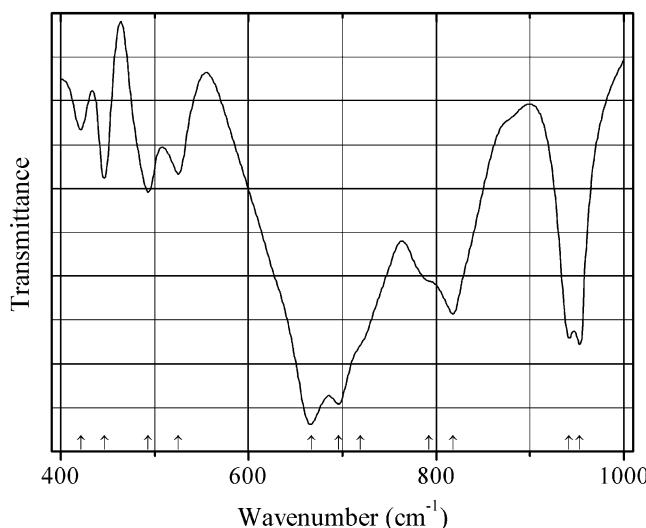
**Origin:** Synthetic.

**Description:** Prepared by heating a mixture of  $V_2O_5$  and defect pyrochlore  $H_2Ta_6O_6 \cdot H_2O$ , first at 873 K for 24 h, and thereafter at 1073 K for 12 h. Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic,  $a = 11.860(3)$ ,  $b = 5.516(1)$ ,  $c = 6.928(1)$  Å. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 5.96 (94) (101, 200), 4.491 (84) (201), 4.310 (100) (011), 4.050 (92) (111, 210), 3.487 (71) (211, 002), 2.845 (71) (112), 2.609 (68) (212, 410, 302).

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Chahboun et al. (1988).

**Wavenumbers (cm⁻¹):** 816s, 684, 418, 351w.

**V142 Tellurium(IV) oxovanadate**  $Te_2V_2O_9$ 

**Origin:** Synthetic.

**Description:** Polycrystalline sample prepared by heating a mixture of  $\text{TeO}_2$  and  $\text{V}_2\text{O}_5$  at 450 °C for 24 h with several intermediate grindings and mixings. Characterized by powder X-ray diffraction data. Orthorhombic. V is in tetrahedral coordination environment with V–O bond lengths ranging from 1.633 to 1.946 Å. Te has threefold coordination.

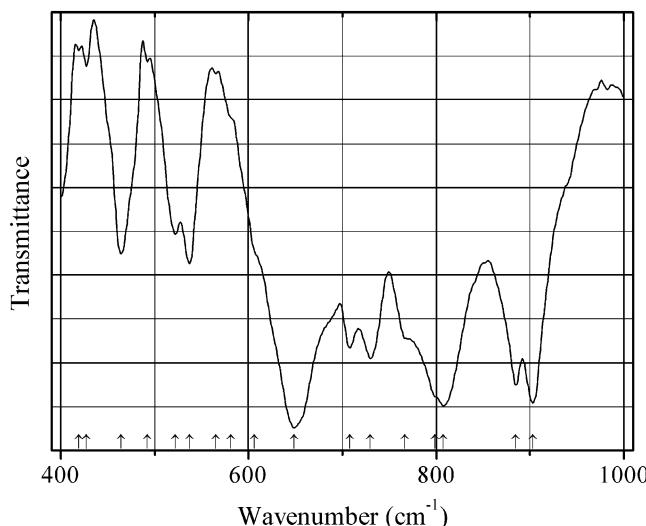
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Zhang et al. (2012b).

**Wavenumbers (cm<sup>-1</sup>):** 953, 942, 818, 792sh, 719sh, 696s, 667s, 525, 493, 446, 421w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

#### V143 Thallium(I) selenite vanadate $\text{TlSeVO}_5$ $\text{TlSeVO}_5$



**Origin:** Synthetic.

**Description:** Yellow crystals prepared hydrothermally from  $\text{Tl}_2\text{CO}_3$  and  $\text{SeO}_2$  at 230 °C for 3 days.

Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group  $Pna2_1$ ,  $a = 7.1639(15)$ ,  $b = 8.6630(19)$ ,  $c = 7.8946(17)$  Å,  $V = 489.95(18)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 5.616$  g/cm<sup>3</sup>. Se and V have three- and sixfold coordination, respectively.

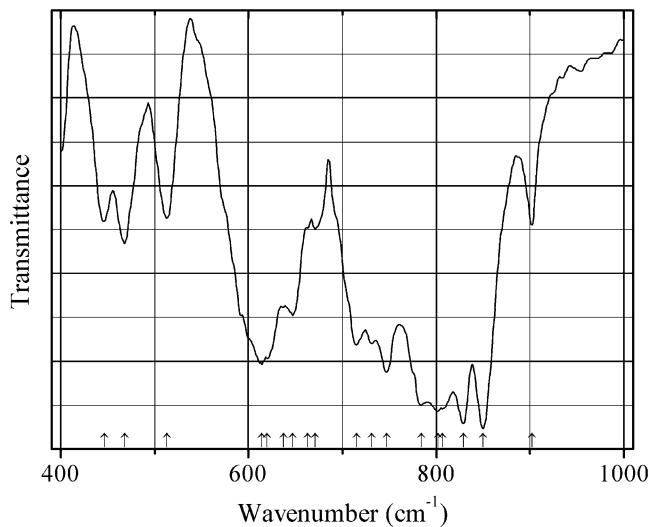
**Kind of sample preparation and/or method of registration of the spectrum:** A sample pressed between two KBr pellets. Transmission.

**Source:** Sivakumar et al. (2007).

**Wavenumbers (IR, cm<sup>-1</sup>):** 903s, 885s, 808s, 799sh, 767sh, 730, 708, 649s, 606, 581w, 565w, 537, 522, 492, 464, 427w, 419w.

**Note:** The wavenumber 649 cm<sup>-1</sup> is erroneously indicated by Sivakumar et al. (2007) as 657 cm<sup>-1</sup>.

The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**V144 Thallium(I) tellurite vanadate  $TlTeVO_5$   $TlTeVO_5$** 

**Origin:** Synthetic.

**Description:** Yellow crystals prepared hydrothermally from  $Tl_2CO_3$  and  $TeO_2$  at 230 °C for 3 days.

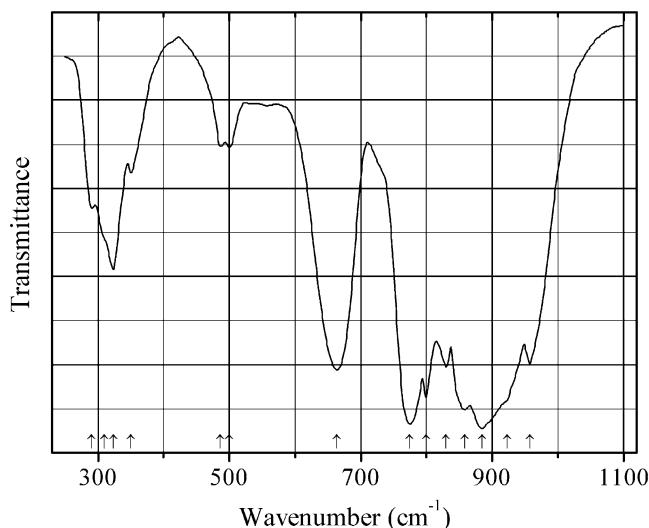
Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group  $Pna2_1$ ,  $a = 7.1639(15)$ ,  $b = 8.6630(19)$ ,  $c = 7.8946(17)$  Å,  $V = 489.95(18)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 6.103$  g/cm<sup>3</sup>. Te and V have three- and sixfold coordination, respectively.

**Kind of sample preparation and/or method of registration of the spectrum:** A sample pressed between two KBr pellets. Transmission.

**Source:** Sivakumar et al. (2007).

**Wavenumbers (IR, cm<sup>-1</sup>):** 902, 850s, 829s, 807s, 802s, 784s, 747, 731, 715, 671, 663, 647, 637, 620, 614, 513, 468, 446.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**V145 Thorium divanadate cubic polymorph  $\alpha$ -Th( $V_2O_7$ )**

**Origin:** Synthetic.

**Description:** Prepared by short-time heating a mixture of  $\text{ThO}_2$  and  $\text{P}_2\text{O}_5$  between 600 and 1000 °C.

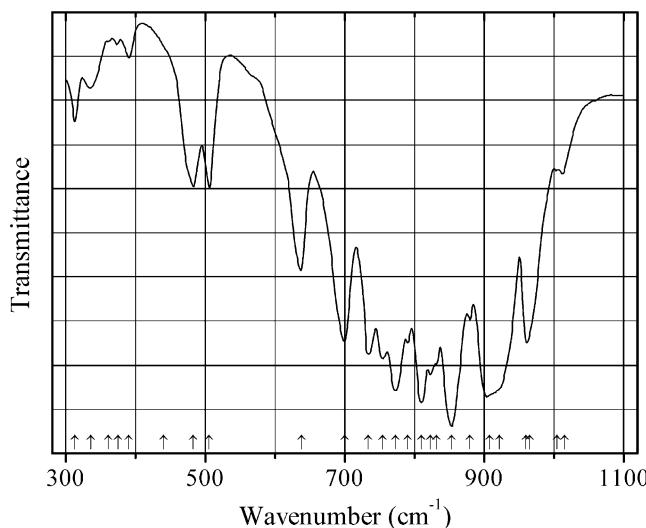
Characterized by powder X-ray diffraction data. Cubic,  $a = 8.72$ ,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Baran et al. (1974).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 958, 923sh, 885s, 858, 830, 799, 774s, 663, 500w, 486w, 350, 323, 310, 290.

## V146 Thorium divanadate orthorhombic polymorph $\beta$ -Th(V<sub>2</sub>O<sub>7</sub>)



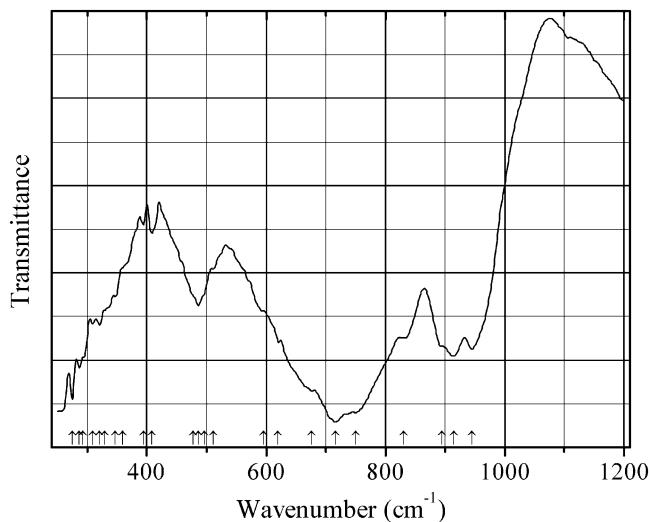
**Origin:** Synthetic.

**Description:** Prepared by long-time heating a mixture of  $\text{ThO}_2$  and  $\text{V}_2\text{O}_5$  at  $600^\circ\text{C}$ . Characterized by powder X-ray diffraction data. Orthorhombic,  $a = 7.216$ ,  $b = 6.964$ ,  $c = 22.800 \text{ \AA}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Baran et al. (1974).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1015w, 1005w, 965sh, 960, 922sh, 908s, 880, 853s, 832sh, 823, 810s, 790, 773s, 754, 734, 700, 638, 505, 482, 440, 390w, 375w, 360w, 335w, 313w.

**V147 Zinc iron(III) orthovanadate  $Zn_3Fe_4(VO_4)_6$** 

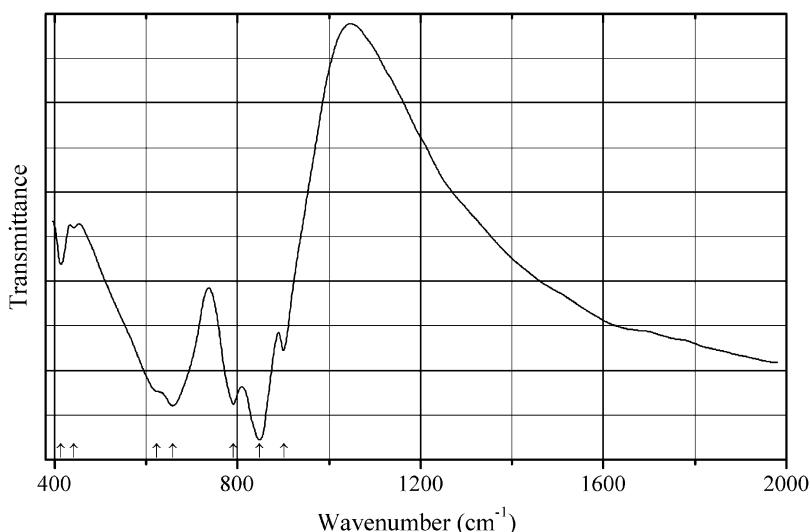
**Origin:** Synthetic.

**Description:** Prepared by stepwise heating a mixture of  $FeVO_4$  and  $Zn_3(VO_4)_2$ , taken in stoichiometric amounts, at 700, 750, and 800 °C, for 24 h at each temperature. Characterized by powder X-ray diffraction data. Triclinic,  $a = 6.681(1)$ ,  $b = 8.021(2)$ ,  $c = 9.778(4)$  Å,  $\alpha = 105.25(4)$ °,  $\beta = 105.00$ °,  $\gamma = 102.20(4)$ °,  $V = 465.8$  Å<sup>3</sup>,  $Z = 1$ .  $D_{\text{calc}} = 3.95$  g/cm<sup>3</sup>. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 3.2713 (34) (-201), 3.1997 (45) (2-10), 3.1368 (56) (0-13), 3.0747 (100) (021), 3.0442 (36) (-202).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.  
**Source:** Kurzawa and Blonska-Tabero (2002).

**Wavenumbers (cm<sup>-1</sup>):** 945s, 915s, 895sh, 830sh, 750s, 716s, 676, 511, 486, 408w, (394w).

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**V148 Zinc orthovanadate  $Zn_3(VO_4)_2$** 

**Origin:** Synthetic.

**Description:** Prepared hydrothermally from  $\text{Zn}(\text{NO}_3)_2$  and  $\text{V}_2\text{O}_5$  in the presence of hexamethylene-tetramine at 120 °C for 24 h with subsequent annealing of the  $\text{Zn}_3(\text{OH})_2\text{V}_2\text{O}_7 \cdot n\text{H}_2\text{O}$  precursor at 600 °C for 10 h. Characterized by powder X-ray diffraction data. Orthorhombic,  $a = 8.299$ ,  $b = 11.52$ ,  $c = 6.111$  Å (see JCPDS card no. 34-0378).

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

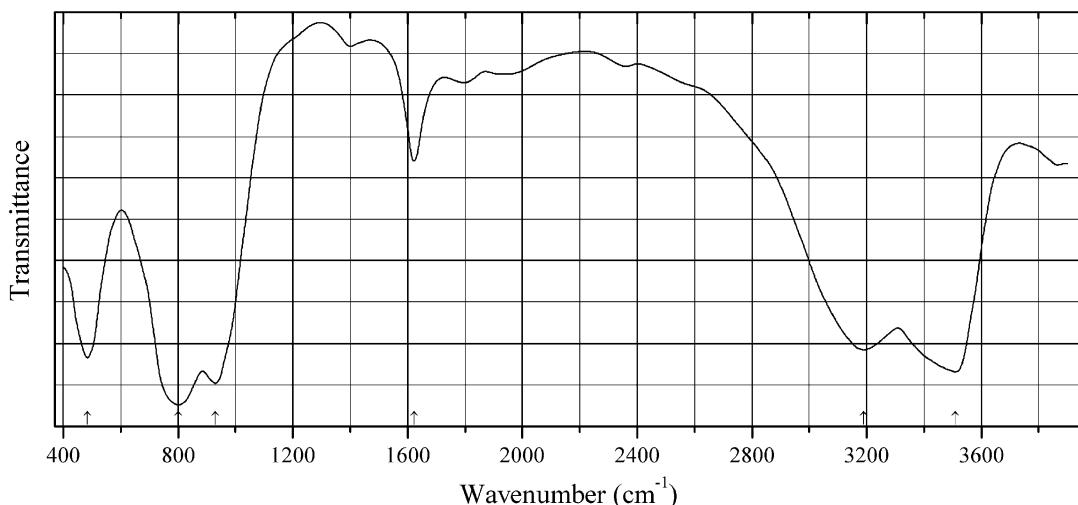
**Source:** Ni et al. (2010b).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 901, 848s, 791s, 658s, 624, 442w, 414.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 961s, 816, 797, 692w, 633w, 457w, 394, 374, 318s, 261, 224, 200w, 179w, 156.

#### V149 Zinc basic pyrovanadate hydrate $\text{Zn}_3(\text{V}_2\text{O}_7)(\text{OH})_2 \cdot 2.5\text{H}_2\text{O}$



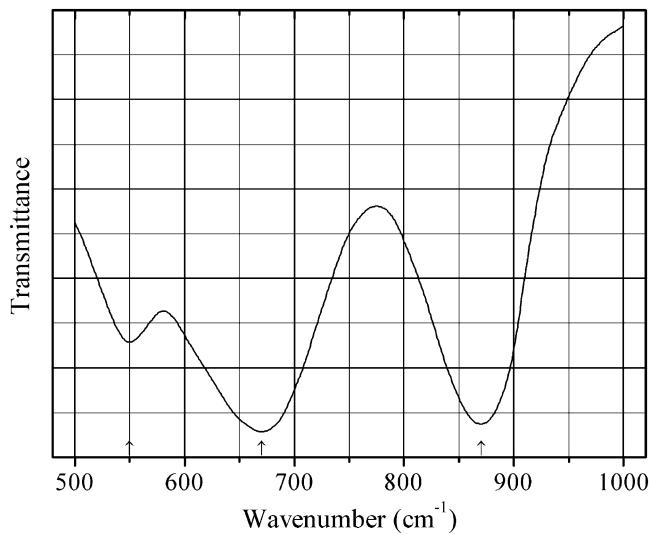
**Origin:** Synthetic.

**Description:** Precipitate obtained by adding 10% aqueous  $(\text{NH}_4)\text{OH}$  to the solution prepared from 30% aqueous  $\text{H}_2\text{O}_2$ ,  $\text{V}_2\text{O}_5$ , and of  $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ . Characterized by powder X-ray diffraction data and TG analysis. Hexagonal.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Melghit et al. (2007).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3510s, 3190, 1622, 930s, 800s, 484.

**V150 Zinc vanadyl oxide  $\text{Zn}(\text{VO}_2)_2\text{O}_2$   $\text{Zn}(\text{VO}_2)_2\text{O}_2$** 

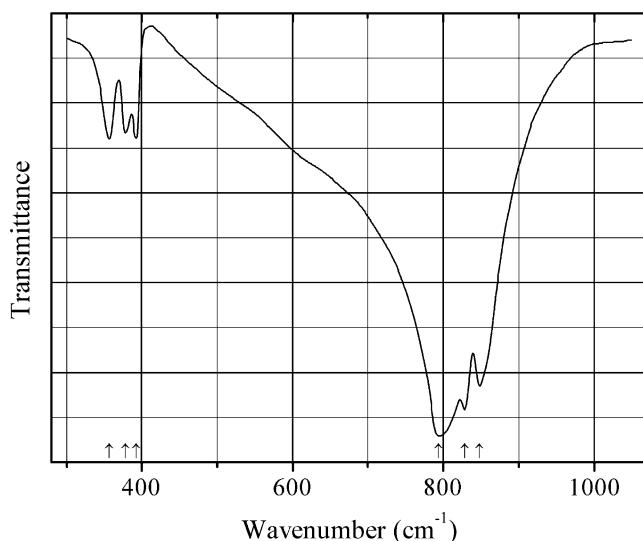
**Origin:** Synthetic.

**Description:** Obtained by the thermal decomposition at 550 °C for 8 h of a precursor prepared from  $\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$  and  $(\text{NH}_4)(\text{VO}_3)$  by a rheological phase reaction method. Characterized by powder X-ray diffraction data. Monoclinic,  $a = 9.223$ ,  $b = 3.511$ ,  $c = 6.552$  Å,  $\beta = 111.23^\circ$ ,  $V = 197.7$  Å<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Liu and Tang (2009).

**Wavenumbers (cm<sup>-1</sup>):** 870s, 670s, 550.

**V151 Alforsite vanadate analogue  $\text{Ba}_5(\text{VO}_4)_3\text{Cl}$** 

**Origin:** Synthetic.

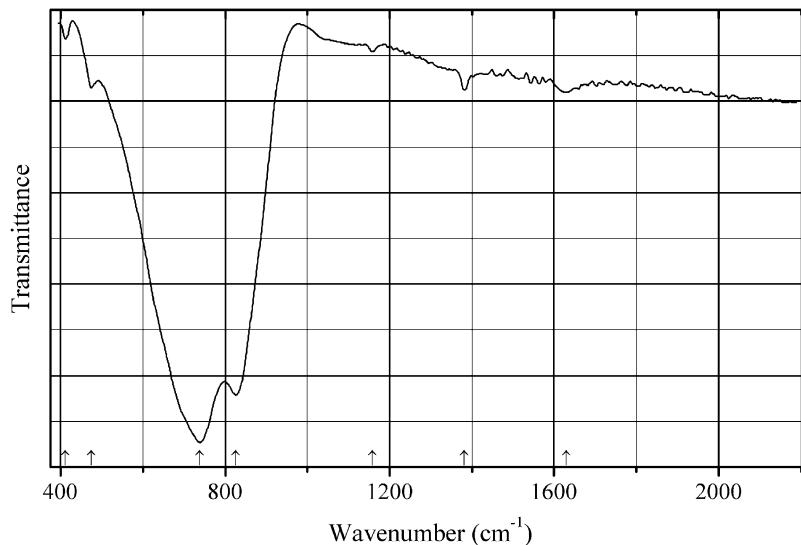
**Description:** Obtained by double-ply heating a mixture of  $\text{Ba}_3(\text{VO}_4)_2$  and  $\text{BaCl}_2$ , taken in stoichiometric molar ratio, at 950–1000 °C for 1–2 h with intermediate grinding. Characterized by powder X-ray diffraction data. Hexagonal, space group  $P6_3/m$ ,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Baran and Aymonino (1972).

**Wavenumbers (cm<sup>-1</sup>):** 848s, 828w, 794s, 393, 378, 357.

### V152 Clinobisvanite $\text{BiVO}_4$



**Origin:** Synthetic.

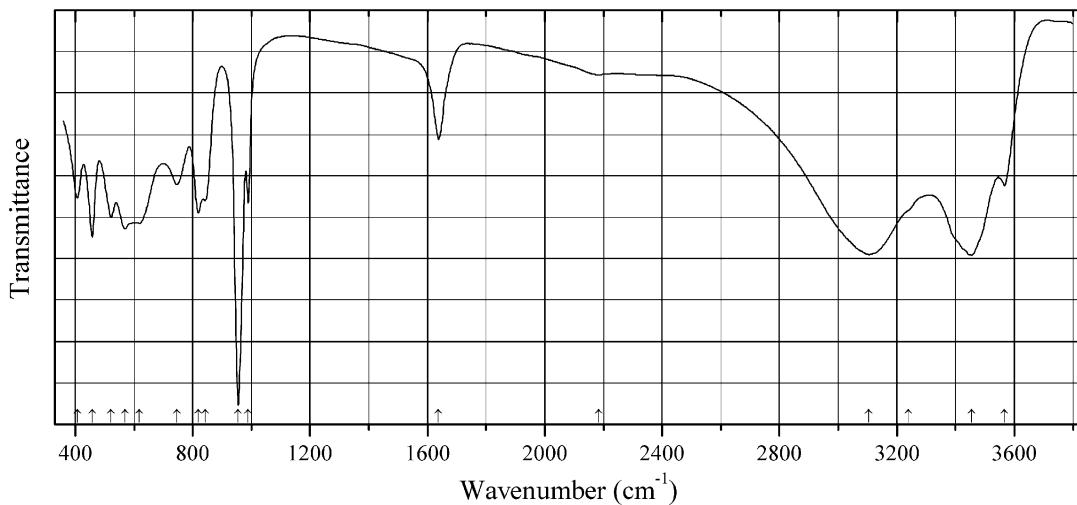
**Description:** Prepared from ammonium vanadate and bismuth nitrate using a complex sol-gel procedure followed by calcination at 600 °C for 2 h. Monoclinic. Characterized by powder X-ray diffraction data and EDX spectroscopy.

**Kind of sample preparation and/or method of registration of the spectrum:** No data.

**Source:** Pookmanee et al. (2013).

**Wavenumbers (cm<sup>-1</sup>):** 1629w, 1382w, 1158w, 826s, 737s, 474w, 412w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. Weak bands with wavenumbers above 1000 cm<sup>-1</sup> may correspond to impurities.

**V153 Magnesiopascoite**  $\text{Ca}_2\text{MgV}^{5+}_{10}\text{O}_{28}\cdot 16\text{H}_2\text{O}$ 

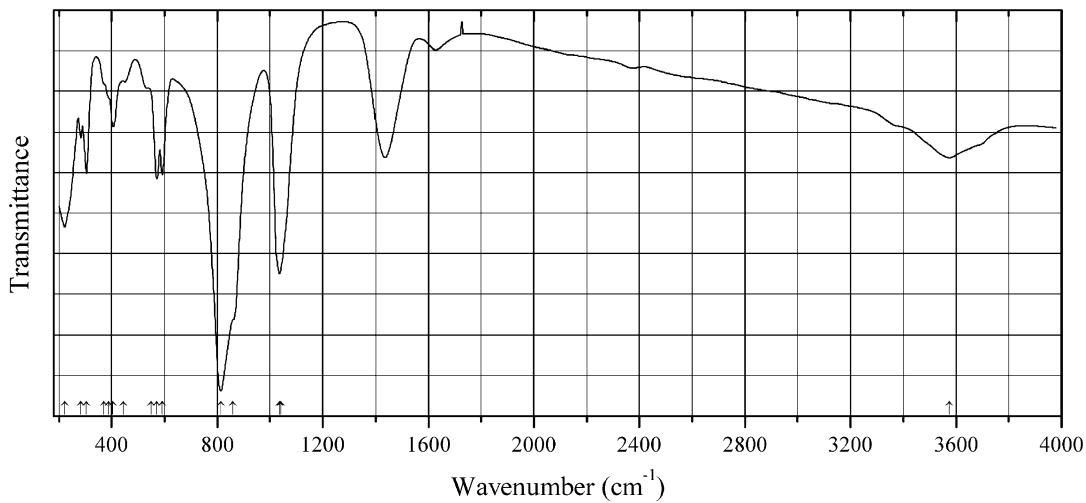
**Origin:** Packrat Mine, Gateway, Gateway District, Mesa Co., Colorado, USA.

**Description:** Orange crust from the association with U,V-oxides. Investigated by A.V. Kasatkin. The empirical formula is (electron microprobe):  $\text{Ca}_{2.07}\text{Mg}_{1.03}\text{V}_{9.90}\text{O}_{28}\cdot n\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3567, 3455s, 3240sh, 3105s, 2184w, 1638, 989, 955s, 842, 819, 746, 619, 569, 522, 458, 407.

**Note:** The spectrum was obtained by N.V. Chukanov.

**V154 Vanadinite Sr,OH-analogue**  $\text{Sr}_{10}(\text{PO}_4)_5(\text{VO}_4)_5(\text{OH})_2$ 

**Origin:** Synthetic.

**Description:** Obtained in the reaction between aqueous solution of  $\text{Sr}(\text{NO}_3)_2$ , containing  $\text{NH}_4\text{OH}$ , and a solution containing  $(\text{NH}_4)_2(\text{HPO}_4)$  and  $(\text{NH}_4)(\text{VO}_3)$  with subsequently heating a precipitate formed first at  $100^\circ\text{C}$  for 2 h and thereafter at  $850^\circ\text{C}$  for 2 h. Characterized by powder X-ray diffraction data.

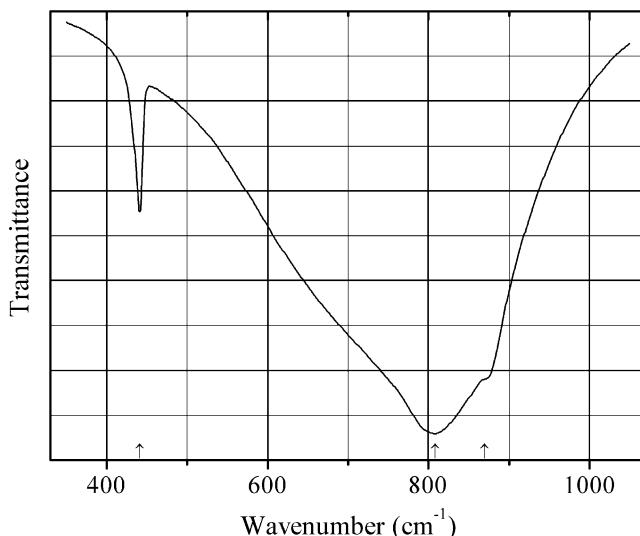
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Galera-Gomez et al. (1982).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3575, 1042s, 858sh, 815s, 592, 572, 550, 443, 405, 390sh, 370sh, 305, 283, 222s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. Bands in the range from 1400 to  $1700\text{ cm}^{-1}$  correspond to impurities.

#### V155 Wakefieldite-(Pr) $\text{PrVO}_4$



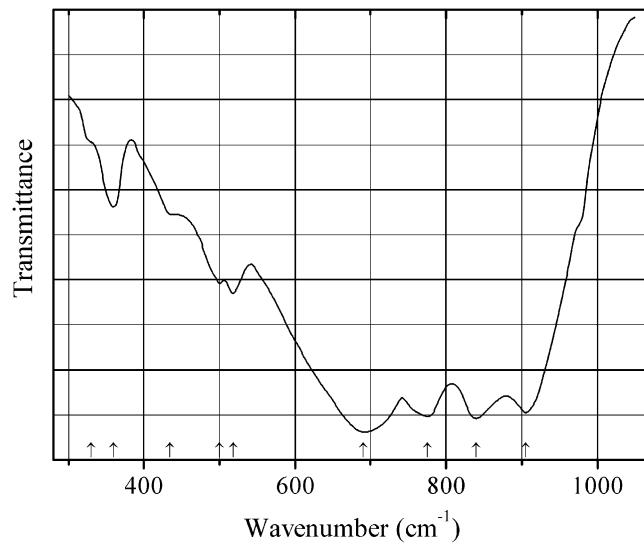
**Origin:** Synthetic.

**Description:** Obtained by heating a stoichiometric mixture of  $\text{Pr}_2\text{O}_3$  and  $\text{V}_2\text{O}_5$  powders in air for several hours, first at  $750^\circ\text{C}$  and thereafter at  $1000^\circ\text{C}$  with intermediate grinding. Tetragonal,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Baran and Aymonino (1971).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 870sh, 808s, 441.

**V156 Ziesite and blossom polymorph Cu<sub>2</sub>V<sub>2</sub>O<sub>7</sub>**

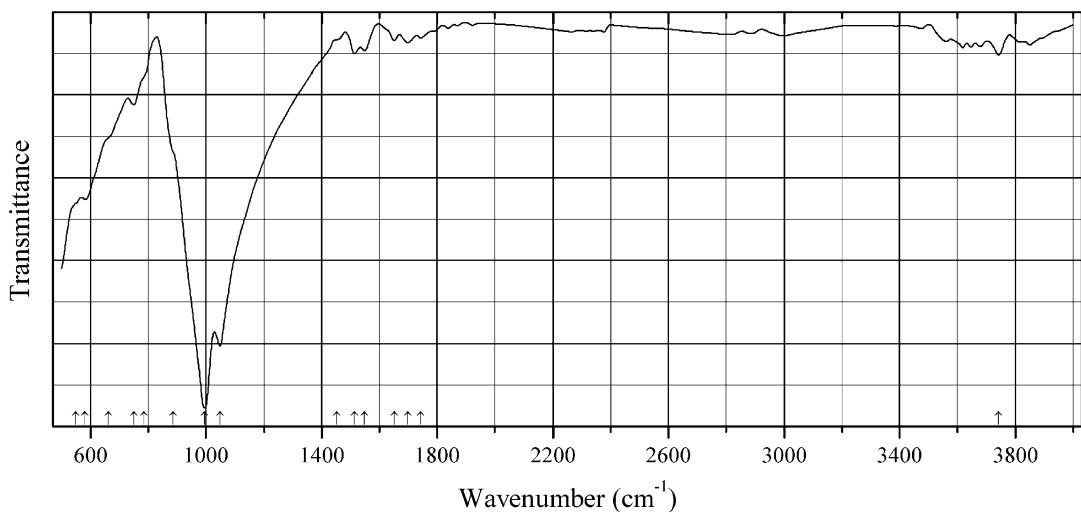
**Origin:** Synthetic.

**Description:** Dark brown powder obtained in a solid-state reaction of CuO and V<sub>2</sub>O<sub>5</sub> at 600 °C for 16 h with intermediate grinding. Characterized by powder X-ray diffraction data. Monoclinic,  $a = 6.87$ ,  $b = 8.11$ ,  $c = 9.16$  Å,  $\beta = 109.5^\circ$ ,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Pedregosa et al. (1974).

**Wavenumbers (cm<sup>-1</sup>):** 905s, 840s, 775s, 690s, 518, 500, 435sh, 360, 330sh.

**V157 Reppiaite Mn<sup>2+</sup><sub>5</sub>(VO<sub>4</sub>)<sub>2</sub>(OH)<sub>4</sub>**

**Origin:** Synthetic.

**Description:** Dark red columnar crystals hydrothermally grown from  $\text{Mn}_2\text{O}_3$  and  $\text{V}_2\text{O}_5$  in 3 M  $\text{CsOH}$  at 580 °C and 1.5 kbar. The crystal structure is solved. Monoclinic, space group  $C2/m$ ,  $a = 9.6568$  (9) Å,  $b = 9.5627(9)$  Å,  $c = 5.4139(6)$  Å,  $\beta = 98.529(8)$ °,  $V = 494.42(9)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 3.846$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

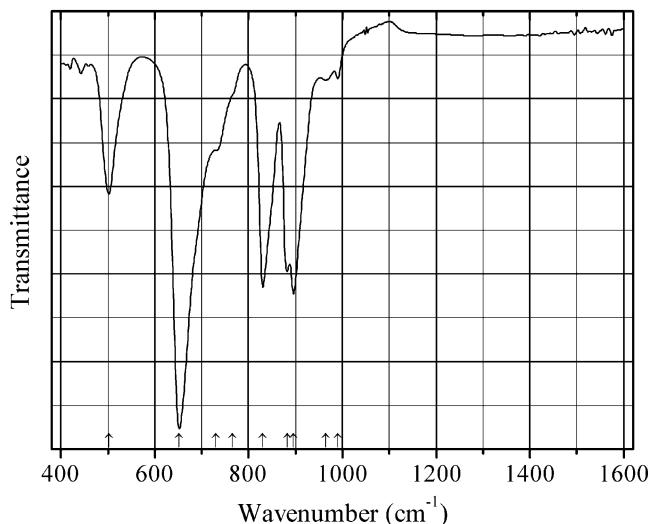
**Source:** Sanjeeva et al. (2016).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3743w, 1743w, 1698w, 1651w, 1549w, 1513w, 1452sh, 1048s, 995s, 886sh, 785sh, 750w, 663sh, 582, 550sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The intensity of the band of O-H-stretching vibrations at 3743 cm<sup>-1</sup> is anomalously low, and the wavenumber is anomalously high. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 789s, 749w, 402w, 315w.

### V158 Ziminaite monoclinic polymorph $\text{Fe}^{3+}(\text{VO}_4)$



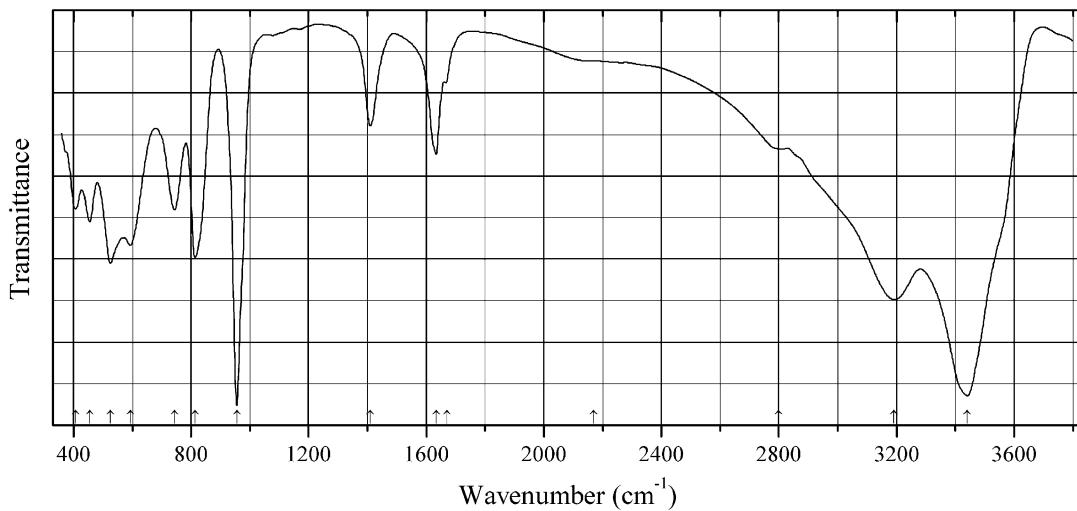
**Origin:** Synthetic.

**Description:** Obtained using a sol-gel technique with subsequently heating the sol at 500 °C. Characterized by electron diffraction. Monoclinic.

**Kind of sample preparation and/or method of registration of the spectrum:** Film on a Si wafer. Absorption.

**Source:** Vuk et al. (2001).

**Wavenumbers (cm<sup>-1</sup>):** 990w, 965w, 896, 882s, 830s, 766sh, 730sh, 652s, 502.

**V159 Wernerbaurite**  $\{(NH_4)_2[Ca_2(H_2O)_{14}](H_2O)_2\}\{V_{10}O_{28}\}$ 

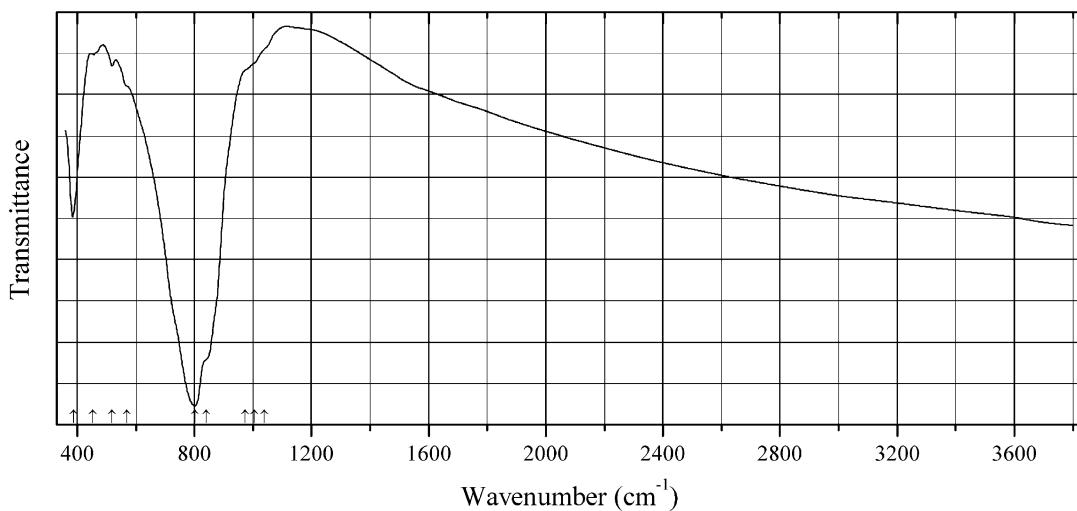
**Origin:** St Jude Mine, Gypsum Valley, Slick Rock District, San Miguel Co., Colorado, USA (type locality).

**Description:** Orange granular aggregate from the association with U,V-oxides. Investigated by A.V. Kasatkin. Characterized by single-crystal X-ray diffraction data. Triclinic,  $a = 9.709(10)$ ,  $b = 10.272(11)$ ,  $c = 10.599(7)$  Å,  $\alpha = 90.05(7)^\circ$ ,  $\beta = 77.09(7)^\circ$ ,  $\gamma = 69.90(9)^\circ$ ,  $V = 964(1)$  Å<sup>3</sup>. The empirical formula is (electron microprobe):  $(NH_4)_xCa_{1.96}V_{10.00}O_{28} \cdot nH_2O$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3441s, 3190s, 2800, 2170w, 1670w, 1635, 1410, 956s, 814, 744, 593, 526, 456, 408.

**Note:** The spectrum was obtained by N.V. Chukanov.

**V160 Schäferite Ni analogue**  $(Ca_2Na)Ni_2(VO_4)_3$ 

**Origin:** Slag dump near the Kamariza mine, Lavrion, mining district, Attikí (Attika, Attica) Prefecture, Greece.

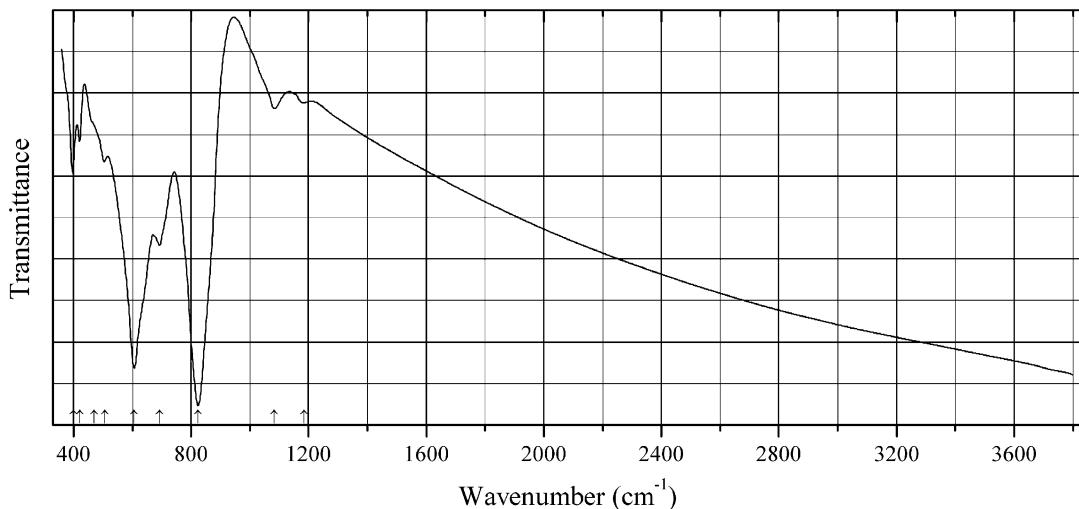
**Description:** Dark olive-green crust from the association with trevorite and liebenbergite. The empirical formula is (electron microprobe):  $(\text{Ca}_{1.93}\text{Na}_{1.04})(\text{Ni}_{1.32}\text{Mg}_{0.44}\text{Fe}_{0.25})(\text{V}_{2.93}\text{P}_{0.06}\text{Cr}_{0.03}\text{Si}_{0.01})\text{O}_{12}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1040sh, 1005sh, 975sh, 840sh, 801s, 570sh, 519w, 454w, 387.

**Note:** The spectrum was obtained by N.V. Chukanov.

### V161 Pucherite $\text{Bi}(\text{VO}_4)$



**Origin:** Neustädtel, Erzgebirge (Ore Mts.), Saxony, Germany.

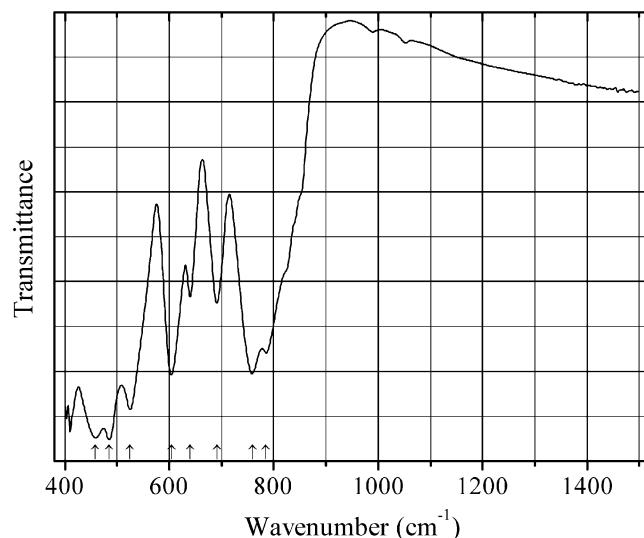
**Description:** Yellowish-brown crystals.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1184w, 1083w, 824s, 693, 606s, 507, 470sh, 421, 400.

**Note:** The spectrum was obtained by N.V. Chukanov.

### V162 Cheremnykhite trigonal dimorph $\text{Pb}_3\text{Zn}_3(\text{TeO}_6)(\text{VO}_4)_2$



**Origin:** Synthetic.

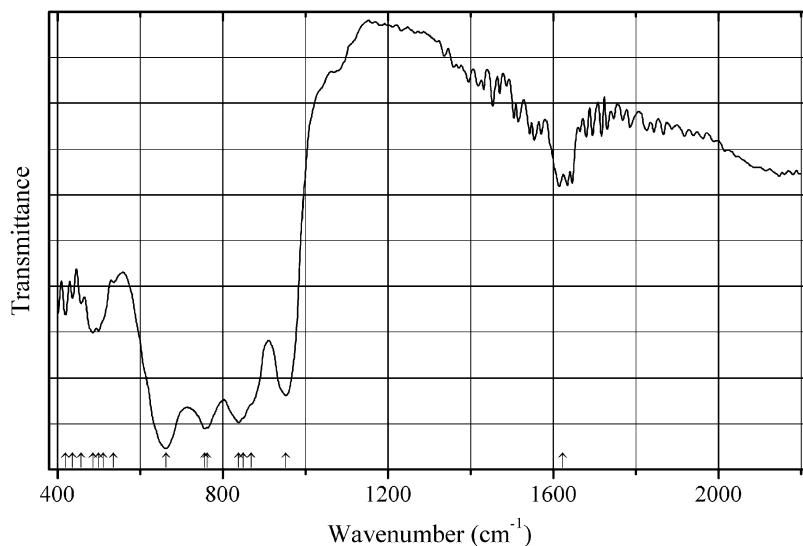
**Description:** Synthesized by conventional solid-state methods from stoichiometric amounts of PbO, ZnO, H<sub>2</sub>TeO<sub>4</sub>·2H<sub>2</sub>O, and V<sub>2</sub>O<sub>5</sub> first at 400 °C for 20 h to decompose H<sub>2</sub>TeO<sub>4</sub>·2H<sub>2</sub>O and thereafter at 700 °C for 5 days, with intermediate grindings. Characterized by powder and single-crystal X-ray diffraction data. Trigonal, space group *P*321, *a* = 8.608(2), *c* = 5.186(3) Å, *V* = 332.8(2) Å<sup>3</sup>, *Z* = 1. *D*<sub>calc</sub> = 6.343 g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Yu et al. (2016).

**Wavenumbers (cm<sup>-1</sup>):** 785, 759s, 691, 640, 604s, 525, 485s, 459s.

### V163 Fervanite (?) Fe<sup>3+</sup><sub>4</sub>V<sup>5+</sup><sub>4</sub>O<sub>16</sub>·5H<sub>2</sub>O



**Origin:** Synthetic.

**Description:** Poor-crystallized yellow powder prepared in the reaction between boiling aqueous solutions of ferric iron nitrate and V<sub>2</sub>O<sub>5</sub>. The empirical formula is FeVO<sub>4</sub>·1.1H<sub>2</sub>O.

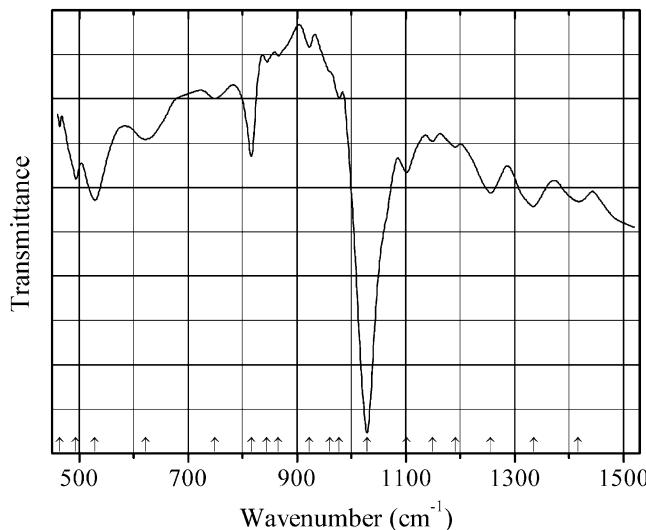
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Melghit and Al-Mungi (2007).

**Wavenumbers (cm<sup>-1</sup>):** 1624, 953, 870sh, 850sh, 839s, 763sh, 757s, 663s, 537w, 511sh, (500), 486, (458), (437), (420).

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

## **V164 Ronneburgite** $K_2MnV_4O_{12}$



**Origin:** Ronneburg, Thuringia, Germany (type locality).

**Description:** Reddish-brown crystals from the association with hummerite, gypsum, epsomite, picromerite and hematite. Holotype sample. The crystal structure contains infinite metavanadate chains of corner-sharing  $\text{VO}_4$  tetrahedra. Monoclinic, space group  $P2_1/n$ ,  $a = 8.183(3)$ ,  $b = 9.247(3)$ ,  $c = 8.651(2)$  Å,  $\beta = 109.74(2)^\circ$ ,  $Z = 2$ .  $D_{\text{meas}} = 2.84$  g/cm $^3$ ,  $D_{\text{calc}} = 2.85$  g/cm $^3$ . Optically biaxial (-),  $\alpha = 1.925(5)$ ,  $\beta = 1.960(10)$ ,  $\gamma = 1.988(4)$ ,  $2V = 82^\circ$ . The empirical formula is  $\text{K}_{1.91}\text{Mn}_{0.93}\text{Mg}_{0.08}\text{V}_{4.00}\text{O}_{11.96}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 3.701 (55) (-211), 3.336 (100) (121), 3.118 (50) (-122), 3.000 (36) (112), 2.878 (64) (-103, 031), 2.752 (68) (-222).

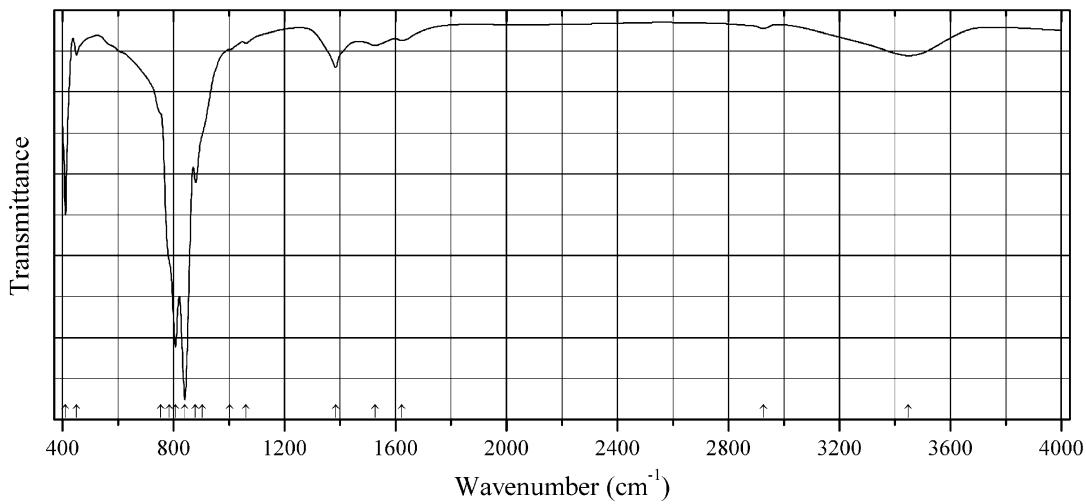
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission of a small plate-like chip using an IR microscope.

Source: Witzke et al. (2001).

**Wavenumbers (IR, cm<sup>-1</sup>):** (1417), (1335), (1256), (1191), (1149), 1102, 1029s, 978w, 961sh, 923w, 866w, 845w, 816, 749, 622, 529, 494, (464).

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. Peaks above 1102 cm<sup>-1</sup> may be due to interference. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 952s, 942sh, 911, 878s, 830w, 658w, 461, 350, 336, 261.

**V165 Wakefieldite-(Y)  $\text{YVO}_4$** 

**Origin:** Synthetic.

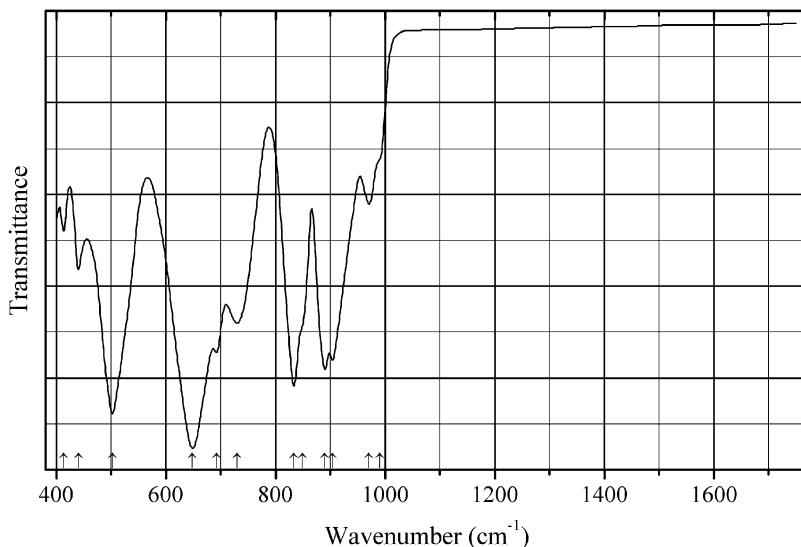
**Description:** Eu-doped sample prepared hydrothermally from sodium orthovanadate and corresponding nitrates at Y: Eu = 9:1. Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** Absorption. Kind of sample preparation is not indicated.

**Source:** Tran et al. (2012).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3449, 2926w, 1624w, 1526w, 1384, 1061w, 1003sh, 905sh, 880, 841s, 808s, 785sh, 755sh, 451w, 426, 411.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The band at 2926  $\text{cm}^{-1}$  corresponds to the admixture of an organic substance. The band at 1384  $\text{cm}^{-1}$  indicates possible admixture of nitrate anions. The bands at 3449 and 1624  $\text{cm}^{-1}$  correspond to adsorbed water molecules.

**V166 Ziminaite  $\text{Fe}^{3+}_6(\text{VO}_4)_6$** 

**Origin:** Synthetic.

**Description:** Nanorods obtained by dehydration of synthetic fervanite at 500 °C. Characterized by powder X-ray diffraction data and Mössbauer spectroscopy. Triclinic.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

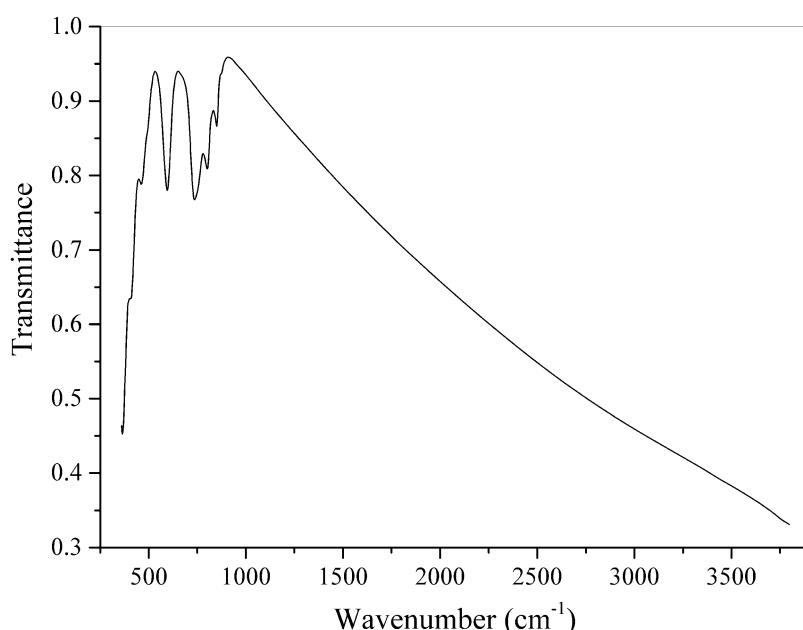
**Source:** Lehnens et al. (2014).

**Wavenumbers (IR, cm<sup>-1</sup>):** 990sh, 970, 904s, 890s, 849sh, 833s, 730, 692, 648s, 502s, 440, 413w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 965, 931s, 907, 895s, 845s, 832s, 770, 736s, 660w, 633w, 502w, 450, 408, 391, 371, 329, 317.

### V167 Janchevite Pb<sub>7</sub>V<sup>5+</sup>(O<sub>8.5</sub>□<sub>0.5</sub>)Cl<sub>2</sub>



**Origin:** Kombat mine, Grootfontein district, Otjozondjupa region, Namibia (type locality).

**Description:** Orange-red, thick tabular anhedral grains from the association with baryte, hausmannite, calcite, magnesite, and kombatite. Holotype sample. Tetragonal, space group *I4/mmm*,  $a = 3.9591$  (5) Å,  $c = 22.6897(3)$  Å,  $V = 355.65(1)$  Å<sup>3</sup>;  $Z = 1$ .  $D_{\text{calc}} = 8.18$  g/cm<sup>3</sup>. The empirical formula is (electron microprobe): Pb<sub>7.20</sub>V<sup>5+</sup><sub>0.38</sub>Mo<sup>6+</sup><sub>0.29</sub>Si<sub>0.13</sub>Cl<sub>2.06</sub>O<sub>8.25</sub>. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å (I, %) ( $hkl$ )] are: 3.889 (24) (011), 3.501 (31) (013), 2.979 (86) (015), 2.833 (25) (008), 2.794 (100) (110), 1.992 (26) (118), 1.988 (49) (020), 1.649 (46) (215).

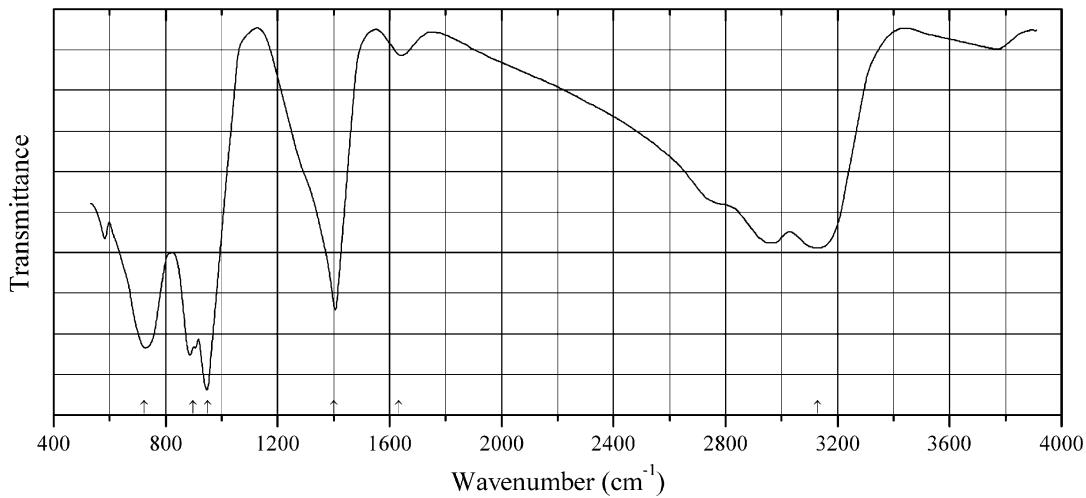
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 870w, 850, 802, 736, 595, 462, 405sh, 366s.

**Note:** The spectrum was obtained by N.V. Chukanov.

## 2.12 Chromates

**Cr21 Ammonium dichromate**  $(\text{NH}_4)_2\text{Cr}_2\text{O}_7$



**Origin:** Synthetic.

**Description:** Analytical grade reactant.

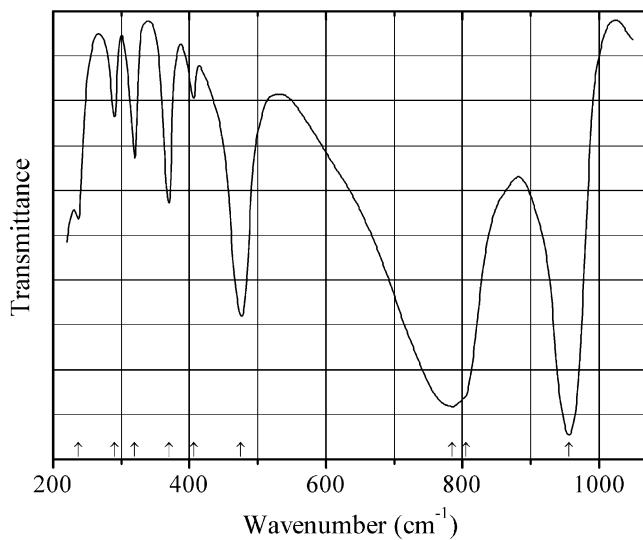
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** De Waal and Heyns (1992).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3128s, 1633w, 1402s, 949s, 898s, 724s.

**Note:** The band at 1633  $\text{cm}^{-1}$  may be due to adsorbed water.

**Cr22 Copper chromate**  $\text{CuCrO}_4$



**Origin:** Synthetic.

**Description:** Prepared hydrothermally from  $\text{CuCO}_3$ ,  $\text{Cu}(\text{OH})_2$ , and  $\text{CrO}_3$  at  $220\text{ }^\circ\text{C}$  for 24 h. Orthorhombic, space group  $Cmcm$ ,  $Z = 4$ . In the crystal structure, strongly distorted  $\text{CuO}_6$  octahedra are present.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

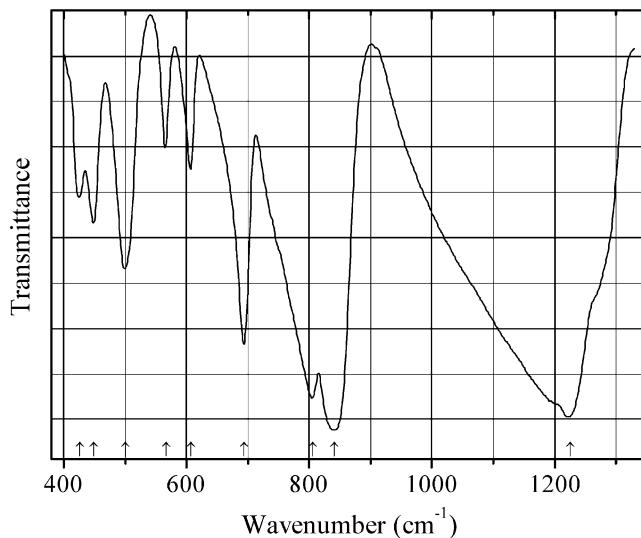
**Source:** Baran (1994).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 956s, 805sh, 785s, 475s, 406w, 370, 320, 290, 237.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 966, 944s, 928, 806s, 412, 386, 342, 254.

### Cr23 Lead orthoborate chromate $\text{Pb}_6(\text{BO}_3)_2(\text{CrO}_4)\text{O}_2$



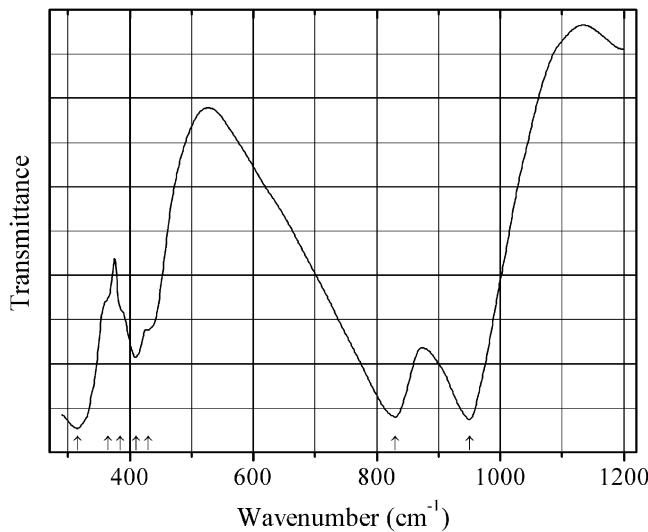
**Origin:** Synthetic.

**Description:** Prepared in a solid-state reaction from the powder mixture of  $\text{PbO}$ ,  $\text{CrO}_3$ , and  $\text{B}_2\text{O}_3$  with the molar ratio 15:2:3. Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group  $Pnma$ ,  $a = 6.4160(13)$ ,  $b = 11.635(2)$ ,  $c = 18.164(4)$  Å,  $V = 1356.0(5)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 7.391$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Chen et al. (2009).

**Wavenumbers (cm<sup>-1</sup>):** 1225s, 841s, 806s, 694s, 608, 567, 500, 449, 426.

**Cr24 Magnesium chromate  $\alpha\text{-Mg}(\text{CrO}_4)$** 

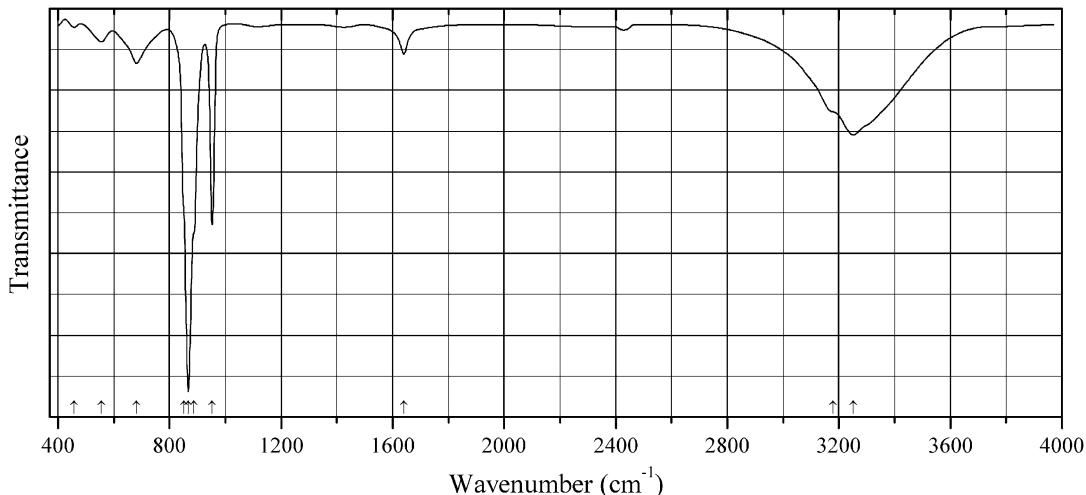
**Origin:** Synthetic.

**Description:** Orthorhombic, space group *Cmcm*,  $Z = 4$  (see Muller et al. 1969b).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Muller et al. (1969a).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 950s, 830s, 430sh, 410, 385sh, 365sh, 315s.

**Cr25 Potassium magnesium chromate hydrate  $\text{K}_2\text{Mg}(\text{CrO}_4)_2 \cdot 2\text{H}_2\text{O}$** 

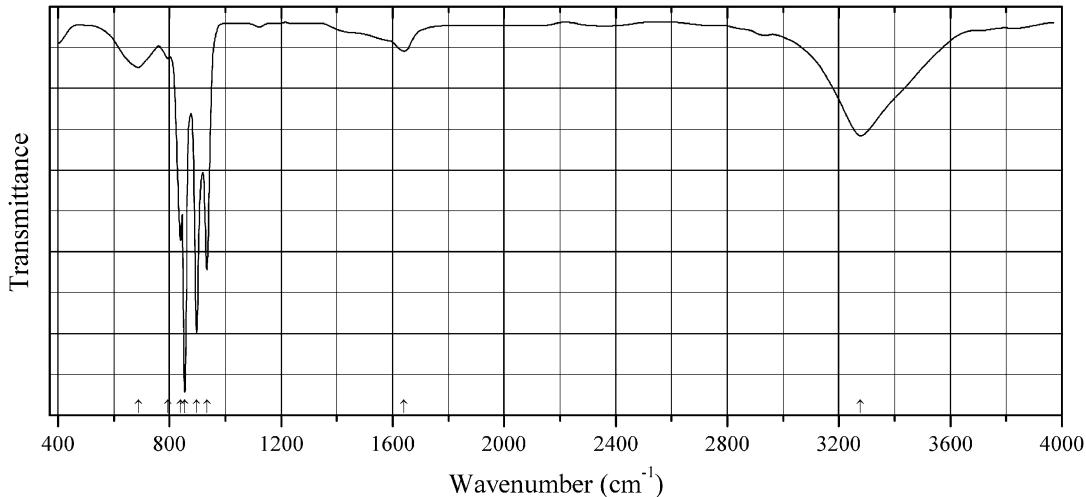
**Origin:** Synthetic.

**Description:** Prepared by precipitation from aqueous solution of magnesium acetate and potassium chromate. Triclinic, space group *P-1*,  $Z = 1$ . Structurally related to kröhnkite.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.  
**Source:** Stoilova et al. (2009).

**Wavenumbers (cm<sup>-1</sup>):** 3251s, 3180sh, 1640, 953s, 887sh, 867s, 852sh, 682, 556, 458w.

**Cr26 Potassium nickel chromate hydrate**  $K_2Ni(CrO_4)_2 \cdot 2H_2O$



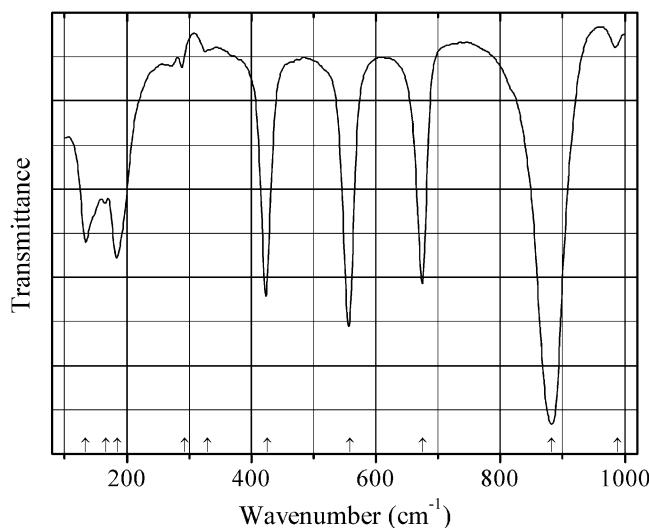
**Origin:** Synthetic.

**Description:** Prepared by precipitation from aqueous solution of nickel acetate and potassium chromate. Triclinic, space group *P*-1, *Z* = 1. Structurally related to kröhnkite.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.  
**Source:** Stoilova et al. (2009).

**Wavenumbers (cm<sup>-1</sup>):** 3278 (broad), 1640w, 934s, 897s, 855s, 840, 793, 688 (broad).

**Cr27 Potassium peroxochromate**  $K_3[Cr(O_2)_4]$



**Origin:** Synthetic.

**Description:** Tetragonal, space group  $I-42m$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

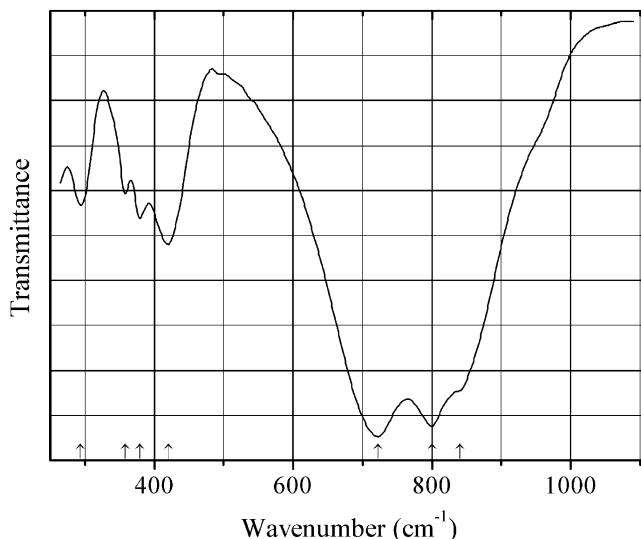
**Source:** Haeuseler and Haxhillazi (2003).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 988w, 883s, 676s, 558s, 426s, 330w, 293w, 185, 166w, 134.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 919s, 879, 838w, 682w, 564s, 526, 464s, 430s, 336, 286, 217w, 183w.

### Cr28 Praseodymium chromate(V) $\text{PrCrO}_4$



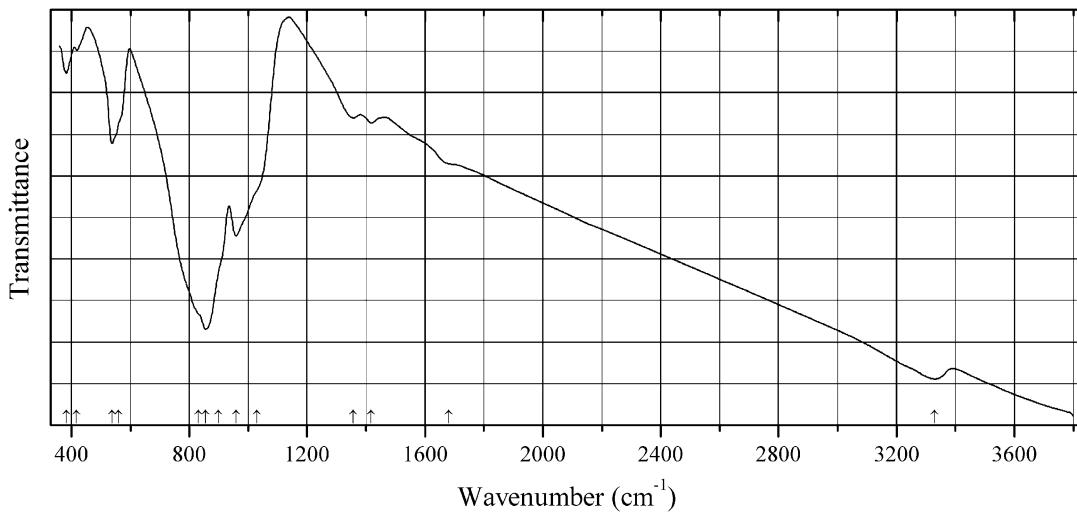
**Origin:** Synthetic.

**Description:** Prepared by heating  $\text{PrCr}(\text{C}_2\text{O}_4)_3 \cdot 8\text{H}_2\text{O}$  at 500 °C for 10 min. Characterized by powder X-ray diffraction data. Triclinic, space group  $P\bar{2}_1/n$ ,  $a = 6.98(2)$ ,  $b = 7.16(1)$ ,  $c = 6.63(1)$  Å,  $\beta = 105.22(10)^\circ$ ,  $V = 319.72$  Å<sup>3</sup>,  $Z = 4$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 3.58 (30) (020, 111), 3.36 (59) (200), 3.162 (100) (120), 2.925 (74) (012), 1.989 (30) (212), 1.921 (34) (-132).

**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc.  
Transmission.

**Source:** Manca and Baran (1981).

**Wavenumbers (cm<sup>-1</sup>):** 840sh, 800s, 722s, 420, 379, 358, 294.

**Cr29 Embreyite**  $(\text{Pb}, \text{Cu}, \square)_2\text{Pb}[(\text{Cr}, \text{P})\text{O}_4]_2 \cdot n\text{H}_2\text{O}$ 

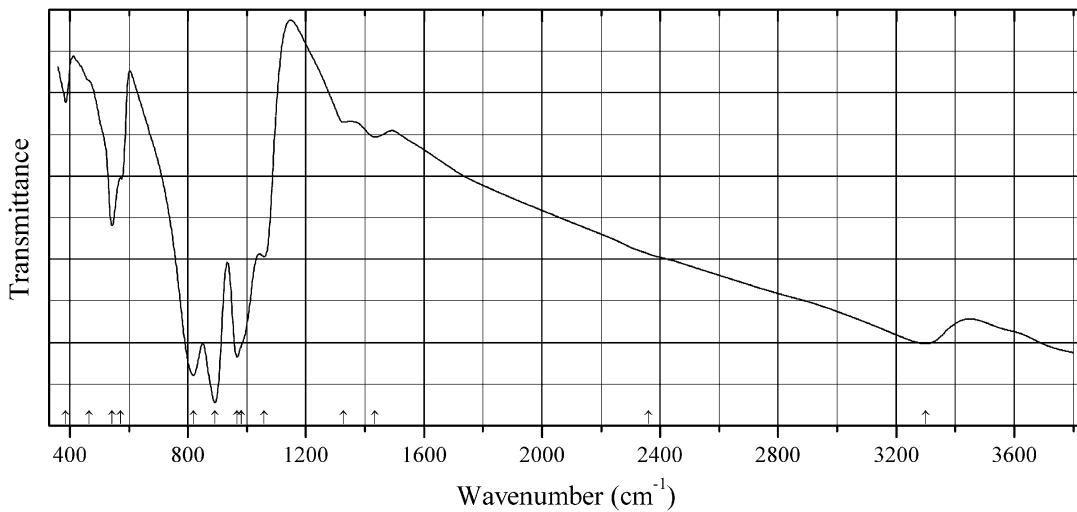
**Origin:** Krokotovyi Shurf (Crocoite Pit), Uspenskaya Mt., Berezovskoe ore field, Middle Urals.

**Description:** Brownish-orange flattened crystals from the association with crocoite, vauquelinite pyromorphite, and goethite. The crystal structure is solved. Monoclinic, space group  $C2/m$ ,  $a = 9.802(16)$ ,  $b = 5.603(9)$ ,  $c = 7.649(12)$  Å,  $\beta = 114.85(3)^\circ$ ,  $V = 381.2(11)$  Å<sup>3</sup>. The empirical formula is (electron microprobe,  $Z = 2$ ):  $\text{Pb}_{1.29}\text{Cu}_{0.07}\text{Cr}_{0.52}\text{P}_{0.43}\text{O}_4 \cdot n\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3329, 1680w, 1418w, 1356w, 1030sh, 959, 900sh, 855s, 830sh, 560sh, 538, 418w, 383.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Cr30 Embreyite**  $(\text{Pb}, \text{Cu}, \square)_2\text{Pb}[(\text{Cr}, \text{P})\text{O}_4]_2 \cdot n\text{H}_2\text{O}$ 

**Origin:** Krokotovyi Shurf (Crocoite Pit), Uspenskaya Mt., Berezovskoe ore field, Middle Urals.

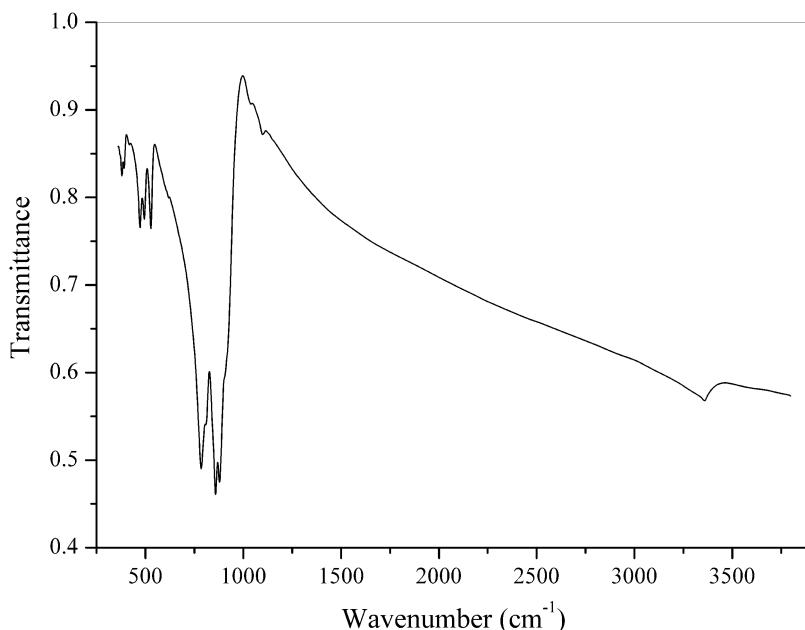
**Description:** Reddish-brown crystals from the association with vauquelinite. A Cu-rich variety. The empirical formula is (electron microprobe, Z = 1):  $\text{Pb}_{2.5}\text{Cu}_{0.3}\text{Cr}_{1.05}\text{P}_{0.95}\text{O}_8 \cdot n\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3301, 1433, 1328w, 1059, 980sh, 966s, 891s, 819s, 572, 543, 465sh, 386.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Cr31 Iranite**  $\text{Pb}_{10}\text{Cu}(\text{CrO}_4)_6(\text{SiO}_4)_2(\text{OH})_2$



**Origin:** Santa Ana mine, Caracoles, Sierra Gorda district, Antofagasta Region, Chile.

**Description:** Brownish-orange lenticular crystals from the association with wulfenite. Confirmed by the IR spectrum and qualitative electron microprobe analyses.

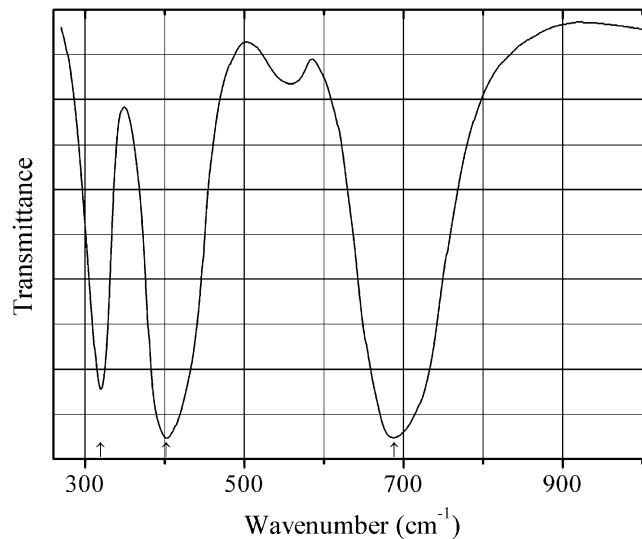
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3359, 1099w, 1037w, 905sh, 879s, 858s, 807, 785s, 620w, 528, 495, 473, 417w, 389, 379.

**Note:** The spectrum was obtained by N.V. Chukanov. The weak bands at 1099, 1037, and 620  $\text{cm}^{-1}$  correspond to trace amounts of  $\text{SO}_4^{2-}$  anions.

## 2.13 Germanates

**Ge4 Brunogeierte**  $\text{Fe}^{2+}\text{Ge}^{4+}\text{O}_4$



**Origin:** Synthetic.

**Description:** Prepared in the solid-state reaction between  $\text{GeO}_2$  and  $\text{FeO}$  at 1000 °C.

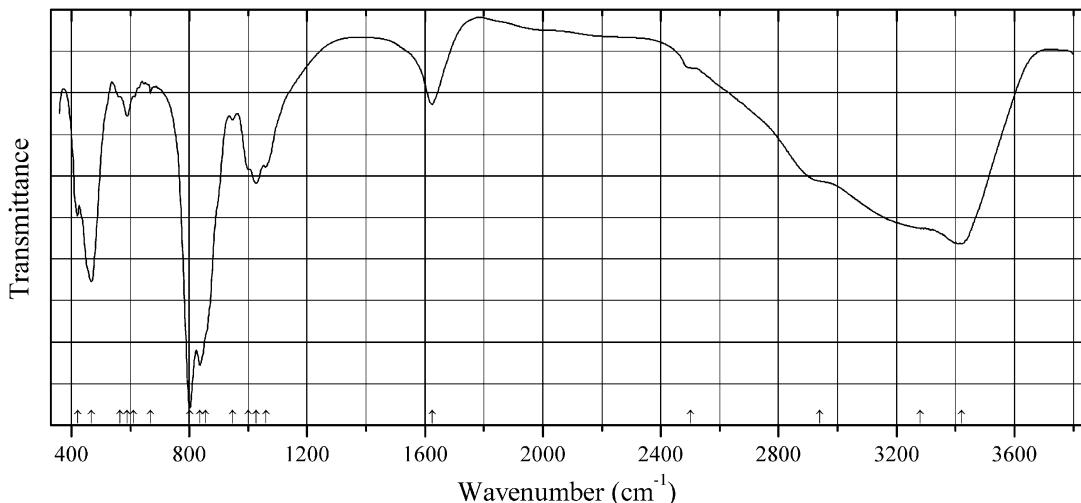
**Kind of sample preparation and/or method of registration of the spectrum:** No data.

**Source:** Tarte (1963).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 688s, 402s, 319.

## 2.14 Arsenides, Arsenites, Arsenates, and Sulfato-Arsenates

**As316 Castellaroite**  $\text{Mn}^{2+}\text{AsO}_4 \cdot 4\text{H}_2\text{O}$



**Origin:** Monte Nero Mine, Rocchetta Vara, La Spezia Province, Liguria, Italy (type locality).

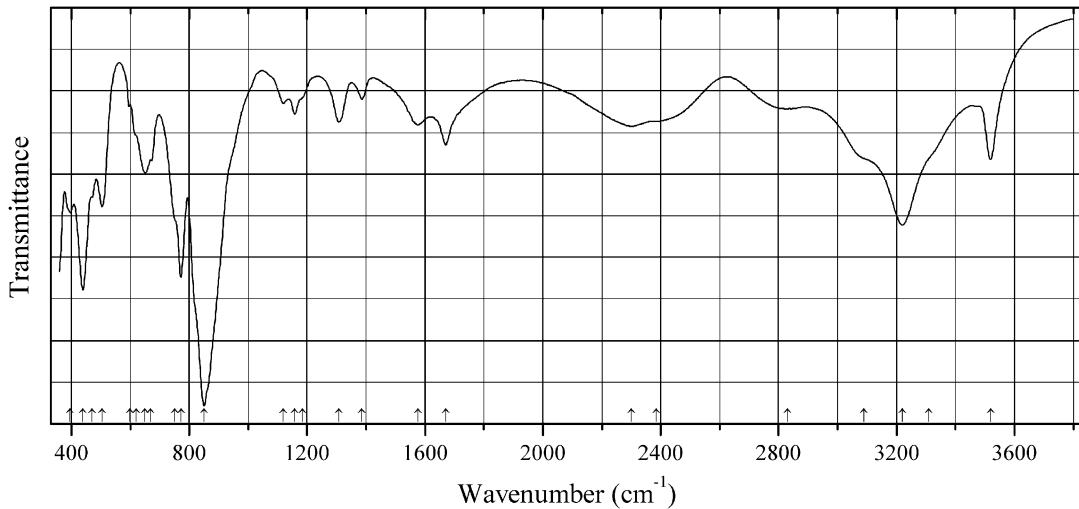
**Description:** White radiated aggregates from the association with rhodochrosite. The sample was received from L. Chiappino, a coauthor of the first description of castellaroite.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3421s (broad), 3280sh, 2940sh, 2500sh, 1624, 1061, 1027, 1001, 948w, 855sh, 836s, 801s, 669w, 610sh, 589, 565sh, 468s, 421.

**Note:** The spectrum was obtained by N.V. Chukanov.

### As317 Magnesiokoritnigite Mg(AsO<sub>3</sub>OH)·H<sub>2</sub>O



**Origin:** Torrecillas mine, Salar Grande, El Tamarugal Province, Tarapacá Region, Chile (type locality).

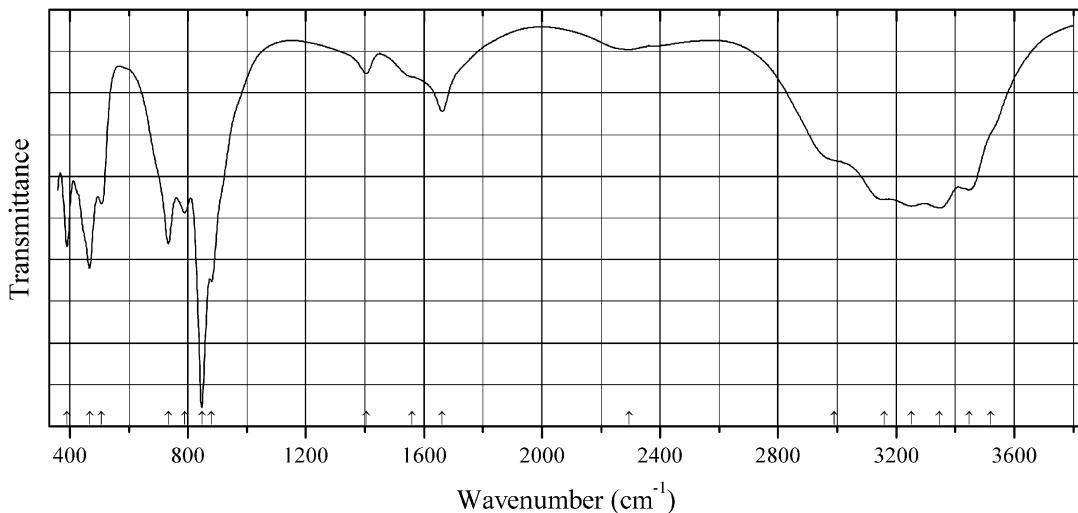
**Description:** Pink crystals from the association with magnesiocanutite. Investigated by I.V. Pekov.

The empirical formula is (electron microprobe): (Mg<sub>0.99</sub>Mn<sub>0.01</sub>)(HAsO<sub>4</sub>)·H<sub>2</sub>O.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3519, 3310sh, 3220s, 3090sh, 2830, 2385, 2301, 1670, 1576, 1386w, 1307, 1185sh, 1158, 1120w, 850s, 772s, 750sh, 670, 650, 620sh, 599w, 504, 470sh, 439s, 395.

**Note:** The spectrum was obtained by N.V. Chukanov.

**As318 Chudobaite**  $(\text{Mg}, \text{Zn})_5(\text{AsO}_4)_2(\text{HAsO}_4)_2 \cdot 10\text{H}_2\text{O}$ 

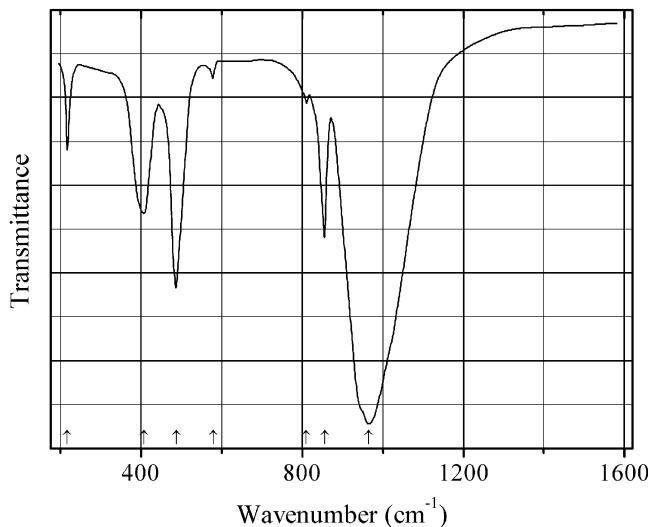
**Origin:** Torrecillas mine, Salar Grande, El Tamarugal Province, Tarapacá Region, Chile.

**Description:** White granular aggregate from the association with hörnésite, gypsum, arsenic, pyrite, dolomite, and quartz. Investigated by I.V. Pekov. Identified by qualitative electron microprobe analyses and powder X-ray diffraction data. The strongest lines of the powder X-ray diffraction pattern [ $d, \text{\AA}$  ( $I, \%$ )] are: 10.26 (100), 7.70 (11), 4.79 (15), 3.423 (15), 2.973 (22), 2.735 (11).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3520sh, 3447, 3346s, 3252, 3160, 2990sh, 2295w, 1662, 1560sh, 1404w, 879s, 847s, 789, 734s, 507, 467s, 301s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**As319 Boron arsenate**  $\text{B}(\text{AsO}_4)$ 

**Origin:** Synthetic.

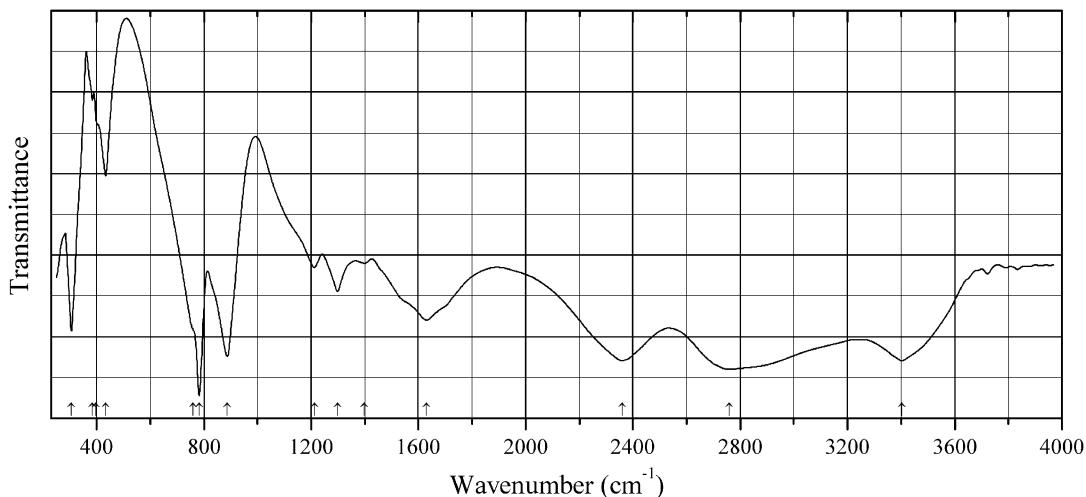
**Description:** Structurally related to cristobalite.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

**Source:** Rulmont et al. (1987).

**Wavenumbers (cm<sup>-1</sup>):** 965s, 857, 809w, 580w, 488s, 408, 217.

### As320 Cesium acid (pentahydrogen) arsenate CsH<sub>5</sub>(AsO<sub>4</sub>)<sub>2</sub>



**Origin:** Synthetic.

**Description:** Produced from an aqueous stoichiometric solution of cesium carbonate and orthoarsenic acid. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 10.983(1)$ ,  $b = 7.943(1)$ ,  $c = 9.844(1)$  Å,  $\beta = 96.15(1)^\circ$ ,  $V = 853.82(6)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 3.235$  g/cm<sup>3</sup>.

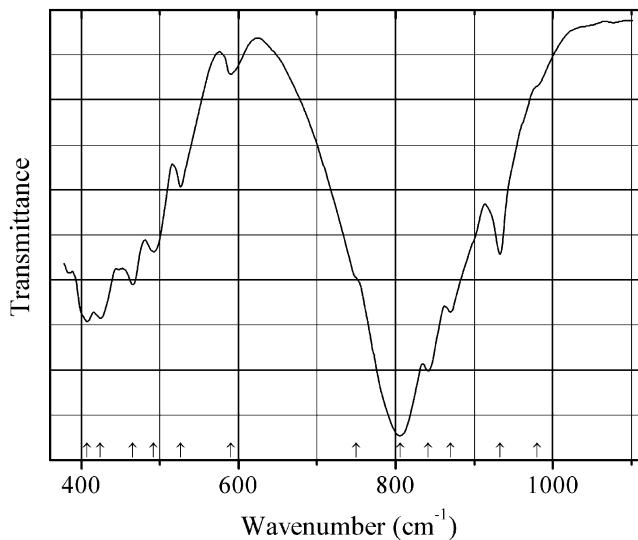
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Naīli et al. (2001).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3402s (broad), 2760s (broad), 2360s (broad), 1631 (broad), 1399, 1299, 1212, 887s, 782s, 760sh, 434, 398sh, 384, 306.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 830s, 767s, 415s, 370, 335, 290, 265, 235, 200sh, 170w, 125w, 100w, 75, 65, 42, 39, 25.

**As321 Cesium iron arsenate  $\text{Cs}_7\text{Fe}_7\text{O}_2(\text{AsO}_4)_8$** 

**Origin:** Synthetic.

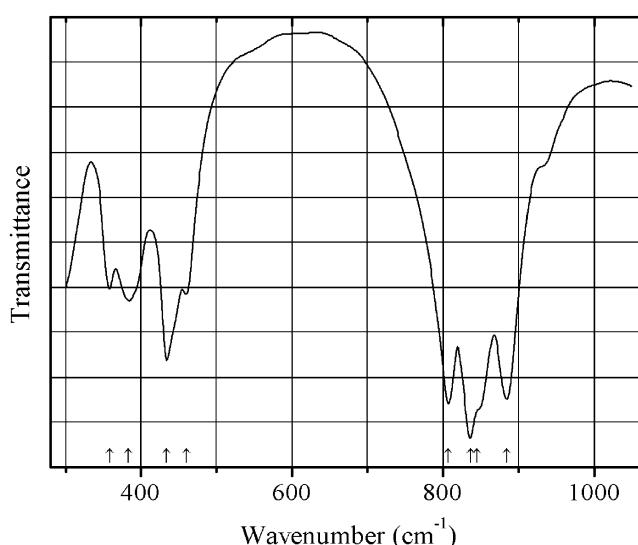
**Description:** Prepared from the mixture of  $\text{Cs}_2\text{CO}_3$ ,  $\text{Fe}_2\text{O}_3$ , and  $(\text{NH}_4)(\text{H}_2\text{AsO}_4)$  in the molar ratio 3:3:4 heated first at 450 °C for 12 h and then at 800 °C for 10 days. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 8.464(2)$ ,  $b = 23.146(5)$ ,  $c = 10.214(3)$  Å,  $\beta = 107.87(2)^\circ$ ,  $V = 1904.5$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 4.298$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Fitouri et al. (2015).

**Wavenumbers (cm<sup>-1</sup>):** 980sh, 933, 870, 841s, 806s, 750sh, 590w, 526, 492, 465, 424, 407.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**As322 Calcium chlorarsenate  $\text{Ca}_2(\text{AsO}_4)\text{Cl}$** 

**Origin:** Synthetic.

**Description:** Crystals grown from melt by means of a reaction flux technique using  $\text{As}_2\text{O}_3$ ,  $\text{CaCl}_2$ , and  $\text{CaCO}_3$  as starting materials. Related to chlor-spodiosite. Orthorhombic, space group  $Pbcm$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

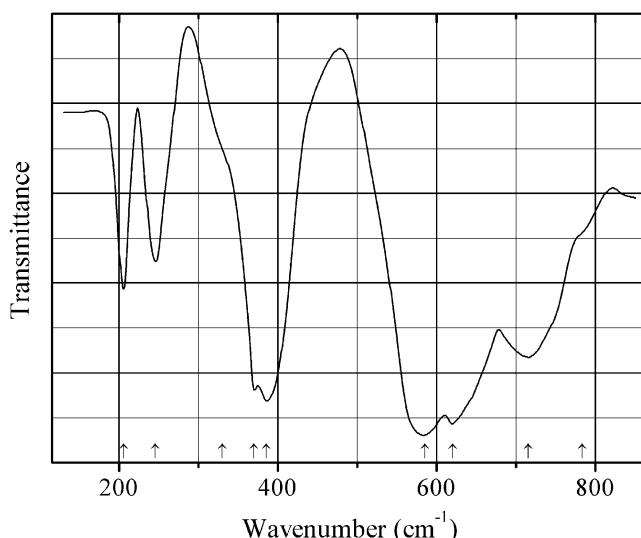
**Source:** Kowalczyk and Condrate Sr (1974).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 885s, 845sh, 837s, 807s, 460, 434s, 383, 359.

**Note:** In the paper by Kowalczyk and Condrate Sr (1974) the wavenumber  $460 \text{ cm}^{-1}$  is erroneously indicated as  $470 \text{ cm}^{-1}$ . In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 878s, 870, 838s, 813, 497w, 466w, 390, 314.

### As323 Calcium arsenate $\text{CaAs}_2\text{O}_6$ $\text{CaAs}_2\text{O}_6$



**Origin:** Synthetic.

**Description:** Obtained in a solid-state reaction between  $\text{CaCO}_3$  and  $\text{As}_2\text{O}_3$ . In the crystal structure,  $\text{AsO}_6$  octahedra are present. Trigonal, space group  $P-31/m$ ,  $a = 4.82$ ,  $c = 5.07 \text{ \AA}$ .

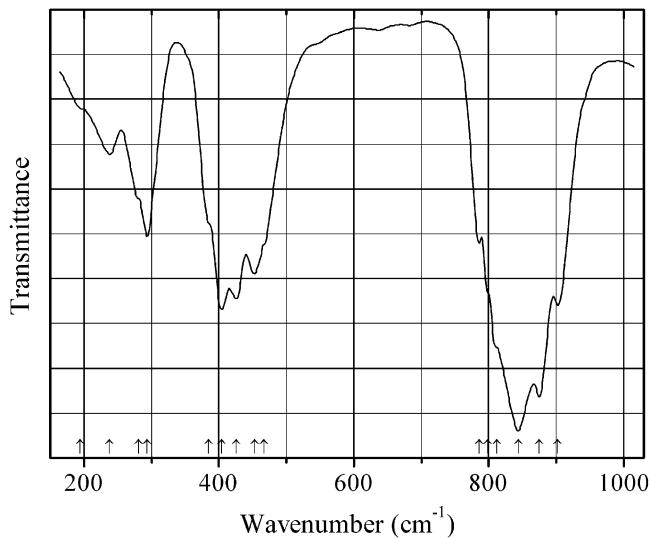
**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc.  
Transmission.

**Source:** Husson et al. (1984).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 783sh, 715, 620s, 585s, 385s, 370s, 330sh, 245, 205.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman, spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 762s, 590w, 570, 426, 397, 286s.

**As324 Calcium orthoarsenate trigonal polymorph**  $\text{Ca}_3(\text{AsO}_4)_2$ 

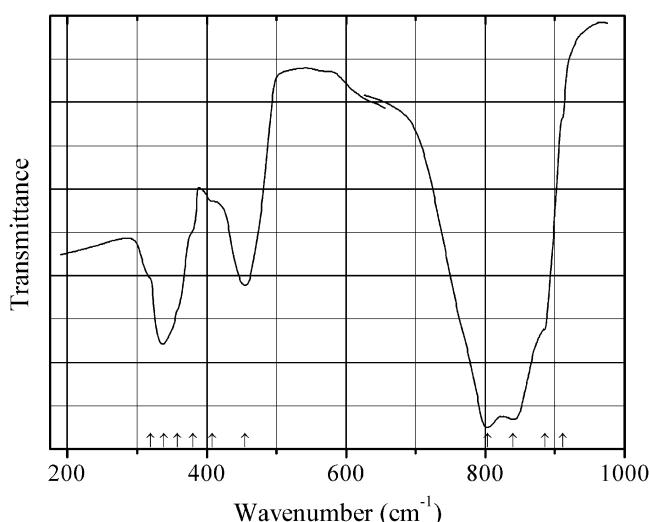
**Origin:** Synthetic.

**Description:** Prepared in a solid-state reaction, from a mixture of  $\text{CaCO}_3$  and  $\text{As}_2\text{O}_5$ , first at  $700\text{ }^\circ\text{C}$  for 7 h and thereafter (after trituration of the product) at  $800\text{ }^\circ\text{C}$  for 3 h. Trigonal, space group  $R\bar{3}c$ ,  $Z = 7$ .

**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc. Transmission.

**Source:** Baran (1976).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 902, 875s, 844s, 812sh, 799sh, 786, 467sh, 453, 426, 404, 385, 294, 281sh, 238, 195w.

**As325 Calcium samarium thorium arsenate**  $\text{CaSmTh}(\text{AsO}_4)_3$ 

**Origin:** Synthetic.

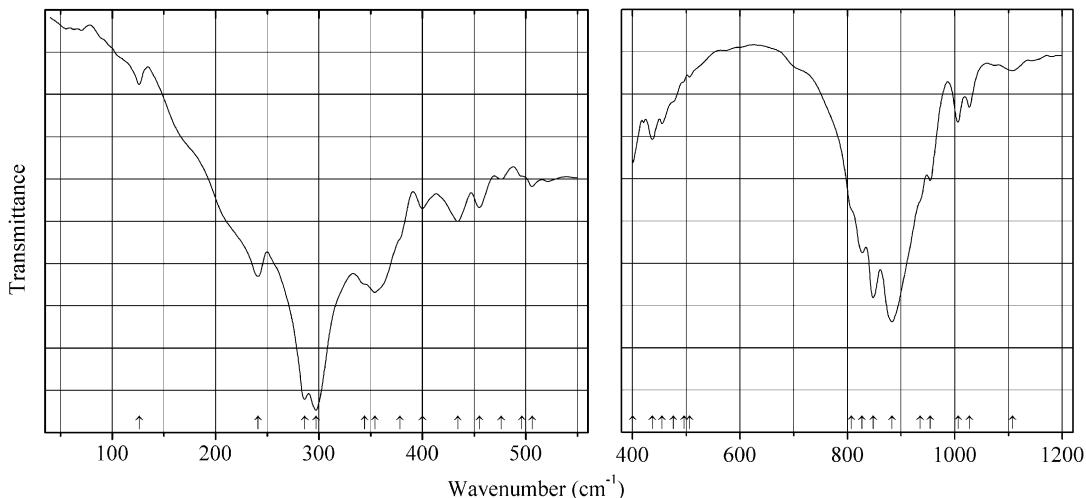
**Description:** Prepared by a standard solid-state method. Structurally related to xenotime-group minerals. Tetragonal, space group  $I4_1/amd$ ,  $a = 7.175(2)$ ,  $c = 6.409(3)$  Å,  $V = 330.0$  Å $^3$ .  $D_{\text{meas}} = 5.61$  g/cm $^3$ ,  $D_{\text{calc}} = 5.63$  g/cm $^3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** CsBr disc. Absorption.

**Source:** Nabar and Sakhardande (1985).

**Wavenumbers (cm $^{-1}$ ):** 911sh, 886sh, 840s, 803s, 455, 408sh, 380sh, 358sh, 338, 319sh.

### As326 Lithium zirconium arsenate $\text{LiZr}_2(\text{AsO}_4)_3$



**Origin:** Synthetic.

**Description:** Synthesized from stoichiometric amounts of  $\text{LiNO}_3$ ,  $\text{ZrOCl}_2$ , and arsenic acid using a precipitation method. In the structure which has a  $P112_1/n$  space group, the arsenic atoms occupy three independent positions.

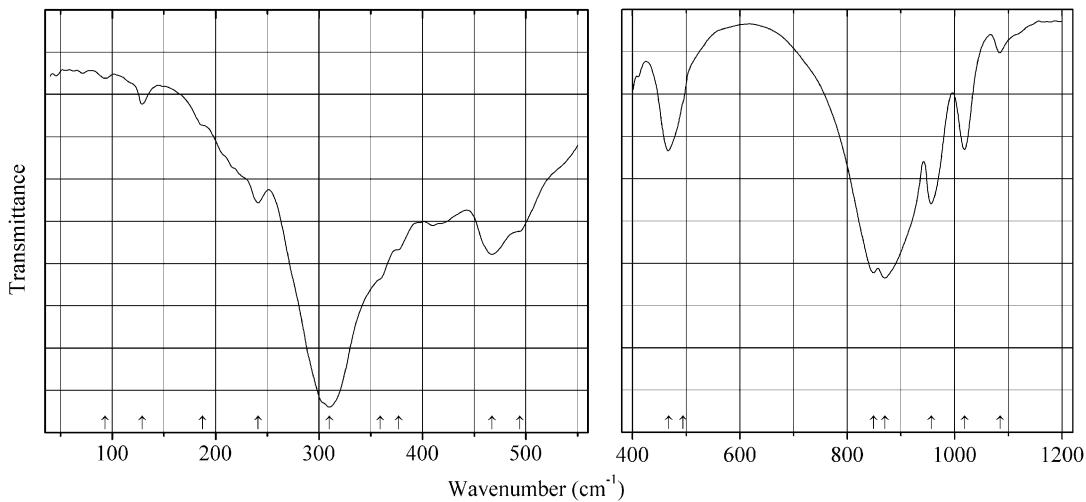
**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Absorption.

**Source:** Borovikova et al. (2014).

**Wavenumbers (IR, cm $^{-1}$ ):** 1107w, 1027w, 1006w, 954, 935sh, 883s, 848s, 827, 807sh, 506w, 496sh, 476sh, 455w, 437w, 400w, 378sh, 354, 344sh, 297s, 286s, 241, 126w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 976s, 953, 938w, 876, 869s, 854s, 848, 820, 805w, 474, 430, 388, 364, 354, 336, 269w, 256, 230, 194, 178w.

**As327 Lithium zirconium arsenate**  $\text{LiZr}_2(\text{AsO}_4)_3$ 

**Origin:** Synthetic.

**Description:** Synthesized from stoichiometric amounts of  $\text{LiNO}_3$ ,  $\text{ZrOCl}_2$ , and arsenic acid using a precipitation method. Hexagonal, space group  $R\bar{3}c$ .

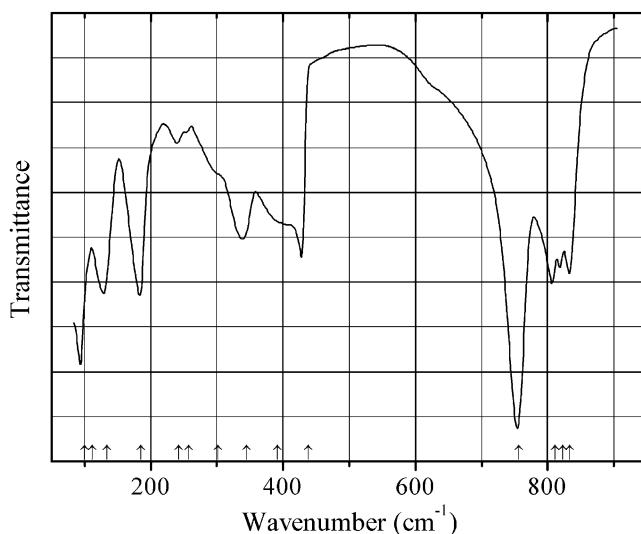
**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Absorption.

**Source:** Borovikova et al. (2014).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1084w, 1018, 956, 870s, 849s, 494sh, 467, 377sh, 359sh, 310s, 241, 187sh, 129w, 93w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 979s, 951, 864s, 857, 473, 445w, 380, 359, 346, 333, 253, 189, 176.

**As328 Mercury(I) orthoarsenate**  $(\text{Hg}_2)_3(\text{AsO}_4)_2$ 

**Origin:** Synthetic.

**Description:** Obtained as precipitate formed in the reaction of aqueous solutions of orthoarsenic acid and  $\text{Hg}_2(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$ . The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

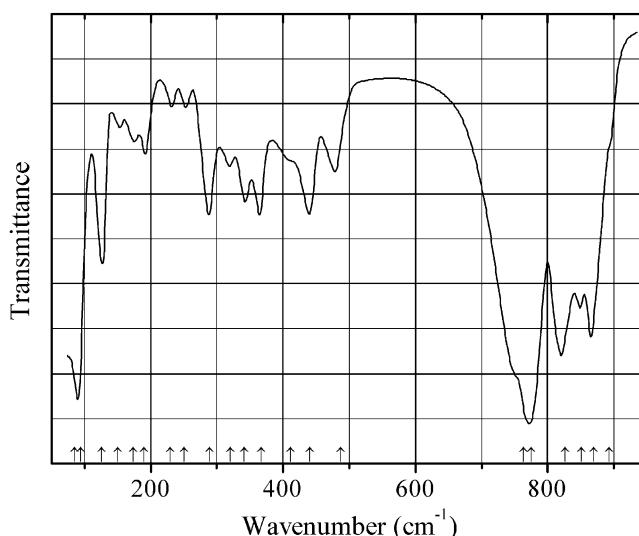
**Source:** Baran et al. (1999b).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 834, 823, 811, 757s, 438, 392sh, 345, 302sh, 258sh, 242w, 185s, 134s, 112sh, 100s.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** ~845sh, 789, 770sh, 814s, 432s, 390sh, 368w, 312w, 253w, 225w, 148s, 129s, 110w, 98s.

### As329 Mercury(II) orthoarsenate $\text{Hg}_3(\text{AsO}_4)_2$



**Origin:** Synthetic.

**Description:** Obtained as precipitate formed in the reaction of aqueous solutions of orthoarsenic acid and  $\text{Hg}(\text{NO}_3)_2 \cdot \text{H}_2\text{O}$ . The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $Z = 4$ .

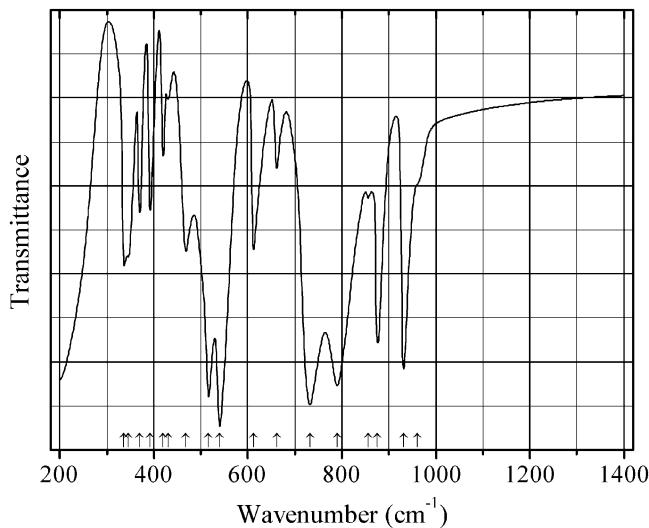
**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

**Source:** Baran et al. (1999b).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 893sh, 869s, 851s, 826s, 775s, 763sh, 487, 440, 411sh, 367, 342, 320w, 289, 250w, 230w, 190, 173w, 150w, 126s, 94s, 85sh.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 876w, 825, 784w, 759, 851s, 501, 415s, 362, 327, 278, 227, 195sh, 170sh, 140s, 110w, 86.

**As330 Potassium antimony oxoarsenate**  $K_2Sb(AsO_4)O_2$ 

**Origin:** Synthetic.

**Description:** Obtained in the solid-state reaction between  $Sb_2O_3$ ,  $As_2O_5$ , and  $K_2CO_3$  at 900 °C for 1 day. Characterized by chemical analyses. The crystal structure is solved. Orthorhombic, space group  $Pnma$ ,  $a = 9.603(6)$ ,  $b = 5.972(5)$ ,  $c = 11.304(8)$  Å,  $V = 648.27$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{meas}} = 3.76$  (5) g/cm<sup>3</sup>,  $D_{\text{calc}} = 3.79$  g/cm<sup>3</sup>.

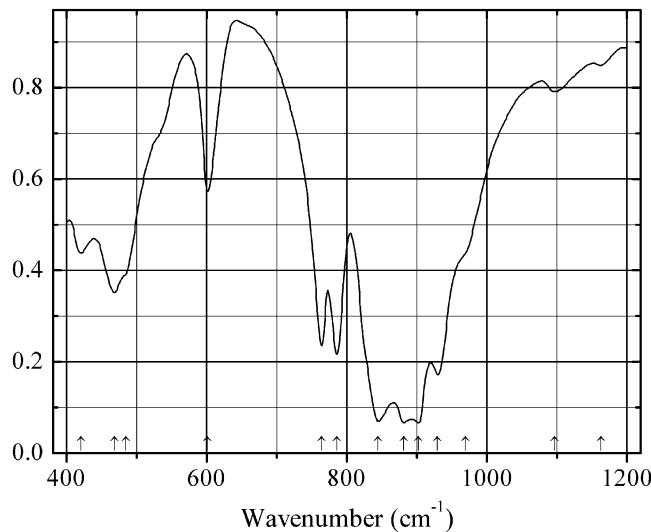
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Botto and Garcia (1989).

**Wavenumbers (IR, cm<sup>-1</sup>):** 960sh, 932s, 876s, 856w, 790s, 732s, 662, 612, 540s, 526s, 468, 430w, 420, 392, 370, 345, 336.

**Note:** The wavenumber 516 cm<sup>-1</sup> is erroneously indicated by Botto and Garcia (1989) as 526 cm<sup>-1</sup>. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 984w, 961, 915, 892w, 872s, 644s, 603w, 533s, 508sh, 475, 419w, 404w, 373, 340, 297, 279, 251.

**As331 Potassium iron diarsenate (pyroarsenate) KFe(As<sub>2</sub>O<sub>7</sub>)**


**Origin:** Synthetic.

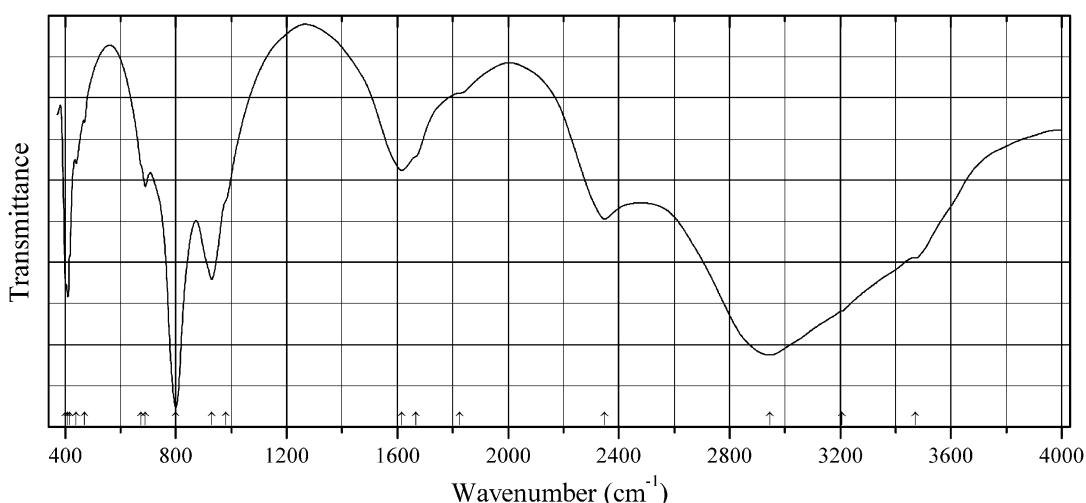
**Description:** Beige single crystals grown from aqueous solution of KNO<sub>3</sub>, Fe(NO<sub>3</sub>)<sub>3</sub>·9H<sub>2</sub>O, and H<sub>3</sub>AsO<sub>4</sub> with the molar ratio of 10:1:20, with subsequent heating up to 700 °C in order to avoid volatile products. Characterized by qualitative EDX analysis. The crystal structure is solved. Triclinic, space group *P*-1, *a* = 7.662(1), *b* = 8.402(2), *c* = 10.100(3) Å,  $\alpha$  = 90.42(3)°,  $\beta$  = 89.74(2)°,  $\gamma$  = 106.39(2)°, *V* = 623.8(3) Å<sup>3</sup>, *Z* = 4. *D*<sub>calc</sub> = 3.799 g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Ouerfelli et al. (2007).

**Wavenumbers (cm<sup>-1</sup>):** 1163w, 1097w, 970sh, 930s, 902s, 882s, 845sh, 786s, 764s, 601, 530sh, 484sh, 468, 420.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**As332 Potassium magnesium arsenate hexahydrate KMg(AsO<sub>4</sub>)·6H<sub>2</sub>O**


**Origin:** Synthetic.

**Description:** Prepared by a simple precipitation procedure of mixing  $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$  and  $\text{K}(\text{H}_2\text{AsO}_4)$  solutions at room temperature. Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group  $Pmn2_1$ ,  $a = 6.99(3)$ ,  $b = 6.22(2)$ ,  $c = 11.26(4)$  Å,  $V = 490.63(3)$  Å<sup>3</sup>,  $Z = 2$ . Isostructural with struvite.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc (?). Absorption.

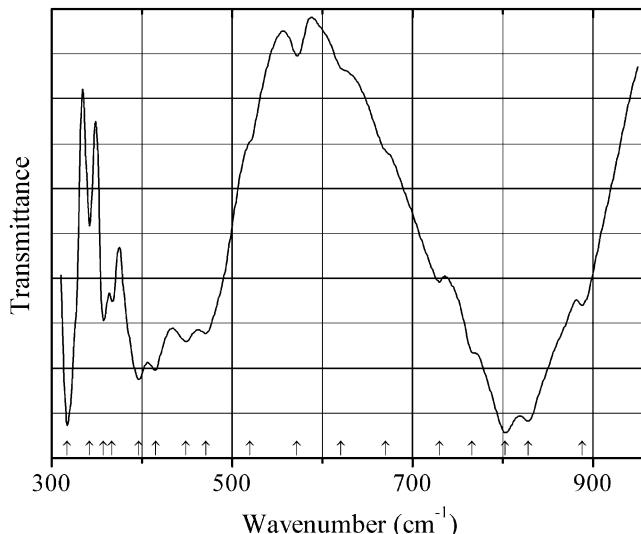
**Source:** Abdija et al. (2014).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3470sh, 3205sh, 2945s, 2348, 1825sh, 1667sh, 1616, 980sh, 930s, 800s, 690, 675sh, 470, 440, 417, 409s, 402s.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 3500–2200s, 1760–1500w, 819s, 458w, 414w, 382, 350w.

**As333 Potassium manganese arsenate**  $\text{K}_2\text{Mn}^{2+}\text{Mn}^{3+}(\text{AsO}_4)_3$



**Origin:** Synthetic.

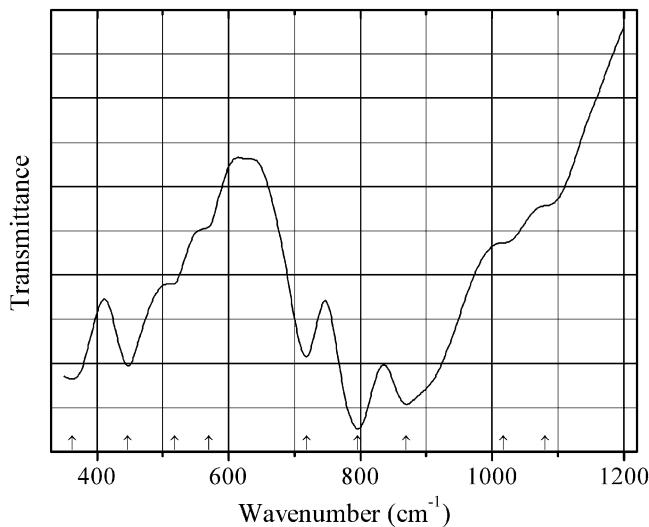
**Description:** Obtained by heating a stoichiometric mixture of manganese oxide, ammonium dihydrogen arsenate, and potassium carbonate first at 400 °C for 4 h and thereafter at 800 °C for 48 h. The crystal structure is solved. Monoclinic, space group  $C2/c$ ,  $a = 12.490(1)$ ,  $b = 13.013(1)$ ,  $c = 6.888(1)$  Å,  $\beta = 114.46(2)^\circ$ ,  $V = 1019.2(8)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{meas}} = 4.28(4)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 4.30$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Chaalia et al. (2012).

**Wavenumbers (cm<sup>-1</sup>):** 888, 828s, 803s, 766sh, 730, 670sh, 621sh, 572w, 520sh, 471, 449, 415, 397, 367, 357, 342, 317s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**As334 Potassium sodium iron arsenate  $\text{Na}_{2.77}\text{K}_{1.52}\text{Fe}_{2.57}(\text{AsO}_4)_4$   $\text{Na}_{2.77}\text{K}_{1.52}\text{Fe}_{2.57}(\text{AsO}_4)_4$** 

**Origin:** Synthetic.

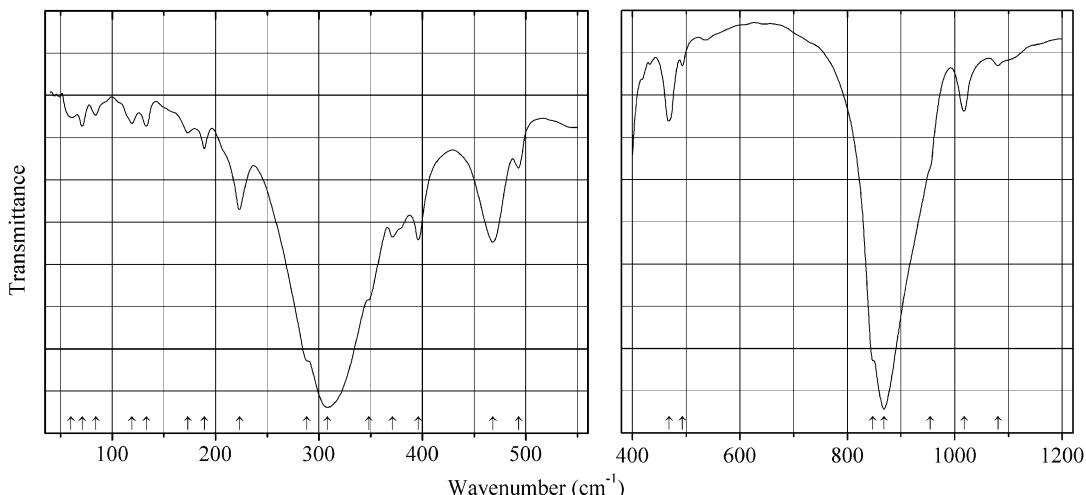
**Description:** Green crystals obtained by solid-state reaction from a mixture of  $\text{Na}_2\text{CO}_3$ ,  $\text{K}_2\text{CO}_3$ ,  $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ , and  $(\text{NH}_4)(\text{H}_2\text{AsO}_4)$  with a Na:K:Fe:As molar ratio of 1:1:1:5, first at 400 °C for 24 h and thereafter (after intermediate grinding) at 850 °C for 72 h. Characterized by powder X-ray diffraction data and EDS analysis. The crystal structure is solved. Orthorhombic, space group  $\text{Cmce}$ ,  $a = 10.854(4)$ ,  $b = 20.985(8)$ ,  $c = 6.536(2)$  Å,  $V = 1488.7(9)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 3.669$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Ouerfelli et al. (2015).

**Wavenumbers (cm<sup>-1</sup>):** 1081sh, 1017sh, 870s, 796s, 718, 570sh, 518sh, 447, 362s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**As335 Potassium zirconium arsenate  $\text{KZr}_2(\text{AsO}_4)_3$** 

**Origin:** Synthetic.

**Description:** Colorless polycrystalline powder obtained by evaporation of aqueous solution containing stoichiometric amounts of  $\text{KNO}_3$ ,  $\text{ZrOCl}_2 \cdot 8\text{H}_2\text{O}$ , and  $\text{H}_3\text{AsO}_4$  at 90 °C, drying at 270 °C and sintering at 600 and 850–950 °C with intermediate grindings. Characterized by powder X-ray diffraction data. Trigonal, space group  $R\text{-}3c$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Absorption.

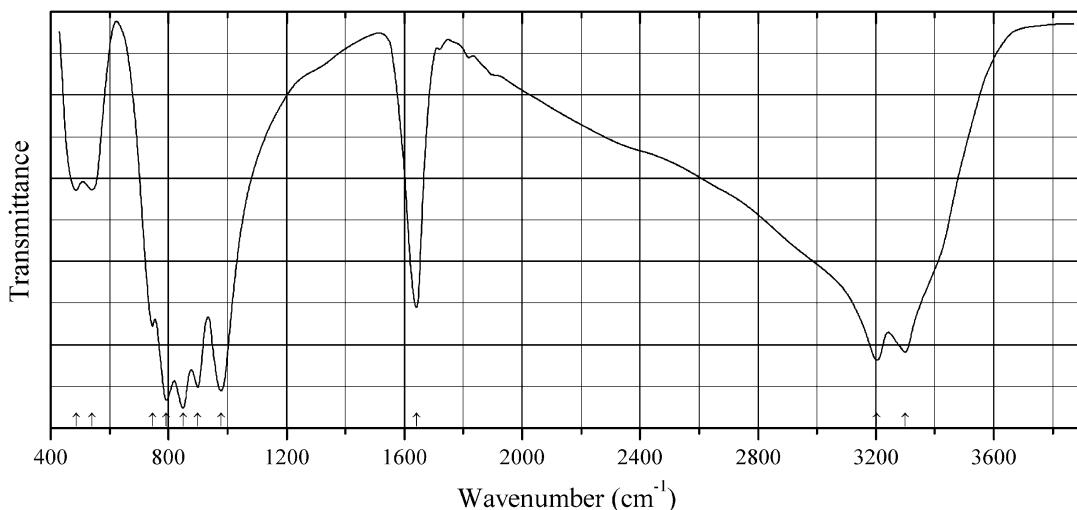
**Source:** Borovikova et al. (2014).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1080w, 1017, 954sh, 868s, 847sh, 493w, 468, 396, 371, 348sh, 308s, 288sh, 223, 189w, 173w, 133w, 119w, 84w, 71w, 60w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 982s, 949, 862s, 857s, 842, 468w, 437, 381w, 358, 255, 237.

### As336 Scandium arsenate monohydrate $\text{Sc}(\text{AsO}_4) \cdot \text{H}_2\text{O}$



**Origin:** Synthetic.

**Description:** Colorless platy crystals prepared from  $\text{Sc}_2\text{O}_3$ , hydrated arsenic acid, and  $\text{Li}_2\text{CO}_3$  by hydrothermal synthesis at 493 K for 7 days. Triclinic, space group  $P\text{-}1$ ,  $Z = 2$ .

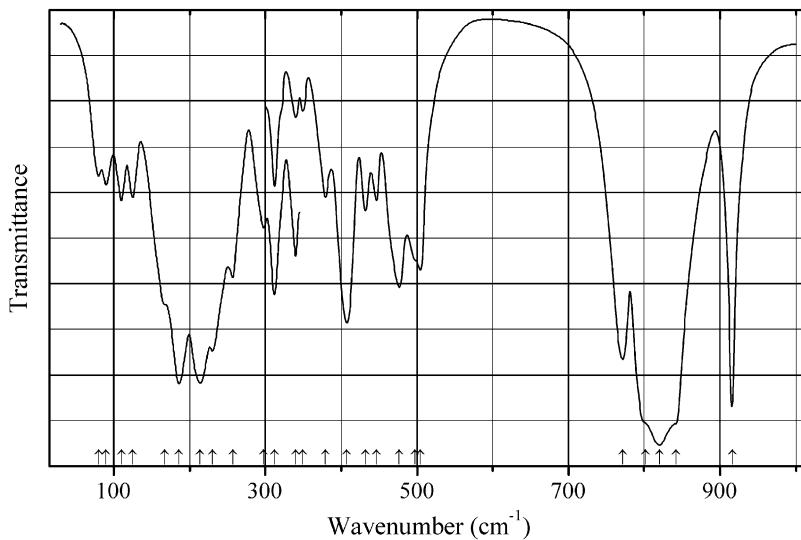
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Baran et al. (2006).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3300s, 3203s, 1641, 978s, 899s, 849s, 793s, 746, 540, 486.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 1638, 935s, 866s, 832s, 805, 744w, 484, 385, 347, 323w, 287, 244w, 188w, 167, 138.

**As337 Sodium indium arsenate (alluaudite-type)  $\text{Na}_3\text{In}_2(\text{AsO}_4)_3$** 


**Origin:** Synthetic.

**Description:**  $\text{Na}_3\text{In}_2(\text{AsO}_4)_3$  was synthesized by a solid-state reaction between  $\text{NaHCO}_3$ ,  $\text{In}_2\text{O}_3$ , and  $(\text{NH}_4)(\text{H}_2\text{AsO}_4)$ , as well as by a chemical attack of the reagents ( $\text{NaHCO}_3$ ,  $\text{In}_2\text{O}_3$ ,  $\text{As}_2\text{O}_3$ ) by nitric acid. Characterized by powder X-ray diffraction data. The crystal structure is solved by the Rietveld method. Monoclinic, space group  $C2/c$ ,  $a = 12.6025(1)$ ,  $b = 13.1699(1)$ ,  $c = 6.8335(1)$  Å,  $\beta = 113.7422(5)^\circ$ ,  $Z = 4$ .

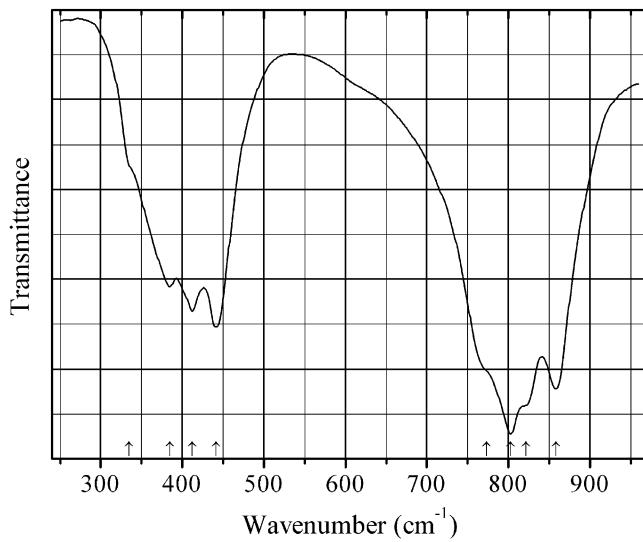
**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

**Source:** Khorari et al. (1997).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 917s, 842sh, 820s, 802sh, 772s, 505s, 497sh, 477s, 447, 432, 407s, 379, 349, 340, 312, 298, 257w, 230w, 214s, 186s, 167sh, 125w, 110w, 90w, 80w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 934s, 907w, 990, 866s, 855, 837, 832sh, 806sh, 796, 773, 480s, 472sh, 419, 397, 378w, 369w, 354w, 328, 284, 271, 231w, 168, 149, 133, 122, 96w, 90w, 86w, 78.

**As338 Sodium lead neodymium arsenate chloride (apatite-type)  $\text{Na}_2\text{Pb}_6\text{Nd}_2(\text{AsO}_4)_6\text{Cl}_2$** 

**Origin:** Synthetic.

**Description:** Prepared by stepwise heating of the mixture of NaCl, PbO, Nd<sub>2</sub>O<sub>3</sub>, and As<sub>2</sub>O<sub>5</sub>, first at 350 °C and thereafter (after intermediate grindings) at 650, 800, and 850 °C for 2 h at each temperature. Characterized by powder X-ray diffraction data. Hexagonal, space group  $P6_3/m$ ,  $a = 10.08(1)$ ,  $c = 7.21(1)$  Å,  $V = 634.4$  Å<sup>3</sup>,  $Z = 1$ .  $D_{\text{meas}} = 6.3$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 6.49$  g/cm<sup>3</sup>. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 4.12 (18) (111), 3.60 (19) (002), 3.294 (27) (210), 2.999 (100) (211), 2.929 (44) (112), 2.906 (53) (300), 1.943 (19) (213), 1.928 (18) (321).

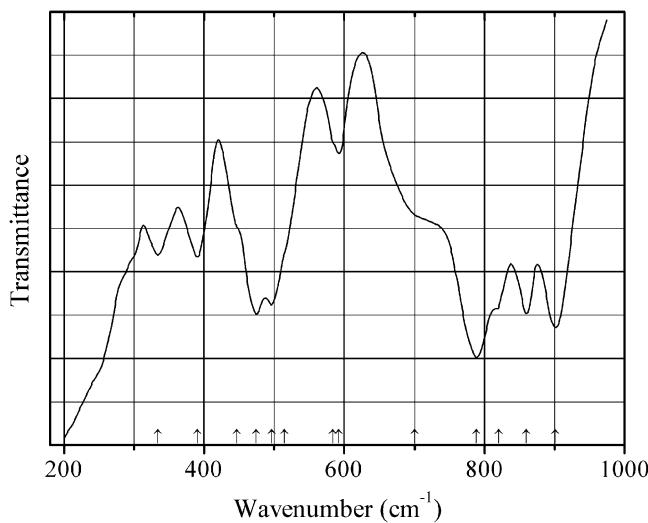
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Escobar and Baran (1982).

**Wavenumbers (IR, cm<sup>-1</sup>):** 858s, 822sh, 803s, 773sh, 441, 412, 385, 335sh.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 850, 822s, 800, 772, 410, 330.

**As339 Sodium nickel iron(III) arsenate  $\text{NaNiFe}_2(\text{AsO}_4)_3$** 

**Origin:** Synthetic.

**Description:** Crystals obtained from a stoichiometric mixture of  $\text{Na}_2\text{CO}_3$ ,  $\text{NiO}$ ,  $\text{Fe}_2\text{O}_3$ , and  $\text{As}_2\text{O}_5$  by solid-state reaction at 800 °C for 15 h with intermediate grindings. Characterized by chemical analyses and powder X-ray diffraction data. Monoclinic, space group  $P2_1/c$ ,  $a = 7.06(1)$ ,  $b = 9.38(1)$ ,  $c = 19.63(1)$  Å,  $\beta = 114.2(1)^\circ$ ,  $V = 1186(2)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{meas}} = 3.40(1)$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 3.42$  g/cm<sup>3</sup>. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 5.63 (56) (−111), 2.847 (98) (−204), 2.815 (100) (−222), 2.654 (56) (220), 2.263 (57) (−227).

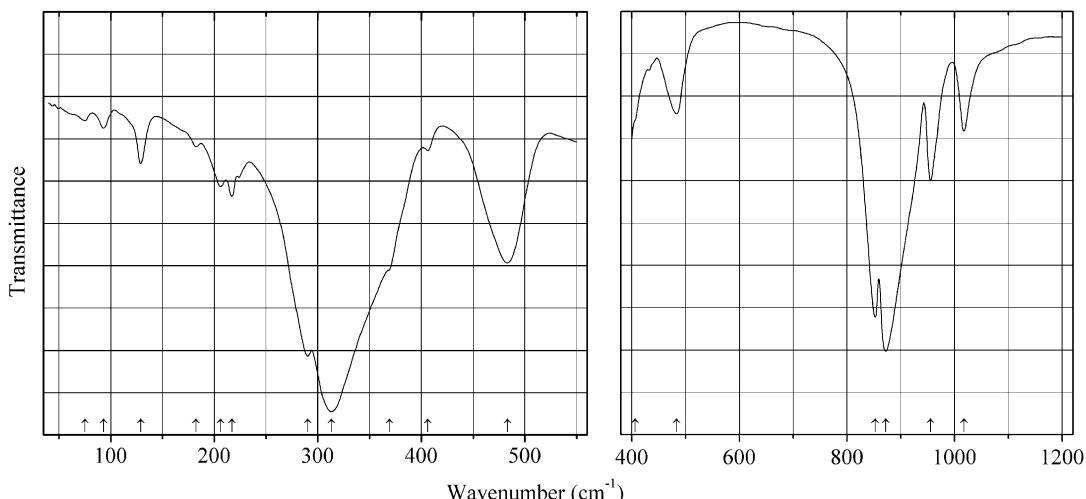
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Augsburger et al. (1992).

**Wavenumbers (cm<sup>−1</sup>):** 901s, 860s, 820sh, 789s, 700sh, 592w, 584sh, 515sh, 496, 474, 447sh, 390, 334.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### As340 Sodium zirconium arsenate $\text{NaZr}_2(\text{AsO}_4)_3$



**Origin:** Synthetic.

**Description:** Obtained by precipitation from aqueous solutions containing stoichiometric amounts of  $\text{NaNO}_3 + \text{ZrOCl}_2 \cdot 8\text{H}_2\text{O}$  and  $\text{H}_3\text{AsO}_4$  with subsequent stepwise heating the precipitate at 90, 270, 600, and 850–950 °C with intermediate grindings. Characterized by powder X-ray diffraction data. Trigonal, space group  $R\bar{3}c$ ,  $Z = 6$ .

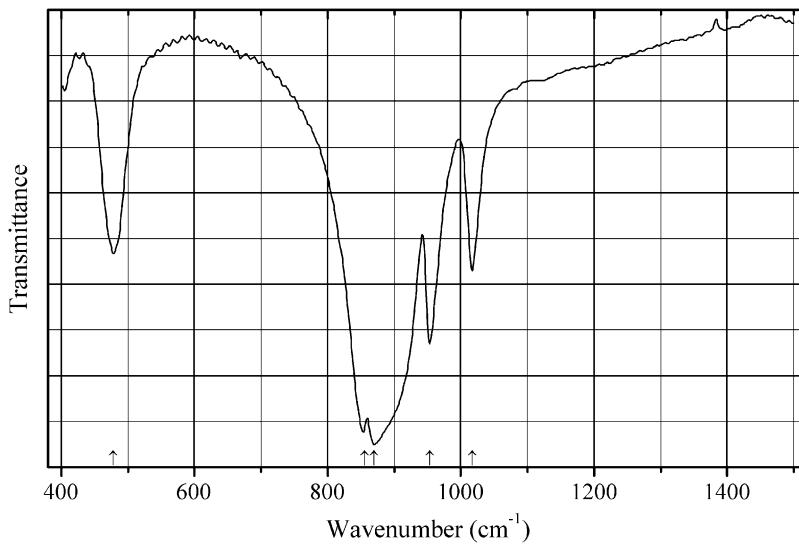
**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Absorption.

**Source:** Borovikova et al. (2014).

**Wavenumbers (IR, cm<sup>−1</sup>):** 1017, 955, 872s, 852s, 483, 406w, 369sh, 313s, 290, 217w, 206w, 182w, 129w, 93w, 75w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>−1</sup>):** 979s, 948, 863s, 856s, 837, 472w, 446, 389, 363, 340, 256.

**As341 Sodium zirconium arsenate**  $\text{NaZr}_2(\text{AsO}_4)_3$ 

**Origin:** Synthetic.

**Description:** Obtained by evaporation of an aqueous solutions containing stoichiometric amounts of  $\text{NaNO}_3$ ,  $\text{ZrOCl}_2 \cdot 8\text{H}_2\text{O}$ , and  $(\text{NH}_4)(\text{H}_2\text{AsO}_4)$  and subsequent stepwise heating the resulting powder up to 800 °C with intermediate grindings. Characterized by powder X-ray diffraction data. The crystal structure is solved. Trigonal, space group  $R-3c$ ,  $a = 9.1518(2)$ ,  $c = 23.1097(4)$  Å,  $V = 1676.26(1)$  Å<sup>3</sup>,  $Z = 6$ .

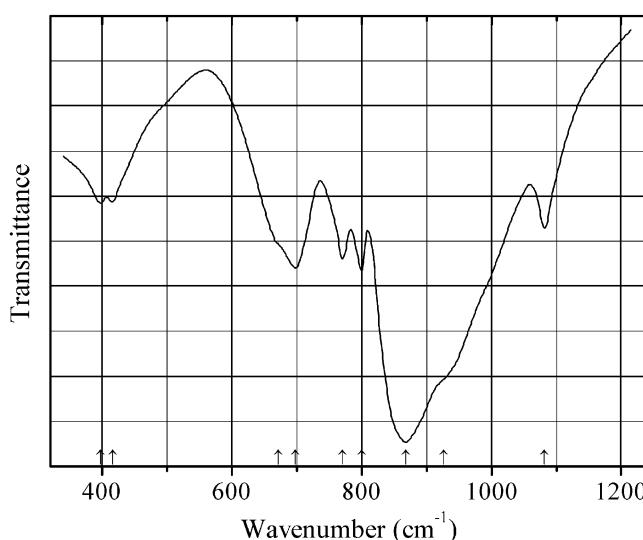
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Chakir et al. (2003).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1017, 953, 870s, 855s, 478.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 978.5s, 949, 863s, 837, 470w, 446, 390w, 362w, 339, 300w, 255, 236w, 179w, 153w, 115, 63.

**As342 Tantalum oxyarsenate**  $\text{Ta}(\text{AsO}_4)\text{O}$ 

**Origin:** Synthetic.

**Description:** Orthorhombic,  $a = 11.57$ ,  $b = 5.31$ ,  $c = 6.66 \text{ \AA}$ .

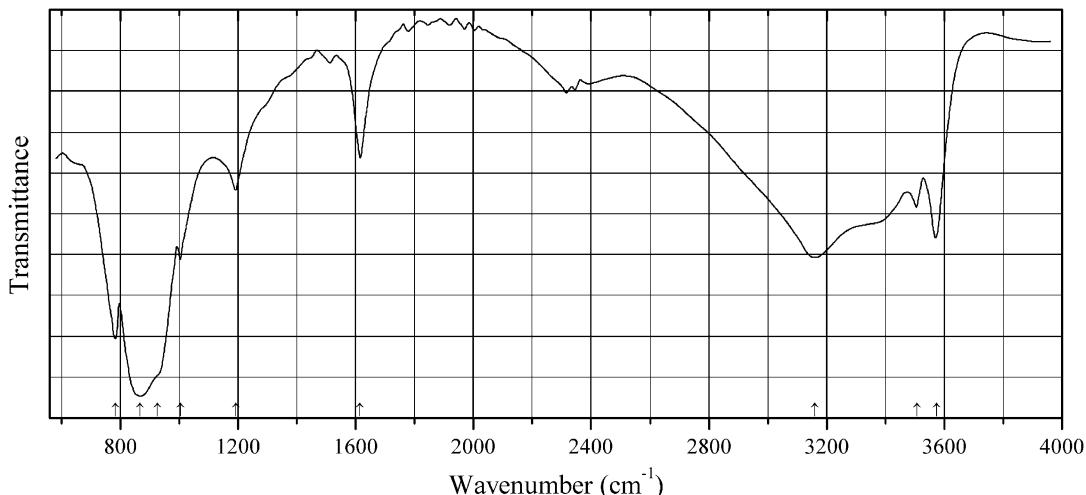
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Chahboun et al. (1988).

**Wavenumbers (cm<sup>-1</sup>):** 1082, 927sh, 868s, 800, 770, 698, 672sh, 416, 398.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### As343 Zirconium acid arsenate monohydrate $\alpha\text{-Zr(HAsO}_4\text{)}_2\cdot\text{H}_2\text{O}$



**Origin:** Synthetic.

**Description:** Prepared in the reaction of zirconyl chloride with a mixture of arsenic and hydrochloric acids with subsequent refluxing and drying at 110 °C. Characterized by DSC and powder X-ray diffraction data. Monoclinic,  $a = 9.146(1)$ ,  $b = 5.381(5)$ ,  $c = 16.61(2) \text{ \AA}$ ,  $\beta = 111.5^\circ$ .

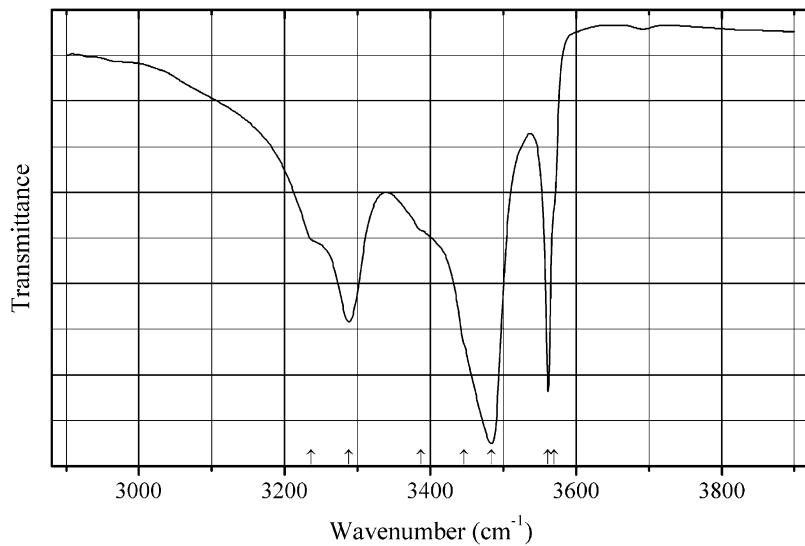
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Slade et al. (1997).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3573, 3508, 3160s, 1615, 1192, 1004, 926sh, 868s, 784.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. Weak bands in the range from 2320 to 2380 cm<sup>-1</sup> correspond to atmospheric CO<sub>2</sub>. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 983, 882s, 869s, 808, 785, 775, 423sh, 410, 363w, 326, 287, 165w, 136, 107w, 78w, 65w, 51w.

**As344 Allactite**  $Mn^{2+} \cdot_7 (AsO_4)_2(OH)_8$ 

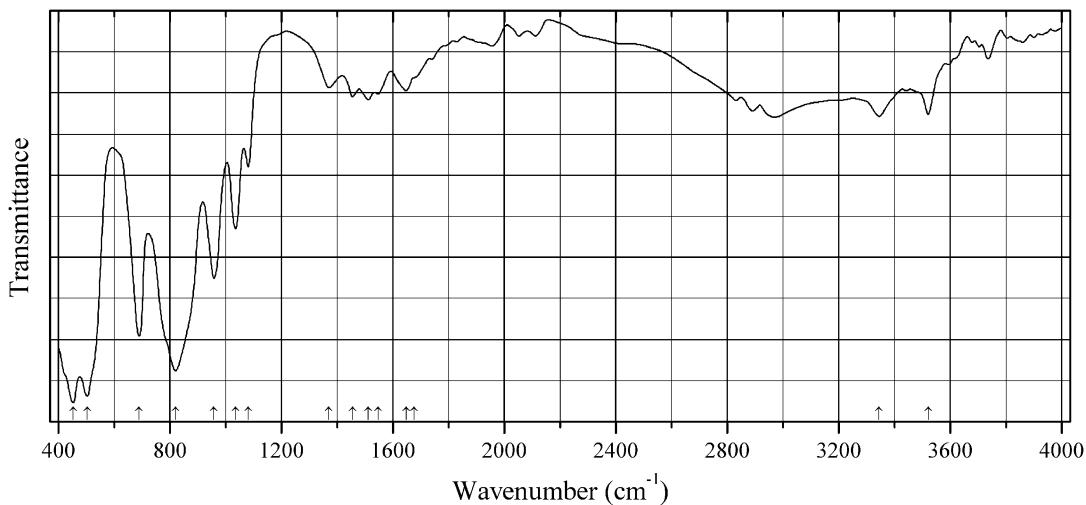
**Origin:** Långban deposit, Bergslagen ore region, Filipstad district, Värmland, Sweden.

**Description:** Red crystals from the association with native lead, calcite, dolomite, domeykite, and pyrochroite. The crystal structure is solved for two prismatic crystals. Monoclinic, space group  $P2_1/n$ ,  $a = 5.482\text{--}5.5225$ ,  $b = 12.153\text{--}12.276$ ,  $c = 10.014\text{--}10.123$  Å,  $\beta = 95.55\text{--}95.63^\circ$ ,  $Z = 2$ .  $D_{\text{calc}} = 3.856$  g/cm<sup>3</sup>. Optically biaxial (-),  $\alpha = 1.554(2)$ ,  $\beta = 1.558(2)$ ,  $\gamma = 1.566(2)$ ,  $2V = 70(5)^\circ$ . The empirical formula is (electron microprobe):  $Mn^{2+}_{6.73}Ca_{0.13}Mg_{0.12}Zn_{0.02})As^{5+}_{2.00}O_{16}H_8$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Gatta et al. (2016).

**Wavenumbers (cm<sup>-1</sup>):** 3570sh, 3562, 3484s, 3446sh, 3387sh, 3288, 3236sh.

**As345 Arhbarite** Cu<sub>2</sub>Mg(AsO<sub>4</sub>)(OH)<sub>3</sub>

**Origin:** Aghbar Mine (Arhbar Mine), Aghbar, Bou Azzer District, Tazenakht, Ouarzazate Province, Morocco (type locality).

**Description:** Blue aggregates from the association with dolomite, hematite, löllingite, pharmacolite, erythrite, talc, and mcguinessite (the type material). Characterized by powder X-ray diffraction data. Triclinic, space group  $P\bar{1}$ ,  $a = 5.315(4)$ ,  $b = 5.978(6)$ ,  $c = 5.030(6)$  Å,  $\alpha = 113.58(6)^\circ$ ,  $\beta = 97.14(7)^\circ$ ,  $\gamma = 89.30(8)^\circ$ ,  $V = 145.2(1)$  Å $^3$ ,  $Z = 1$ . The empirical formula is (electron microprobe): Cu<sub>1.98</sub>(Mg<sub>0.88</sub>Cu<sub>0.09</sub>Ni<sub>0.01</sub>Co<sub>0.01</sub>)(AsO<sub>4</sub>)<sub>1.02</sub>(OH)<sub>2.92</sub>.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

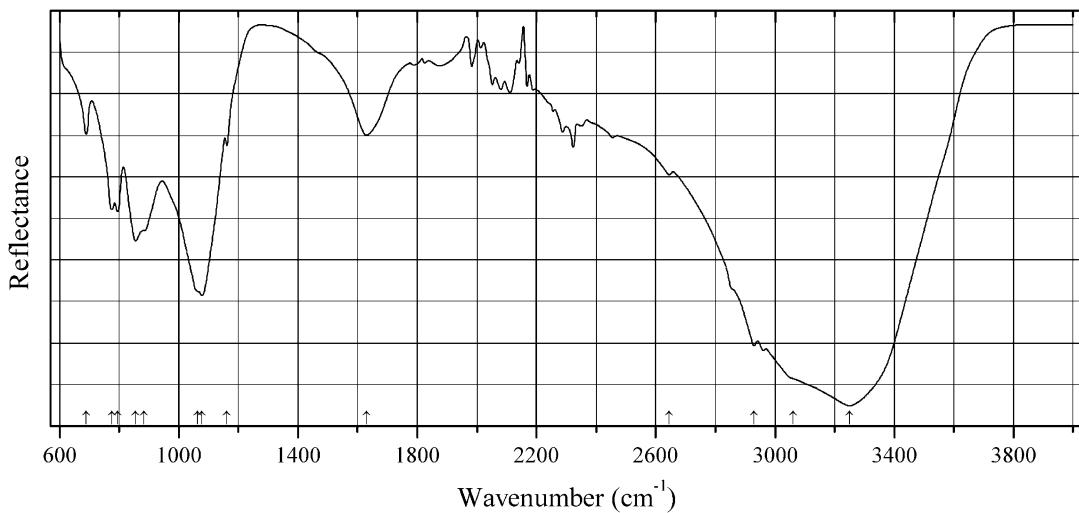
**Source:** Krause et al. (2003).

**Wavenumbers (IR, cm $^{-1}$ ):** 3520, 3345, 1676sh, 1647, 1547, 1512, 1456, 1371, 1081, 1036, 958, 820s, 690, 504s, 453s, as well as bands in the ranges 3600–3800, 2800–3200, and 1800–2200 cm $^{-1}$ .

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The bands in the ranges 1800–3000 and 1300–1500 cm $^{-1}$  indicate possible presence of acid arsenate groups. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 3525, 3355w, 956w, 840s, 820, 681w, 512sh, 489, 464s, 409w, 331, 318, 141.

#### As346 Bettertonite Al<sub>6</sub>(AsO<sub>4</sub>)<sub>3</sub>(OH)<sub>9</sub>·16H<sub>2</sub>O



**Origin:** Penberthy Croft Mine, St Hilary, Mount's Bay District, Cornwall, England, UK (type locality).

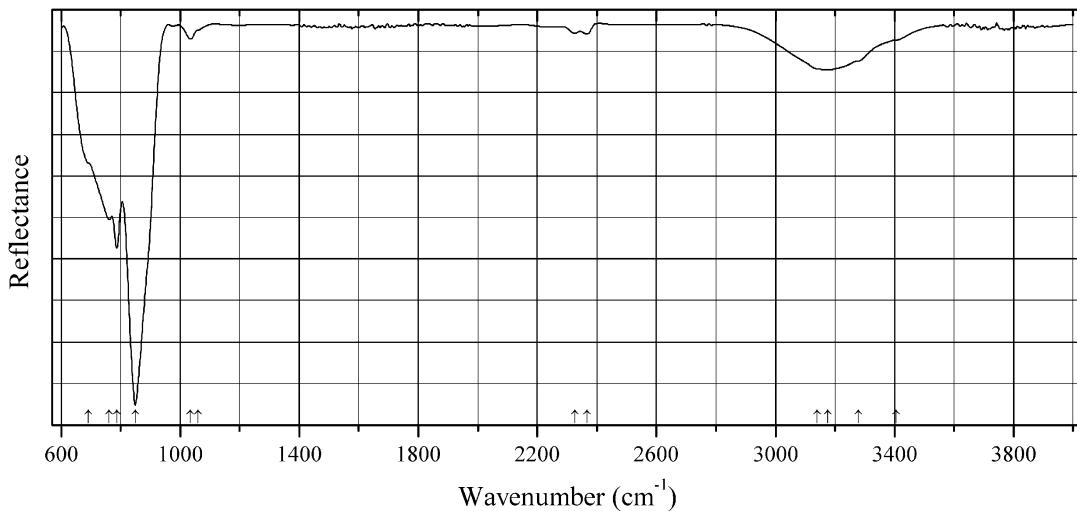
**Description:** No data. Possibly, type material.

**Kind of sample preparation and/or method of registration of the spectrum:** Powdered sample. Absorption.

**Source:** Grey et al. (2016b).

**Wavenumbers (cm $^{-1}$ ):** 3250s, 3060sh, (2960), (2930), (2855), 2645w, 1630, 1162w, 1078s, 1064sh, 884sh, 855, 795, 775, 690w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The band denoted by Grey et al. (2016b) as 1070 cm $^{-1}$  was identified as a doublet (1078+1064 cm $^{-1}$ ).

**As347 Canosioite**  $\text{Ba}_2\text{Fe}^{3+}(\text{AsO}_4)_2(\text{OH})$ 

**Origin:** Valletta mine, Maira Valley, Cuneo Province, Piedmont, Italy (type locality).

**Description:** Reddish-brown granules from the association with aegirine, baryte, calcite, hematite, Mn-bearing muscovite, as well as unidentified Mn oxides and arsenates. Holotype sample. The crystal structure is solved. Monoclinic, space group  $P2_1/m$ ,  $a = 7.8642(4)$ ,  $b = 6.1083(3)$ ,  $c = 9.1670(5)$  Å,  $\beta = 112.874(6)^\circ$ ,  $V = 405.73(4)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 4.943$  g/cm<sup>3</sup>. Optically biaxial (+),  $2V = 84(2)^\circ$ . The empirical formula is (electron microprobe):  $(\text{Ba}_{1.92}\text{Pb}_{0.05}\text{Sr}_{0.02}\text{Na}_{0.01})(\text{Fe}^{3+}_{0.52}\text{Mn}^{3+}_{0.29}\text{Al}_{0.16}\text{Mg}_{0.06})[(\text{As}_{0.64}\text{V}_{0.36})\text{O}_4]_2(\text{OH})_{0.92}\text{F}_{0.01}\cdot 0.07\text{H}_2\text{O}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 3.713 (18) (111), 3.304 (100) (21–1), 3.058 (31) (020), 3.047 (59) (10–3), 2.801 (73) (112), 2.337 (24) (220), 2.158 (24) (12–3).

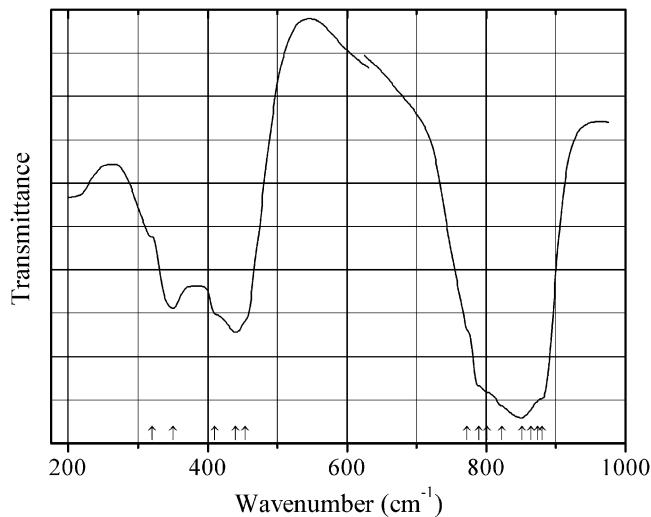
**Kind of sample preparation and/or method of registration of the spectrum:** Reflection using IR microscope. Kind of sample preparation is not indicated.

**Source:** Cámara et al. (2016a).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3405sh, 3278sh, 3175, 3139sh, (2366), (2326), 1061sh, 1035, 849s, 787s, 762, 692sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. Weak bands in the range from 2300 to 2400 cm<sup>-1</sup> correspond to atmospheric CO<sub>2</sub>. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 896s, 862s, 838s, 820sh, 779w, 719sh, 686, 595w, 507, 478, 457, 368s, 326, 282, 234, 187, 163, 147, 133.

**As348 Cheralite La-bearing CaLaTh(AsO<sub>4</sub>)<sub>3</sub>**

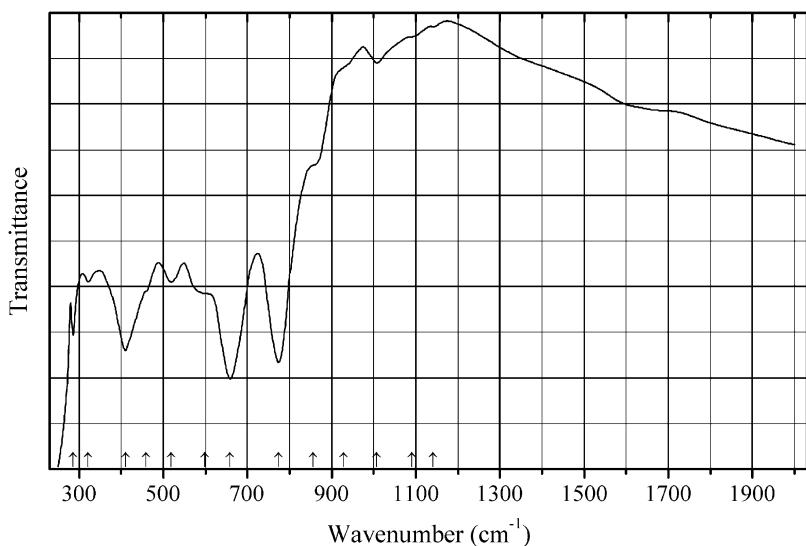
**Origin:** Synthetic.

**Description:** Prepared using a solid-state reaction technique. Characterized by powder X-ray diffraction data. Monoclinic, isostructural with monazite, space group  $P2_1/m$ ,  $a = 6.883(5)$ ,  $b = 7.070(6)$ ,  $c = 6.674(7)$  Å,  $\beta = 104.74(8)^\circ$ ,  $V = 314.1$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{meas}} = 5.80$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 5.83$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** CsBr disc. Transmission.

**Source:** Nabar and Sakhardande (1985).

**Wavenumbers (cm<sup>-1</sup>):** 880sh, 874sh, 864sh, 851s, 823sh, 801sh, 790sh, 772sh, 454sh, 440s, 410sh, 350, 320sh.

**As349 Fetiasite (Fe<sup>2+</sup>,Fe<sup>3+</sup>,Ti<sup>4+</sup>)<sub>3</sub>(As<sup>3+</sup><sub>2</sub>O<sub>5</sub>)O<sub>2</sub>**

**Origin:** Cervandone Mt., Val Devero, Baceno, Verbano-Cusio-Ossola province, Piedmont, Italy (type locality).

**Description:** Brown to black aggregates from the association with asbecasite, cafarsite, cervandonite, etc. Holotype sample. The crystal structure is solved. Monoclinic, space group  $P2_1/m$ ,  $a = 10.614(2)$ ,  $b = 3.252(1)$ ,  $c = 8.945(1)$  Å,  $\beta = 108.95(2)^\circ$ ,  $V = 291.9(2)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{meas}} = 4.6$  g/cm $^3$ ,  $D_{\text{calc}} = 4.76\text{--}4.80$  g/cm $^3$ . The empirical formula is (electron microprobe):  $(\text{Fe}^{2+}_{1.38}\text{Fe}^{3+}_{0.92}\text{Ti}_{0.54}\text{Mn}_{0.08})(\text{As}^{3+}_{2}\text{O}_5)\text{O}_2$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 2.985 (67) (−103), 2.811 (94) (202, 301), 2.749 (100) (−211, 210), 2.391 (85) (112), 1.779 (48) (−504, −511), 1.709 (35) (510, −603).

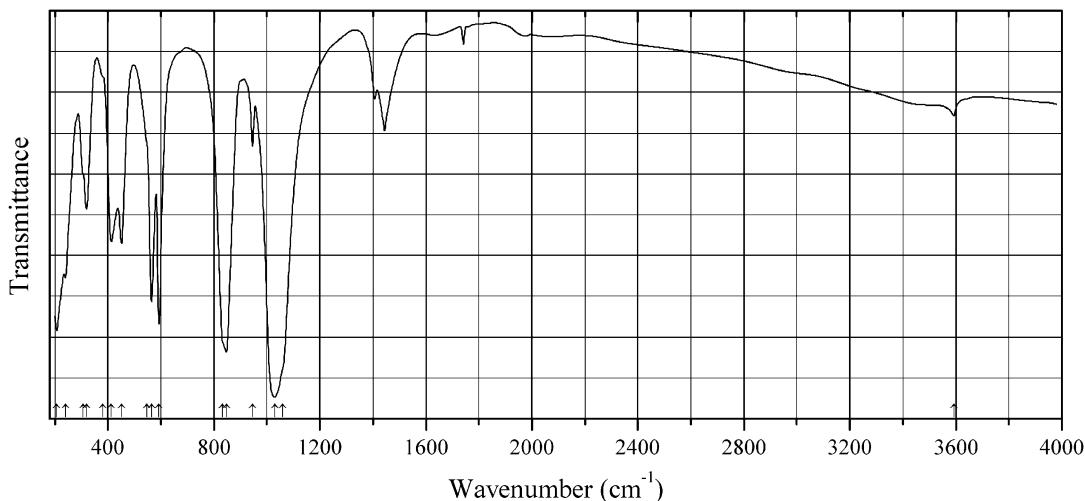
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Graeser et al. (1994).

**Wavenumbers (cm $^{-1}$ ):** 1142w, 1090sh, 1007w, 929sh, 856sh, 774s, 659s, 599sh, 519w, 459sh, 410, 322w, (286).

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. No data on absorptions above 2000 cm $^{-1}$  are given. Consequently, the presence of OH groups in fetiasite cannot be excluded.

### As350 Johnbaumite Sr-analogue $\text{Sr}_5[(\text{AsO}_4)_2(\text{PO}_4)](\text{OH})$



**Origin:** Synthetic.

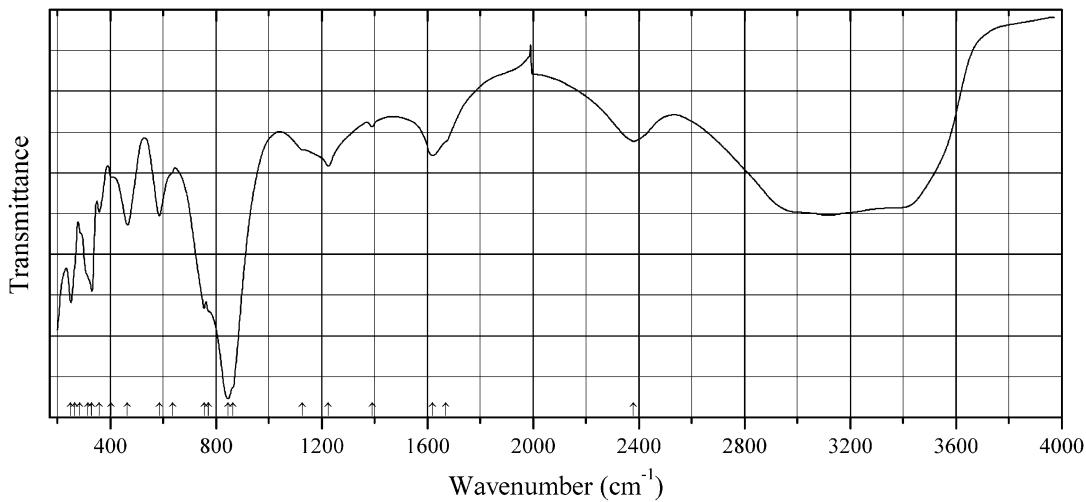
**Description:** Apatite-type compound prepared from aqueous solutions of  $\text{Sr}(\text{NO}_3)_2$ ,  $(\text{NH}_4)_2(\text{HPO}_4)$ , and  $\text{Na}_3(\text{AsO}_4)\cdot\text{H}_2\text{O}$  and  $(\text{NH}_4)(\text{OH})$  with subsequently heating a precipitate first at 100 °C for 2 h and thereafter at 850 °C for 2 h. Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Galera-Gomez et al. (1982).

**Wavenumbers (cm $^{-1}$ ):** 3593w, 1061sh, 1030s, 946, 848s, 832sh, 593s, 565s, 548sh, 452, 413, 380, 320, 307, (240), (207s), and bands in the range of 1400–1500 cm $^{-1}$ .

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. Bands in the range of 1400–1500 cm $^{-1}$  correspond to carbonate groups.

**As351 Kaatialaite**  $\text{Fe}^{3+}(\text{H}_2\text{AsO}_4)_3 \cdot 5\text{H}_2\text{O}$ 

**Origin:** Synthetic.

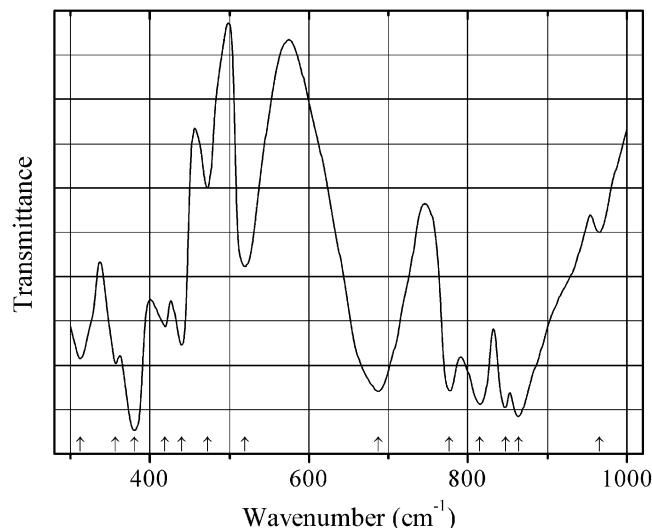
**Description:** Greenish blue aggregates. Monoclinic, space group  $P2_1$  or  $P2_1/m$ ,  $a = 15.363(5)$ ,  $b = 19.844(5)$ ,  $c = 4.736(2)$  Å,  $\beta = 91.77(3)^\circ$ ,  $Z = 4$ .  $D_{\text{meas}} = 2.62(3)$  g/cm $^3$ ,  $D_{\text{calc}} = 2.62$  g/cm $^3$ . Optically biaxial (+),  $\alpha = 1.581(2)$ ,  $\beta = 1.582$  (calculated),  $\gamma = 1.625(2)$ ,  $2V = 15(2)^\circ$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 9.94 (50) (020), 8.33 (100) (120), 7.68 (70) (200), 6.08 (40) (130), 3.410 (40) (231), 3.153 (45) (24-1).

**Kind of sample preparation and/or method of registration of the spectrum:** KI disc. Transmission.

**Source:** Raade et al. (1984).

**Wavenumbers (cm $^{-1}$ ):** 2380, 1670sh, 1620, 1390w, 1225w, 1125sh, 865sh, 845s, 770sh, 755, 635sh, 585, 465, 403sh, 358w, 330, 315sh, 285sh, 265sh, 250.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**As352 Katiarsite**  $\text{KTi}(\text{AsO}_4)\text{O}$ 

**Origin:** Synthetic.

**Description:** Prepared by heating a mixture of  $K_2CO_3/KNO_3$ ,  $TiO_2$ , and  $(NH_4)(H_2AsO_4)$  powders taken in stoichiometric amounts first at  $500\text{ }^\circ C$  for 12 h and thereafter at  $900\text{ }^\circ C$  for 24 h with intermediate grinding. Characterized by powder X-ray diffraction data. Orthorhombic, space group  $Pna2_1$ ,  $a = 12.815(8)$ ,  $b = 6.402(4)$ ,  $c = 10.589(6)\text{ \AA}$ ,  $V = 868.7\text{ \AA}^3$ .

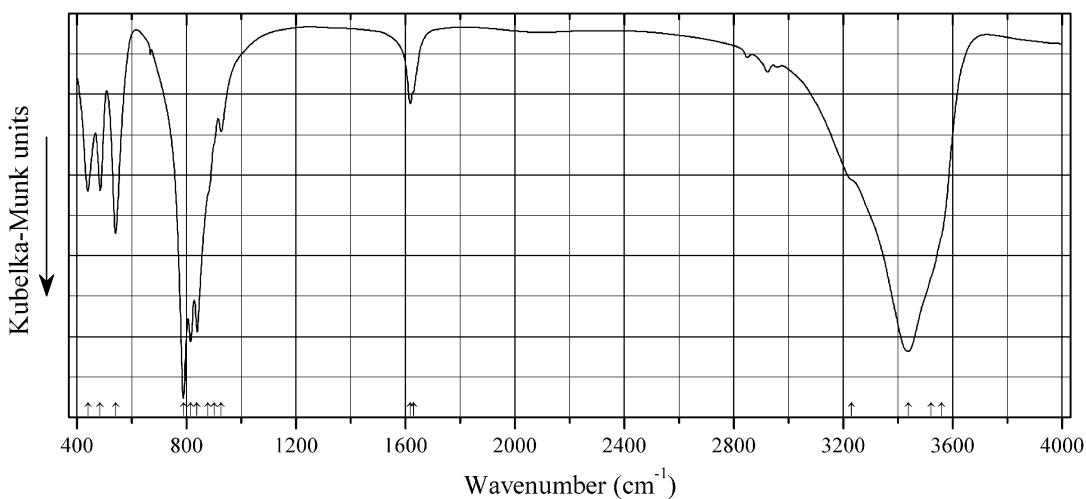
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Rangan et al. (1993).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 965w, 864s, 847s, 815s, 777s, 687s, 520, 473w, 440, 419, 381s, 357, 313.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

### As353 Lemanskiite $NaCaCu_5(AsO_4)_4Cl \cdot 5H_2O$



**Origin:** Abundancia mine, El Guanaco miningdistrict, Region II, Antofagasta province, Chile (type locality).

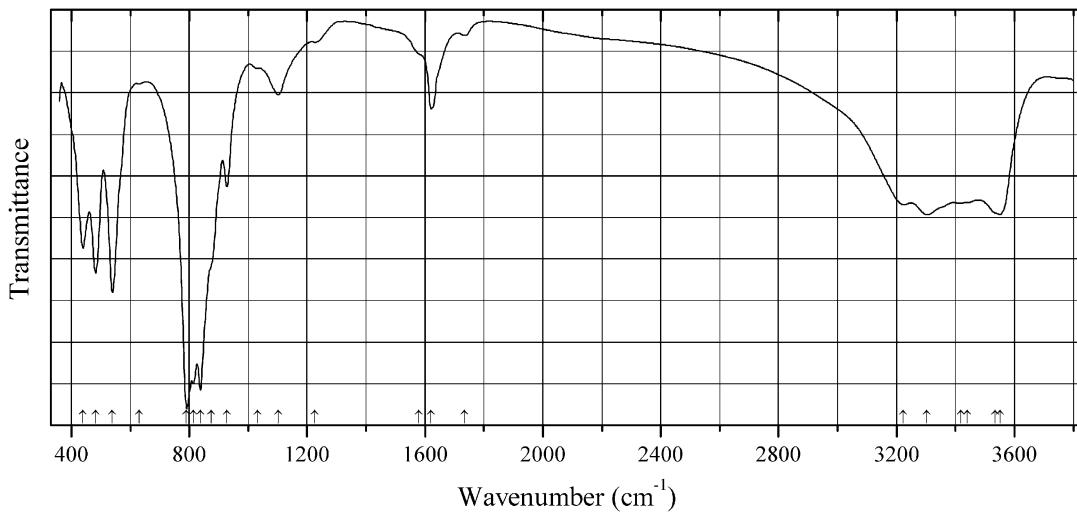
**Description:** Dark sky blue massive nodule from the association with lammerite, olivenite, mansfieldite, sénarmontite, a mineral of the crandallite group, rutile, anatase, and talc. Holotype sample. Described as tetragonal ( $P4_122$  or  $P4_322$ ) mineral with  $a = 9.9758(4)$ ,  $c = 36.714(1)\text{ \AA}$ ,  $V = 653.6(2)\text{ \AA}^3$ ,  $Z = 8$ .  $D_{meas} = 3.78(1)\text{ g/cm}^3$ ,  $D_{calc} = 3.863(5)\text{ g/cm}^3$ . Optically uniaxial (-),  $\epsilon = 1.647(2)$ ,  $\omega = 1.749(2)$ . The empirical formula is  $Na_{1.04}Ca_{1.00}Cu_{5.01}(AsO_4)_{4.00}Cl_{0.96}(OH)_{0.11} \cdot 4.93H_2O$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ ,  $\text{\AA}$  ( $I$ , %) ( $hkl$ )] are: 9.60 (9) (101), 9.177 (100) (004), 4.588 (32) (008), 4.167 (10) (108), 3.059 (15) (0.0.12).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Ondruš et al. (2006).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3559sh, 3521sh, 3437s, 3229sh, 1630sh, 1618, 927, 902sh, 880sh, 839s, 815s, 789s, 541, 485, 440.

**Note:** Weak bands in the range from 2800 to 3000  $\text{cm}^{-1}$  correspond to the admixture of an organic substance.

**As354 Lemanskiite**  $\text{NaCaCu}_5(\text{AsO}_4)_4\text{Cl}\cdot 3\text{H}_2\text{O}$ 

**Origin:** Perseverancia deposit, Guanaco, Antofagasta, Chile.

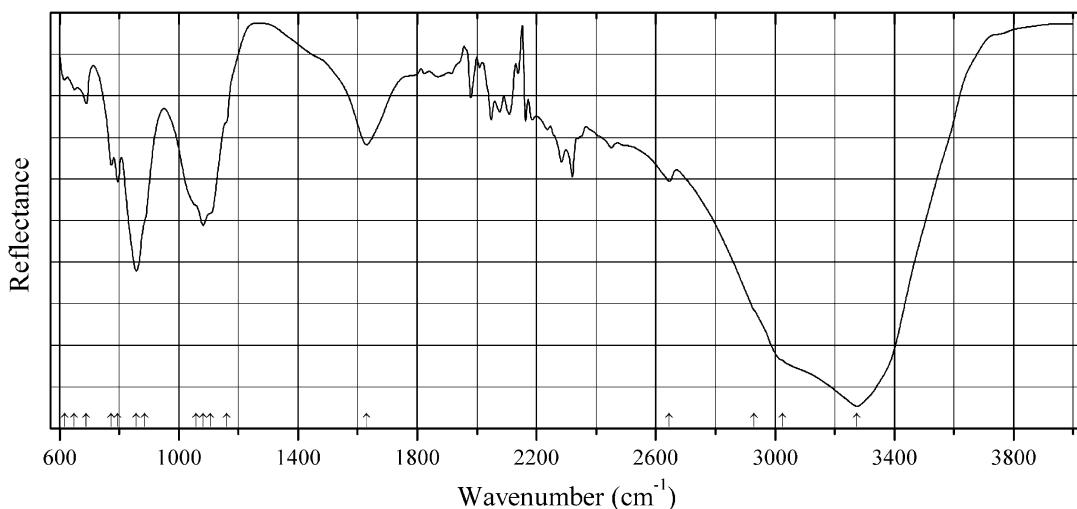
**Description:** Blue crystals. A sample used for the revision of the lemanskiite chemical formula.

Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2_1/m$ ,  $a = 9.250(2)$ ,  $b = 10.0058(10)$ ,  $c = 10.0412(17)$  Å,  $\beta = 97.37(3)^\circ$ ,  $V = 921.7(3)$  Å<sup>3</sup>,  $Z = 2$ . The empirical formula is  $\text{Na}_{0.98}(\text{Ca}_{0.98}\text{Sr}_{0.03})\text{Cu}_{5.07}\text{As}_{3.97}\text{O}_{15.97}\text{Cl}_{1.03}\cdot 3\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3551s, 3535sh, 3441, 3419, 3303s, 3224, 1734w, 1621, 1580sh, 1225w, 1102w, 928, 875sh, 838s, 813s, 791s, 629w, 539s, 483s, 439.

**Note:** The spectrum was obtained by N.V. Chukanov.

**As355 Penberthycroftite**  $\text{Al}_6(\text{AsO}_4)_3(\text{OH})_9\cdot 13\text{H}_2\text{O}$ 

**Origin:** Penberthy Croft mine, St. Hilary, Cornwall, England, UK (type locality).

**Description:** White rectangular laths from the association with arsenopyrite, bettertonite, bulachite, cassiterite, chalcopyrite, chamosite, goethite, liskeardite, pharmacoalumite–pharmacosiderite, and quartz. Holotype sample. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 7.753$  (2) Å,  $b = 24.679(5)$  Å,  $c = 15.679(3)$  Å,  $\beta = 94.19(3)^\circ$ ,  $V = 2991.9(12)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 2.18$  g/cm $^3$ . The empirical formula is  $\text{Al}_{5.96}\text{Fe}_{0.04}[(\text{As}_{0.97}\text{Al}_{0.03})\text{O}_4]_3(\text{SO}_4)_{0.26}(\text{OH})_{8.30} \cdot 13.24\text{H}_2\text{O}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 13.264 (46) (011), 12.402 (16) (020), 9.732 (100) (021), 7.420 (28) (110), 5.670 (8) (130), 5.423 (6) (−131).

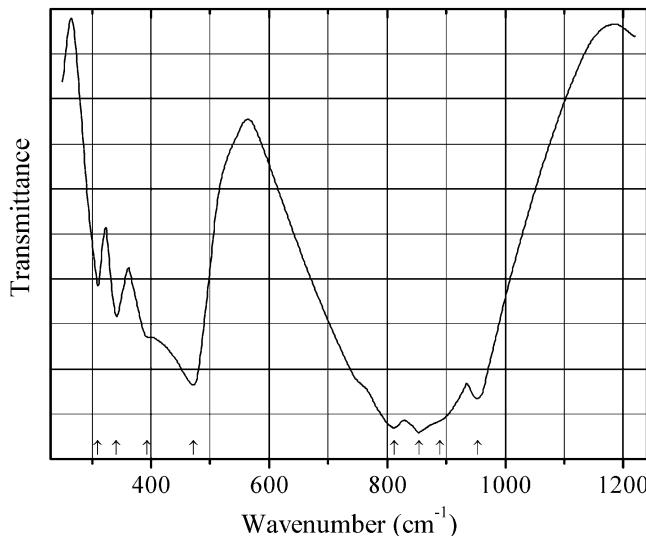
**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of powdered mineral.

**Source:** Grey et al. (2016a).

**Wavenumbers (cm $^{-1}$ ):** 3275s, 3025sh, 2930sh, 2645w, 1630, 1160sh, 1105sh, 1082, 1057sh, 885sh, 858, 796, 774, 690w, 650w, 617w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

#### As356 Petewilliamsite-related Cd diarsenate $\text{Cd}_2\text{As}_2\text{O}_7$



**Origin:** Synthetic.

**Description:** Prepared by solid-state reaction of CdO and  $\text{As}_2\text{O}_5$  at 873 K for 10–12 days. Monoclinic, space group  $C2/m$ ,  $Z = 2$ .

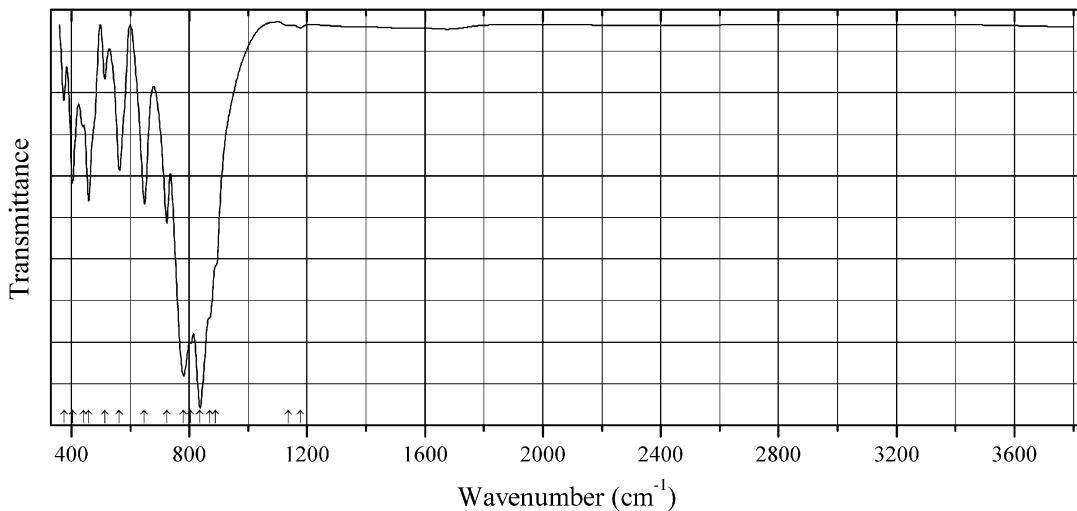
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Baran and Weil (2004).

**Wavenumbers (IR, cm $^{-1}$ ):** 953, 890sh, 854s, 812s, 472, 393, 341, 310.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 880s, 810w, 489w, 358, 423, 323, 294, 216w.

**As357 Bradaczekite**  $\text{NaCu}_4(\text{AsO}_4)_3$ 

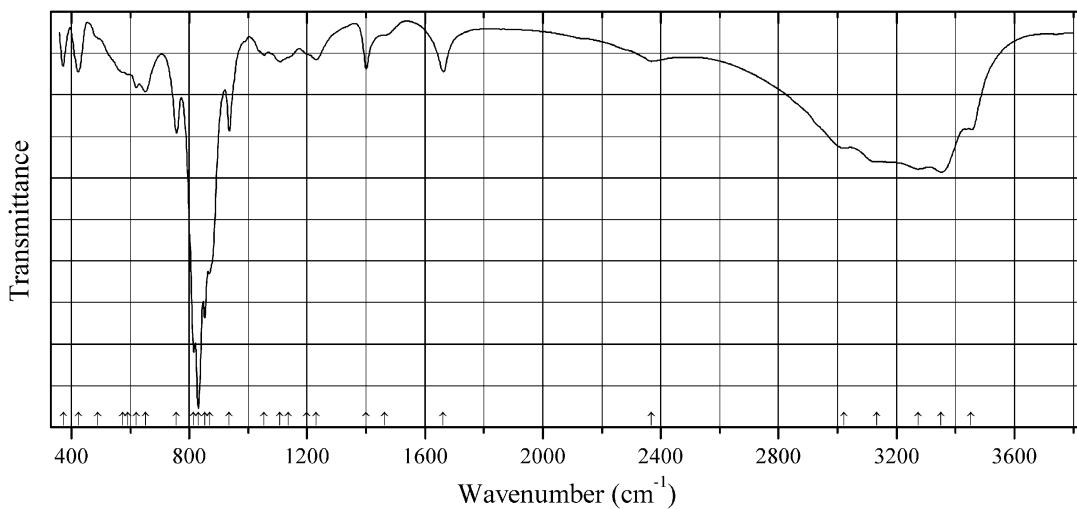
**Origin:** Arsenatnaya fumarole, North Breach of the Great Fissure Tolbachik volcano, Kamchatka peninsula, Russia.

**Description:** Deep blue coarse crystals. Investigated by I.V. Pekov.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption. Baseline correction has been applied.

**Wavenumbers (cm<sup>-1</sup>):** 1176w, 1135w, 890sh, 870sh, 837s, 805, 781s, 724, 648, 563, 513w, 459, 442w, 404, 375.

**Note:** The spectrum was obtained by N.V. Chukanov.

**As358 Vysokýite**  $\text{U}^{4+}(\text{H}_2\text{AsO}_4)_4 \cdot 4\text{H}_2\text{O}$ 

**Origin:** Geschieber vein, Svornost shaft, Jáchymov, Krušné Hory Mts. (Ore Mts.), Czech Republic (type locality).

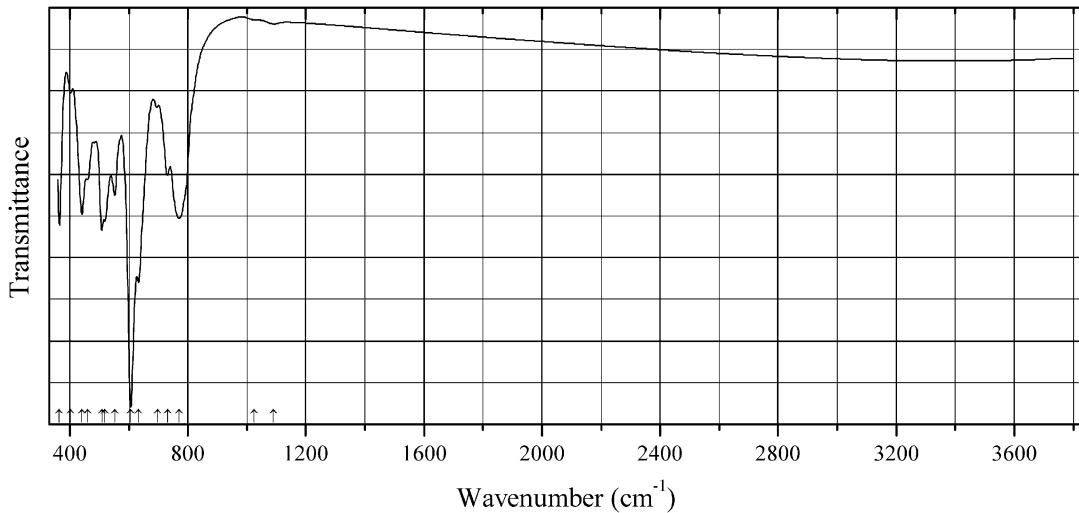
**Description:** Aggregates of green acicular crystals from the association with štěpite. The sample was received from the authors of the first description of vysokýite.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3452, 3350, 3273, 3132, 3022, 2368w, 1662, 1463w, 1401, 1231, 1200sh,

1135sh, 1108, 1053w, 936, 869, 853s, 831s, 815s, 757, 651, 621, 591, 575sh, 490sh, 424, 373.

**Note:** The spectrum was obtained by N.V. Chukanov.



**Origin:** Tsumeb mine, Tsumeb, Namibia (type locality).

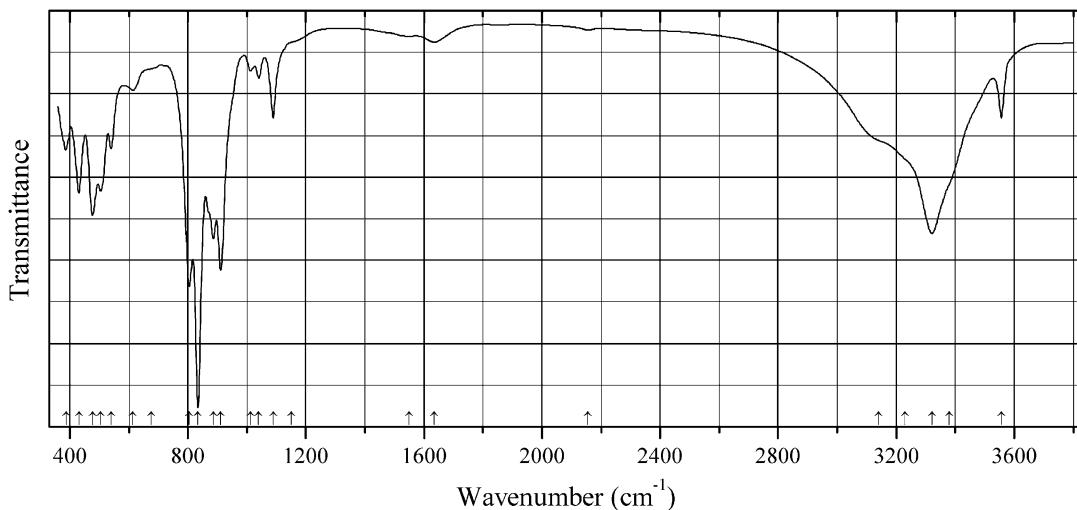
**Description:** Brownish-red acicular crystals from a sulfide aggregate. Investigated by A.V. Kasatkin.

Holotype sample. The empirical formula is (electron microprobe):  $Pb_{1.00}Fe_{3.65}As_{10.35}O_{22}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 1090w, 1025w, 770, 731, 697w, 632s, 606s, 552, 519, 508, 460, 441, 403w, 365.

**Note:** The spectrum was obtained by N.V. Chukanov.

**As360 Kamarizaite**  $\text{Fe}^{3+}_3(\text{AsO}_4)_2(\text{OH})_3 \cdot 3\text{H}_2\text{O}$ 

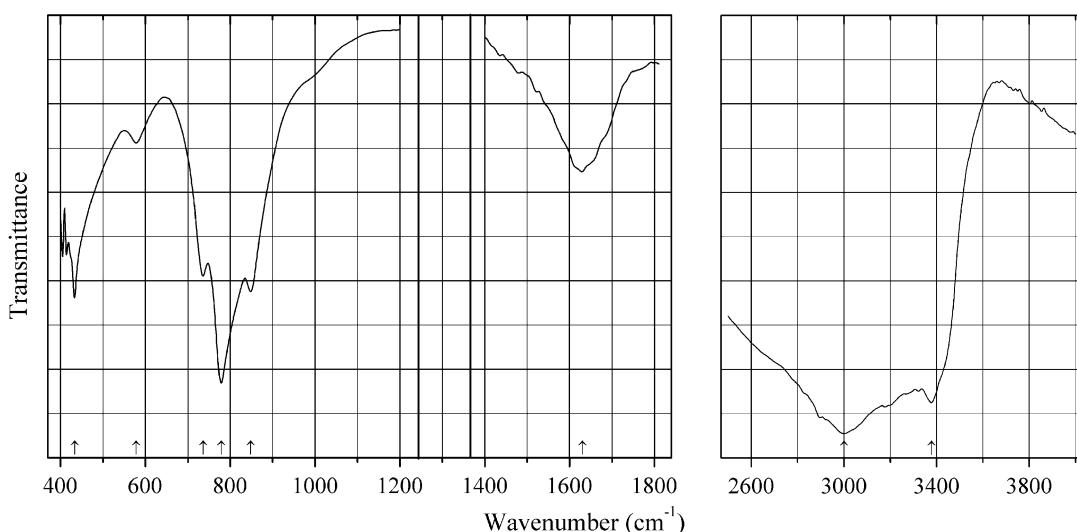
**Origin:** Hilarion mine, Agios Konstantinos, Lavrion mining District, Attikí (Attika, Attica) Prefecture, Greece.

**Description:** Fine-grained, porcelain-like yellow pseudomorphs after grains of an unknown ore mineral from the association with goethite, scorodite, and jarosite. Investigated by I.V. Pekov.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3556, 3380sh, 3321s, 3230sh, 3140sh, 2156w, 1635, 1550w, 1150sh, 1089, 1040, 1013, 911s, 886, 870sh, 834s, 805s, 675sh, 614, 540, 505, 477, 431, 387.

**Note:** The spectrum was obtained by N.V. Chukanov.

**As361 Symplesite**  $\text{Fe}^{2+}_3(\text{AsO}_4)_2 \cdot 8\text{H}_2\text{O}$ 

**Origin:** Saubach, near Mildenberg, Vogtland, Saxony, Germany.

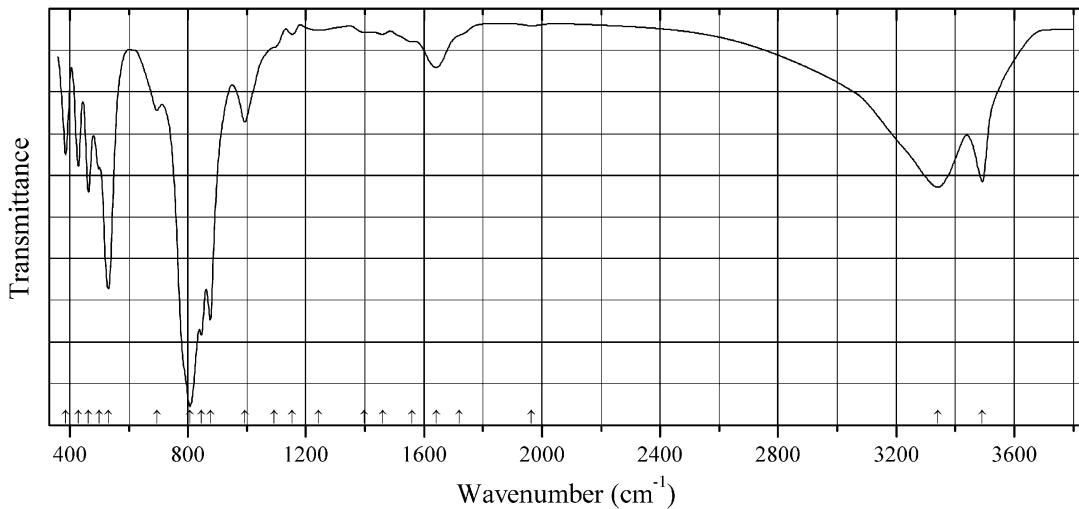
**Description:** Black acicular crystals. Characterized by powder X-ray diffraction data. Triclinic, space group  $P\bar{1}$ ,  $a = 7.785$ ,  $b = 9.259$ ,  $c = 4.751$  Å,  $\alpha = 93.053^\circ$ ,  $\beta = 98.139^\circ$ ,  $\gamma = 106.379^\circ$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Makreski et al. (2015b).

**Wavenumbers (cm<sup>-1</sup>):** 3377, 3000s, 1630, 848, 779s, 736, 578w, 433.

### As362 Agardite-(Ce) CeCu<sup>2+</sup><sub>6</sub>(AsO<sub>4</sub>)<sub>3</sub>(OH)<sub>6</sub>·3H<sub>2</sub>O



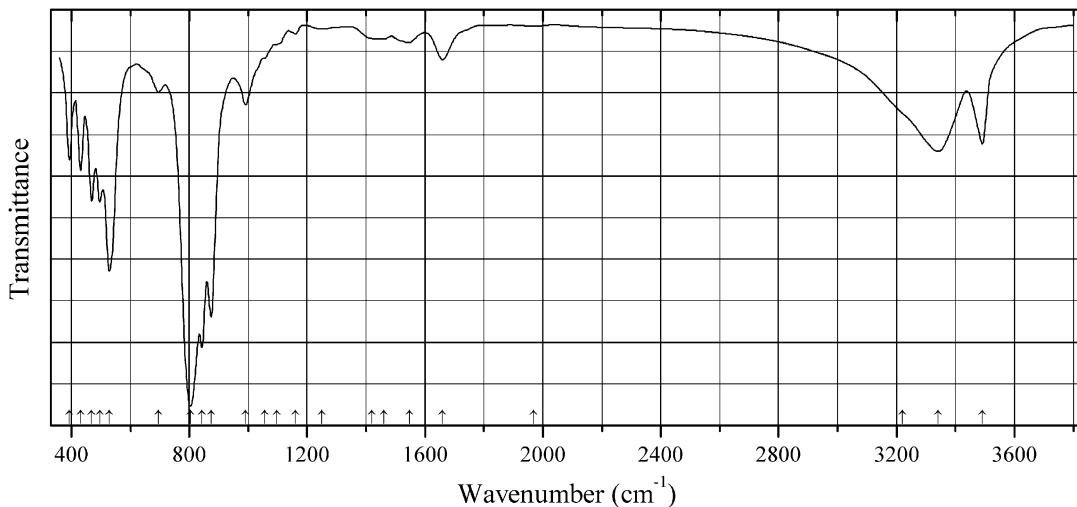
**Origin:** Clara Mine, Schwarzwald, Germany (type locality).

**Description:** Random aggregates of olive green acicular hexagonal crystals growing on fluorite. The crystal structure is solved. Hexagonal, space group  $P6_3/m$ ,  $a = 13.598(6)$  Å,  $c = 5.954(3)$  Å,  $V = 953.5(2)$  Å<sup>3</sup>,  $Z = 2$ . The empirical formula is (electron microprobe): [(Ce<sub>0.32</sub>La<sub>0.19</sub>Nd<sub>0.15</sub>Pr<sub>0.06</sub>Gd<sub>0.04</sub>Y<sub>0.04</sub>Sm<sub>0.03</sub>Eu<sub>0.02</sub>)Ca<sub>0.20</sub>Sr<sub>0.06</sub>](Cu<sub>5.74</sub>Fe<sup>3+</sup><sub>0.16</sub>Mn<sup>2+</sup><sub>0.02</sub>)[(AsO<sub>4</sub>)<sub>2.89</sub>(PO<sub>4</sub>)<sub>0.04</sub>(SiO<sub>4</sub>)<sub>0.04</sub>(SbO<sub>4</sub>)<sub>0.03</sub>](OH)<sub>5.97</sub>O<sub>0.03</sub>·3H<sub>2</sub>O.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3492, 3340, 1965w, 1720sh, 1641, 1560w, 1460w, 1397w, 1243w, 1154w, 1092w, 993, 876s, 846s, 807s, 695, 530s, 499, 464, 429, 385.

**Note:** The spectrum was obtained by N.V. Chukanov. The weak bands in the range from 1092 to 1560 cm<sup>-1</sup> correspond to isolated H<sup>+</sup> cations that do not form strong covalent bonds with coordinating O atoms.

**As363 Agardite-(Nd)  $\text{NdCu}^{2+}_6(\text{AsO}_4)_3(\text{OH})_6 \cdot 3\text{H}_2\text{O}$** 

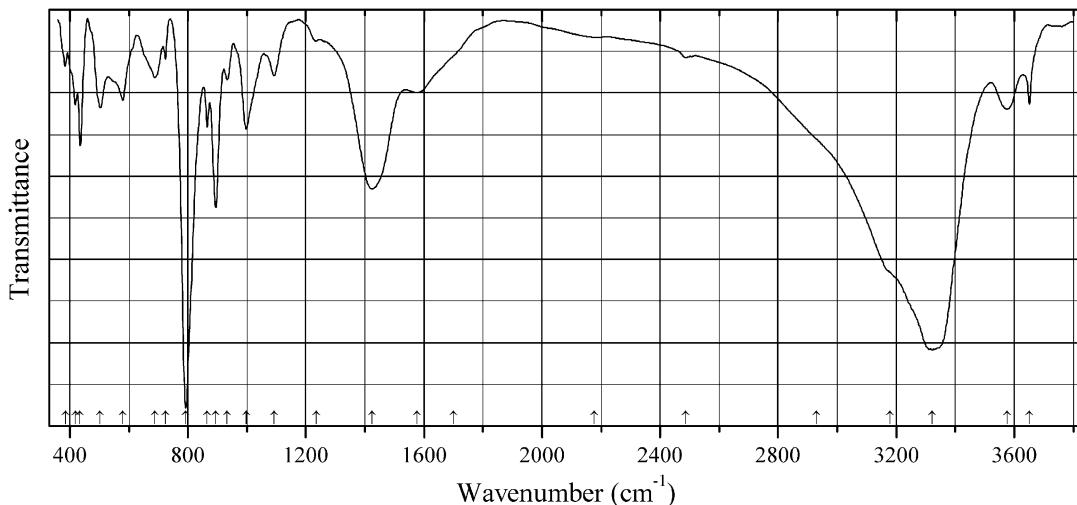
**Origin:** Hilarion Mine, Agios Konstantinos (Kamariza), Lavrion District, Attikí Prefecture.

**Description:** Bluish green acicular crystals growing [with zones of agardite-(La)] from the association with zincolivenite, azurite, malachite, and calcite. Holotype sample. Hexagonal, space group  $P6_3/m$ ,  $a = 13.548(8)$  Å,  $c = 5.894(6)$  Å,  $V = 937(2)$  Å<sup>3</sup>,  $Z = 2$ . The empirical formula is  $[(\text{Nd}_{0.19}\text{La}_{0.14}\text{Y}_{0.12}\text{Pr}_{0.05}\text{Gd}_{0.02}\text{Ce}_{0.02}\text{Sm}_{0.02}\text{Dy}_{0.02})\text{Ca}_{0.39}](\text{Cu}_{5.49}\text{Zn}_{0.44})(\text{AsO}_4)_3(\text{OH})_{5.38} \cdot 2.64\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3491, 3340, 3220sh, 1968w, 1660, 1547w, 1460w, 1420w, 1250w, 1160w, 1098w, 1057w, 991, 874s, 843s, 804s, 695, 529s, 496, 469, 432, 393.

**Note:** The spectrum was obtained by N.V. Chukanov. The weak bands in the range from 1057 to 1547 cm<sup>-1</sup> correspond to isolated H<sup>+</sup> cations that do not form strong covalent bonds with coordinating O atoms.

**As364 Chlorophoenicite  $\text{Mn}_3\text{Zn}_2(\text{HAsO}_4)(\text{OH})_8$** 

**Origin:** Sterling Hill, New Jersey, USA.

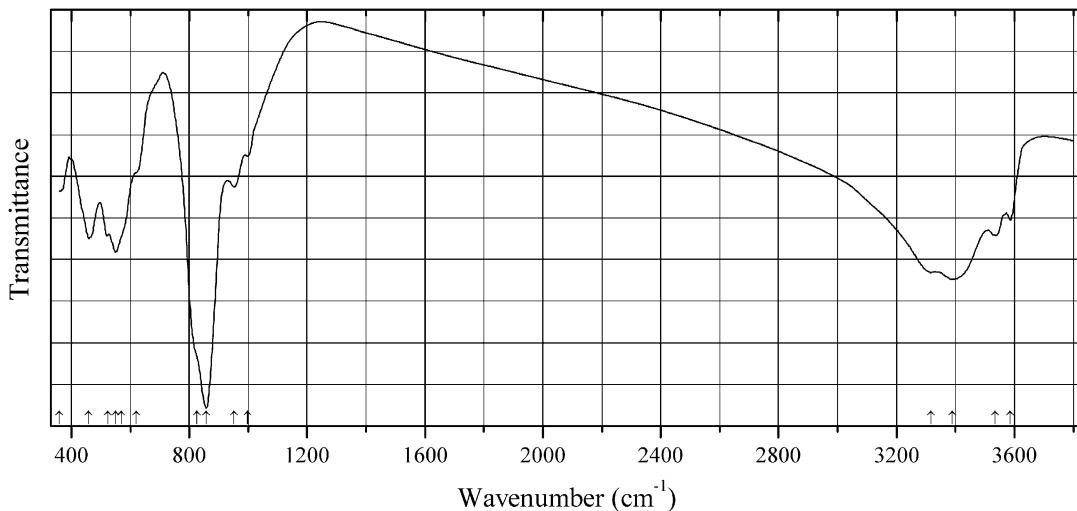
**Description:** White fibrous aggregate on rhodochrosite. The empirical formula is (electron microprobe):  $(\text{Mn}_{2.68}\text{Mg}_{0.24}\text{Fe}_{0.02})\text{Zn}_{2.06}[\text{H}(\text{As}_{0.98}\text{S}_{0.02})\text{O}_4]_8(\text{OH})_8$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3651, 3575, 3322s, 3180sh, 2930sh, 2487w, 2186w, 1700sh, 1577, 1235w, 1092, 998, 933w, 894, 793s, 688, 580, 503, 435, 419, 385w.

**Note:** The spectrum was obtained by N.V. Chukanov. Additional bands at 1424, 866, and 724  $\text{cm}^{-1}$  correspond to admixed rhodochrosite.

### As365 Gerdtremmelite $\text{ZnAl}_2(\text{AsO}_4)_5(\text{OH})_5$



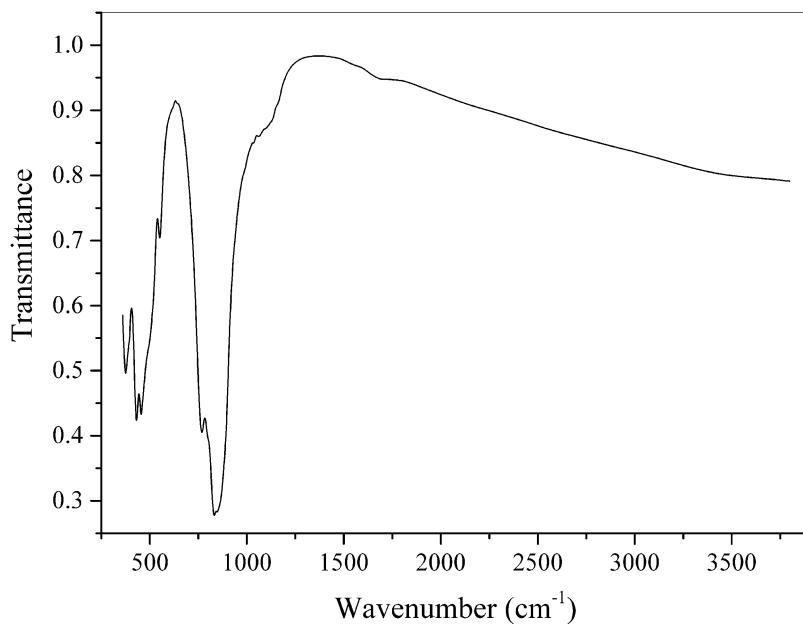
**Origin:** Tsumeb Mine, Tsumeb, Oshikoto Region, Namibia (type locality).

**Description:** Brown crust. Cotype sample received from Gerd Tremmel.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3586, 3535, 3389s, 3318, 999, 953, 857s, 825sh, 620sh, 570sh, 550s, 523, 459, (360).

**Note:** The spectrum was obtained by N.V. Chukanov.

**As367 Badalovite**  $\text{Na}_2\text{Mg}_2\text{Fe}^{3+}(\text{AsO}_4)_3$ 

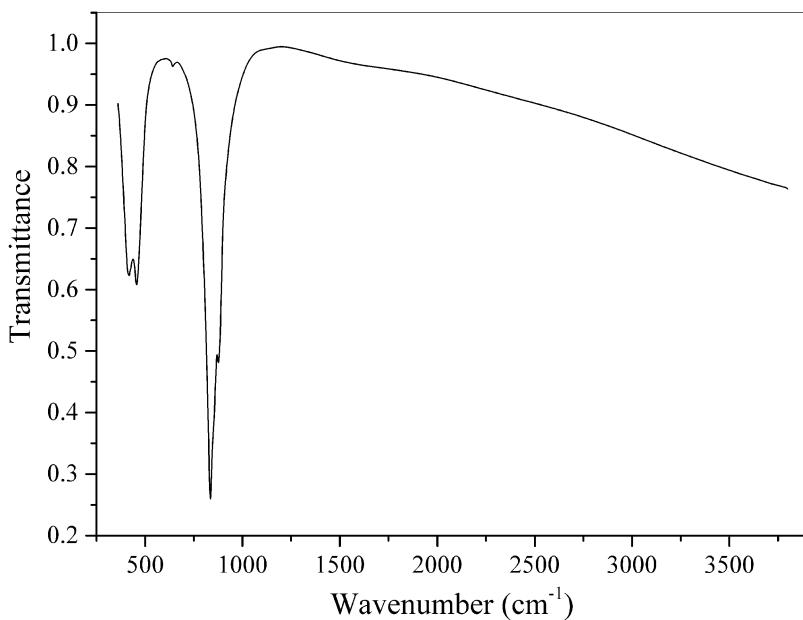
**Origin:** Arsenatnaya fumarole, North Breach of the Great Fissure Tolbachik volcano, Kamchatka peninsula, Russia (type locality).

**Description:** Yellow prismatic crystals from the association with calciojohillerite, hematite, fluorphlogopite, aphthitalite, and cassiterite. Investigated by I.V. Pekov. Characterized by single-crystal X-ray diffraction data. Monoclinic, space group  $C2/c$ ,  $a = 11.90$ ,  $b = 12.78$ ,  $c = 6.66 \text{ \AA}$ ,  $\beta = 112.52^\circ$ ,  $V = 936.6 \text{ \AA}^3$ ,  $Z = 4$ . The empirical formula is (electron microprobe):  $(\text{Na}_{1.61}\text{Ca}_{0.33}\text{K}_{0.03})(\text{Mg}_{1.78}\text{Zn}_{0.05}\text{Mn}_{0.03}\text{Cu}_{0.01})(\text{Fe}_{0.85}\text{Al}_{0.13})[(\text{AsO}_4)_{2.94}(\text{PO}_4)_{0.04}(\text{VO}_4)_{0.01}(\text{SO}_4)_{0.01}]$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 1695w, 1160sh, 1125sh, 1063w, 1033w, 850s, 832s, 805sh, 769s, 551, 490sh, 455s, 431s, 390sh, 375.

**Note:** The spectrum was obtained by N.V. Chukanov.

**As368 Svabite**  $\text{Ca}_5(\text{AsO}_4)_3\text{F}$ 

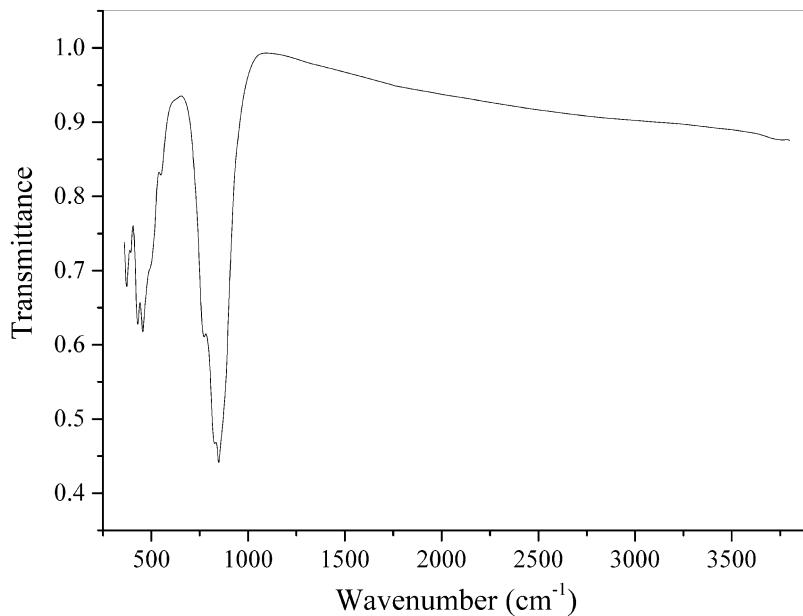
**Origin:** Arsenatnaya fumarole, North Breach of the Great Fissure Tolbachik volcano, Kamchatka peninsula, Russia.

**Description:** White radiated aggregates from the association with calciojohillerite, anhydrite, berzelite, diopside, and hematite. Investigated by I.V. Pekov. A V-bearing variety (As: V ≈ 94:6). Characterized by single-crystal X-ray diffraction data. Hexagonal, space group  $P6_3/m$ ,  $a = 9.785$ ,  $c = 6.946$  Å,  $V = 576.1$  Å<sup>3</sup>,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm⁻¹):** 877, 835s, 643w, 456, 418.

**Note:** The spectrum was obtained by N.V. Chukanov.

**As369 Calciojohillerite**  $\text{NaCaMg}_3(\text{AsO}_4)_3$ 

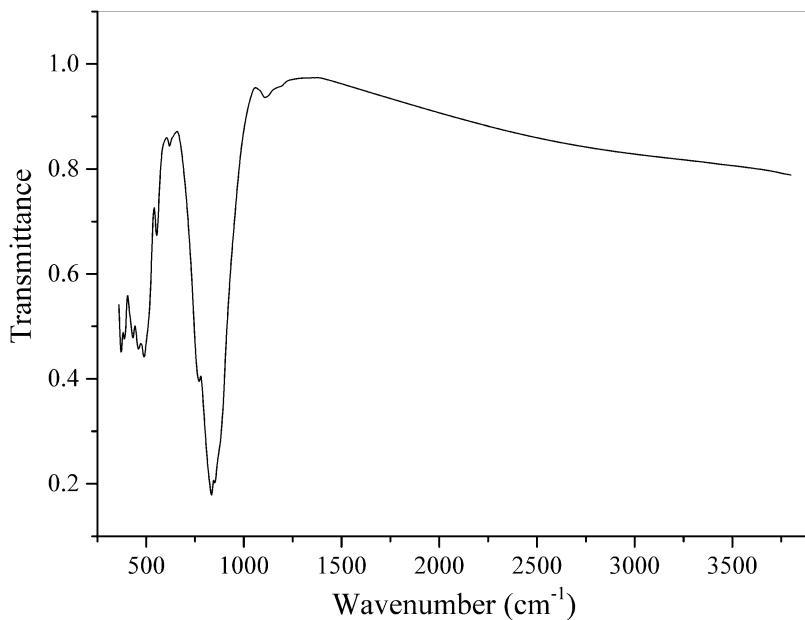
**Origin:** Arsenatnaya fumarole, North Breach of the Great Fissure Tolbachik volcano, Kamchatka peninsula, Russia (type locality).

**Description:** Greenish-brown prismatic crystals from the association with hematite, tenorite, cassiterite, johillerite, bradaczekite, hatertite, nickenichite, badalovite (IMA2016-053), aphthitalite, langbeinite, calciolangbeinite, etc. Investigated by I.V. Pekov.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 848s, 830s, 549w, 495sh, 455, 429, 393, 373.

**Note:** The spectrum was obtained by N.V. Chukanov.

**As370 Nickenichite**  $\text{Na}(\square,\text{Ca})(\square,\text{Cu})(\text{Mg},\text{Fe}^{3+})_3(\text{AsO}_4)_3$ 

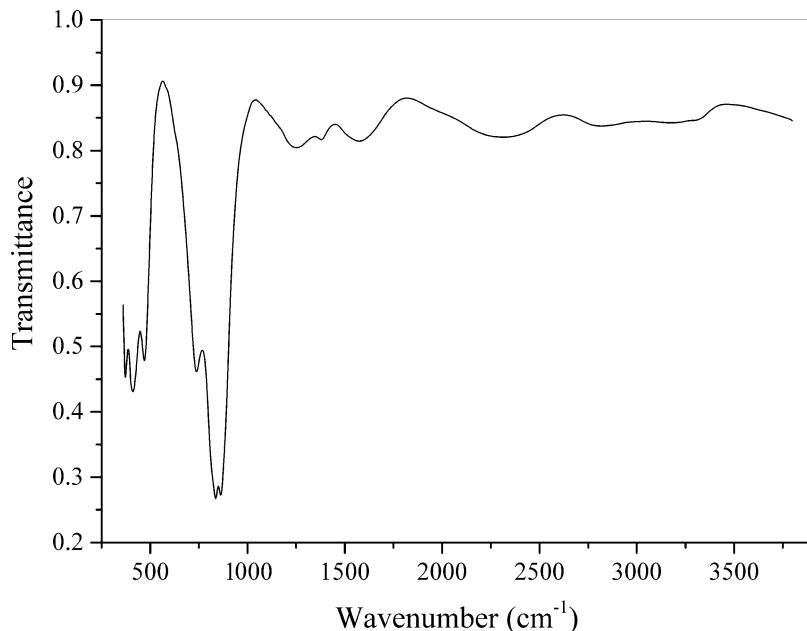
**Origin:** Arsenatnaya fumarole, North Breach of the Great Fissure Tolbachik volcano, Kamchatka peninsula, Russia (type locality).

**Description:** Violet prismatic crystals from the association with hematite, tenorite, johillerite, aphthitalite, etc. Investigated by I.V. Pekov. The empirical formula is (electron microprobe):  $\text{Na}_{1.41}\text{K}_{0.03}\text{Ca}_{0.38}\text{Cu}_{0.17}\text{Mg}_{2.89}\text{Fe}_{0.31}\text{Al}_{0.09}[(\text{As}_{2.86}\text{P}_{0.03}\text{V}_{0.01}\text{Si}_{0.01})\text{O}_{12}]$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 1175sh, 1109w, 852s, 835s, 772, 619w, 554, 489, 463, 432, 390, 374.

**Note:** The spectrum was obtained by N.V. Chukanov. The bands at 1175, 1109, and 619 cm<sup>-1</sup> correspond to trace amounts of  $\text{SO}_4^{2-}$  groups.

**As371 Magnesiocanutite**  $\text{NaMnMg}_2[\text{AsO}_4]_2[\text{AsO}_2(\text{OH})_2]$ 

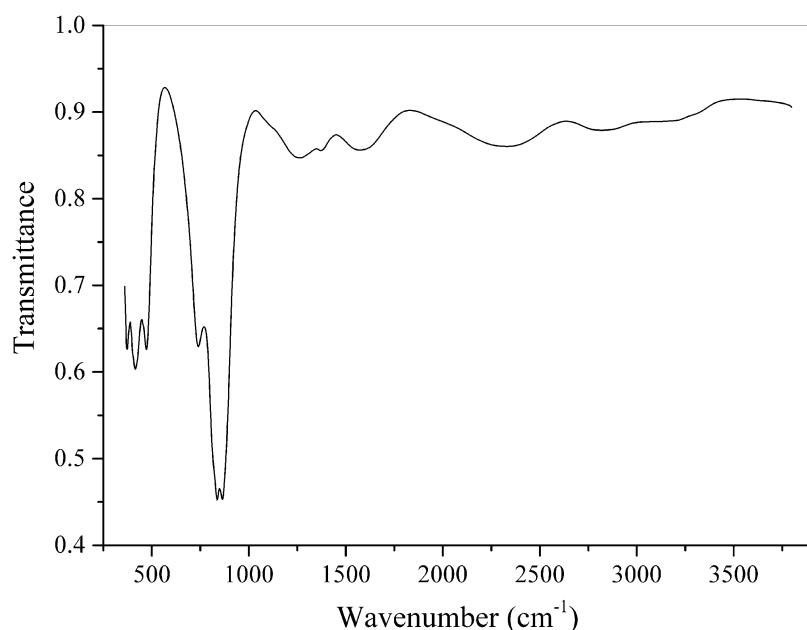
**Origin:** Torrecillas mine, Salar Grande, El Tamarugal Province, Tarapacá Region, Chile (type locality).

**Description:** Brown crystals from the association with magnesiokoritnigite and lavendulan. The empirical formula is (electron microprobe):  $\text{H}_2\text{Na}_{1.0}\text{Mn}_{1.0}(\text{Mg}_{1.8}\text{Mn}_{0.15}\text{Cu}_{0.05})\text{As}_{3.0}\text{O}_{12}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3290sh, 3180, 2820, 2309, 1577, 1380, 1254, 863s, 837s, 738, 470, 411, 375.

**Note:** The spectrum was obtained by N.V. Chukanov.

**As372 Magnesiocanutite**  $\text{NaMnMg}_2[\text{AsO}_4]_2[\text{AsO}_2(\text{OH})_2]$ 

**Origin:** Torrecillas mine, Salar Grande, El Tamarugal Province, Tarapacá Region, Chile (type locality).

**Description:** Light brown crystals from the association with magnesiokoritnigite. A Mn-rich variety.

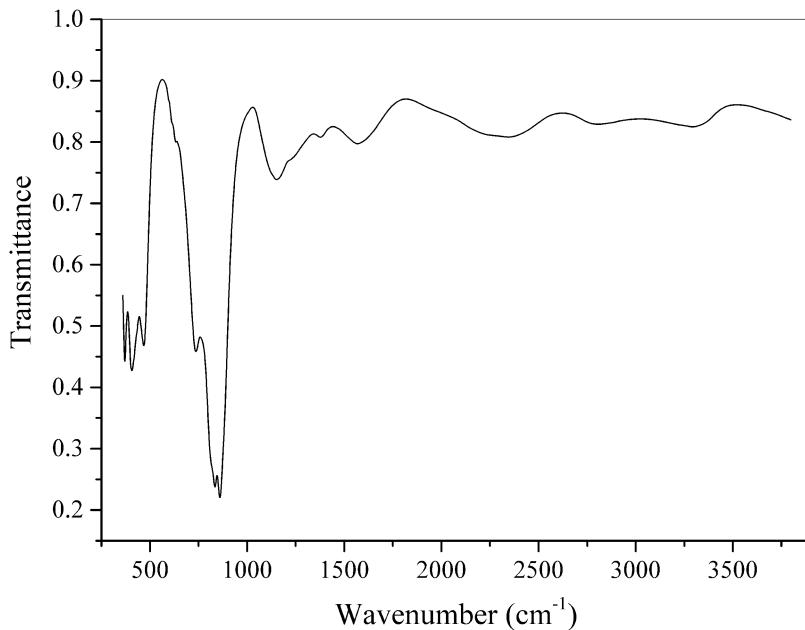
The empirical formula is (electron microprobe):  $H_2Na_{1.0}Mn_{1.0}(Mg_{1.2}Mn_{0.8})As_{3.0}O_{12}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3290sh, 3110sh, 2825, 2338, 1577, 1372, 1263, 1120sh, 864s, 837s, 740, 472, 414, 374.

**Note:** The spectrum was obtained by N.V. Chukanov.

### As373 Canutite $NaMnMn_2[AsO_4]_2[AsO_2(OH)_2]$



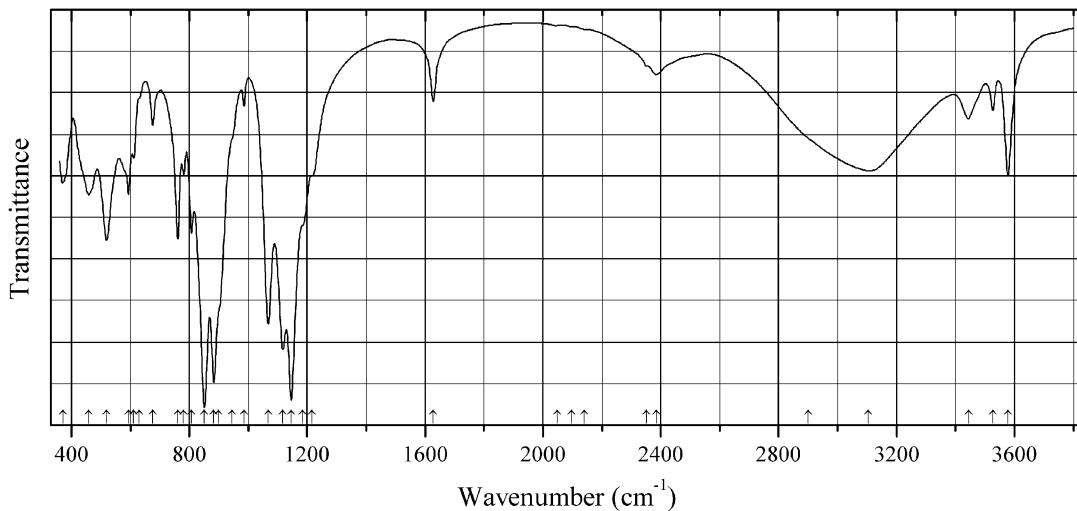
**Origin:** Torrecillas mine, Salar Grande, El Tamarugal Province, Tarapacá Region, Chile (type locality).

**Description:** Brown crystals. The empirical formula is (electron microprobe):  $H_2Na_{1.0}Mn_{1.0}(Mn_{1.2}Mg_{0.7}Cu_{0.2})As_{3.0}O_{12}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3290sh, 3110sh, 2825, 2338, 1577, 1372, 1263, 1120sh, 864s, 837s, 740, 472, 414, 374.

**Note:** The spectrum was obtained by N.V. Chukanov.

**AsS27 Juansilvaite**  $\text{Na}_5\text{Al}_3(\text{HAsO}_4)_2(\text{H}_2\text{AsO}_4)_2(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ 

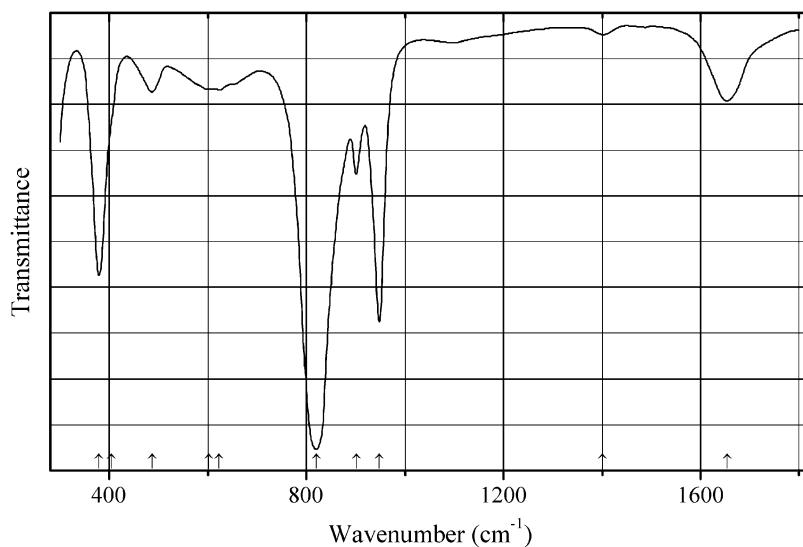
**Origin:** Torrecillas mine, Salar Grande, El Tamarugal Province, Tarapacá Region, Chile (type locality).

**Description:** Pink crystals. Investigated by I.V. Pekov.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3578, 3527, 3444, 3105, 2900sh, 2385, 2350w, 2140w, 2098w, 2049w, 1627, 1215sh, 1185sh, 1146s, 1117s, 1068s, 985w, 945sh, 900sh, 883s, 851s, 807, 781, 761, 675, 630sh, 611, 593, 519, 459, 372.

**Note:** The spectrum was obtained by N.V. Chukanov.

**UAs23 Uranospinite**  $\text{Ca}(\text{UO}_2)_2(\text{AsO}_4)_2 \cdot 10\text{H}_2\text{O}$ 

**Origin:** Synthetic.

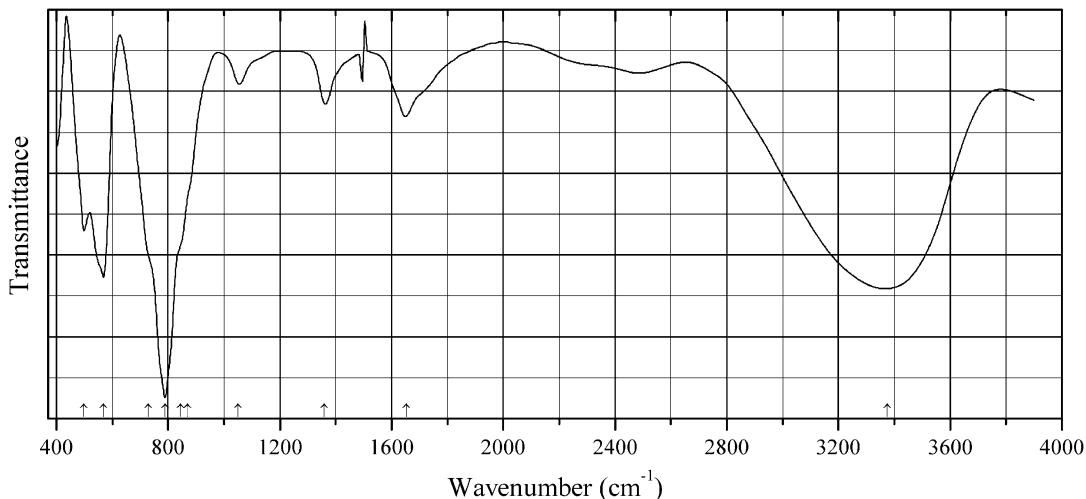
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Wilkins (1971).

**Wavenumbers (cm<sup>-1</sup>):** 1654, 1400w, 948s, 901, 820s, 623, 602, 487, 405sh, 379s.

## 2.15 Selenides, Selenites, and Selenates

**Se51 Aluminium acid selenite hydrate** AlH(SeO<sub>3</sub>)<sub>2</sub>·2H<sub>2</sub>O



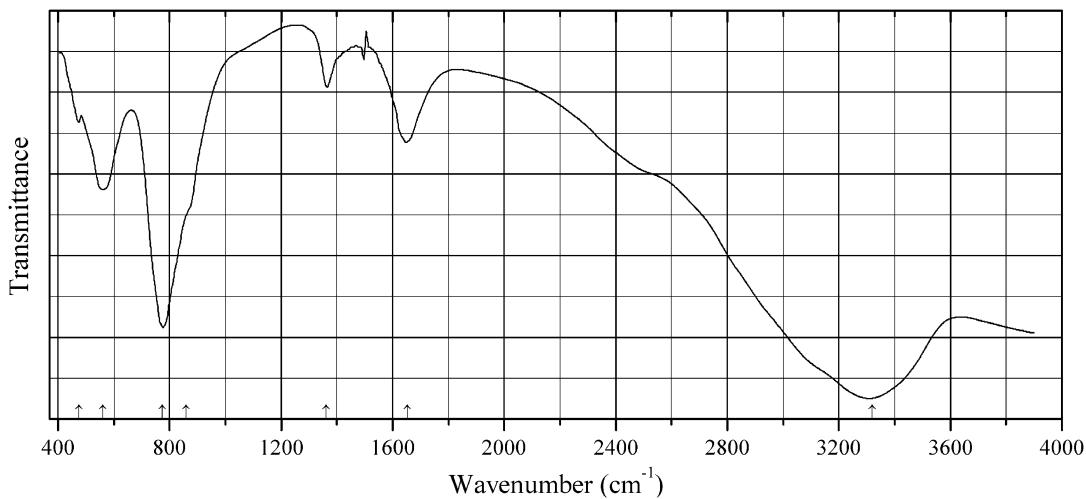
**Origin:** Synthetic.

**Description:** Prepared hydrothermally from a mixture of Al(NO<sub>3</sub>)<sub>3</sub>·9H<sub>2</sub>O and H<sub>2</sub>SeO<sub>3</sub> at 70 °C. The crystal structure is solved. Monoclinic, space group *P2<sub>1</sub>/n*, *a* = 7.3853(5), *b* = 6.4895(6), *c* = 7.3958(7) Å, β = 106.28(9)°, *V* = 340.24 Å<sup>3</sup>, *Z* = 2. *D*<sub>calc</sub> = 3.054 g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** No data.

**Source:** Morris et al. (1991).

**Wavenumbers (cm<sup>-1</sup>):** 3376s, 1654, 1360, 1051, 870sh, 845sh, 790s, 730sh, 569s, 499, and a series of bands in the range from 2000 to 2800 cm<sup>-1</sup>.

**Se52 Aluminium selenite hydrate**  $\text{Al}_2(\text{SeO}_3)_3 \cdot 6\text{H}_2\text{O}$ 


**Origin:** Synthetic.

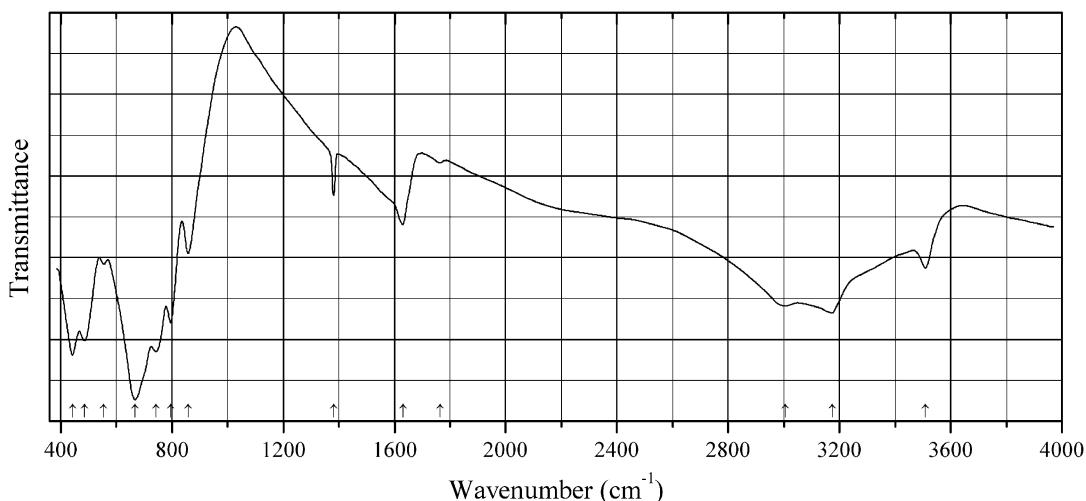
**Description:** Prepared hydrothermally from a mixture of  $\text{Al}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$  and  $\text{H}_2\text{SeO}_3$  at 70 °C. The crystal structure is solved. Trigonal, space group  $P31c$ ,  $a = 8.8020(6)$ ,  $c = 10.7070(8)$  Å,  $V = 718.39$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 2.468$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** No data.

**Source:** Morris et al. (1991).

**Wavenumbers (cm<sup>-1</sup>):** 3320s, 1652, 1362, 860sh, 775s, 560, 475w.

**Note:** The band at 1362 cm<sup>-1</sup> may correspond to an impurity.

**Se53 Barium cobalt selenite hydrate**  $\text{BaCo}_2(\text{SeO}_3)_3 \cdot 3\text{H}_2\text{O}$ 


**Origin:** Synthetic.

**Description:** Purple hexagonal prismatic crystals. Structurally related to zemannite. Hexagonal, space group  $P6_3$ ,  $a = 18.0430(6)$ ,  $c = 7.6120(2)$  Å,  $V = 2146.08(12)$  Å<sup>3</sup>,  $Z = 8$ .  $D_{\text{calc}} = 4.272$  g/cm<sup>3</sup>.

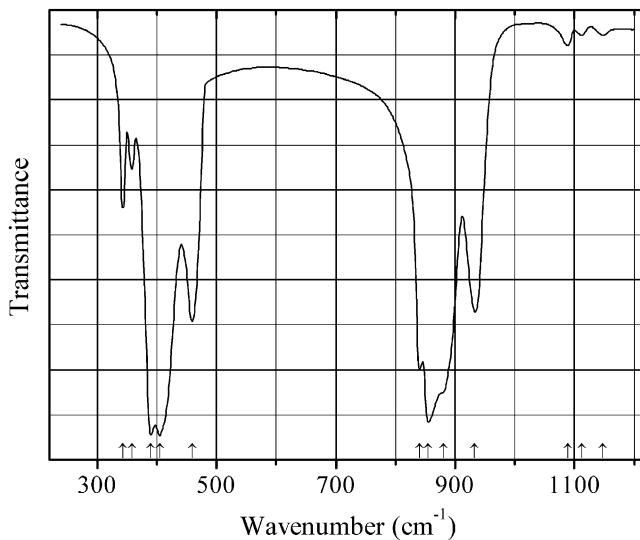
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Johnston and Harrison (2011).

**Wavenumbers (cm<sup>-1</sup>):** 3510, 3175, 3005, 1764w, 1630, (1381), 859, 795, 743s, 667s, 555w, 486s, 442s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The band at 1381 cm<sup>-1</sup> may be due to the admixture of potassium nitrate in the KBr disc.

#### Se54 Baryte selenate analogue Ba(SeO<sub>4</sub>)



**Origin:** Synthetic.

**Description:** Prepared by precipitation from aqueous solutions of sodium selenate and strontium chloride. The precipitate was dried at 150 °C. Isostructural with baryte. Orthorhombic, space group *Pnma*, *a* = 9.006, *b* = 5.690, *c* = 7.353 Å, *Z* = 2.

**Kind of sample preparation and/or method of registration of the spectrum:** Thin film on a CsBr plate. Transmission.

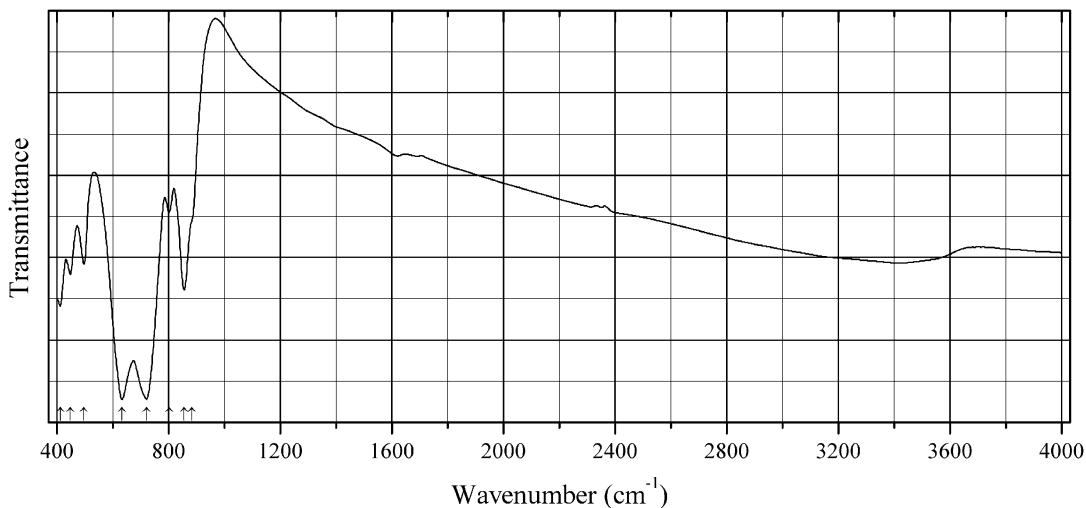
**Source:** Scheuermann and Schutte (1973b).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1148w, 1112w, 1089w, 933, 880sh, 855s, 840s, 459, 405s, 390s, 358, 343.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 915, 905sh, 901, 898, 874, 866, 846s, 465, 437w, 423, 421, 418sh, 352s, 338s, 333.

**Note:** The authors of the cited paper write: “There appears to be no combination of observed bands which would explain the three bands at 1089, 1112, and 1148 cm<sup>-1</sup> satisfactorily.” However, these bands may correspond to a sulfate impurity, which is typical for selenate reactants.

**Se55 Bismuth(III) tellurite selenate  $\text{Bi}_2(\text{TeO}_3)_2(\text{SeO}_4)$** 

**Origin:** Synthetic.

**Description:** Prepared hydrothermally from  $\text{Bi}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$ ,  $\text{TeO}_2$ , and  $\text{H}_2\text{SeO}_4$  at 230 °C for 4 days.

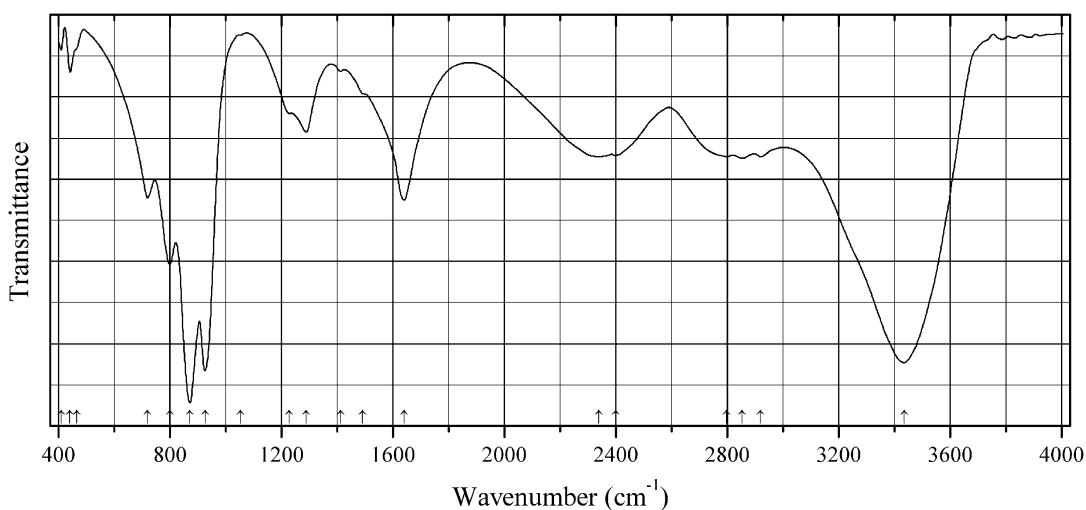
Monoclinic, space group  $I2/a$ ,  $a = 8.0995(2)$ ,  $b = 7.4835(2)$ ,  $c = 14.8219(5)$  Å,  $\beta = 97.824(3)$ °,  $V = 890.03(4)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 6.807$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Lee et al. (2013).

**Wavenumbers (cm<sup>-1</sup>):** 883sh, 856, 802w, 721s, 634s, 497, 449, 412.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Se56 Cesium acid arsenate selenate  $\text{Cs}_4(\text{SeO}_4)(\text{HSeO}_4)_2(\text{H}_3\text{AsO}_4)$** 

**Origin:** Synthetic.

**Description:** Synthesized by evaporation of aqueous solution of  $\text{CsHSeO}_4$ ,  $\text{Cs}_3\text{H}(\text{SeO}_4)_2$ , and  $\text{H}_3\text{AsO}_4$  at room temperature. Monoclinic, space group  $P2_1$ ,  $a = 5.973(1)$ ,  $b = 13.691(3)$ ,  $c = 11.910(3)$  Å,  $\beta = 94.867(1)^\circ$ ,  $V = 970.39(4)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{meas}} = 3.782$  g/cm $^3$ ,  $D_{\text{calc}} = 3.780$  g/cm $^3$ . Characterized by DSC and TG data.

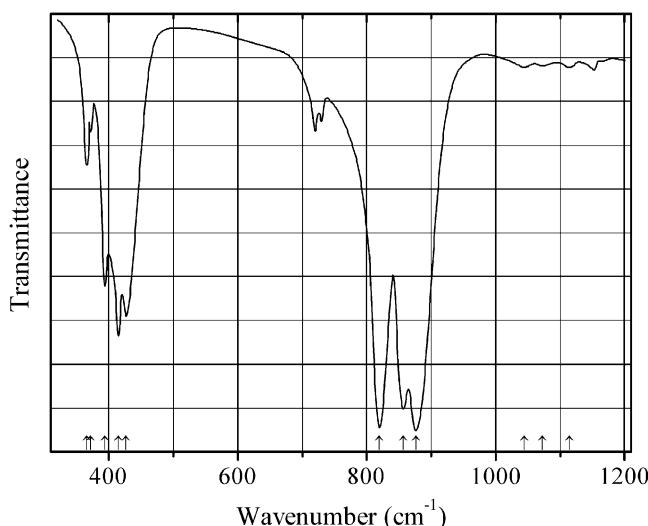
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Amri et al. (2009).

**Wavenumbers (cm $^{-1}$ ):** 3434s (broad), 2920, 2854, 2798, 2400, 2338 (broad), 1640, 1492sh, 1414w, 1290, 1228sh, 1054w, 926s, 872s, 800s, 720, 465sh, 442w, 410w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### Se58 Lead selenate $\text{PbSeO}_4$



**Origin:** Synthetic.

**Description:** Prepared by precipitation from aqueous solutions of sodium selenate and lead acetate. Monoclinic, space group  $P2_1/n$ ,  $a = 7.153$ ,  $b = 7.403$ ,  $c = 6.957$  Å,  $\beta = 103.27^\circ$ ,  $Z = 4$ .

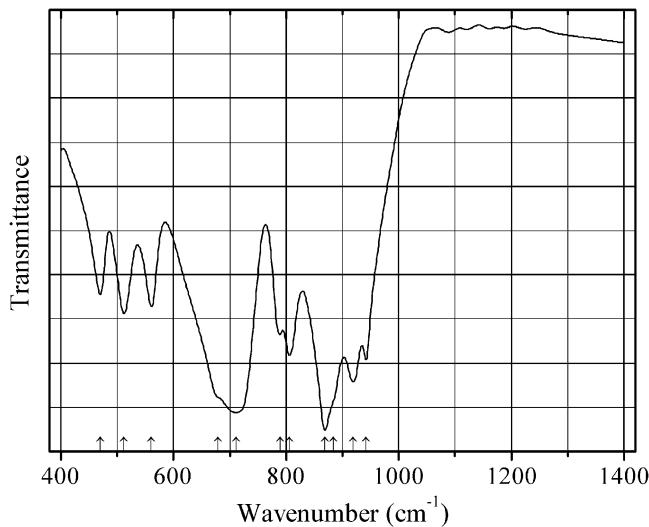
**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull. Transmission.

**Source:** Scheuermann and Schutte (1973b).

**Wavenumbers (IR, cm $^{-1}$ ):** 1114w, 1073w, 1044w, 876s, 857s, 820s, 427, 415, 394, 372, 366.

**Note:** The weak bands between 700 and 730 cm $^{-1}$  may correspond to Nujol. The weak bands at 1114, 1073, and 1044 cm $^{-1}$  assigned by Scheuermann and Schutte (1973b) to combination modes may actually correspond to the admixture of  $\text{SO}_4^{2-}$  anions. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 861, 844, 829, 818, 435, 428, 422, 411, 402, 385, 357, 326, 314.

**Se59 Copper molybdate selenite**  $\text{Cu}_2(\text{MoO}_4)(\text{SeO}_3)$ 

**Origin:** Synthetic.

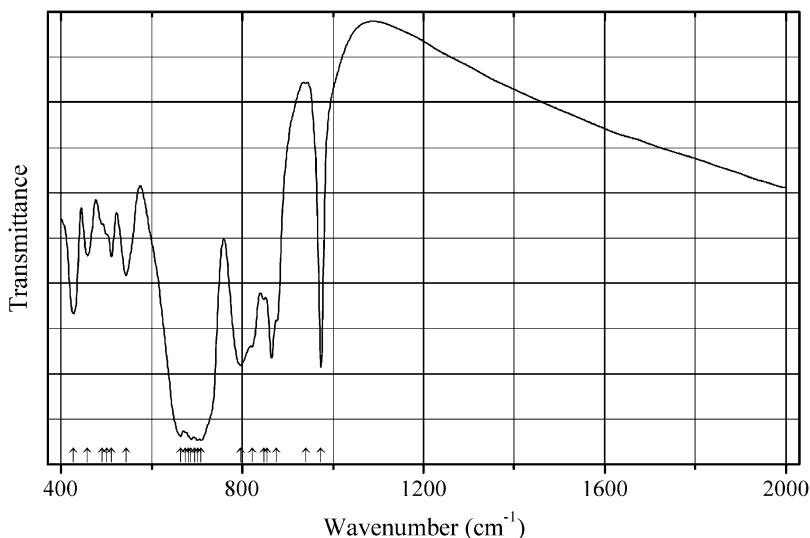
**Description:** Synthesized hydrothermally from  $\text{MoO}_3$ ,  $\text{CuO}$ , and  $\text{SeO}_2$  at  $210^\circ\text{C}$  for 4 days. Monoclinic, space group  $P2_1/c$ ,  $a = 8.148(5)$ ,  $b = 9.023(5)$ ,  $c = 8.392(5)$  Å,  $\beta = 91.141(6)^\circ$ ,  $V = 104.675(12)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 4.607$  g/cm<sup>3</sup>. In the crystal structure, Cu occupies two sites, each five-coordinated by three selenite oxygens and molybdate oxygens in a square pyramidal geometry.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Zhang et al. (2009c).

**Wavenumbers (cm<sup>-1</sup>):** 942, 919s, 884sh, 869s, 806, 789, 711s, 679sh, 561, 512, 470.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Se60 Indium vanadate selenite**  $\text{In}(\text{VSe}_2\text{O}_8)$   $\text{In}(\text{VSe}_2\text{O}_8)$ 

**Origin:** Synthetic.

**Description:** Prepared from  $\text{In}_2\text{O}_3$ ,  $\text{V}_2\text{O}_5$ , and  $\text{SeO}_2$  by a standard solid-state reaction technique.

The crystal structure is silved. Monoclinic, space group  $Pm$ ,  $a = 4.6348(9)$ ,  $b = 6.9111(14)$ ,  $c = 10.507(2)$  Å,  $\beta = 97.77(3)^\circ$ ,  $V = 333.48(11)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{calc}} = 4.498$  g/cm $^3$ .

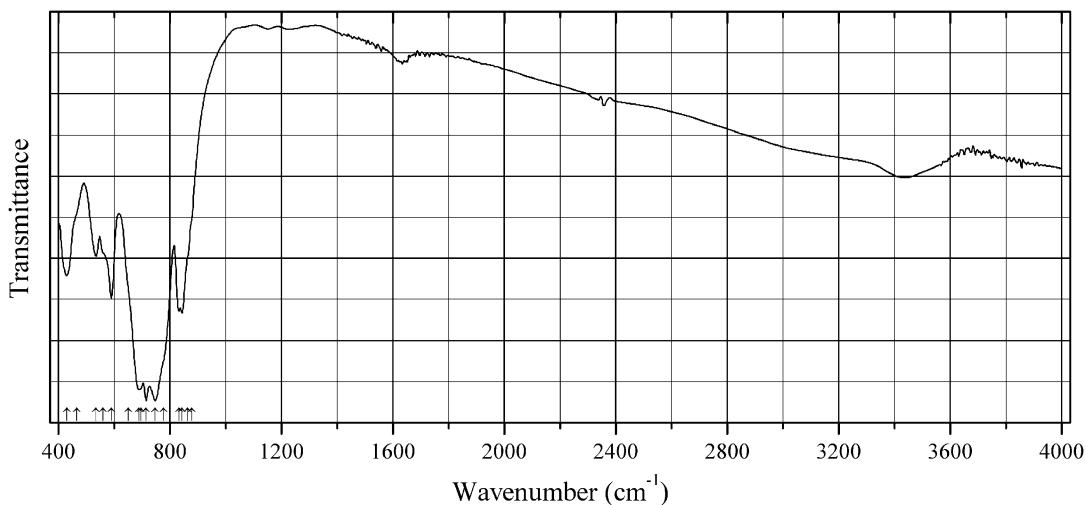
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Lee et al. (2011).

**Wavenumbers (cm $^{-1}$ ):** 974, 940, 876sh, 854, 847, 822, 796, 709s, 701s, 695sh, 687s, 681sh, 674sh, 663, 543, 511, 501sh, 491sh, 458, 427.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

### Se61 Indium zinc selenite $\text{In}_2\text{Zn}(\text{SeO}_3)_4$ $\text{In}_2\text{Zn}(\text{SeO}_3)_4$



**Origin:** Synthetic.

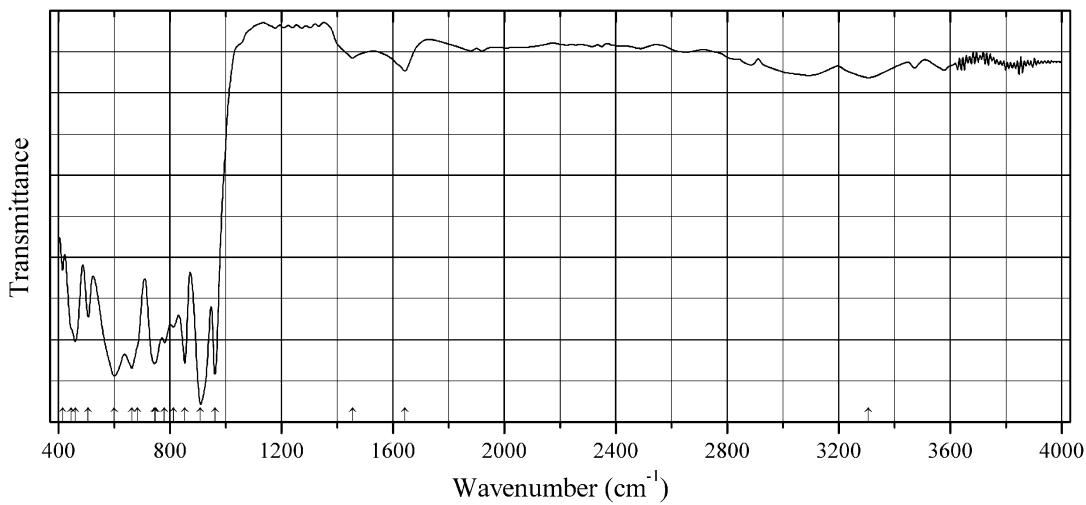
**Description:** Obtained by a standard solid-state reaction from  $\text{ZnO}$ ,  $\text{In}_2\text{O}_3$ , and  $\text{SeO}_2$ . Monoclinic, space group  $P2_1/n$ ,  $a = 8.4331(7)$ ,  $b = 4.7819(4)$ ,  $c = 14.6583(13)$  Å,  $\beta = 101.684(6)^\circ$ ,  $V = 578.87$  (9) Å $^3$ ,  $Z = 2$ .  $D_{\text{calc}} = 4.606$  g/cm $^3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Lee et al. (2012).

**Wavenumbers (cm $^{-1}$ ):** 878sh, 864sh, 844, 832, 777sh, 747s, 715s, 696sh, 690s, 650sh, 589, 561sh, 535, 465sh, 430.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Se62 Iron dimolybdate selenite hydrate  $\text{Fe}_2(\text{Mo}_2\text{O}_7)(\text{SeO}_3)_2 \cdot \text{H}_2\text{O}$   $\text{Fe}_2(\text{Mo}_2\text{O}_7)(\text{SeO}_3)_2 \cdot \text{H}_2\text{O}$** 

**Origin:** Synthetic.

**Description:** Prepared hydrothermally from  $\text{MoO}_3$ ,  $\text{Fe}_2\text{O}_3$ , and  $\text{SeO}_2$  at  $230^\circ\text{C}$  for 4 days.

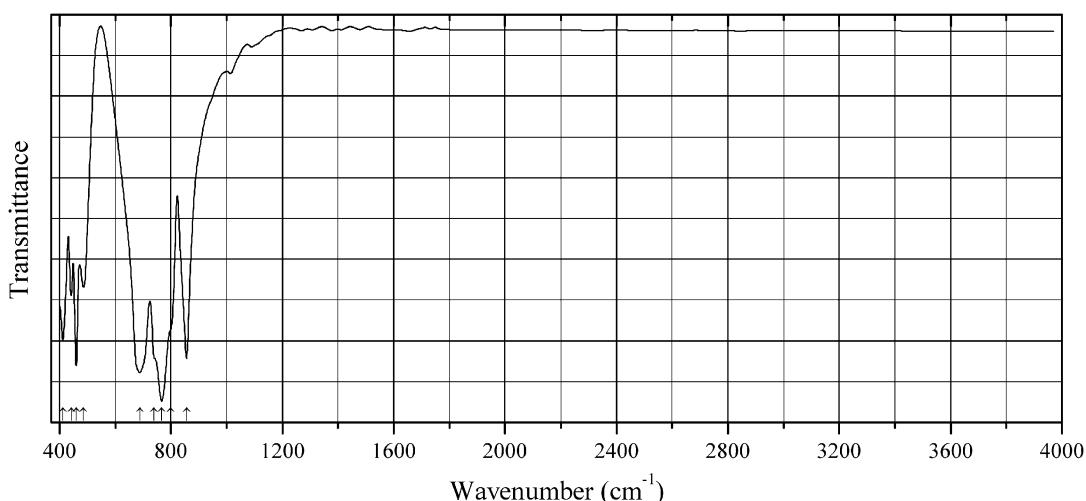
Characterized by TG and powder X-ray diffraction data. Monoclinic, space group  $C2/c$ ,  $a = 19.898(12)$ ,  $b = 5.469(3)$ ,  $c = 13.400(9)$  Å,  $\beta = 132.140(13)^\circ$ ,  $V = 1081.3(12)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 4.223$  g/cm $^3$ . The crystal structure features a pillared-layered architecture composed of iron (III) selenite layers interconnected by  $\text{Mo}_2\text{O}_{10}$  dimers.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Zhang et al. (2009c).

**Wavenumbers (cm $^{-1}$ ):** 3305w, 1643, 1456w, 962s, 910s, 854s, 812, 781, 750sh, 744s, 685sh, 663s, 601s, 507, 460, 446sh, 415.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Se63 Lanthanum selenite  $\text{La}_2(\text{SeO}_3)_3$** 

**Origin:** Synthetic.

**Description:** Obtained by thermal decomposition of  $\text{La}_2(\text{Se}_2\text{O}_5)(\text{SeO}_3)_2$ . Monoclinic, space group  $P2_1/m$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc (above  $400 \text{ cm}^{-1}$ ) and polyethylene disc (below  $400 \text{ cm}^{-1}$ ). Transmission.

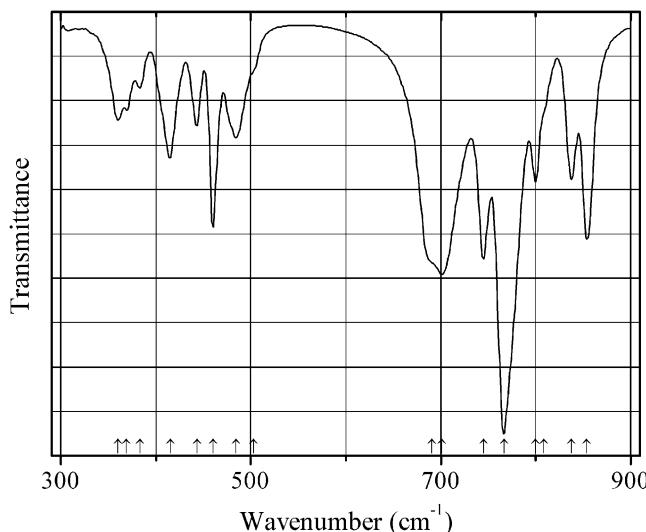
**Source:** Gopinath et al. (1998).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 856s, 800sh, 767s, 740sh, 688s, 486, 460s, 442, 412, 382, 368, 241, 201, 157, 96w, 79w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 852s, 812s, 790w, 744s, 480, 450s, 430sh, 408, 389, 365w, 250, 219sh, 203, 176, 167, 137w, 89w.

#### Se64 Lanthanum selenite $\text{La}_2\text{Se}_3\text{O}_9$



**Origin:** Synthetic.

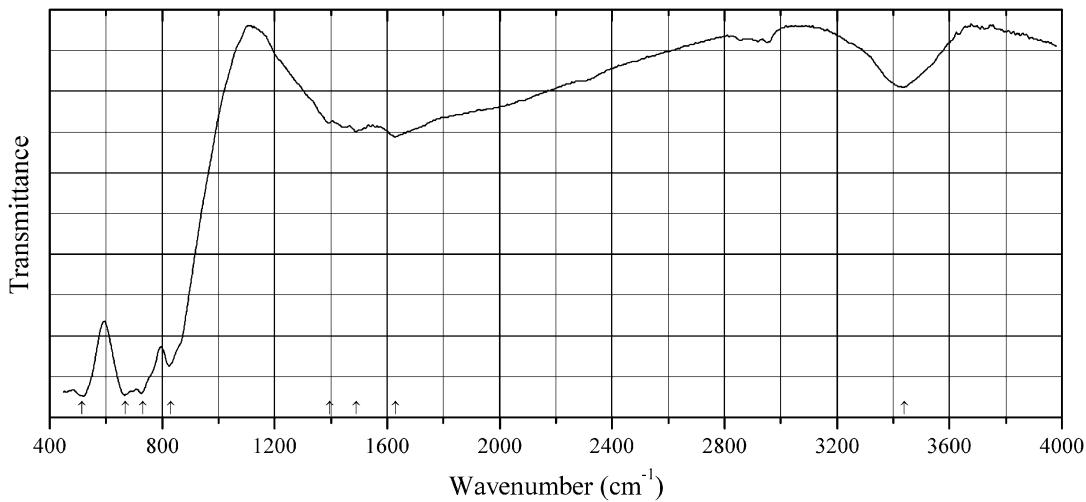
**Description:** Monoclinic, space group  $P2_1/m$ ,  $a = 14.47(8)$ ,  $b = 6.98(4)$ ,  $c = 8.21(5) \text{ \AA}$ ,  $\beta = 91.0(7)^\circ$ ,  $Z = 4$ . Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** Absorption. Kind of sample preparation is not indicated.

**Source:** Pedro et al. (1995).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 854s, 838, 809sh, 800, 767s, 745s, 701s, 691sh, 503sh, 484, 460, 443, 415, 383w, 369, 360.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**Se65 Lithium zinc selenite  $\text{Li}_2\text{Zn}_3(\text{SeO}_3)_4 \cdot 2\text{H}_2\text{O}$   $\text{Li}_2\text{Zn}_3(\text{SeO}_3)_4 \cdot 2\text{H}_2\text{O}$** 

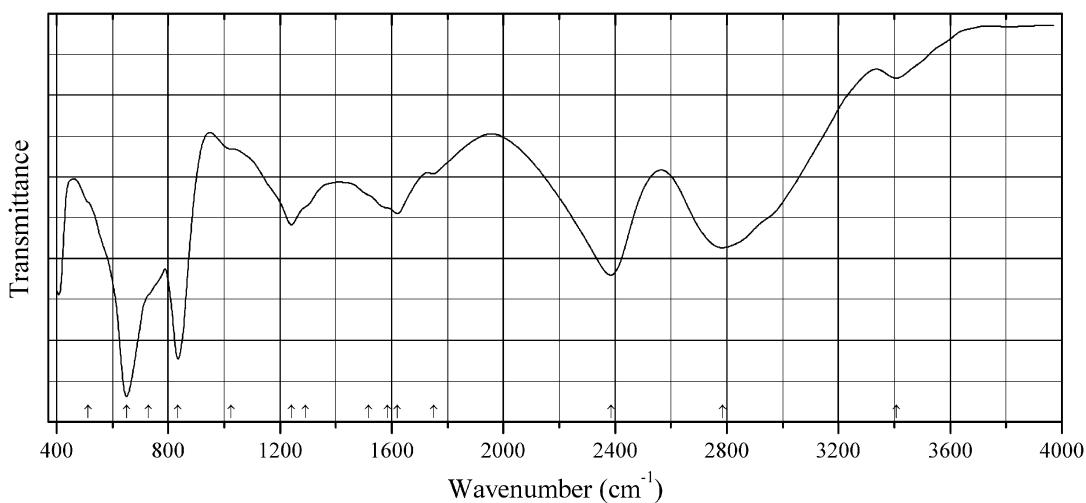
**Origin:** Synthetic.

**Description:** Prepared hydrothermally from corresponding metal carbonates and  $\text{SeO}_2$  at 230 °C for 6 days. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 8.123(4)$ ,  $b = 9.139(4)$ ,  $c = 7.938(3)$  Å,  $\beta = 12.838(9)$ °,  $V = 543.1(4)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 4.501$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Liu et al. (2015c).

**Wavenumbers (cm<sup>-1</sup>):** 3440, 1630, 1490, 1395, 830, 730s, 670s, 515s.

**Se66 Potassium acid selenite  $\text{K}(\text{HSeO}_3)$** 

**Origin:** Synthetic.

**Description:** Crystals grown by slow evaporation of an aqueous solution formed by dissolving 2 moles of SeO and 1 mole of K<sub>2</sub>CO<sub>3</sub>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

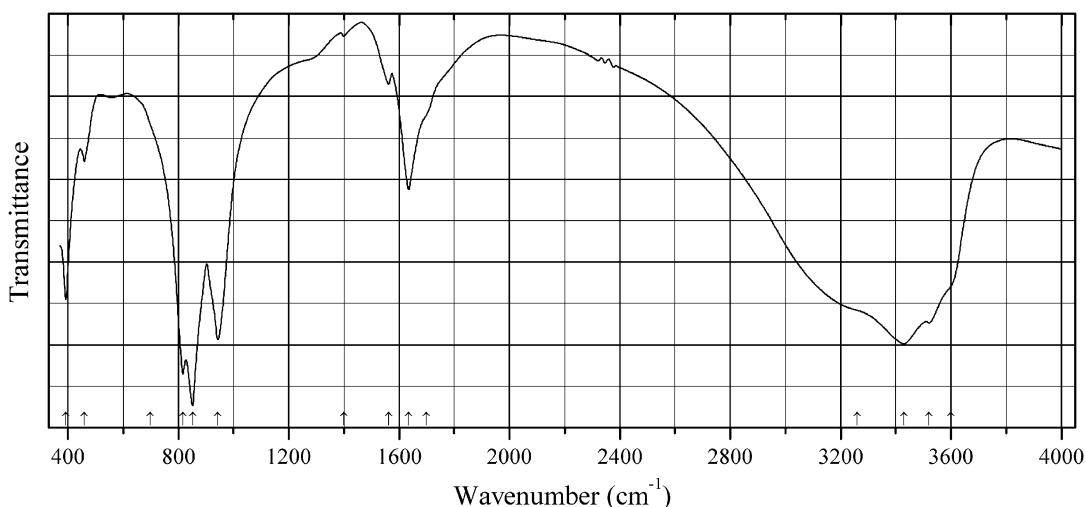
**Source:** Cody et al. (1978).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3408w, 2784s, 2385s, 1750w, 1621, 1584sh, 1517sh, 1292sh, 1240, 1024, 835s, 728sh, 650s, 512sh, 408.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 826s, 665, 423, 403, 351, 341.

### Se67 Potassium hydronium uranyl selenate hydrate K<sub>3</sub>(H<sub>3</sub>O)(UO<sub>2</sub>)<sub>4</sub>(SeO<sub>4</sub>)<sub>6</sub>·9H<sub>2</sub>O



**Origin:** Synthetic.

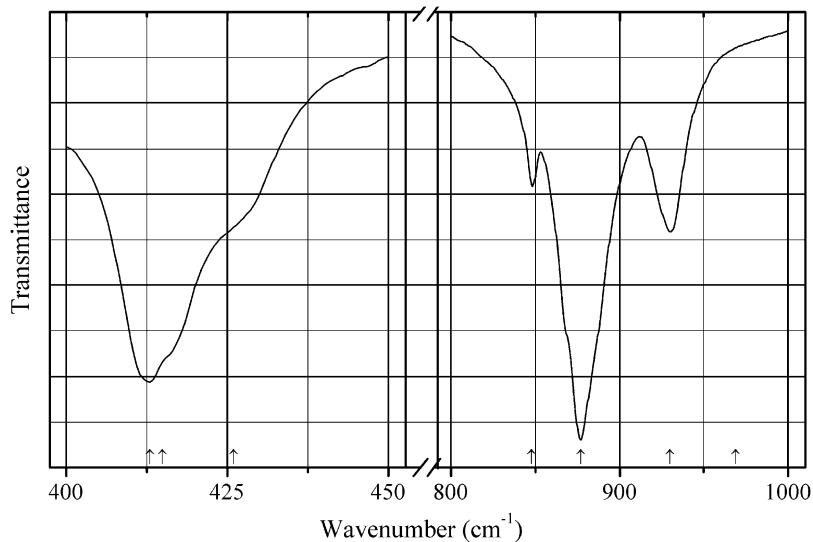
**Description:** Yellow-green crystals prepared by evaporation of the mixture of an aqueous solution containing uranyl nitrate, selenic acid, potassium carbonate, and carbamide. The crystal structure is solved. Triclinic, space group P2<sub>1</sub>/m,  $a = 12.001(3)$ ,  $b = 13.613(3)$ ,  $c = 13.753(3)$  Å,  $\beta = 109.187(4)^\circ$ ,  $V = 2122.0(8)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 3.467$  g/cm<sup>3</sup>. The structure contains two kinds of uranyl cations which are coordinated by five and three O atoms.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Gurzhiy et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 3600sh, 3520, 3430s, 3260sh, 1698sh, 1635, 1561w, 1399w, 943s, 851s, 816s, ~680sh, 459, 392.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The weak band 1399 cm<sup>-1</sup> indicates that H<sub>3</sub>O<sup>+</sup> groups are partly dissociated into H<sub>2</sub>O and H<sup>+</sup>.

**Se68 Potassium sodium selenate  $K_3Na(SeO_4)_2$** 

**Origin:** Synthetic.

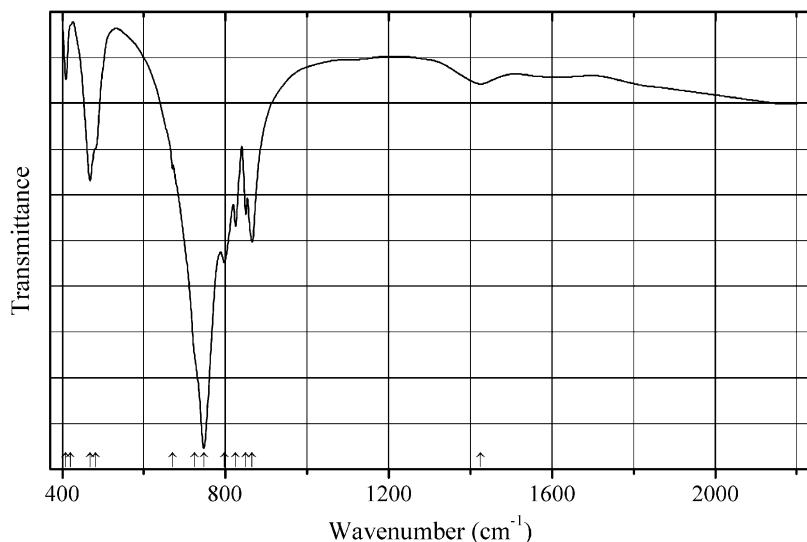
**Description:** Colorless crystals obtained at 300 K from a stoichiometric solution of sodium and potassium hydroxides and selenium acid with subsequent recrystallization from an aqueous solution. Trigonal, space group  $P-3m1$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Kaczmarski et al. (2000).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 930, 877, 869sh, 848, 426sh, 415sh, 413.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Se69 Potassium yttrium selenite  $KY(SeO_3)_2$** 

**Origin:** Synthetic.

**Description:** Synthesized hydrothermally from  $K_2CO_3$ ,  $Y(NO_3)_3 \cdot 6H_2O$ , and  $SeO_2$  at 230 °C for 4 days. Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group  $Pnma$ ,  $a = 13.3838(2)$ ,  $b = 5.70270(10)$ ,  $c = 8.6759(2)$  Å,  $V = 662.18(2)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 3.831$  g/cm<sup>3</sup>.

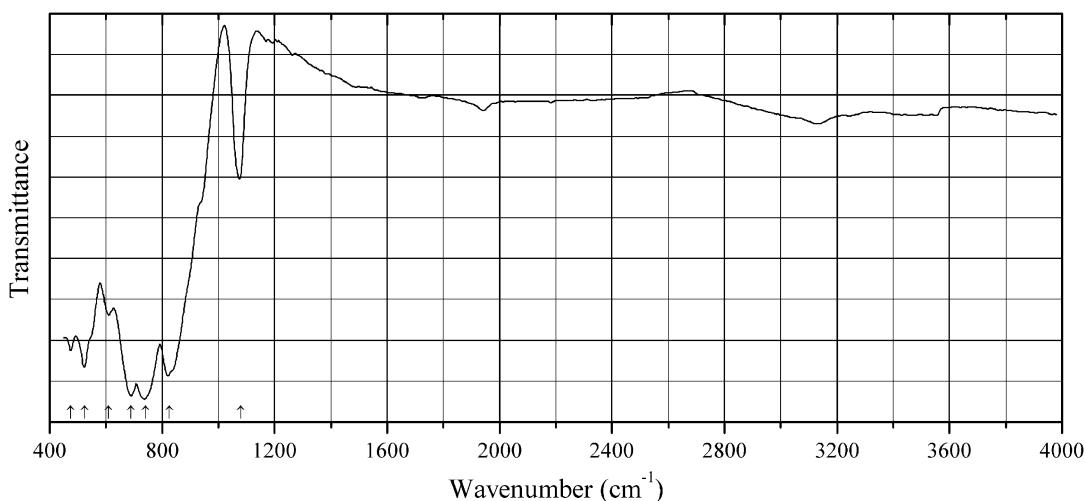
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Bang et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 1425, 865, 850, 825, 797, 747s, 725sh, 670, 482sh, 468, 420sh, 409w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### Se70 Potassium zinc selenite $K_2Zn_3(SeO_3)_4$ $K_2Zn_3(SeO_3)_4$



**Origin:** Synthetic.

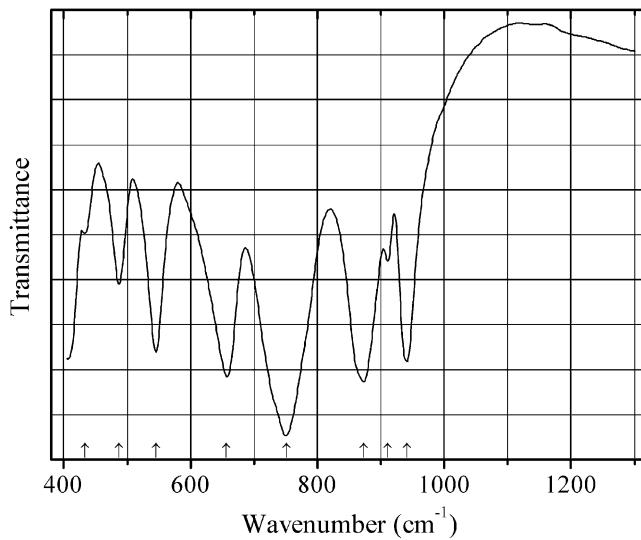
**Description:** Prepared hydrothermally from  $K_2CO_3$ ,  $ZnCO_3$ , and  $SeO_2$  at 230 °C for 6 days. The crystal structure is solved. Monoclinic, space group  $C2/c$ ,  $a = 11.3584(12)$ ,  $b = 8.6091(9)$ ,  $c = 13.6816(14)$  Å,  $\beta = 93.456(2)^\circ$ ,  $V = 1335.4(2)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 3.890$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Liu et al. (2015c).

**Wavenumbers (cm<sup>-1</sup>):** 1080, 825s, 740s, 690s, 609, 525s, 474.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The band at 1080 cm<sup>-1</sup> was assigned by the authors to Se–O vibrations. However this band as well as weak bands above 1080 cm<sup>-1</sup> should be assigned to impurities.

**Se71 Scandium vanadyl selenite  $\alpha\text{-ScVSe}_2\text{O}_8$** 

**Origin:** Synthetic.

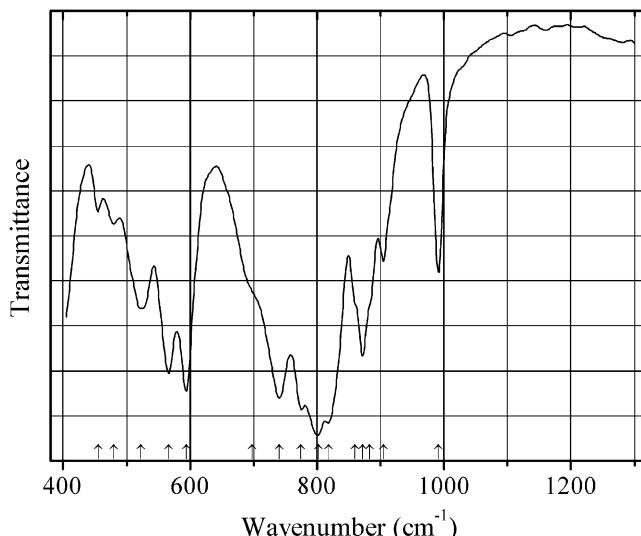
**Description:** Prepared hydrothermally from  $\text{Sc}_2\text{O}_3$ ,  $\text{V}_2\text{O}_5$ , and  $\text{SeO}_2$  at  $230^\circ\text{C}$  for 4 days. The crystal structure is solved. Monoclinic, space group  $P2_1/n$ ,  $a = 8.96460(10)$ ,  $b = 5.12600(10)$ ,  $c = 14.4802(2)$  Å,  $\beta = 104.5740(10)^\circ$ ,  $V = 570.09(10)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 3.938$  g/cm $^3$ . The  $\text{Sc}^{3+}$  cations are in distorted octahedral coordination.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Kim et al. (2013).

**Wavenumbers (cm $^{-1}$ ):** 941, 911w, 873s, 751s, 657s, 545, 487, 433w.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**Se72 Scandium vanadyl selenite  $\beta\text{-ScVSe}_2\text{O}_8$** 

**Origin:** Synthetic.

**Description:** Prepared by a solid-state reaction from  $\text{Sc}_2\text{O}_3$ ,  $\text{V}_2\text{O}_5$ , and  $\text{SeO}_2$ , first at  $350^\circ\text{C}$  for 5 h, and thereafter at  $450^\circ\text{C}$  for 48 h. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 6.59040(10)$ ,  $b = 15.9098(3)$ ,  $c = 6.63740(10) \text{ \AA}$ ,  $\beta = 92.2790(10)^\circ$ ,  $V = 695.39(2) \text{ \AA}^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 3.647 \text{ g/cm}^3$ . The structure is composed of  $\text{ScO}_7$ ,  $\text{VO}_5$ , and  $\text{SeO}_3$  coordination polyhedra.

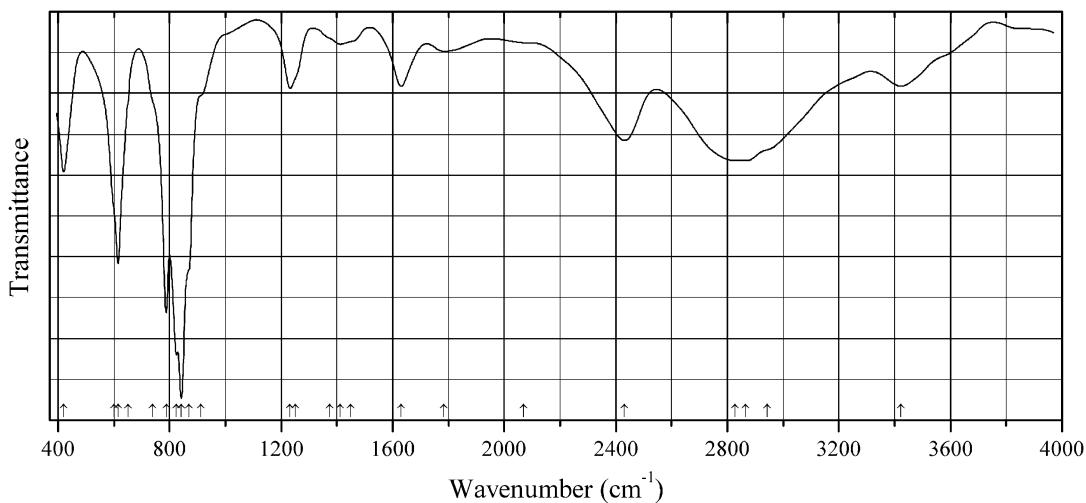
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Kim et al. (2013).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 991, 905, 883sh, 872, 860sh, 818s, 802s, 775s, 740s, 698sh, 594s, 566, 523, 480w, 455w.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

### Se73 Sodium acid selenite $\text{Na}(\text{HSeO}_3)$



**Origin:** Synthetic.

**Description:** Crystals grown by slow evaporation of an aqueous solution containing 2 moles of  $\text{SeO}_2$  and 1 mole of  $\text{Na}_2\text{CO}_3$ .

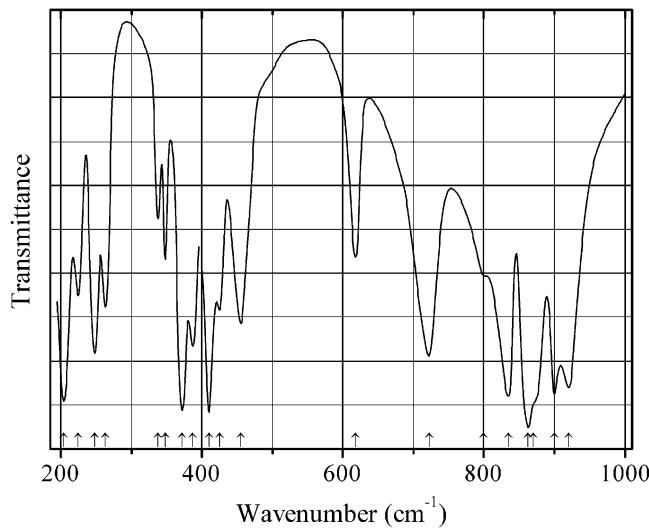
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Cody et al. (1978).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3423, 2942sh, 2865, 2827sh, 2430, 2070sh, 1783w, 1630, 1450sh, 1412w, 1375sh, 1252sh, 1231, 912sh, 870sh, 842s, 825sh, 788s, 738sh, 650sh, 615s, 600sh, 420.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 871s, 845s, 813s, 785, 601, 583, 449, 439, 378, 353, 337, 319.

**Se74 Sodium cadmium selenate hydrate**  $\text{NaCd}(\text{SeO}_4)_2 \cdot 2\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Monoclinic, space group  $P2_1/c$ .

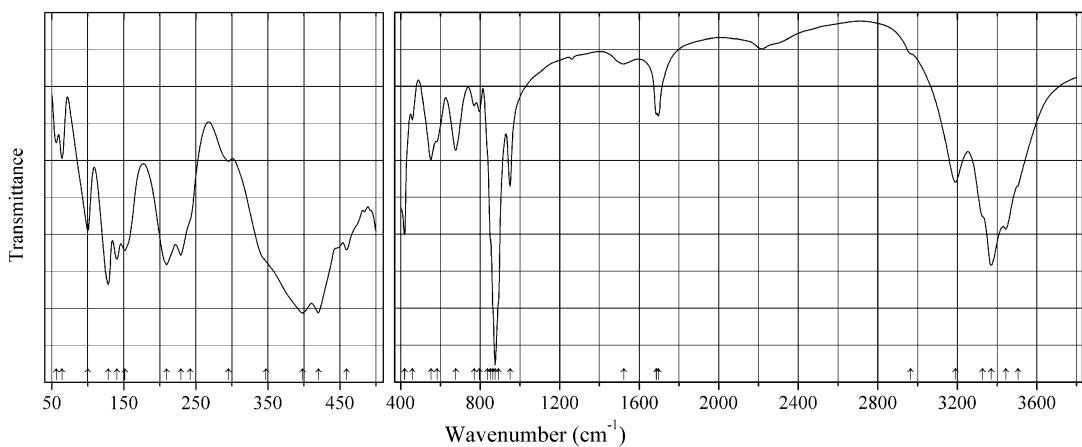
**Kind of sample preparation and/or method of registration of the spectrum:** CsI or KBr disc.  
Transmission.

**Source:** Peytavin et al. (1972a).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 920s, 900s, 870sh, 863s, 835s, 800sh, 722s, 618, 455, 425, 410s, 387, 372s, 348, 338, 263, 248s, 225, 204s.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 909, 889s, 882, 843s, 831s, 600w, 460, 433, 411, 357, 337, 308sh, 255w, 241sh, 168s.

**Se75 Sodium lithium selenate hydrate**  $\text{Na}_3\text{Li}(\text{SeO}_4)_2 \cdot 6\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Colorless crystals grown by evaporation of an aqueous solution of  $\text{Na}_2\text{SeO}_4$  and  $\text{Li}_2\text{SeO}_4$  with a 1:1 ratio at 300 K. Trigonal, space group  $R\bar{3}c$ ,  $Z = 2$ . Confirmed by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc and Nujol mull. Absorption.

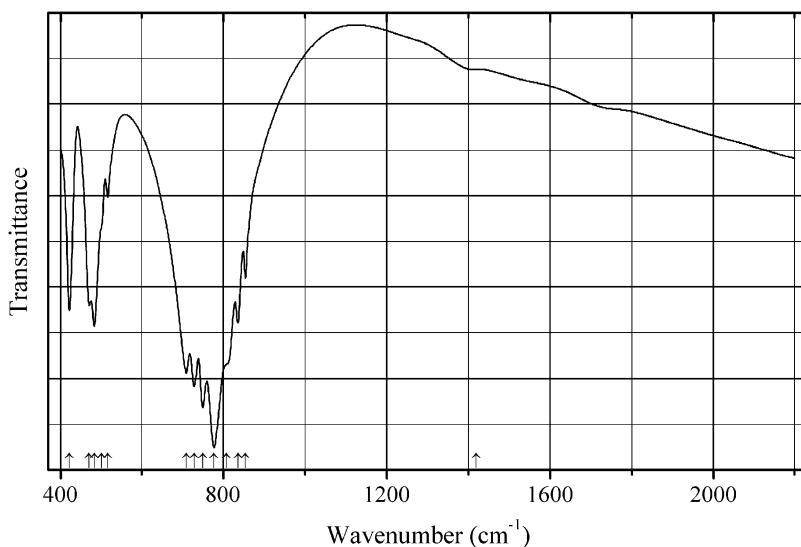
**Source:** Hanuza et al. (2008a).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3505sh, 3443, 3370s, 3327, 3190, 2964sh, 1696, 1686, 1522w, 950, 892sh, 875s, 864sh, 852sh, 836sh, 796w, 770w, 677, 583sh, 553, 459w, 420, 398, 347sh, 295w, 242sh, 229, 209, 151, 140, 128, 100, 64w, 56w.

**Note:** In the cited paper, polarized Raman spectra are given.

**Wavenumbers (Raman, with the  $z(xx)z$  polarization,  $\text{cm}^{-1}$ ):** 3440, 3372, 3215, 1690w, 903w, 866sh, 853s, 835s, 807, 454, 419sh, 398, 354, 346sh, 283, 205, 190, 167, 153, 144, 114.

### Se76 Sodium yttrium selenite $\text{NaY}(\text{SeO}_3)_2$



**Origin:** Synthetic.

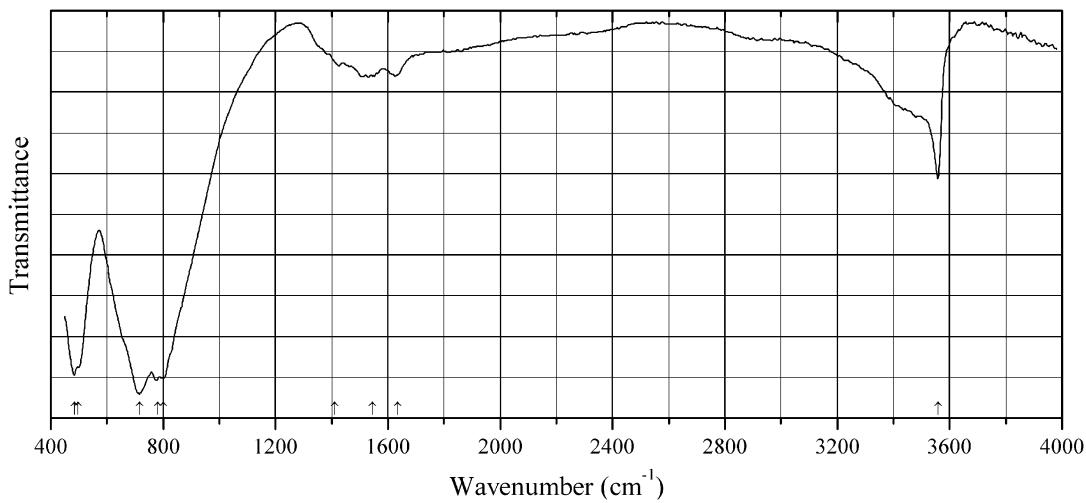
**Description:** Colorless crystals prepared hydrothermally from  $\text{Na}_2\text{CO}_3$ ,  $\text{Y}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ , and  $\text{SeO}_2$  at 230 °C for 4 days. Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group  $P2_1cn$ ,  $a = 5.397(2)$ ,  $b = 8.525(2)$ ,  $c = 12.765(2)$  Å,  $V = 587.3(3)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 4.132$  g/cm<sup>3</sup>. The structure is based on a 3D framework consisting of  $\text{YO}_7$  monocapped trigonal prisms and  $\text{SeO}_3$  trigonal pyramids.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Bang et al. (2014).

**Wavenumbers ( $\text{cm}^{-1}$ ):** (1420sh), 854, 835, 808sh, 777s, 749s, 728s, 708s, 516w, 500sh, 483, 471, 422.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Se77 Sodium zinc selenite  $\text{Na}_2\text{Zn}_3(\text{SeO}_3)_4 \cdot 2\text{H}_2\text{O}$   $\text{Na}_2\text{Zn}_3(\text{SeO}_3)_4 \cdot 2\text{H}_2\text{O}$** 

**Origin:** Synthetic.

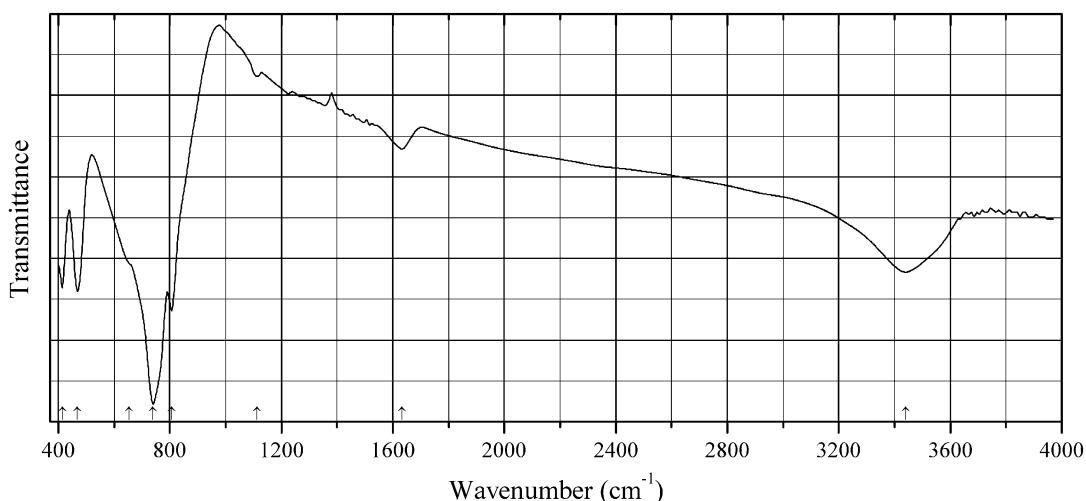
**Description:** Prepared hydrothermally from  $\text{Na}_2\text{CO}_3$ ,  $\text{ZnCO}_3$ , and  $\text{SeO}_2$  (with the molar ratio 1:1:2) at 230 °C for 6 days. The crystal structure is solved. Monoclinic, space group  $C2/c$ ,  $a = 15.7940(18)$ ,  $b = 6.5744(8)$ ,  $c = 14.6787(17)$  Å,  $\beta = 107.396(3)$ °,  $V = 1454.5(3)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 3.589$  g/cm<sup>3</sup>. The structure contains 2D  $[\text{Zn}_3(\text{SeO}_3)_4]^{2-}$  sheets.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Liu et al. (2015c).

**Wavenumbers (cm<sup>-1</sup>):** 3560, 1635w, 1545w, 1410w, 800s, 780s, 715s, 496sh, 485s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Se78 Strontium bismuth(III) selenite hydrate  $\text{Sr}_3\text{Bi}_2(\text{SeO}_3)_6 \cdot \text{H}_2\text{O}$** 

**Origin:** Synthetic.

**Description:** Crystals grown hydrothermally using  $\text{SrCO}_3$ ,  $\text{Bi}_2\text{O}_3$ , and  $\text{SeO}_2$  as starting reactants, at  $230^\circ\text{C}$  for 4 days. Characterized by powder X-ray diffraction and TG data. The crystal structure is solved. Monoclinic, space group  $P2_1/m$ ,  $a = 7.0054(10)$ ,  $b = 17.5092(3)$ ,  $c = 7.3053(10)$  Å,  $\beta = 92.299(10)^\circ$ ,  $V = 895.34(2)$  Å $^3$ ,  $Z = 2$ .  $D_{\text{calc}} = 5.418$  g/cm $^3$ .  $\text{Bi}^{3+}$  has sevenfold coordination.

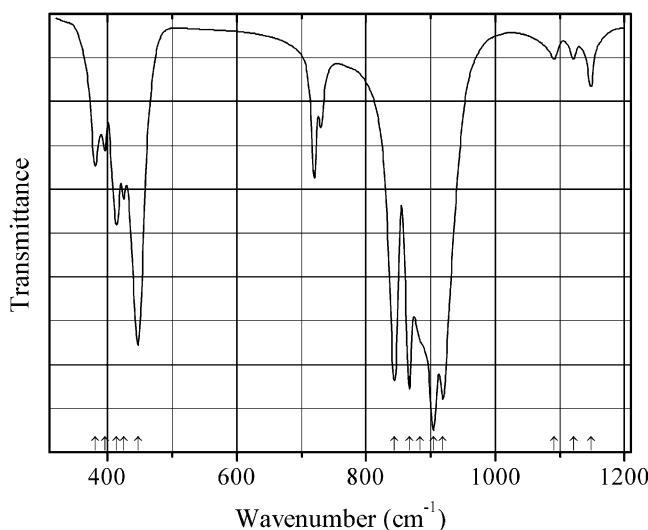
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Ahn et al. (2015).

**Wavenumbers (cm $^{-1}$ ):** 3440, 1633w, 1114w, 807, 740s, 654sh, 469, 414.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### Se79 Strontium selenate $\text{SrSeO}_4$



**Origin:** Synthetic.

**Description:** Prepared by precipitation from hot aqueous solutions of sodium selenate and lead acetate.

Monoclinic, space group  $P2_1/n$ ,  $a = 7.087$ ,  $b = 7.317$ ,  $c = 6.862$  Å,  $\beta = 103.55^\circ$ .

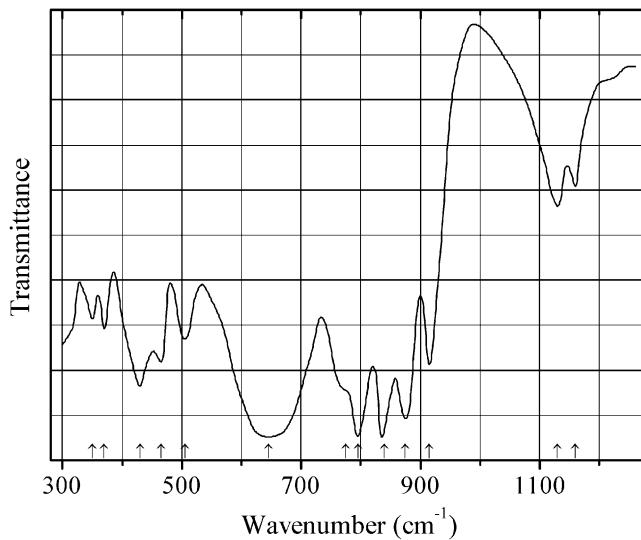
**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull. Transmission.

**Source:** Scheuermann and Schutte (1973b).

**Wavenumbers (IR, cm $^{-1}$ ):** 1148, 1121w, 1091w, 919s, 904s, 884sh, 867s, 844s, 447s, 425, 414, 396, 381.

**Note:** The bands in the range from 1000 to 1200 cm $^{-1}$  may correspond to the admixture of a sulfate. Bands near 720 cm $^{-1}$  may correspond to Nujol. In the cited paper, powder Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 913, 905, 898, 887, 882, 852, 464, 465, 445, 424, 396, 376, 340, 326.

**Se80 Tellurium(IV) oxyselenate**  $\text{Te}_2(\text{SeO}_4)\text{O}_3$ 

**Origin:** Synthetic.

**Description:** Prepared by heating a mixture of Te or  $\text{Na}_2(\text{TeO}_3)$  with 80% selenic acid at  $160^\circ\text{C}$ .

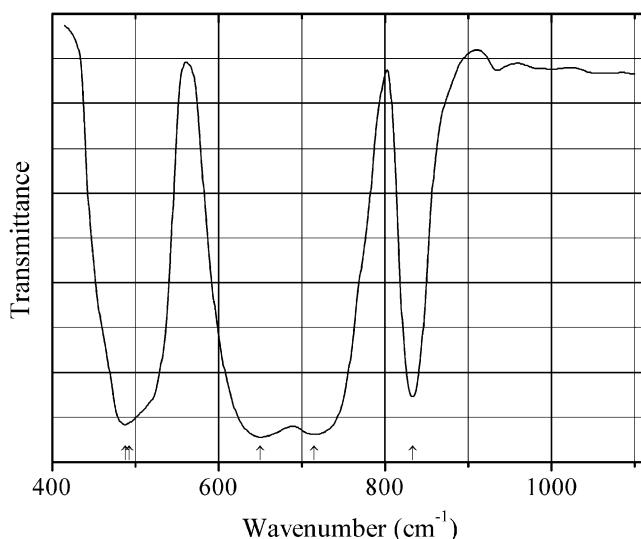
Characterized by chemical analyses and powder X-ray diffraction data. Orthorhombic, space group  $P2_1mn$ ,  $a = 4.807$ ,  $b = 8.628$ ,  $c = 7.346 \text{ \AA}$ ,  $V = 304.67 \text{ \AA}^3$ ,  $Z = 2$ .  $D_{\text{meas}} = 4.82 \text{ g/cm}^3$ ,  $D_{\text{calc}} = 4.85 \text{ g/cm}^3$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ ,  $\text{\AA}$  ( $I$ , %) ( $hkl$ )] are: 4.028 (100) (101), 3.724 (80) (021), 3.649 (70) (111), 2.943 (70) (121), 2.921 (75) (102), 2.450 (75) (003).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Gaitán et al. (1985).

**Wavenumbers (cm<sup>-1</sup>):** 1160w, 1130w, 915, 875s, 840s, 795s, 775sh, 645s, 505, 465, 430, 370, 350.

**Note:** The bands above  $1100 \text{ cm}^{-1}$  may correspond to the admixture of a sulfate.

**Se81 Tellurium oxyselenite**  $\text{Te}(\text{SeO}_3)\text{O}$ 

**Origin:** Synthetic.

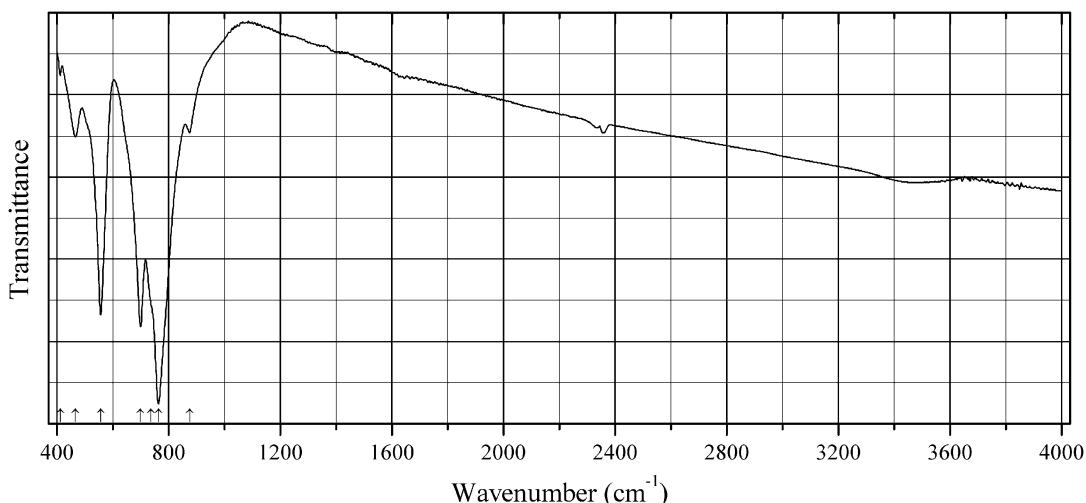
**Description:** Prepared by heating a mixture of  $\text{TeO}_2$  and  $\text{SeO}_2$  (with the 1:1.15 molar ratio) at  $370\text{ }^\circ\text{C}$  for 3 days. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group *Ia*,  $a = 4.3568(8)$ ,  $b = 12.465(3)$ ,  $c = 6.7176(15)$  Å,  $\beta = 90.825(4)^\circ$ ,  $V = 364.77(14)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 4.927$  g/cm<sup>3</sup>. Te has fivefold coordination.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Porter et al. (2001).

**Wavenumbers (cm<sup>-1</sup>):** 833, 715s, 650s, ~510, 488s.

### Se82 Vanadium(III) antimony(V) selenite $\text{VSb}(\text{SeO}_3)_4$



**Origin:** Synthetic.

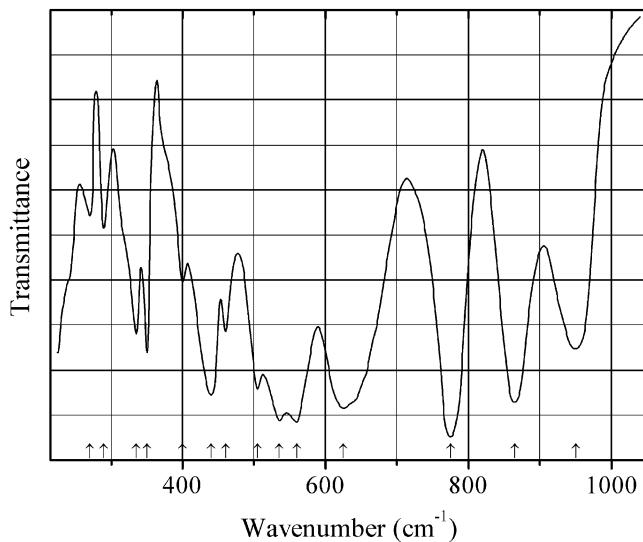
**Description:** Prepared by heating a mixture of appropriate amounts of  $\text{V}_2\text{O}_5$ ,  $\text{Sb}_2\text{O}_3$ , and  $\text{SeO}_2$ , first at  $380\text{ }^\circ\text{C}$  for 5 h and thereafter at  $600\text{ }^\circ\text{C}$  for 48 h. After cooling the product to  $400\text{ }^\circ\text{C}$  at a rate of  $6\text{ }^\circ\text{C}/\text{h}$  it was quenched to room temperature. Characterized by powder X-ray diffraction data. The crystal structure is solved. Cubic, space group *Pa-3*,  $a = 8.0301(7)$  Å,  $V = 517.80(8)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 4.365$  g/cm<sup>3</sup>. The structure is based on a 3D framework consisting of  $(\text{V},\text{Sb})\text{O}_6$  octahedra and  $\text{SeO}_3$  groups.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Shin et al. (2013).

**Wavenumbers (cm<sup>-1</sup>):** 875w, 764s, 738sh, 700s, 557s, 466, 412w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Se83 Vanadyl selenite (VO)(SeO<sub>3</sub>)**

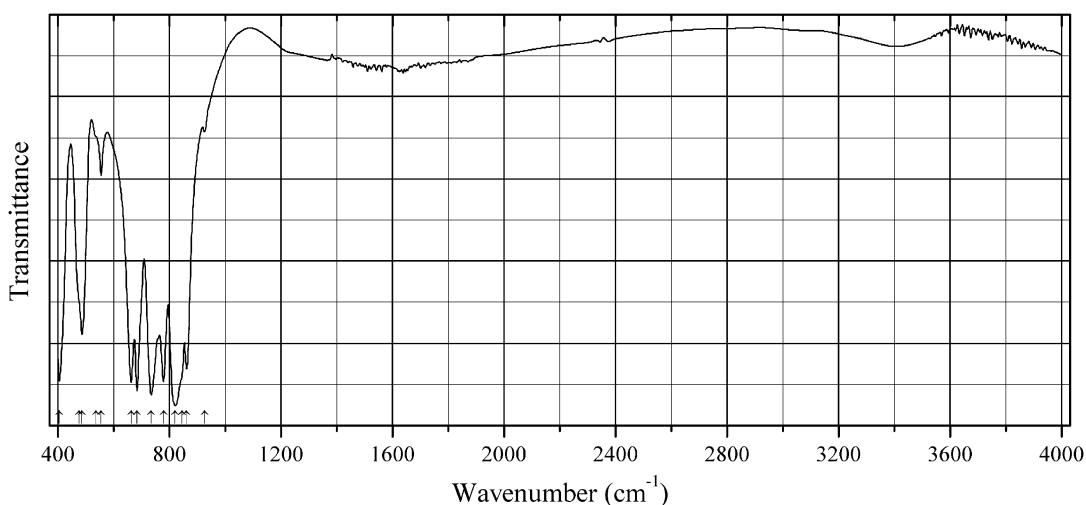
**Origin:** Synthetic.

**Description:** Prepared by heating a mixture of SeO<sub>2</sub> and VO<sub>2</sub>, taken in stoichiometric amounts, at 400 °C for 24 h. Characterized by powder X-ray diffraction data. The crystal structure contains dimers [V<sub>2</sub>O<sub>8</sub>]<sup>8-</sup> consisting of two square pyramids linked via common edge.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Rocha and Baran (1988).

**Wavenumbers (cm<sup>-1</sup>):** 950, 865s, 775s, 625s, 560s, 535s, 505, 460, 440s, 400, 350, 335, 290w, 270w.

**Se84 Yttrium vanadyl oxyselenite Y(VO)(SeO<sub>3</sub>)<sub>2</sub>O**

**Origin:** Synthetic.

**Description:** Crystals grown hydrothermally from  $\text{Y}_2\text{O}_3$ ,  $\text{V}_2\text{O}_5$ , and  $\text{SeO}_2$  at  $450^\circ\text{C}$  for 48 h with three intermediate regrindings. Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group  $\text{Am}b2$ ,  $a = 10.4036(4)$ ,  $b = 7.5904(3)$ ,  $c = 7.8341(3)$  Å,  $V = 618.64(4)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 4.571$  g/cm $^3$ .  $\text{V}^{5+}$  has sixfold coordination with one short V–O bond.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Kim et al. (2014).

**Wavenumbers (cm $^{-1}$ ):** 926w, 862s, 845sh, 821s, 779s, 735s, 684s, 663s, 555, 538sh, 487, 477sh, 406s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### Se85 Alfredopetrovite $\text{Al}_2(\text{Se}^{4+}\text{O}_3)_3 \cdot 6\text{H}_2\text{O}$

**Origin:** Synthetic.

**Description:** Hexagonal, space group  $P62c$ ,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

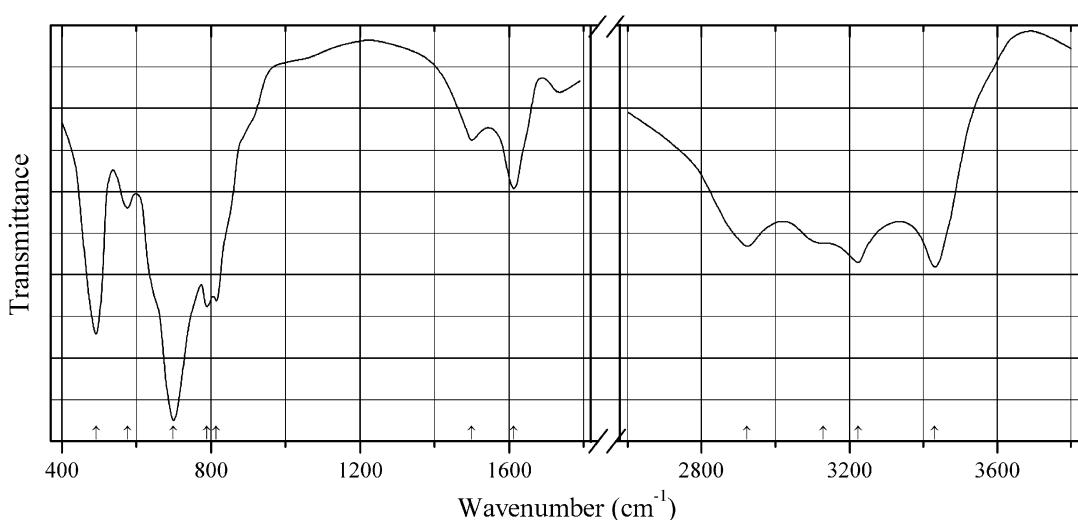
**Source:** Ratheesh et al. (1997).

**Wavenumbers (IR, cm $^{-1}$ ):** 3286–2900s (broad), 1638 (broad), 1372w, 857sh, 770s, 570, 546 (broad), 492w (broad), 460, 421w, 372sh, 360, 310, 295sh, 241w, 221w.

**Note:** The band at  $1372\text{ cm}^{-1}$  may correspond to the admixture of  $\text{NO}_3^-$  in KBr. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 3165s, 3024s, 1640w, 1329w, 874s, 831s, 750w, 722w, 704, 566w, 542, 532, 478w, 439w, 412, 347, 329w, 310w, 232, 191w, 174w, 123, 110, 92w, 74w.

### Se86 Cobaltomenite $\text{Co}(\text{SeO}_3) \cdot 2\text{H}_2\text{O}$



**Origin:** Synthetic.

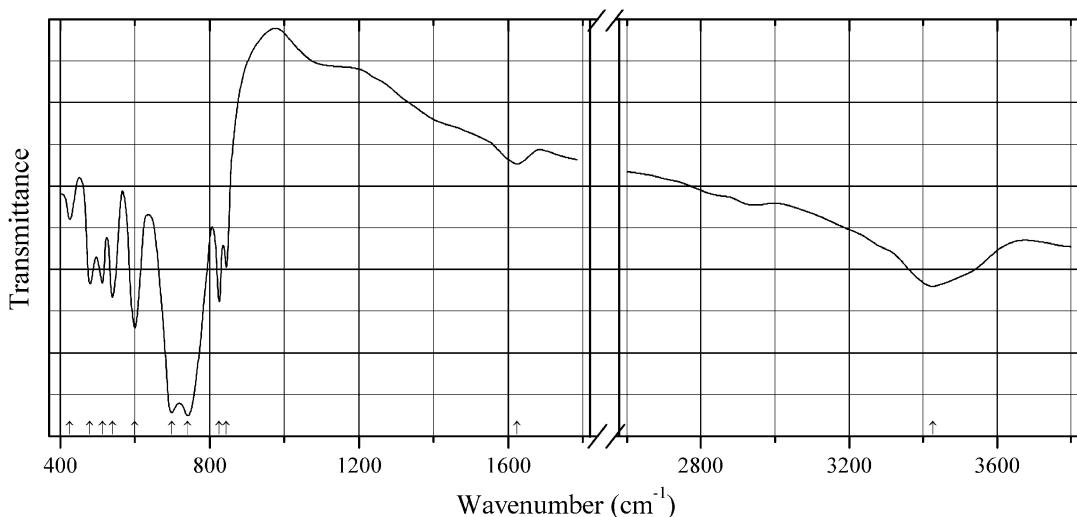
**Description:** Prepared by precipitating an aqueous solution of cobalt(II) nitrate with aqueous solution of sodium selenite at 298 K. Characterized by powder X-ray diffraction data and chemical analyses. Monoclinic, space group  $P2_1/n$ ,  $a = 6.5322$ ,  $b = 8.8251$ ,  $c = 7.6455$  Å,  $\beta = 80.478^\circ$ ,  $V = 434.67$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 3.392$  g/cm $^3$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 5.7388 (100) (011), 4.4125 (29) (020), 3.7770 (50) (002), 3.2488 (39) (112), 2.7393 (55) (122), 2.6546 (26) (202), 2.5421 (30) (212), 2.4740 (27) (103), 2.3731 (41) (22-1).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Vlaev et al. (2005).

**Wavenumbers (cm $^{-1}$ ):** 3430s, 3224s, 3129sh, 2924s, 1613, 1500, 815s, 790s, 700s, 576, 492s.

### Se87 Cobalt selenite Co(SeO<sub>3</sub>)



**Origin:** Synthetic.

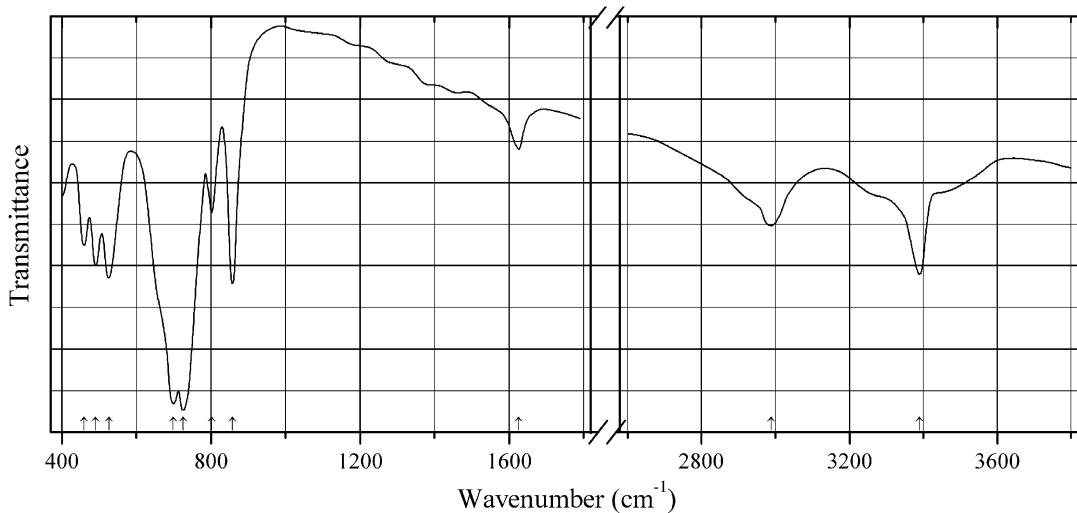
**Description:** Prepared by dehydration of Co(SeO<sub>3</sub>)·2H<sub>2</sub>O. Characterized by powder X-ray diffraction data and chemical analyses. Monoclinic, space group  $C2/c$ ,  $a = 14.5378$ ,  $b = 9.9880$ ,  $c = 14.0460$  Å,  $\beta = 107.369^\circ$ ,  $V = 1946.53$  Å $^3$ .  $D_{\text{calc}} = 4.525$  g/cm $^3$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 7.3205 (40) (200), 4.1775 (26) (22-1), 3.7518 (24) (221), 3.6602 (32) (400), 2.8914 (100) (42-3), 2.8751 (87) (51-3), 2.8090 (77) (510), 2.7865 (31) (313), 2.4868 (29) (040).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Vlaev et al. (2005).

**Wavenumbers (cm $^{-1}$ ):** (3426), (1624w), 845, 826, 742s, 700s, 600, 540, 513, 480, 426w.

**Note:** The bands at 3426 and 1624 cm $^{-1}$  may correspond to adsorbed water.

**Se88 Cobalt selenite hydrate**  $\text{Co}(\text{SeO}_3) \cdot 1/3\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Prepared by partial dehydration of  $\text{Co}(\text{SeO}_3) \cdot 2\text{H}_2\text{O}$ . Characterized by powder X-ray diffraction data and chemical analyses. Triclinic, space group  $P-1$ ,  $a = 8.1197$ ,  $b = 8.4383$ ,  $c = 8.5345$  Å,  $\alpha = 123.816^\circ$ ,  $\beta = 90.538^\circ$ ,  $\gamma = 111.591^\circ$ ,  $V = 434.02$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 3.392$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Vlaev et al. (2005).

**Wavenumbers (cm<sup>-1</sup>):** 3390, 2988, 1626w, 858, 802, 726s, 700s, 526, 491, 460.

**Se90 Orlandiite**  $\text{Pb}_3\text{Cl}_4(\text{Se}^{4+}\text{O}_3) \cdot \text{H}_2\text{O}$ 

**Origin:** Baccu Locci mine, near Villaputzu, Sardinia, Italy (type locality).

**Description:** White aggregates from the association with chalcomenite, pseudoboléite, anglesite, etc. Holotype sample. Triclinic,  $a = 8.290(8)$ ,  $b = 10.588(13)$ ,  $c = 13.587(15)$  Å,  $\alpha = 124.47(8)^\circ$ ,  $\beta = 110.60(9)^\circ$ ,  $\gamma = 63.26(9)^\circ$ ,  $Z = 2$ .  $D_{\text{calc}} = 5.55$  g/cm<sup>3</sup>. The empirical formula is  $\text{Pb}_3[\text{Cl}_{3.68}(\text{OH})_{0.32}](\text{SeO}_3) \cdot \text{H}_2\text{O}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 4.000 (100) (002), 3.258 (75) (-121), 3.188 (75) (-201), 3.818 (55) (201), 3.731 (44) (122), 2.103 (40) (142).

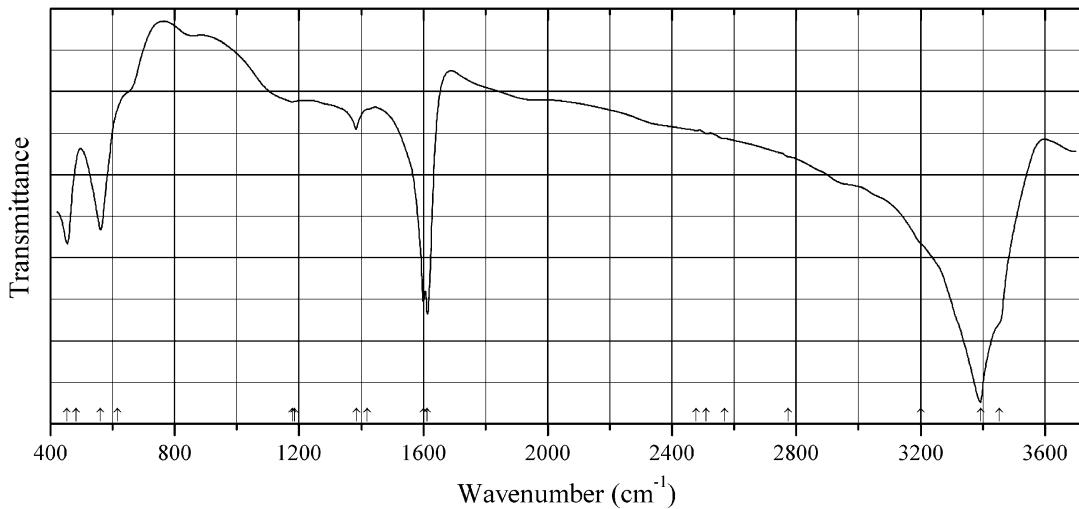
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Campostrini et al. (1999).

**Wavenumbers (cm<sup>-1</sup>):** 3410–3160 (broad), 1586, 788, 724.

## 2.16 Bromides

**Br3 Barium bromide dihydrate**  $\text{BaBr}_2 \cdot 2\text{H}_2\text{O}$



**Origin:** Synthetic.

**Description:** Obtained by crystallization from aqueous solution at room temperature. Monoclinic, space group  $C2/c$ ,  $a = 10.449$ ,  $b = 7.204$ ,  $c = 8.385$  Å,  $\beta = 113.48^\circ$ ,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

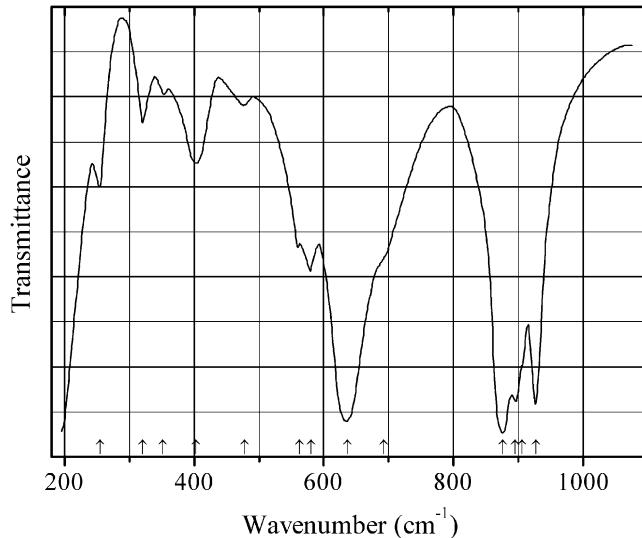
**Source:** Lutz et al. (1978).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3453sh, 3387s, 3200sh, 2775sh, 1613s, 1600s, 1417–1419, 1178–1186, 616sh, 561–566, (452), 420s.

**Note:** In the cited paper, Raman spectrum is given.

## 2.17 Molybdates

**Mo40 Ammonium cuprooxopolymolybdate** ( $\text{NH}_4)_4[\text{H}_6\text{CuMo}_6\text{O}_{24}]\cdot 4\text{H}_2\text{O}$  ( $\text{NH}_4)_4[\text{H}_6\text{CuMo}_6\text{O}_{24}] \cdot 4\text{H}_2\text{O}$ )



**Origin:** Synthetic.

**Description:** Obtained by precipitation in aqueous solution. Characterized by powder X-ray diffraction data. The crystal structure has been published elsewhere. In the cluster  $[\text{H}_6\text{CuMo}_6\text{O}_{24}]$ , both Cu and Mo have octahedral coordination. Six protons are bonded to the O atoms of the  $\text{CuO}_6$  central polyhedron.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

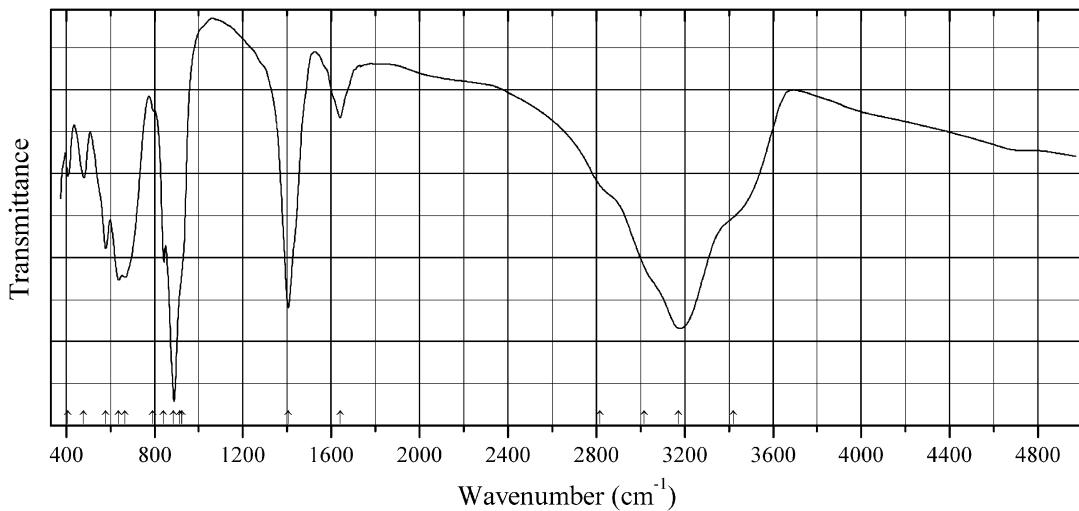
**Source:** Botto et al. (1994).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3388s, 3144s, 2768sh, 2070w, 1631w, 1399s, 927s, 906, 895sh, 876s, 692sh, 637s, 581, 562, 478w, 403, 352w, 321, 255.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 3120w (broad), 936s, 916, 873, 690w, 574w, 495w, 344, 252.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectra.

**Mo41 Ammonium heptamolybdate**  $(\text{NH}_4)_6\text{Mo}_7\text{O}_{24} \cdot 4\text{H}_2\text{O}$ 

**Origin:** Synthetic.

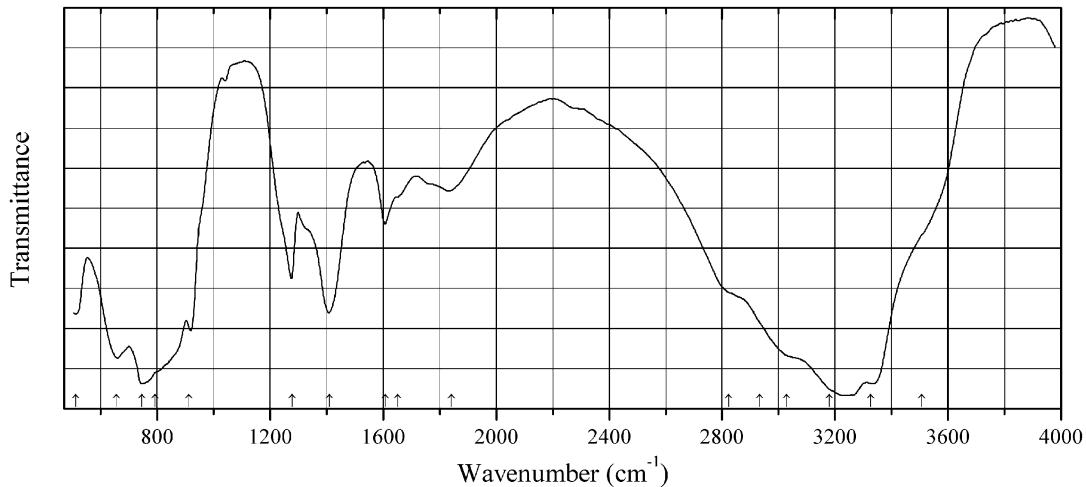
**Description:** Commercial reactant characterized by powder and single-crystal X-ray diffraction data.

Monoclinic,  $a = 8.395(7)$ ,  $b = 36.204(3)$ ,  $c = 10.4765$  Å,  $\beta = 115.884^\circ$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Wienold et al. (2003).

**Wavenumbers (cm<sup>-1</sup>):** 3420sh, 3173s, 3017sh, 2817sh, 1642, 1406s, 925sh, 915sh, 887s, 840, 792w, 667, 636s, 578, 479, 406.

**Mo42 Ammonium nickel molybdate**  $(\text{NH}_4)_2\text{Ni}_2(\text{HMoO}_4)(\text{MoO}_4)(\text{OH})_2$   $(\text{NH}_4)\text{Ni}_2(\text{HMoO}_4)(\text{MoO}_4)(\text{OH})_2$ 

**Origin:** Synthetic.

**Description:** Prepared as a green precipitate by adding concentrated ammonium hydroxide to the solution of  $(\text{NH}_4)_6\text{Mo}_7\text{O}_{24} \cdot 4\text{H}_2\text{O}$  and nickel nitrate containing 0.10 mol of Mo and 0.10 mol of Ni. The crystal structure is solved. Trigonal, space group  $R-3m$ ,  $a = 6.0147(4)$ ,  $c = 21.8812(13)$  Å,  $V = 685.53(7)$  Å $^3$ ,  $Z = 3$ .  $D_{\text{calc}} = 3.446$  g/cm $^3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Photoacoustic Fourier-transform IR spectroscopy.

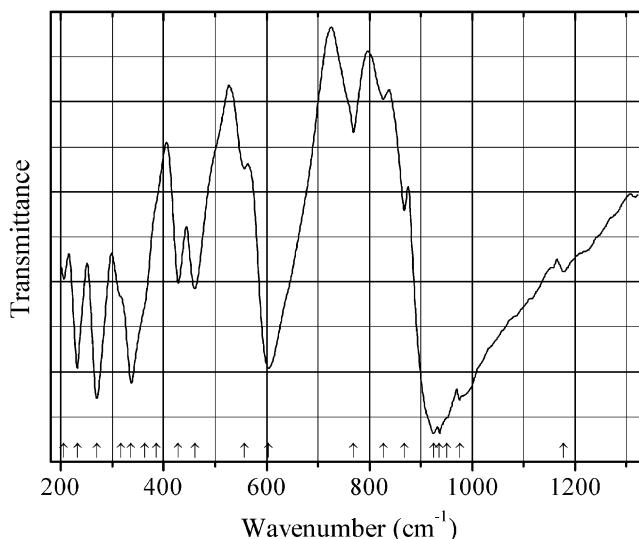
**Source:** Levin et al. (1996).

**Wavenumbers (IR, cm $^{-1}$ ):** 3508sh, 3326, 3180, 3028, 2933, 2823, 1842, 1651, 1608, 1410, 1277, 913, 793, 746, 655, 512.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 904, 321.

### Mo43 Bismuth(III) ferrite dimolybdate $\text{Bi}_3(\text{FeO}_4)(\text{MoO}_4)_2$



**Origin:** Synthetic.

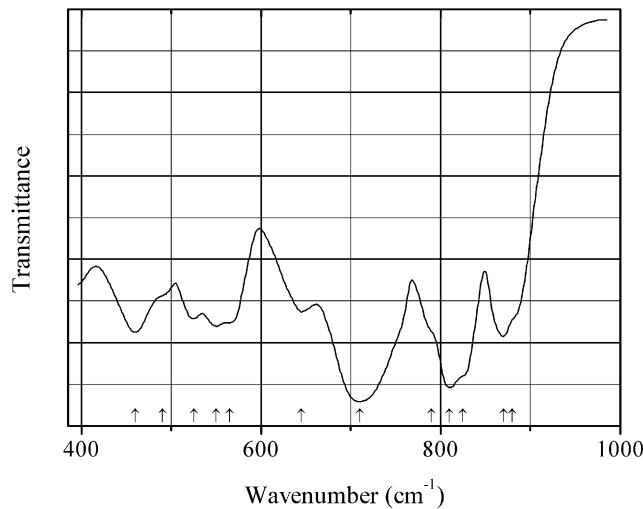
**Description:** Synthesized from aqueous solution of ferric nitrate, bismuth nitrate, and ammonium molybdate heated first at 250 °C and then from 600 to 920 °C for 10 h. Characterized by powder X-ray diffraction data and Mössbauer spectrum. Monoclinic,  $a = 16.904(1)$ ,  $b = 11.653(1)$ ,  $c = 5.2544(6)$  Å,  $\beta = 107.15(1)^\circ$ ,  $V = 989.0(1)$  Å $^3$ .  $D_{\text{calc}} = 7.16$  g/cm $^3$ . In the crystal structure, Fe and Mo are ordered.

**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull. Transmission.

**Source:** Jeitschko et al. (1976).

**Wavenumbers (cm $^{-1}$ ):** 1178w, 977s, 951sh, (936s), 925s, 868w, 827w, 769w, 603s, 557w, 461, 428, 386sh, 364sh, 337s, 316sh, 270s, 232, 206.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**Mo44 Bismuth molybdate**  $\text{Bi}_2\text{MoO}_6$ 

**Origin:** Synthetic.

**Description:** Characterized by powder X-ray diffraction data. Orthorhombic, space group  $B2cb$ .

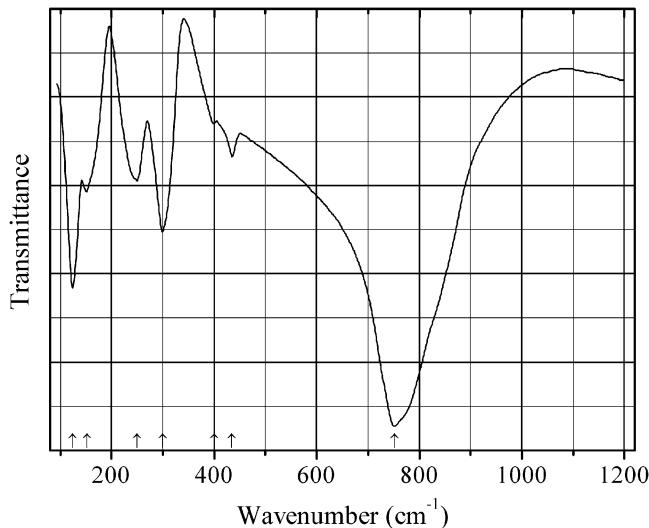
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission.

**Source:** Bode et al. (1973).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 880sh, 870, 825sh, 810s, 790sh, 710s, 645, 565, 550, 525, 490sh, 460, 380, 335, 295, 250.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 905, 885, 870, 830, 795, 730, 400, 380, 320, 265, 230, 210, 180.

**Mo45 Cadmium molybdate**  $\text{CdMoO}_4$ 

**Origin:** Synthetic.

**Description:** Prepared hydrothermally from corresponding oxides at 473 K for 48 h. Characterized by powder X-ray diffraction data and Rietveld crystal structure refinement. Isostructural with scheelite. Tetragonal, space group  $I4_1/a$ ,  $a = 5.156(1)$ ,  $c = 11.196(1)$  Å.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

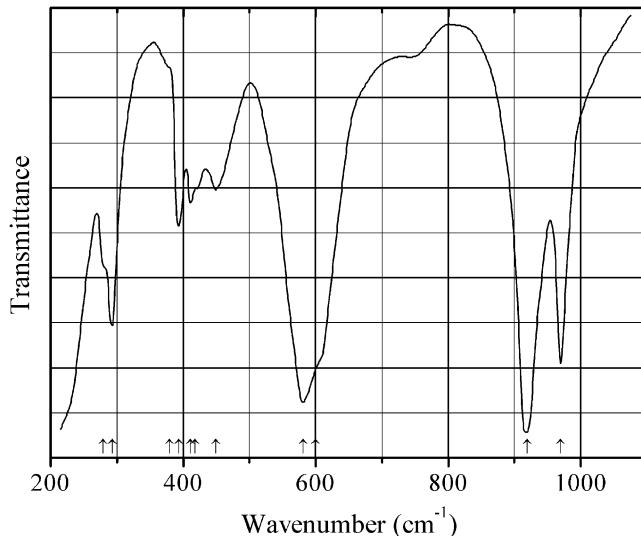
**Source:** Daturi et al. (1997).

**Wavenumbers (IR, cm<sup>-1</sup>):** 752s, 435w, 400w, 300, 250, 152, 125.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 863s, 822, 759, 403, 392, 323s, 268, 205, 191, 144, 112, 83.

#### Mo46 Cesium fluormolybdate $\text{CsMoO}_2\text{F}_3$ $\text{CsMoO}_2\text{F}_3$



**Origin:** Synthetic.

**Description:** Produced from  $\text{Cs}_2\text{CO}_3$ ,  $\text{MoO}_3 \cdot \text{H}_2\text{O}$ , and HF. Characterized by powder X-ray diffraction data. Orthorhombic,  $a = 5.492(1)$ ,  $b = 6.457(1)$ ,  $c = 14.124(2)$  Å,  $Z = 4$ .  $D_{\text{meas}} = 4.19$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 4.21$  g/cm<sup>3</sup>.

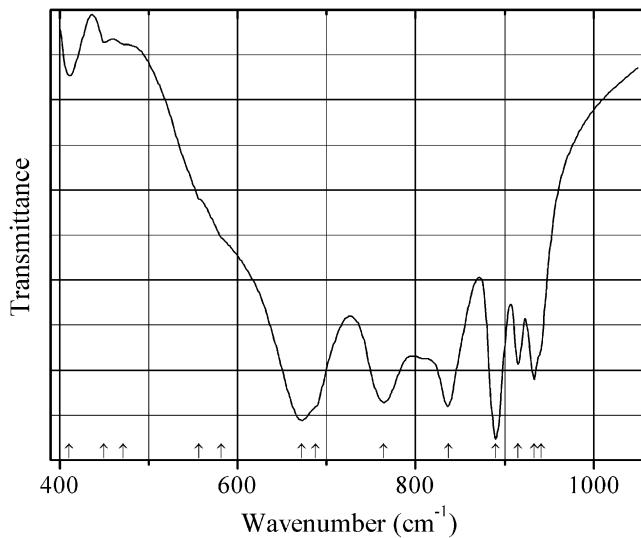
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Mattes et al. (1972).

**Wavenumbers (IR, cm<sup>-1</sup>):** 970, 919s, 600sh, 581s, 449, 418, 411, 393, 380sh, 293, 279sh.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 974s, 912s, 580w, 403, 308, 282, 268, 242.

**Mo47 Cesium thorium molybdate**  $\text{Cs}_2\text{Th}(\text{MoO}_4)_3$ 

**Origin:** Synthetic.

**Description:** Colorless crystals prepared by cooling down the melt of a mixture of  $\text{Th}(\text{NO}_3)_4 \cdot 5\text{H}_2\text{O}$ ,  $\text{CsNO}_3$ , and  $\text{MoO}_3$  from 1050 to 400 °C at a rate of 5 °C/h in air. The crystal structure is solved. Orthorhombic, space group  $Pnnm$ ,  $a = 5.2569(3)$ ,  $b = 9.7336(8)$ ,  $c = 26.8467(16)$  Å,  $V = 1373.71$  (16) Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 4.727$  g/cm<sup>3</sup>.

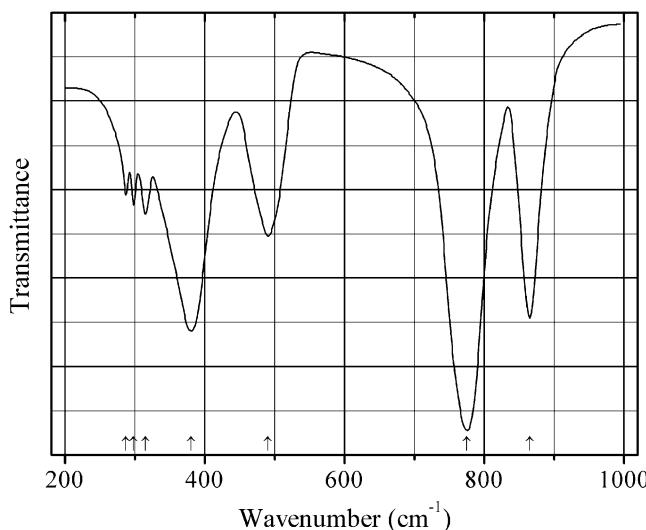
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Xiao et al. (2014).

**Wavenumbers (IR, cm<sup>-1</sup>):** 941sh, 933, 915, 890s, 837s, 764s, 688sh, 672s, 582sh, 557sh, 472w, 450w, 411w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 959s, 954, 948s, 942, 930, 924, 918, 911, 885, 866s, 828, 775, 751, 693, 465, 421, 405, 373, 360, 344, 334, 300, 292, 276, 187, 168, 144, 136, 124, 110, 98.

**Mo48 Lanthanum molybdate**  $\text{La}_2\text{MoO}_6$ 

**Origin:** Synthetic.

**Description:** Tetragonal, space group  $I-42m$ . The crystal structure can be described as a succession of  $\text{La}_2\text{O}_2$  and  $\text{MoO}_4$  layers. The  $\text{MoO}_4$  layer consists of  $\text{MoO}_4$  tetrahedra.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

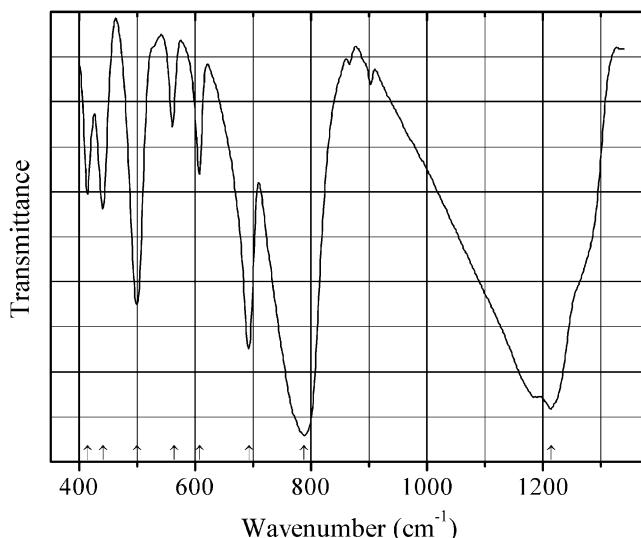
**Source:** Bode et al. (1973).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 865s, 775s, 490, 380s, 315w, 298w, 287w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 875s, 860sh, 800, 765, 695, 490, 455, 435, 375w, 325, 295, 275s, 240, 220.

#### Mo49 Lead orthoborate molybdate $\text{Pb}_6(\text{BO}_3)_2(\text{MoO}_4)\text{O}_2$



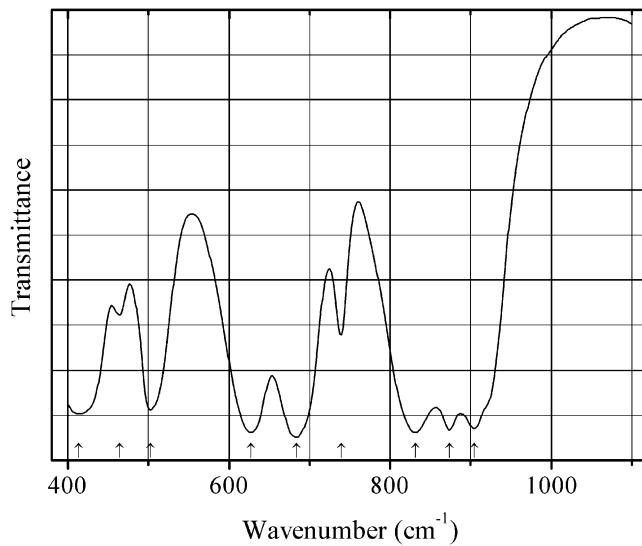
**Origin:** Synthetic.

**Description:** Prepared in a solid-state reaction from the powder mixture of  $\text{PbO}$ ,  $\text{MoO}_3$ , and  $\text{H}_3\text{BO}_3$  with the molar ratio 15:2:3. Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group  $Cncm$ ,  $a = 18.446(4)$ ,  $b = 6.3557(13)$ ,  $c = 11.657(2)$  Å,  $V = 1366.6(5)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 7.546$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Chen et al. (2009).

**Wavenumbers (cm<sup>-1</sup>):** 1215s, 788s, 693, 608, 564, 500, 441, 414.

**Mo50 Lithium molybdate tellurite**  $\text{Li}_2(\text{MoTeO}_6)$ 

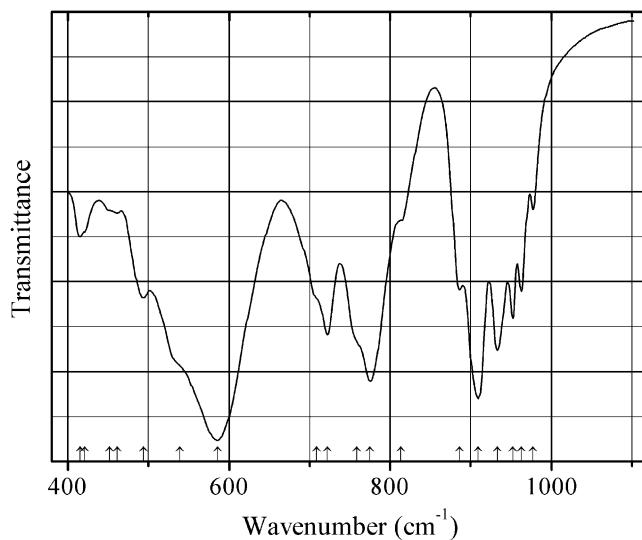
**Origin:** Synthetic.

**Description:** Prepared from  $\text{Li}_2\text{CO}_3$ ,  $\text{TeO}_2$ , and  $\text{MoO}_3$  by a solid-state technique. Monoclinic, space group  $P2_1/n$ ,  $a = 5.3830(5)$ ,  $b = 13.0027(11)$ ,  $c = 6.9814(6)$  Å,  $\beta = 94.7420(10)^\circ$ ,  $V = 486.97(7)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 4.548$  g/cm<sup>3</sup>. In the crystal structure, each  $\text{MoO}_6$  octahedron is connected to three  $\text{TeO}_3$  groups, and each  $\text{TeO}_3$  group is connected to three  $\text{MoO}_6$  octahedra to form a layer.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Nguyen and Halasyamani (2012).

**Wavenumbers (cm<sup>-1</sup>):** 904s, 874s, 831s, 739, 684s, 627s, 503, 464w, 414.

**Mo51 Lithium dimolybdate selenite**  $\text{Li}_6(\text{Mo}_2\text{O}_5)_3(\text{SeO}_3)_6$ 

**Origin:** Synthetic.

**Description:** Crystals prepared from a mixture of  $\text{Li}_2\text{MoO}_4$  and  $\text{SeO}_2$  by a solid-state technique. Orthorhombic, space group  $Pmn2_1$ ,  $a = 8.2687(4)$ ,  $b = 16.6546(7)$ ,  $c = 19.2321(8)$  Å,  $V = 2648.5(2)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 4.060$  g/cm $^3$ . In the crystal structure, the  $\text{Mo}_2\text{O}_{10}$  dimers are connected by  $\text{SeO}_3$  groups to form a layer.

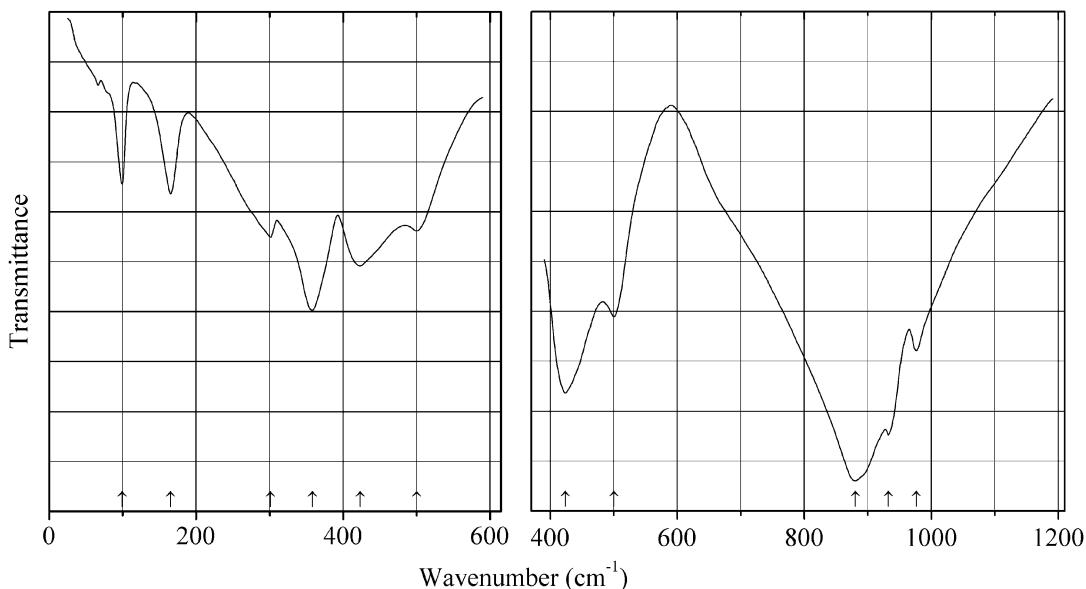
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Nguyen and Halasyamani (2012).

**Wavenumbers (cm $^{-1}$ ):** 977w, 963, 952, 933, 909s, 886, 813, 775s, 759sh, 722, 709sh, 586s, 539sh, 494, 461, 452sh, 421sh, 415w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### Mo52 Potassium aluminium molybdate $\text{KAl}(\text{MoO}_4)_2$



**Origin:** Synthetic.

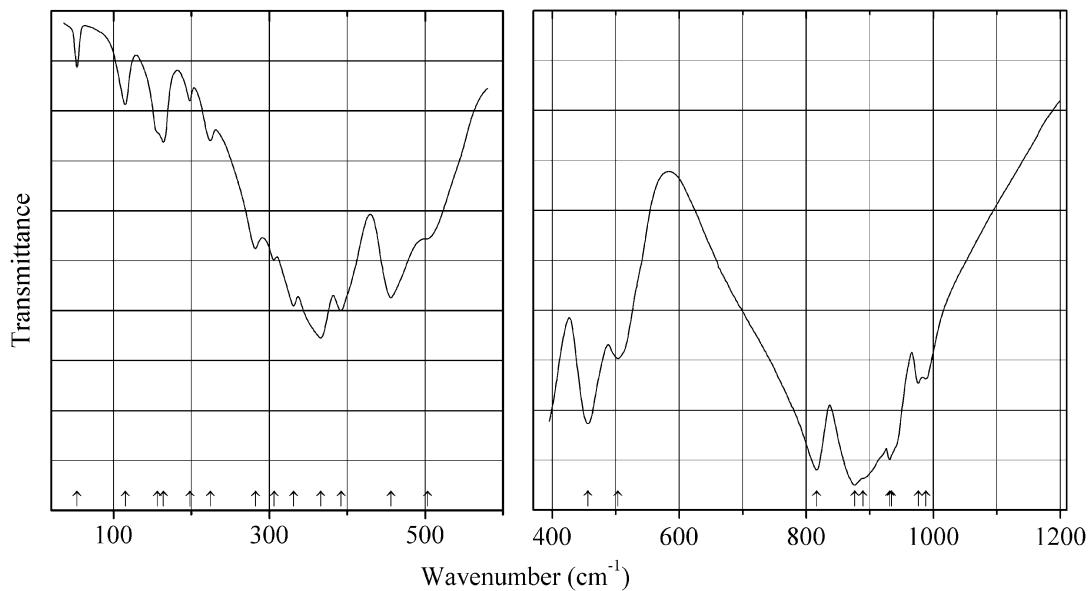
**Description:** Trigonal, space group  $P-3m1$ ,  $Z = 1$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Maczka et al. (1999).

**Wavenumbers (cm $^{-1}$ ):** 976, 932s, 880s, 500, 423s, 358s, 301, 165, 99.

**Mo53 Sodium aluminium molybdate** NaAl(MoO<sub>4</sub>)<sub>2</sub>



**Origin:** Synthetic.

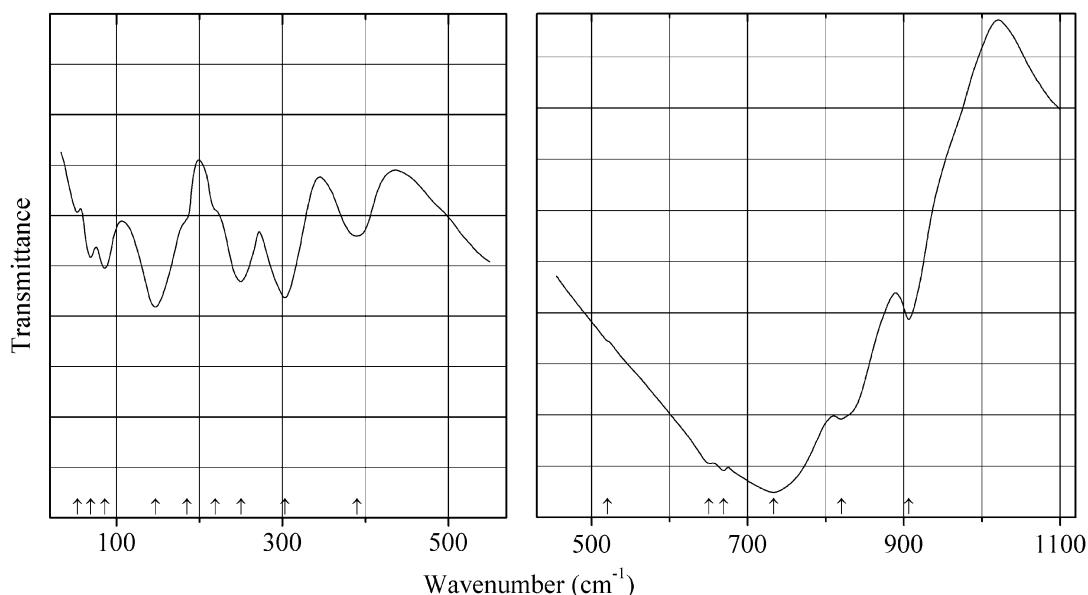
**Description:** Monoclinic, pseudo-orthorhombic, space group  $C2/c$  or  $C2/m$ . Structurally related to yavapaitite.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc and Nujol mull. Transmission.

**Source:** Maczka et al. (1999).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 988, 976, 934sh, 931s, 889sh, 876s, 816s, 503, 456s, 392s, 366s, 331s, 306, 282, 224w, 198w, 164, 156sh, 115w, 53w.

## **Mo54 Sodium bismuth molybdate scheelite-type $\text{NaBi}(\text{MoO}_4)_2$**



**Origin:** Synthetic.

**Description:** Colorless crystals grown at *ca.* 1100 K from the melt prepared from a stoichiometric mixture of  $\text{Na}_2\text{CO}_3$ ,  $\text{Bi}_2\text{O}_3$ , and  $\text{MoO}_3$ . The crystal structure is solved. Tetragonal, space group  $I-4$ ,  $a = 5.267$ ,  $c = 11.565 \text{ \AA}$ ,  $V = 320.83(10) \text{ \AA}^3$ ,  $Z = 2$ .  $D_{\text{calc}} = 5.713 \text{ g/cm}^3$ . Structurally related to scheelite.

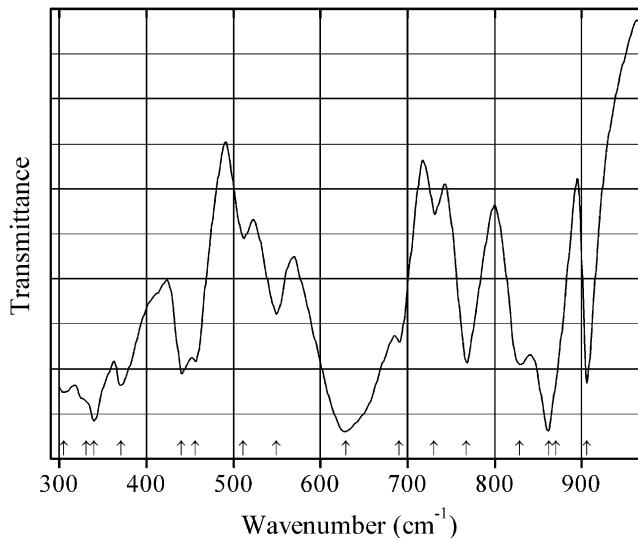
**Source:** Hanuza et al. (1997).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 906, 820, 733s, 669, 650sh, 520sh, 390, 303, 250, 219sh, 185sh, 147, 86, 69, 53w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, polarized Raman spectra are given.

**Wavenumbers (Raman, for the  $x(zz)-x$  polarization,  $\text{cm}^{-1}$ ):** 924sh, 909sh, 878s, 857sh, 760w, 409, 320, 192w, 130w, 88w, 54w.

### Mo55 Tellurium oxumolybdate $\alpha\text{-Te}_2\text{MoO}_7$



**Origin:** Synthetic.

**Description:** Prepared by heating a mixture of  $\text{TeO}_2$  and  $\text{MoO}_3$ , taken in stoichiometric amounts, at 550–600 °C for 10 h. Characterized by powder X-ray diffraction data. The crystal structure is solved.

Monoclinic, space group  $P2_1/c$ ,  $a = 4.286(2)$ ,  $b = 8.618(3)$ ,  $c = 15.945(5) \text{ \AA}$ ,  $\beta = 95.68(1)^\circ$ ,  $Z = 4$ .

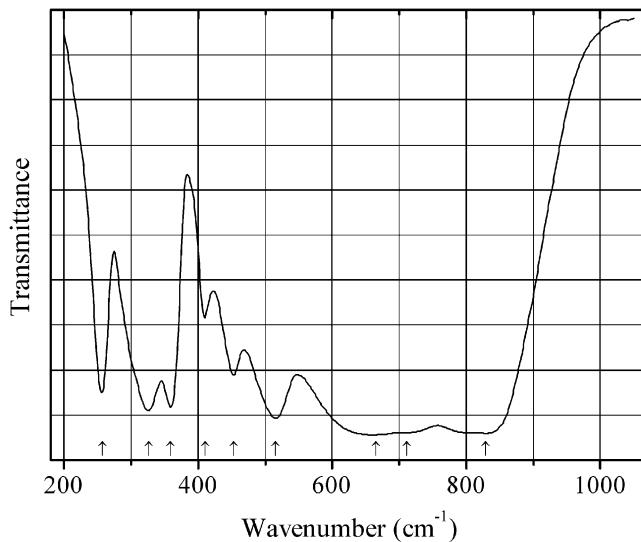
**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc. Transmission.

**Source:** Baran et al. (1981).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 906, 870sh, 862s, 829, 767, 730w, 690, 629s, 549, 511w, 456sh, 440, 371, 340, 331, 305, 296, 244, 230sh, 218.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 911s, 867s, 818s, 737, 619, 548w, 513w, 460sh, 439, 365, 335w, 312w, 290sh, 283, 261w, 218s, 199w, 183w, 183sh, 173s.

**Mo56 Zinc molybdate**  $\beta\text{-Zn}(\text{MoO}_4)$ 

**Origin:** Synthetic.

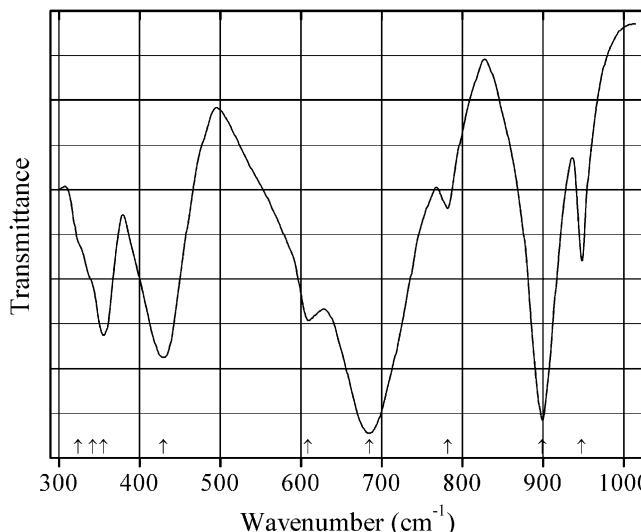
**Description:** Light gray powder prepared hydrothermally from sodium molybdate and zinc nitrate at 140 °C for 8 h. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2/c$ ,  $a = 4.6987(3)$ ,  $b = 5.7487(2)$ ,  $c = 4.9044(2)$  Å,  $\beta = 90.3312^\circ$ ,  $V = 132.47$  Å<sup>3</sup>,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Cavalcante et al. (2013).

**Wavenumbers (cm<sup>-1</sup>):** 829s, 712sh, 665s, 516, 453, 410w, 359, 326, 257.

**Note:** For the IR spectrum of  $\beta\text{-Zn}(\text{MoO}_4)$  see also Jiang et al. (2014).

**Mo57 Zinc telluromolybdate** ZnTeMoO<sub>6</sub>

**Origin:** Synthetic.

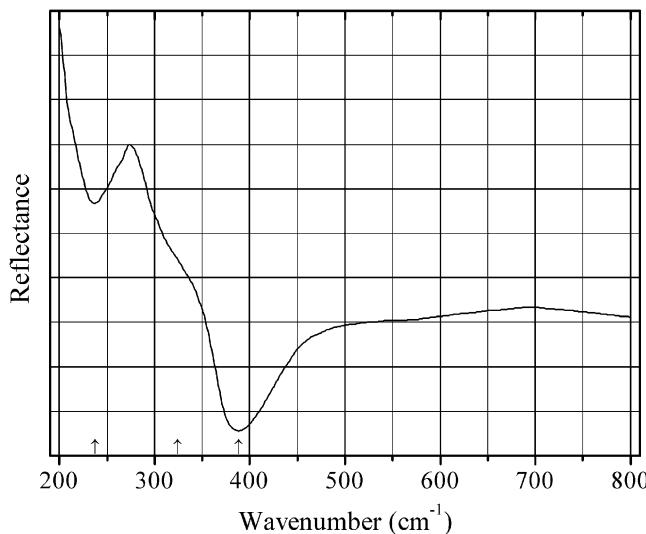
**Description:** Orthorhombic, space group  $P2_12_12_1$ ,  $a = 5.255$ ,  $b = 5.044$ ,  $c = 8.909 \text{ \AA}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc.  
Transmission.

**Source:** Baran et al. (1981).

**Wavenumbers (cm<sup>-1</sup>):** 948, 899s, 782w, 685s, 609, 430, 356, 342sh, 324sh.

### Mo58 Zirconium molybdenum oxide (monoclinic) $\text{ZrMo}_2\text{O}_8$



**Origin:** Synthetic.

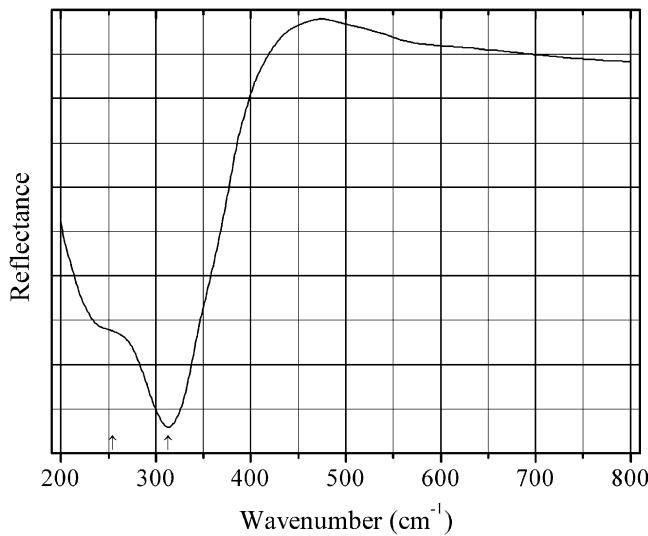
**Description:** Prepared by heating a mixture of  $\text{ZrO}_2$  and  $\text{MoO}_3$  taken in the molar ratio of 1:2, at  $600^\circ\text{C}$  for 64 h. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $C2/c$ ,  $a = 11.4243(19)$ ,  $b = 7.9297(6)$ ,  $c = 7.4610(14) \text{ \AA}$ ,  $\beta = 122.15(2)^\circ$ ,  $V = 572.3(2) \text{ \AA}^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 4.771 \text{ g/cm}^3$ . Mo has fivefold coordination. Two  $\text{MoO}_5$  polyhedra share edges with each other forming  $\text{Mo}_2\text{O}_8$  moieties.

**Kind of sample preparation and/or method of registration of the spectrum:** Diffuse reflectance of a powdered sample.

**Source:** Sahoo et al. (2009).

**Wavenumbers (cm<sup>-1</sup>):** 388s, 324sh, 237.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**Mo59 Zirconium molybdenum oxide (trigonal)  $\text{ZrMo}_2\text{O}_8$** 

**Origin:** Synthetic.

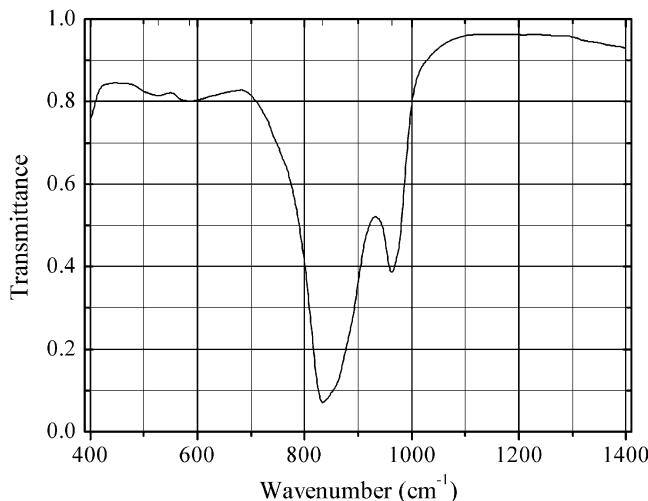
**Description:** The crystal structure is solved. Trigonal, space group  $P-31c$ ,  $a = 10.1391(6)$ ,  $c = 11.7084(8)$  Å,  $Z = 6$ . Mo has fourfold coordination.

**Kind of sample preparation and/or method of registration of the spectrum:** Diffuse reflectance of a powdered sample.

**Source:** Sahoo et al. (2009).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 313, 254sh.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. The wavenumber of the main band ( $313 \text{ cm}^{-1}$ ) is anomalously low for the  $\text{MoO}_4$  tetrahedra.

**Mo60 Vanadyl molybdate (VO)(MoO<sub>4</sub>)**

**Origin:** Synthetic.

**Description:** Obtained by heating a stoichiometric mixture of  $\text{VO}_2$  and  $\text{MoO}_3$  at 700 °C for 48 h. Tetragonal, space group  $P4/n$ .

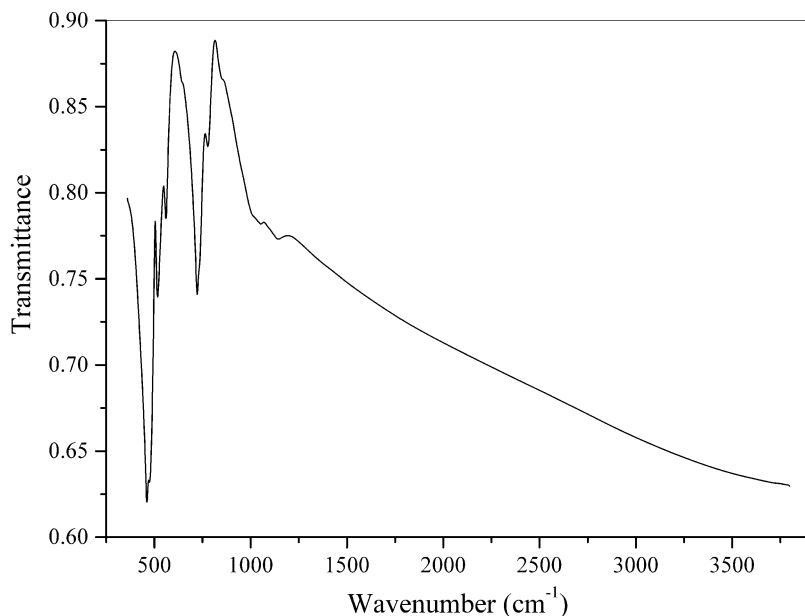
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Stranford and Condrate Sr (1984a).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 963, 834s, 586w, 528w.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. In the cited paper, a figure of Raman spectrum is given.

### Mo61 Kamiokite $\text{Fe}^{2+} \text{Mo}^{4+} \text{O}_8$



**Origin:** Kamioka mine, Hida City, Chubu Region, Honshu Island, Japan (type locality).

**Description:** Black crystals with submetallic lustre. Investigated by A.V. Kasatkin. Confirmed by electron microprobe analyses.

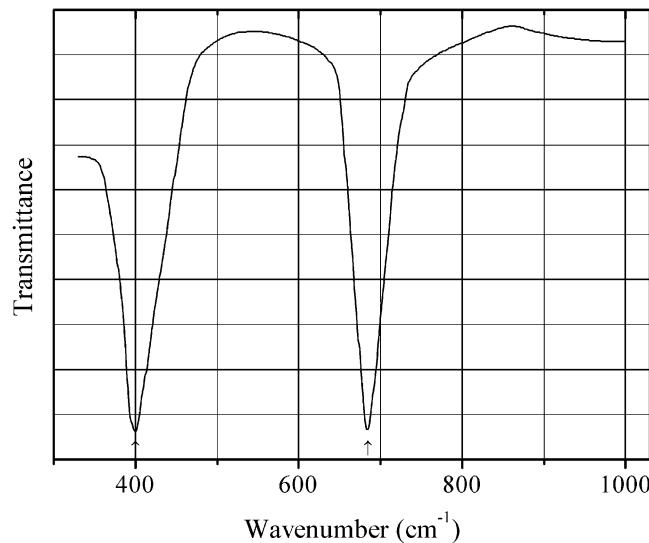
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 1147, 1055, 1020sh, 855sh, 778, 723, 645sh, 560, 517, 475s, 461s.

**Note:** The spectrum was obtained by N.V. Chukanov.

## 2.18 Tellurides, Tellurites, and Tellurates

**Te52 Barium calcium tellurate**  $\text{Ba}_2\text{CaTeO}_6$



**Origin:** Synthetic.

**Description:** Perovskite-type compound.  $D_{\text{calc}} = 6.04 \text{ g/cm}^3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

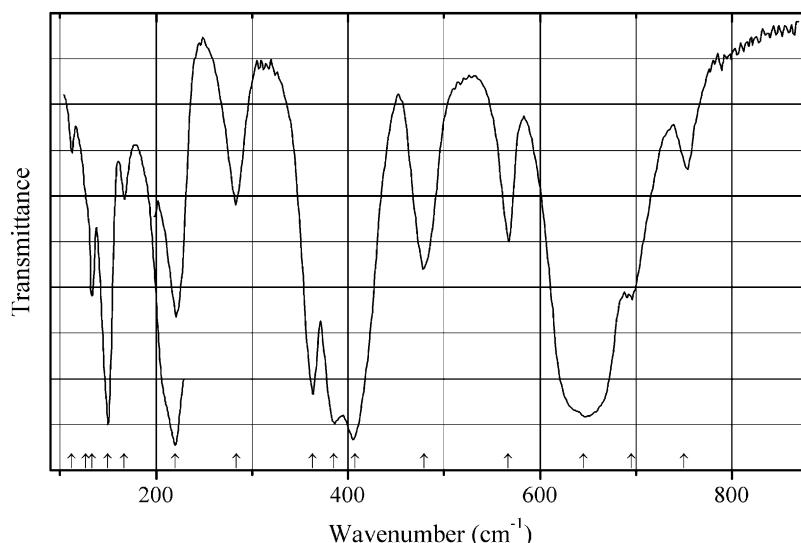
**Source:** Corsmit and Blasse (1974).

**Wavenumbers (IR, cm⁻¹):** 685, 400.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm⁻¹):** 752, 618, 412.

**Te53 Barium cobalt tellurate**  $\text{Ba}_2\text{CoTeO}_6$



**Origin:** Synthetic.

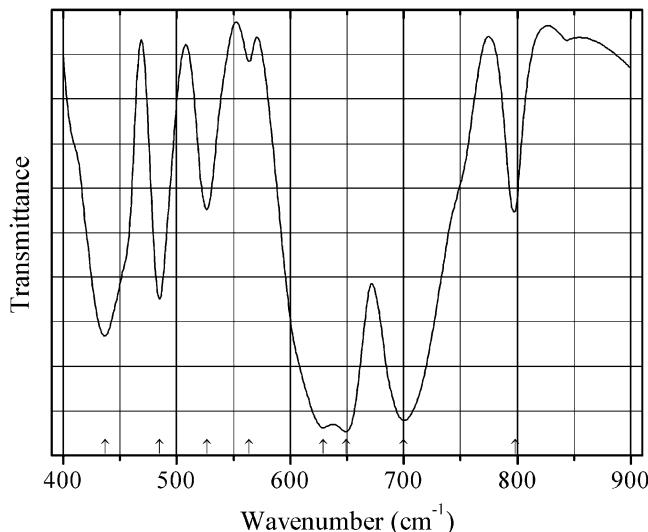
**Description:** A compound with ordered hexagonal perovskite-type structure.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

**Source:** Liegeois-Duyckaerts (1985).

**Wavenumbers (cm<sup>-1</sup>):** 750, 695, 645s, 567, 479, 407s, 385s, 363s, 284, 220, 167w, 150, (133), (127), 112w.

#### Te54 Barium copper tellurate tellurite BaCuTe<sub>2</sub>O<sub>7</sub>



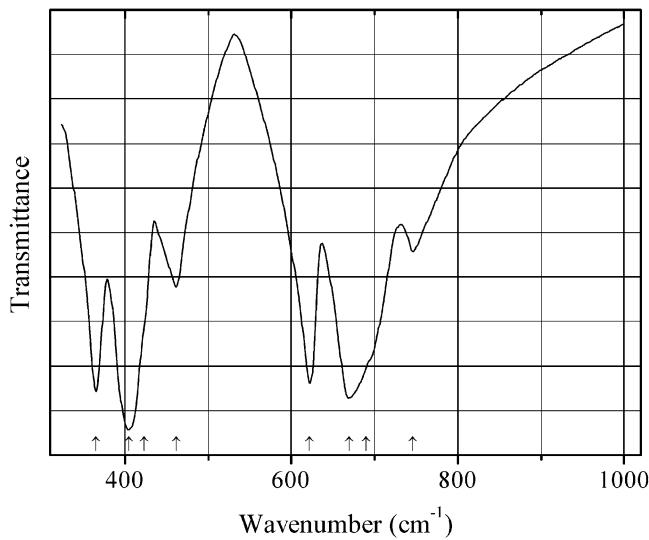
**Origin:** Synthetic.

**Description:** Prepared by solid-state method from the stoichiometric mixture of BaCO<sub>3</sub>, CuO, TeO<sub>2</sub>, and H<sub>2</sub>TeO<sub>4</sub>·2H<sub>2</sub>O at 650 °C. Orthorhombic, space group *Ama*2, *a* = 5.4869(8), *b* = 15.4120(8), *c* = 7.2066(4) Å, *V* = 609.42(10) Å<sup>3</sup>, *Z* = 4. *D*<sub>meas</sub> = 2.39(3) g/cm<sup>3</sup>, *D*<sub>calc</sub> = 2.391 g/cm<sup>3</sup>. Characterized by powder X-ray diffraction, piezoelectric, and polarization measurements.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Yeon et al. (2011).

**Wavenumbers (cm<sup>-1</sup>):** 798, 700s, 649s, 629s, 564w, 527, 485, 437.

**Te55 Barium nickel tellurate**  $\text{Ba}_2\text{NiTeO}_6$ 

**Origin:** Synthetic.

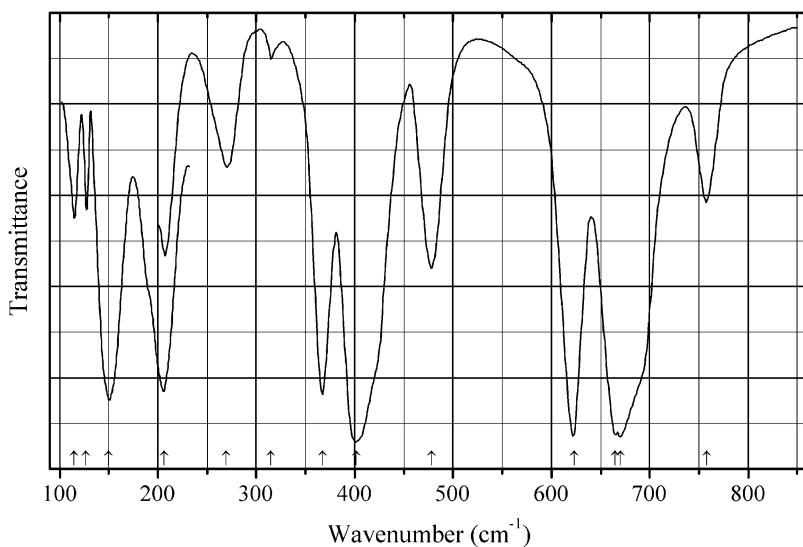
**Description:** Perovskite-type compound. Hexagonal, space group  $R-3m$ ,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Corsmit and Blasse (1974).

**Wavenumbers (cm⁻¹):** 746, 690sh, 670s, 622s, 462, 423sh, 405s, 365s.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Te56 Barium zinc tellurate**  $\text{Ba}_2\text{ZnTeO}_6$ 

**Origin:** Synthetic.

**Description:** Synthesized by solid-state reaction. The stoichiometric mixture of the necessary oxides and carbonates was heated at 600 °C for about 1 night, then reground and heated up to 1100 °C for 1 day. A compound with perovskite-type cubic structure.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

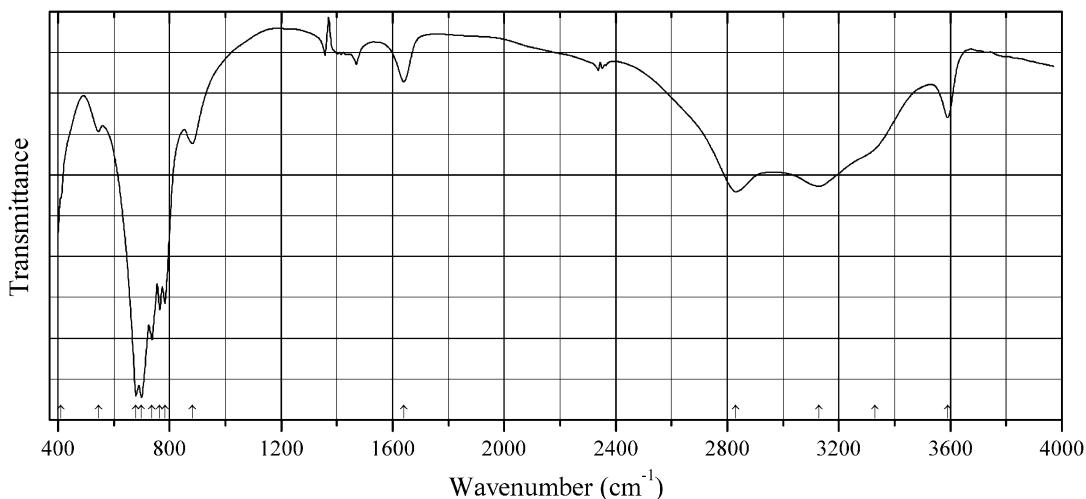
**Source:** Liegeois-Duyckaerts (1975).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 758, 670s, 665s, 623s, 478, 402s, 367, 315w, 269, 206sh, 150, 127w, 115w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 769s, 691s, 620, 575, 473w, 406, 399, 385, 122, 105.

### Te57 Calcium tellurite monohydrate $\text{Ca}(\text{TeO}_3)\cdot\text{H}_2\text{O}$



**Origin:** Synthetic.

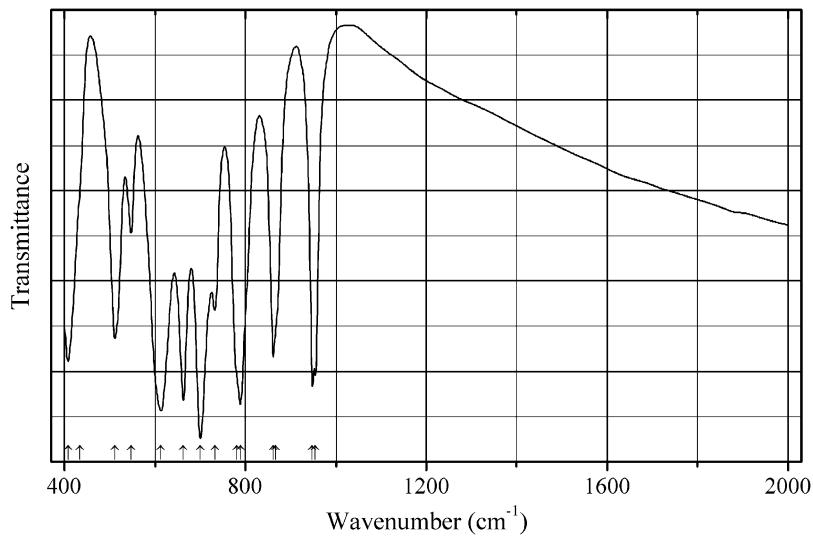
**Description:** Obtained from  $\text{Ca}(\text{NO}_3)_2$  and  $\text{TeO}_2$ , in the presence of  $\text{NaOH}$ , by microwave-assisted hydrothermal synthesis at 185 °C for 1 h. The crystal structure is solved. Orthorhombic, space group  $P2_1cn$ ,  $a = 14.78549(4)$ ,  $b = 6.79194(3)$ ,  $c = 8.06261(3)$  Å,  $V = 809.665(6)$  Å<sup>3</sup>,  $Z = 8$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Poupon et al. (2015).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3590, 3330sh, 3130, 2830, 1641w, 882, 783, 765, 737s, 700s, 680s, 545w, 411sh.

**Note:** The strong band centered at 698  $\text{cm}^{-1}$  and the shoulders at 740 and 770  $\text{cm}^{-1}$  indicated by the authors of the cited paper were determined by us as bands at 680, 700, 737, 765, and 783  $\text{cm}^{-1}$ .

**Te58 Indium vanadate tellurite  $\text{In}(\text{VTe}_2\text{O}_8)$   $\text{In}(\text{VTe}_2\text{O}_8)$** 

**Origin:** Synthetic.

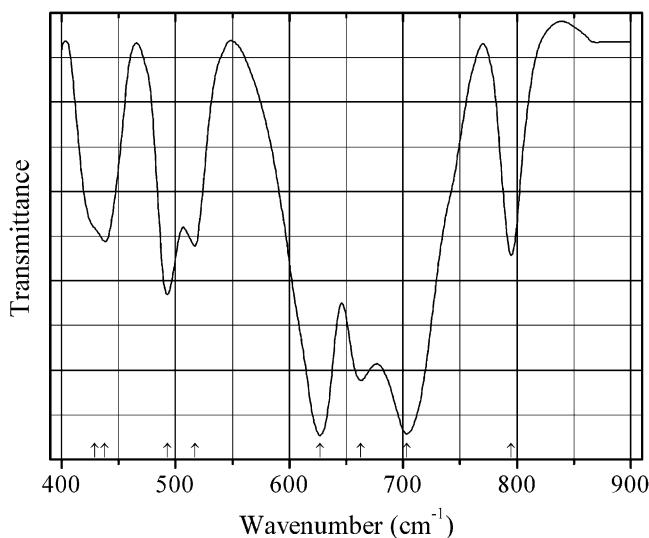
**Description:** Prepared from  $\text{In}_2\text{O}_3$ ,  $\text{V}_2\text{O}_5$ , and  $\text{TeO}_2$  by a standard solid-state reaction. The crystal structure is solved. Monoclinic, space group  $P2_1/n$ ,  $a = 7.8967(16)$ ,  $b = 5.1388(10)$ ,  $c = 16.711(3)$  Å,  $\beta = 94.22(3)^\circ$ ,  $V = 676.3(2)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 5.391$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Lee et al. (2011).

**Wavenumbers (cm<sup>-1</sup>):** 955, 948s, 867sh, 861, 789s, 781sh, 732s, 700s, 662s, 613, 547, 511, 433sh, 407.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**Te59 Lead copper tellurate tellurite  $\text{PbCuTe}_2\text{O}_7$** 

**Origin:** Synthetic.

**Description:** Prepared by a conventional solid-state method from stoichiometric amounts of PbO, CuO, TeO<sub>2</sub>, and H<sub>2</sub>TeO<sub>4</sub>·2H<sub>2</sub>O. Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group *Pbcm*,  $a = 7.2033(5)$ ,  $b = 15.0468(10)$ ,  $c = 5.4691(4)$  Å,  $V = 592.78(7)$  Å<sup>3</sup>,  $Z = 4$ .

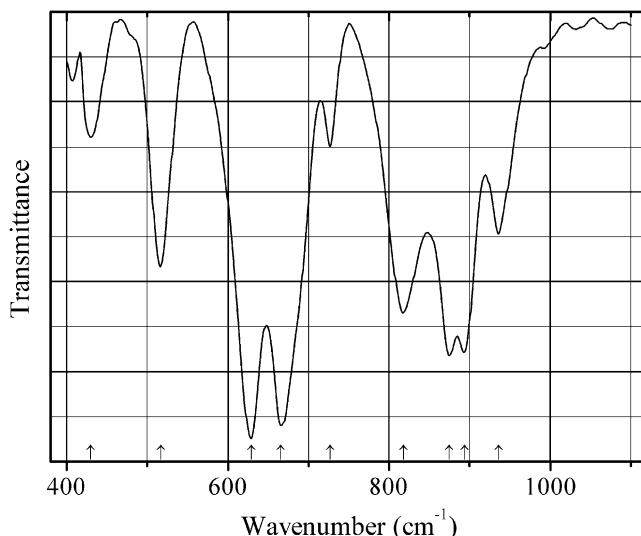
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Yeon et al. (2011).

**Wavenumbers (cm<sup>-1</sup>):** 795, 703s, 663, 627s, 517, 493, 438, 429sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

#### Te60 Lithium tungstate tellurite Li<sub>2</sub>(WTeO<sub>6</sub>)



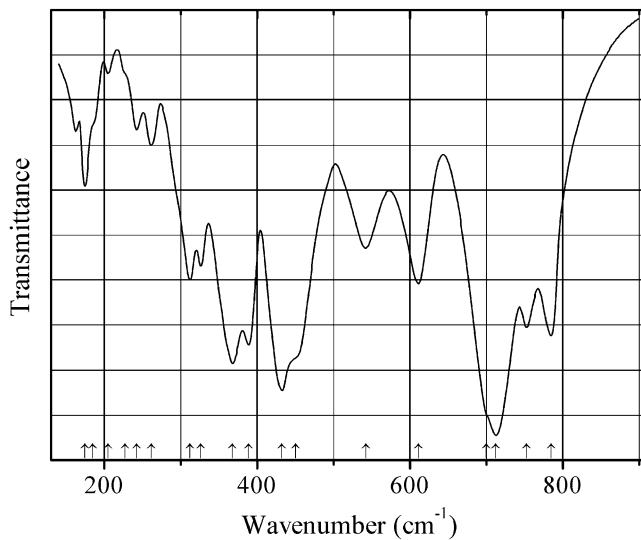
**Origin:** Synthetic.

**Description:** Prepared from Li<sub>2</sub>CO<sub>3</sub>, TeO<sub>2</sub>, and WO<sub>3</sub> by a solid-state technique. Monoclinic, space group *P2<sub>1</sub>/n*,  $a = 5.3950(5)$ ,  $b = 12.9440(12)$ ,  $c = 7.0149(7)$  Å,  $\beta = 94.2510(10)^\circ$ ,  $V = 488.52$  (8) Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 5.729$  g/cm<sup>3</sup>. In the crystal structure, each WO<sub>6</sub> octahedron is connected to three TeO<sub>3</sub> groups, and each TeO<sub>3</sub> group is connected to three WO<sub>6</sub> octahedra to form a layer.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Nguyen and Halasyamani (2012).

**Wavenumbers (cm<sup>-1</sup>):** 936, 894s, 875s, 818, 727s, 666s, 629, 517, 430w.

**Te61 Magnesium tellurite  $MgTe_2O_5$   $MgTe_2O_5$** 

**Origin:** Synthetic.

**Description:** Obtained in the solid-state reaction between MgO and TeO<sub>2</sub> at 680 °C. Characterized by powder X-ray diffraction data. Orthorhombic, Z = 4.

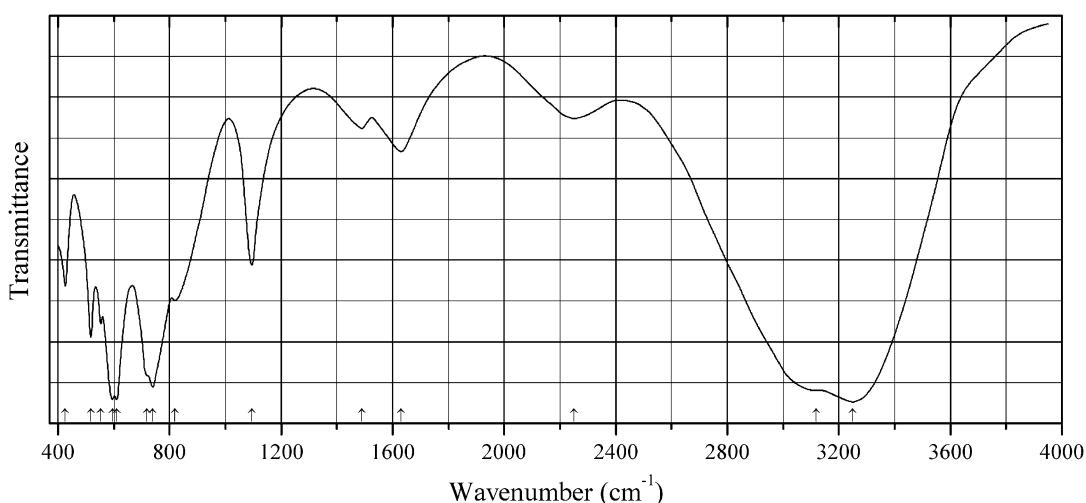
**Kind of sample preparation and/or method of registration of the spectrum:** CsI disc. Transmission.

**Source:** Baran (1978).

**Wavenumbers (IR, cm<sup>-1</sup>):** 785, 752, 712s, 700sh, 611, 542, 450sh, 432s, 389, 367s, 326, 312, 261, 242w, 227sh, 205w, 185sh, 174w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 810s, 725, 698s, 540, 437s, 405, 385, 345sh, 330, 267s, 253, 237w, 222s, 200, 185w, 115.

**Te62 Potassium acid tellurate hydrate  $K_2[TeO_2(OH)_4] \cdot 3H_2O$   $K_2[TeO_2(OH)_4] \cdot 3H_2O$** 

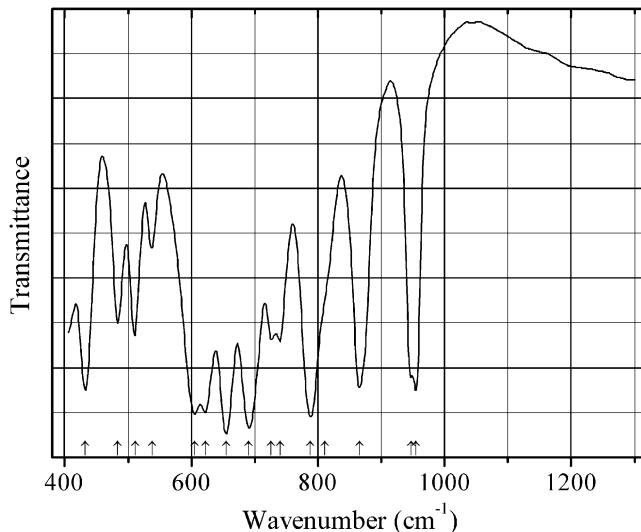
**Origin:** Synthetic.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Siebert (1959).

**Wavenumbers (cm<sup>-1</sup>):** 3250s, 3120sh, 2250, 1630, 1490w, 1095, 820, 740s, 720sh, 610s, 595s, 554, 518, 426.

### Te63 Scandium vanadate tellurite $\text{ScVTe}_2\text{O}_8$



**Origin:** Synthetic.

**Description:** Prepared by a solid-state reaction from  $\text{Sc}_2\text{O}_3$ ,  $\text{V}_2\text{O}_5$ , and  $\text{TeO}_2$ , first at 350 °C for 5 h, and thereafter at 450 °C for 48 h. The crystal structure is solved. Monoclinic, space group  $P2_1/n$ ,  $a = 7.9774(2)$ ,  $b = 5.08710(10)$ ,  $c = 16.5654(4)$  Å,  $\beta = 93.400(2)^\circ$ ,  $V = 671.07(3)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 4.742$  g/cm<sup>3</sup>. The structure is composed of  $\text{ScO}_6$  octahedra,  $\text{VO}_4$  tetrahedra, and asymmetric  $\text{TeO}_4$  polyhedra that are connected via common O atoms.

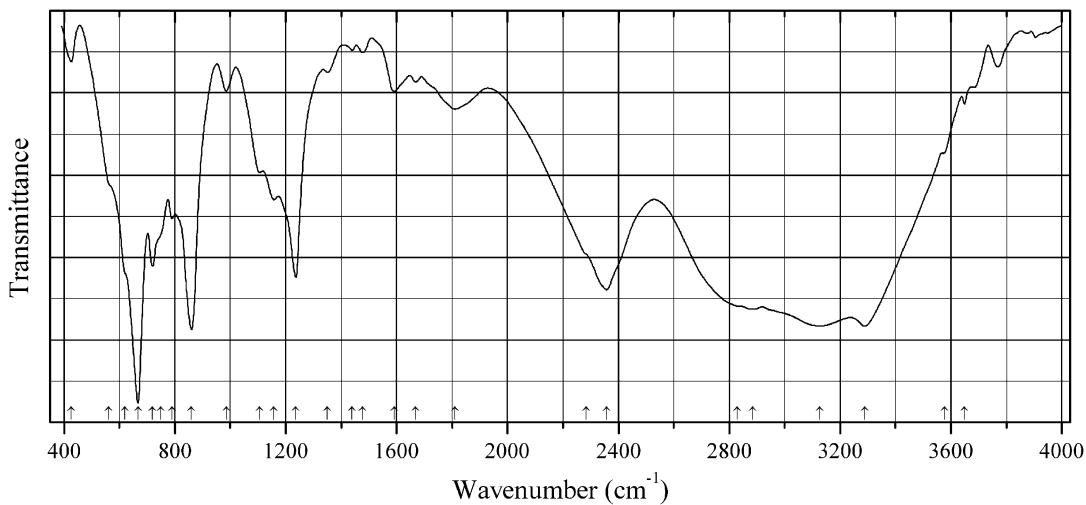
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Transmission.

**Source:** Kim et al. (2013).

**Wavenumbers (cm<sup>-1</sup>):** 955s, 947, 866s, 811sh, 788s, 740, 726, 691s, 655s, 622s, 605s, 538w, 511, 483, 432s.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**Te64 Sodium acid diarsenite tellurite  $\text{Na}_2(\text{H}_4\text{As}_2\text{O}_5)(\text{H}_2\text{TeO}_4)$**



**Origin:** Synthetic.

**Description:** Prepared by slow evaporation of an aqueous solution containing stoichiometric amounts of  $\text{Te}(\text{OH})_6$ ,  $\text{Na}_2\text{CO}_3$ , and  $\text{H}_3\text{AsO}_4$ . Characterized by EDS and thermal analysis. The crystal structure is solved. Tetragonal, space group  $I-4$ ,  $a = 5.576(2)$ ,  $c = 7.773(5)$  Å,  $V = 241.8(2)$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 5.72$  g/cm<sup>3</sup>.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

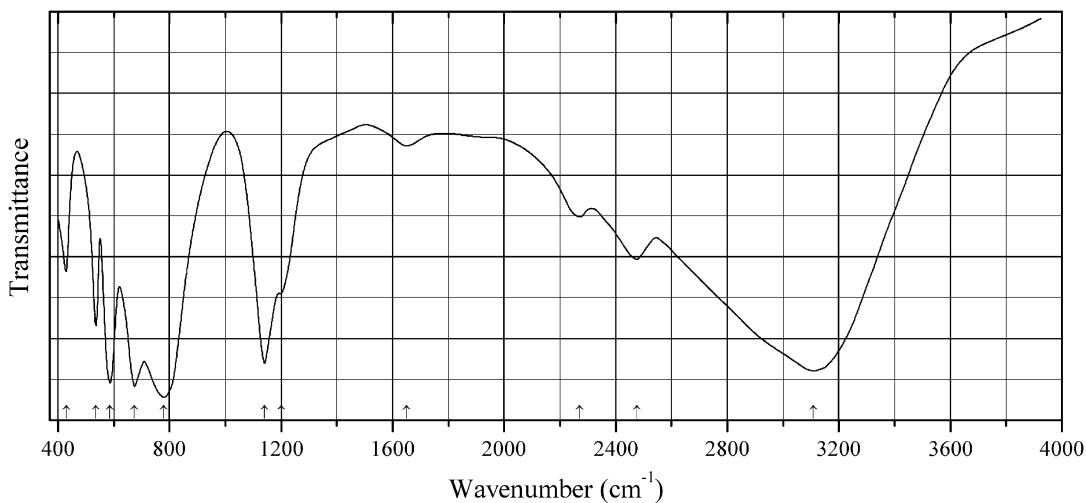
**Source:** Bechibani et al. (2014).

**Wavenumbers (IR, cm<sup>-1</sup>):** 3649w, 3578w, 3289s, 3127s, 2885s, 2830sh, 2358s, 2285sh, 1811, 1669w, 1592, 1478w, 1440w, 1350w, 1236s, 1158, 1106, 985, 860s, 790, 750, 720, 667s, 620sh, 560sh, 427w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 1327w, 1237w, 835, 718, 664sh, 650s, 623, 429, 423, 415, 372, 327, 321, 295w, 244w.

**Te65 Sodium acid tellurate  $\text{Na}_2[\text{TeO}_2(\text{OH})_4]$   $\text{Na}_2[\text{TeO}_2(\text{OH})_4]$**



**Origin:** Synthetic.

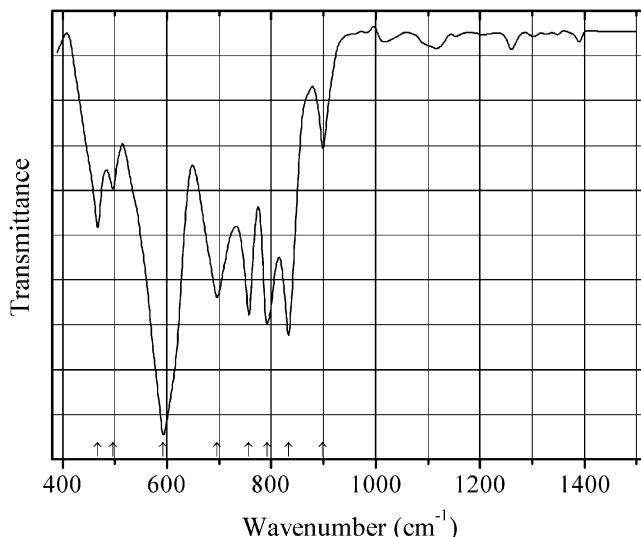
**Description:** Obtained in the reaction of  $\text{Te(OH)}_6$  with excess of NaOH in aqueous solution. Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Siebert (1959).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3110s, 2475, 2270, 1650w, 1200sh, 1141s, 780s, 675s, 587s, 536, 429.

### Te66 Sodium molybdenum(VI) tellurite $\text{Na}_2\text{MoTe}_4\text{O}_{12}$



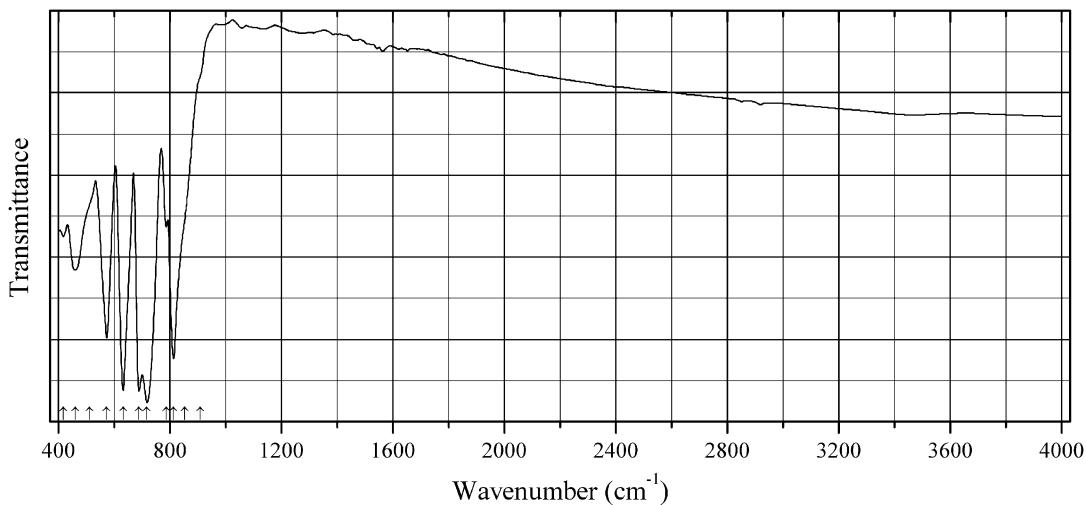
**Origin:** Synthetic.

**Description:** Synthesized hydrothermally from  $\text{Na}_2\text{MoO}_4 \cdot 2\text{H}_2\text{O}$  and  $\text{TeO}_2$  (with the ratio Na:Mo:Te = 6:3:1) at 225 °C for 4 days with subsequent cooling to room temperature over a period of 36 h. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $C2/c$ ,  $a = 17.341(4)$ ,  $b = 5.8262(11)$ ,  $c = 11.268(2)$  Å,  $\beta = 104.38(2)^\circ$ ,  $V = 1102.7(4)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 5.086$  g/cm<sup>3</sup>. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 5.500 (28) (110), 4.194 (29) (400), 4.028 (77) (31-1), 2.976 (49) (51-1), 2.911 (100) (020), 2.618 (29) (221), 2.085 (29) (422).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Balraj and Vidyasagar (1999).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 899, 833s, 792s, 757s, 696s, 593s, 496, 467.

**Te67 Sodium tellurite  $\beta\text{-Na}_2\text{Te}_4\text{O}_9$   $\beta\text{-Na}_2\text{Te}_4\text{O}_9$** 

**Origin:** Synthetic.

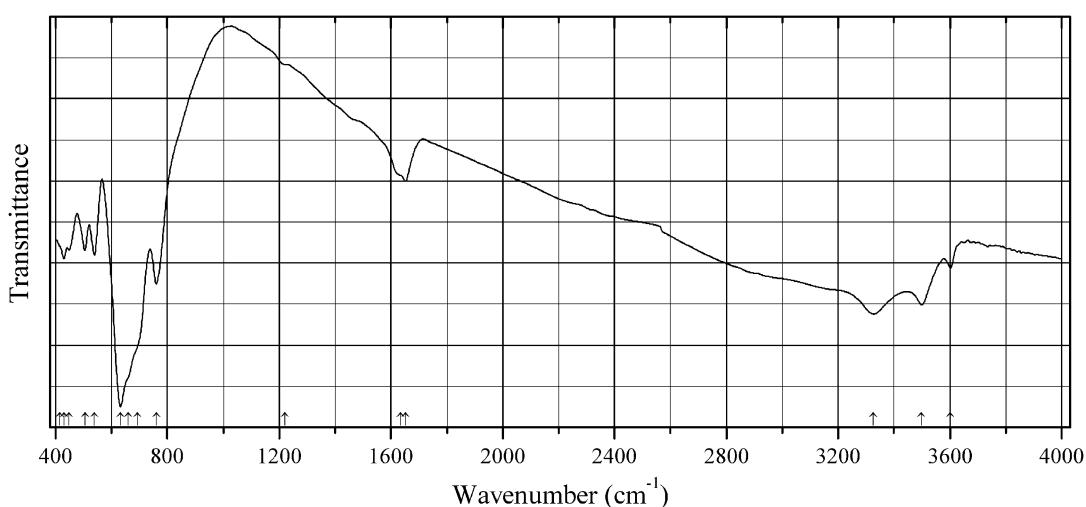
**Description:** Prepared hydrothermally from  $\text{Na}_2\text{CO}_3$  and  $\text{TeO}_2$  at 230 °C for 4 days. The crystal structure is solved. Orthorhombic, space group  $Pccn$ ,  $a = 16.317(2)$ ,  $b = 10.4544(10)$ ,  $c = 10.8874(10)$  Å,  $V = 1857.2(3)$  Å<sup>3</sup>,  $Z = 8$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Lee and Ok (2014).

**Wavenumbers (cm<sup>-1</sup>):** 908sh, 853sh, 814s, 787, 718s, 689s, 632s, 573, 512sh, 460, 419w.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**Te68 Sodium tellurate tellurite hydrate  $\text{Na}_2\text{Te}_2\text{O}_6 \cdot 1.5\text{H}_2\text{O}$   $\text{Na}_2\text{Te}_2\text{O}_6 \cdot 1.5\text{H}_2\text{O}$** 

**Origin:** Synthetic.

**Description:** Prepared hydrothermally from  $\text{Na}_2\text{CO}_3$  and  $\text{TeO}_2$  at 230 °C for 4 days. The crystal structure is solved. Monoclinic, space group  $C2/c$ ,  $a = 8.9884(19)$ ,  $b = 14.3739(19)$ ,  $c = 10.387(3)$  Å,  $\beta = 99.429(11)^\circ$ ,  $V = 1323.9(5)$  Å<sup>3</sup>,  $Z = 4$ .

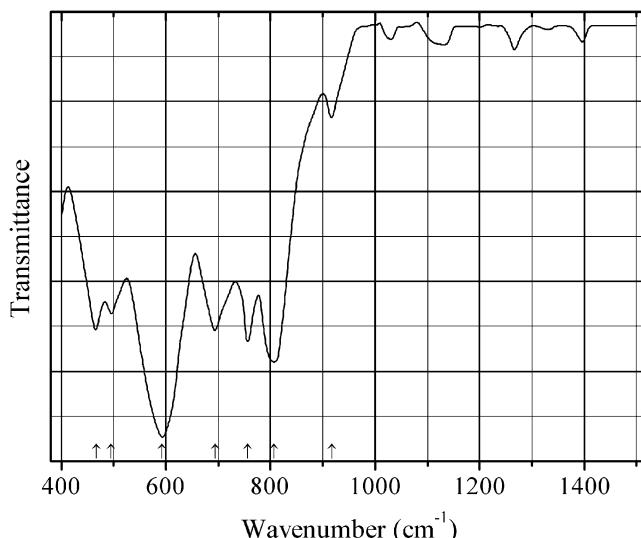
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Lee and Ok (2014).

**Wavenumbers (cm<sup>-1</sup>):** 3602w, 3498, 3327, 1651, 1635sh, 1221sh, 760s, 692sh, 659sh, 632s, 539, 505, 449, 430, 415sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

### Te69 Sodium tungsten tellurite $\text{Na}_2\text{WTe}_4\text{O}_{12}$



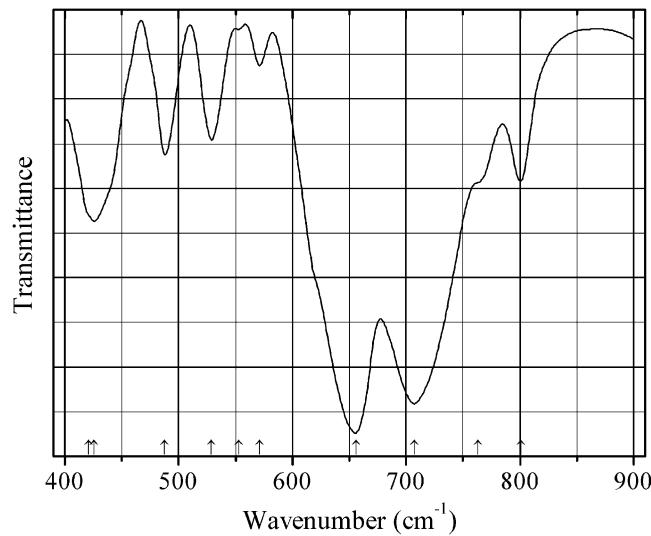
**Origin:** Synthetic.

**Description:** Tiny pale yellow crystals. Synthesized hydrothermally from  $\text{Na}_2\text{WO}_4 \cdot 2\text{H}_2\text{O}$  and  $\text{TeO}_2$  (with the ratio Na:W:Te = 6:3:1) at 225 °C for 4 days with subsequent cooling to room temperature over a period of 36 h. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $C2/c$ ,  $a = 17.348(3)$ ,  $b = 5.7755(10)$ ,  $c = 11.269(3)$  Å,  $\beta = 104.33(2)^\circ$ ,  $V = 1094.0(4)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 5.660$  g/cm<sup>3</sup>. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 4.007 (100) (100), 3.144 (49) (11–3), 2.966 (72) (51–1), 2.883 (48) (020), 2.597 (59) (221).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Balraj and Vidyasagar (1999).

**Wavenumbers (cm<sup>-1</sup>):** 917w, 807s, 756, 694, 593s, 495, 467.

**Te70 Strontium copper tellurate tellurite  $\text{SrCuTe}_2\text{O}_7$** 

**Origin:** Synthetic.

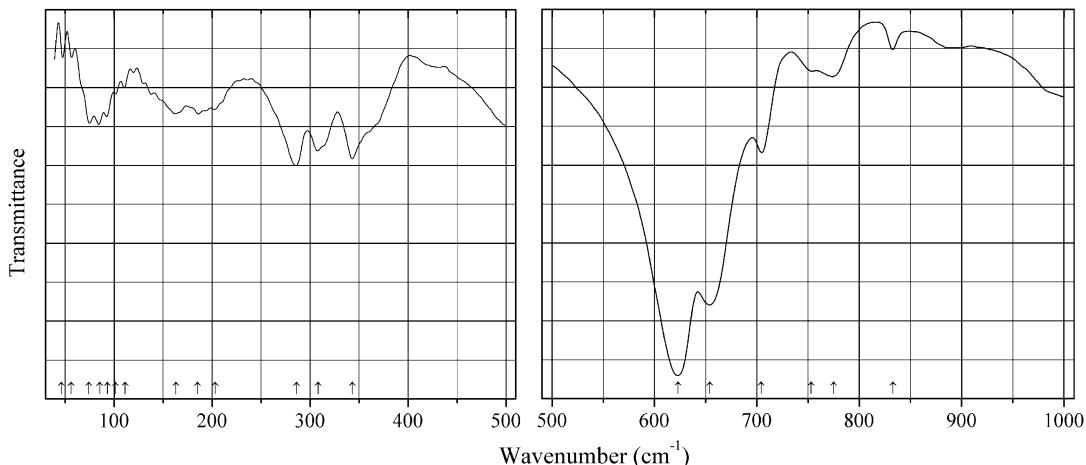
**Description:** Prepared by heating a mixture of  $\text{SrCO}_3$ ,  $\text{CuO}$ ,  $\text{TeO}_2$ , and  $\text{H}_2\text{TeO}_4$ , taken in stoichiometric amounts. Characterized by powder X-ray diffraction data. The crystal structure is solved. Orthorhombic, space group  $Pbcm$ ,  $a = 7.1464(7)$  Å,  $b = 15.0609(15)$  Å,  $c = 5.4380(5)$  Å,  $V = 585.30(10)$  Å<sup>3</sup>,  $Z = 4$ . The structure is based on 2D layers consisting of corner-shared  $\text{CuO}_5$  square pyramids,  $\text{TeO}_6$  octahedra, and  $\text{TeO}_4$  disphenoids.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Yeon et al. (2011).

**Wavenumbers (cm<sup>-1</sup>):** 801, 763sh, 707s, 656s, 571w, 553w, 529, 488, 426, 421sh.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Te71 Thallium tellurite  $\beta\text{-Tl}_2\text{TeO}_3$** 

**Origin:** Synthetic.

**Description:** Light yellow to brown aggregates of crystals prepared by heating a mixture of  $\text{Ti}_2\text{CO}_3$  and  $\text{TeO}_2$ , taken in stoichiometric amounts, at 160 °C for 3 days. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 8.9752(18)$ ,  $b = 4.8534(6)$ ,  $c = 11.884(2)$  Å,  $\beta = 109.67(2)^\circ$ ,  $V = 487.47(15)$  Å<sup>3</sup>,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

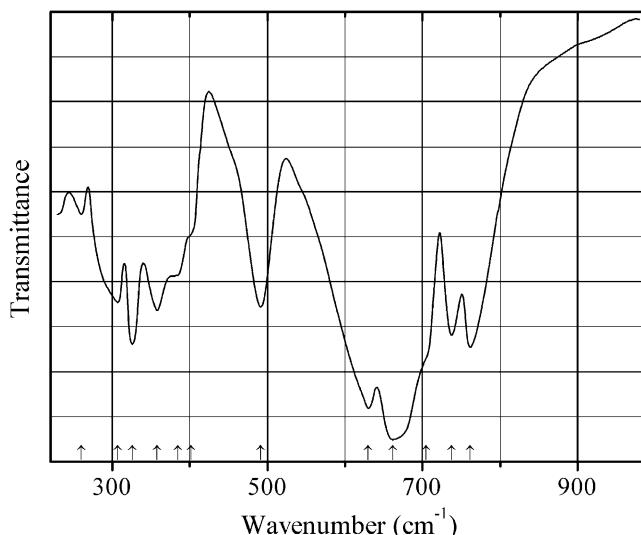
**Source:** Rieger and Mudring (2007).

**Wavenumbers (IR, cm<sup>-1</sup>):** 833w, 775w, 753w, 704, 654s, 623s, 343, 308, 286, 203, 185, 163, 111w, 101, 93, 85, 74, 56w, 46w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 708s, 646, 346w, 296, 172sh, 150, 117, 93s, 66w.

### Te72 Thorium tellurite $\text{ThTe}_2\text{O}_6$



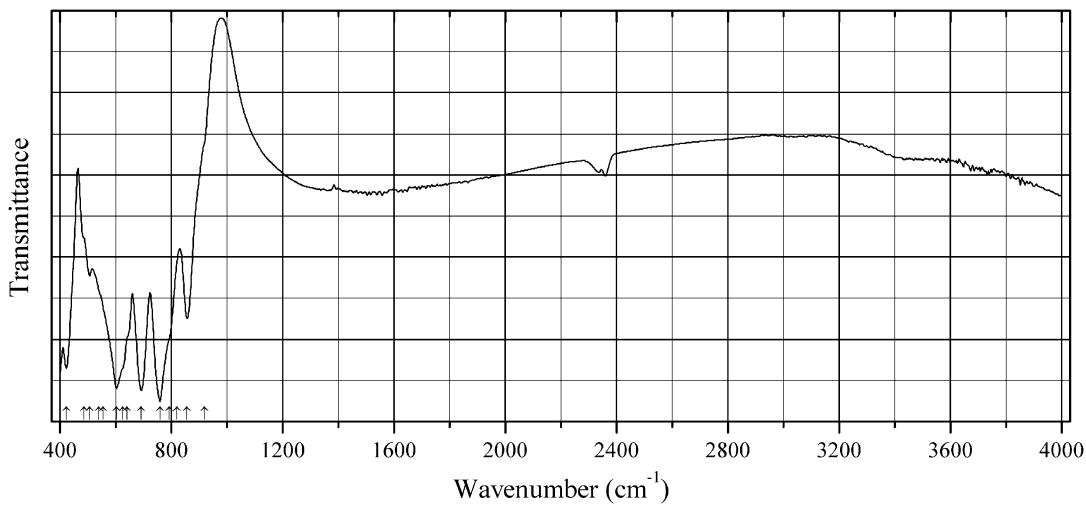
**Origin:** Synthetic.

**Description:** Prepared by heating a mixture of  $\text{TeO}_2$  and  $\text{ThO}_2$  (with the molar ratio 1:2) at 600 °C for 48 h. Characterized by powder X-ray diffraction data. Cubic,  $a = 21.838(8)$ ,  $V = 10414.5$  Å<sup>3</sup>,  $Z = 64$ .  $D_{\text{meas}} = 5.7$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 5.95$  g/cm<sup>3</sup>. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 3.53 (53) (611), 3.432 (72) (540), 3.167 (100) (444), 2.977 (41) (721), 2.849 (53) (731), 2.028 (35) (864).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Botto and Baran (1982).

**Wavenumbers (cm<sup>-1</sup>):** 762, 738, 705sh, 662s, 630s, 491, 402sh, 385sh, 358, 326, 307, 260w.

**Te73 Yttrium vanadyl oxytellurite  $\text{Y}(\text{VO})(\text{TeO}_3)_2\text{O}$** 

**Origin:** Synthetic.

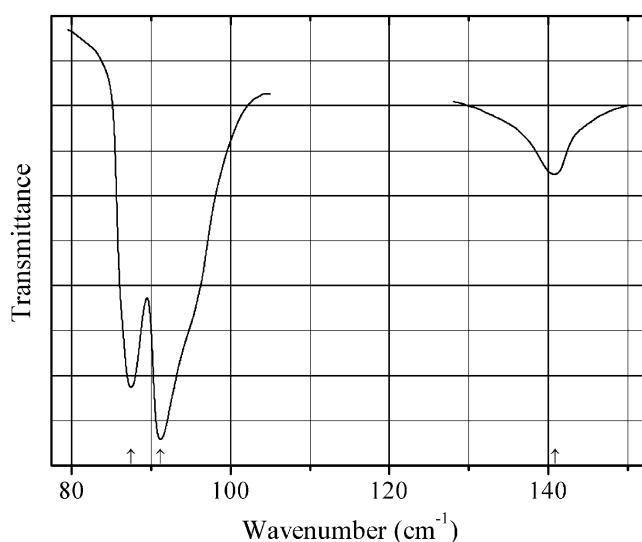
**Description:** Crystals grown hydrothermally from  $\text{Y}_2\text{O}_3$ ,  $\text{V}_2\text{O}_5$ , and  $\text{TeO}_2$  at 550 °C for 48 h with three intermediate regrindings. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $C2/m$ ,  $a = 7.9396(10)$ ,  $b = 7.5625(10)$ ,  $c = 21.282(2)$  Å,  $\beta = 90.010(10)^\circ$ ,  $V = 1277.85(3)$  Å<sup>3</sup>,  $Z = 8$ .  $D_{\text{calc}} = 5.438$  g/cm<sup>3</sup>.  $\text{V}^{5+}$  has sixfold coordination with one short V–O bond.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Kim et al. (2014).

**Wavenumbers (cm<sup>-1</sup>):** 920sh, 857, 821sh, 792sh, 759s, 692s, 640sh, 625sh, 603s, 555sh, 540sh, 507w, 487sh, 423.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Te74 Tellurium Te**

**Origin:** Synthetic.

**Description:** A sample prepared by deposition of evaporated Te on crystalline quartz.

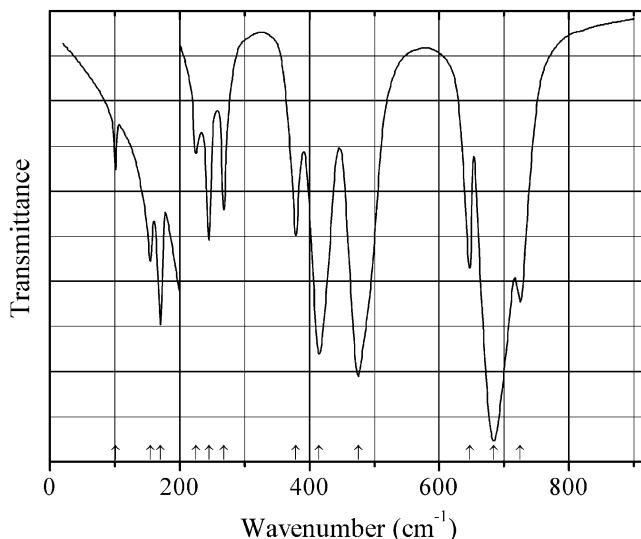
**Kind of sample preparation and/or method of registration of the spectrum:** Polycrystalline film

1500 Å thick. Transmission.

**Source:** Grosse and Richter (1970).

**Wavenumbers (cm<sup>-1</sup>):** 140.8, 91.2, 87.5.

**Te75 Yafsoanite** Ca<sub>3</sub>Zn<sub>3</sub>Te<sup>6+</sup><sub>2</sub>O<sub>12</sub>



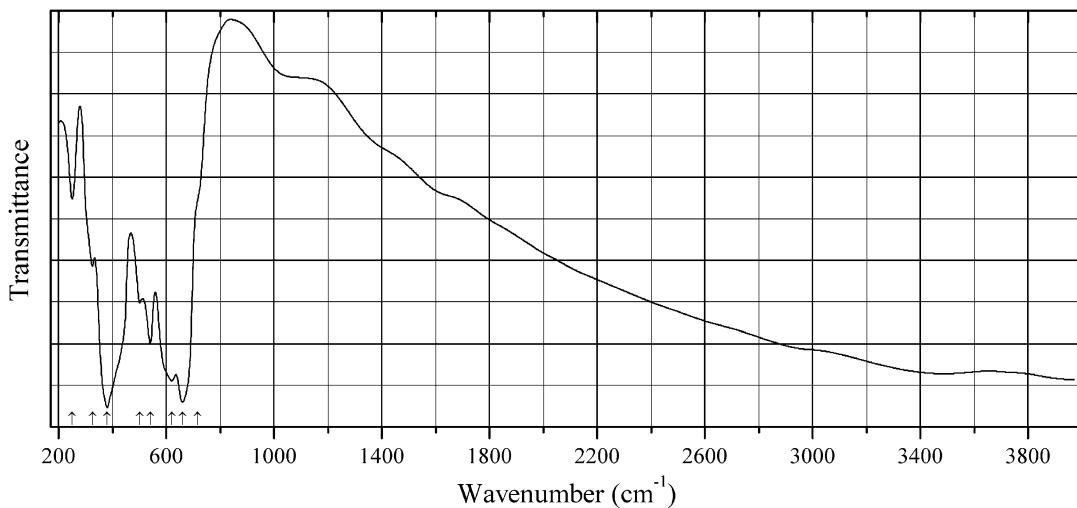
**Origin:** Synthetic.

**Description:** Synthesized by solid-state reaction, starting from CaCO<sub>3</sub>, ZnO, and TeO<sub>2</sub>. Confirmed by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

**Source:** Rulmont et al. (1992).

**Wavenumbers (cm<sup>-1</sup>):** 725, 684s, 647, 475s, 415s, 379, 268, 245, 225w, 171, 155, 101w.

**Te76 Pingguite  $\text{Bi}_6\text{Te}^{4+}_2\text{O}_{13}$** 

**Origin:** Yangjiava, Pinggu Co., Beijing Municipality, China (type locality).

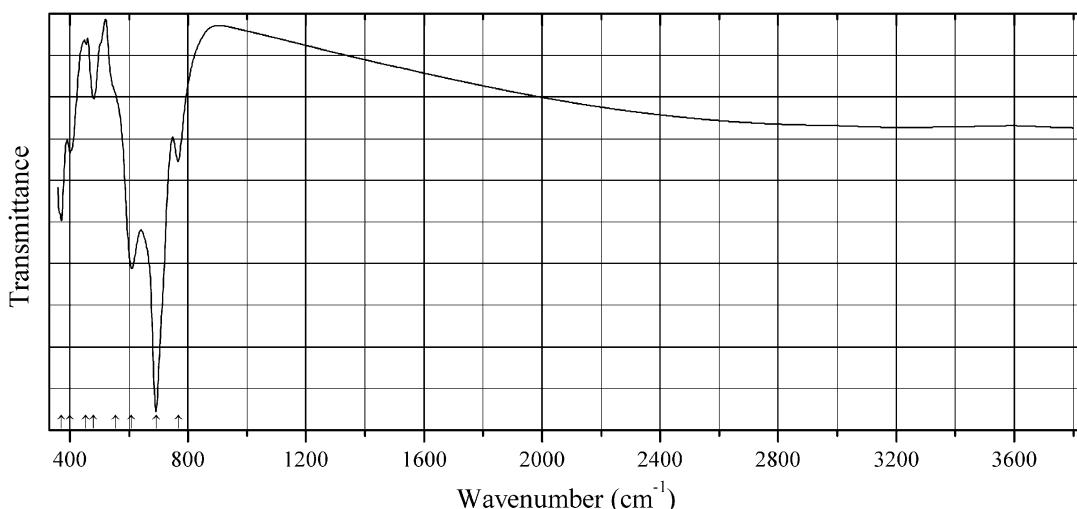
**Description:** Yellowish green aggregate from the association with malachite, pyromorphite, bismutite, etc. Holotype sample. Orthorhombic,  $a = 5.689(1)$ ,  $b = 10.791(1)$ ,  $c = 5.308(1)$  Å,  $Z = 1$ .  $D_{\text{meas}} = 8.44$  g/cm<sup>3</sup>,  $D_{\text{calc}} = 8.64$  g/cm<sup>3</sup>. Optically biaxial (−),  $\alpha = 1.554(2)$ ,  $\beta = 1.558(2)$ ,  $\gamma = 1.566(2)$ ,  $2V = 70(5)$ °. The empirical formula is  $\text{Bi}_{5.80}\text{Te}_{2.15}\text{O}_{13}$ . The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %) ( $hkl$ )] are: 3.146 (100) (121), 2.841 (80) (200), 2.694 (20) (040), 1.695 (20) (321), 1.956 (10) (240), 1.631 (10) (161).

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Sun et al. (1994).

**Wavenumbers (cm<sup>-1</sup>):** 715sh, 660s, 620, 540, 500, 380s, 325, 250.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

**Te77 Denningite  $\text{CaMn}^{2+}\text{Te}^{4+}_4\text{O}_{10}$** 

**Origin:** Moctezuma (La Bambolla) mine, Moctezuma, Sonora, Mexico (type locality).

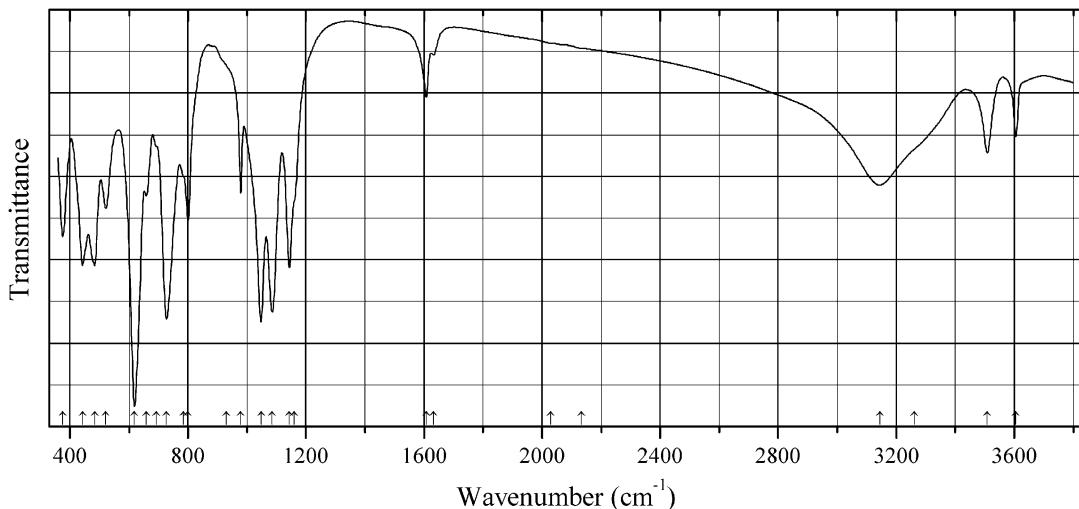
**Description:** Pale yellowish-green granular aggregate from the association with muscovite. The empirical formula is (electron microprobe):  $\text{Ca}_{0.79}\text{Mn}_{1.15}\text{Mg}_{0.05}\text{Te}_{4.00}\text{O}_5$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 767, 692s, 609s, 555sh, 481, 454w, 401, 372.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Te78 Poughite**  $\text{Fe}^{3+} \cdot_2(\text{Te}^{4+}\text{O}_3)_2(\text{SO}_4) \cdot 3\text{H}_2\text{O}$



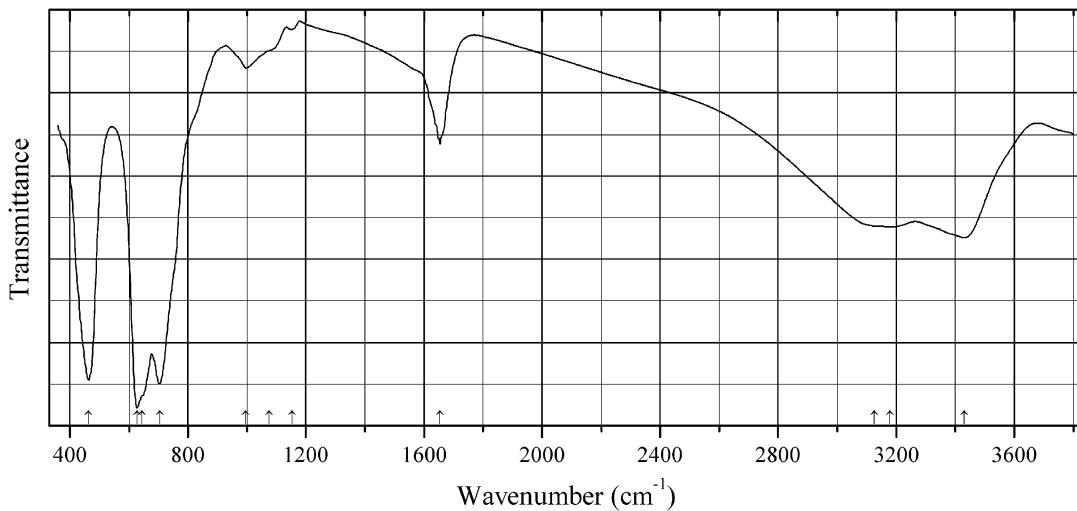
**Origin:** Moctezuma (La Bambolla) mine, Moctezuma, Sonora, Mexico (type locality).

**Description:** Yellow spherulites on quartz. The empirical formula is (electron microprobe):  $(\text{Fe}_{0.92}\text{Al}_{0.08})(\text{TeO}_3)_{1.99}(\text{SO}_4)_{1.02} \cdot n\text{H}_2\text{O}$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc.  
Absorption.

**Wavenumbers ( $\text{cm}^{-1}$ ):** 3606, 3508, 3260sh, 3144, 2134w, 2028w, 1633, 1608, 1160sh, 1144s, 1086s, 1048s, 979, 930sh, 800, 785sh, 728s, 693sh, 659, 619s, 522, 484s, 443s, 375.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Te79 Zemannite**  $Mg_{0.5}ZnFe^{3+}(Te^{4+}O_3)_3 \cdot 4.5H_2O$ 

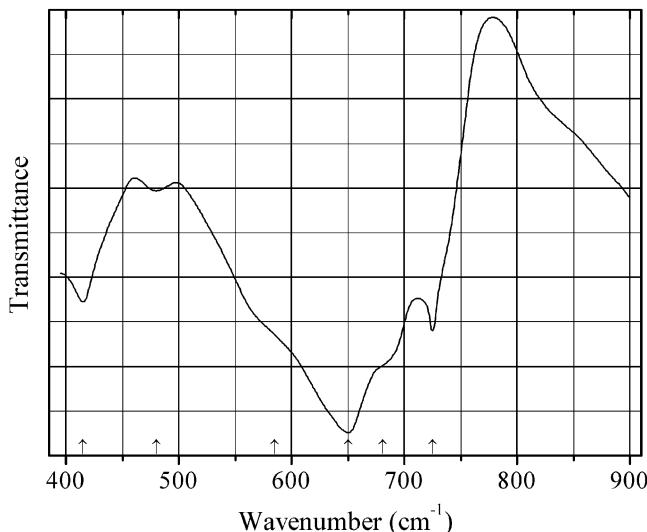
**Origin:** Moctezuma (La Bambolla) mine, Moctezuma, Sonora, Mexico (type locality).

**Description:** Brown acicular crystals from the association with dickite and quartz. The empirical formula is (electron microprobe):  $Mg_{0.63}Zn_{0.84}Fe_{0.98}Al_{0.02}Ti_{0.02}(TeO_3)_3 \cdot nH_2O$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3430s, 3180, 3125sh, 1654, 1152w, 1075sh, 996, 704s, 645sh, 627s, 464s.

**Note:** The spectrum was obtained by N.V. Chukanov.

**Te80 Plumbotellurite**  $Pb(Te^{4+}O_3)$ 

**Origin:** Synthetic.

**Description:** Synthesized by crystallization above the solidus temperature of the PbO–TeO<sub>2</sub> system.

Characterized by powder X-ray diffraction data and electron microprobe analysis.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

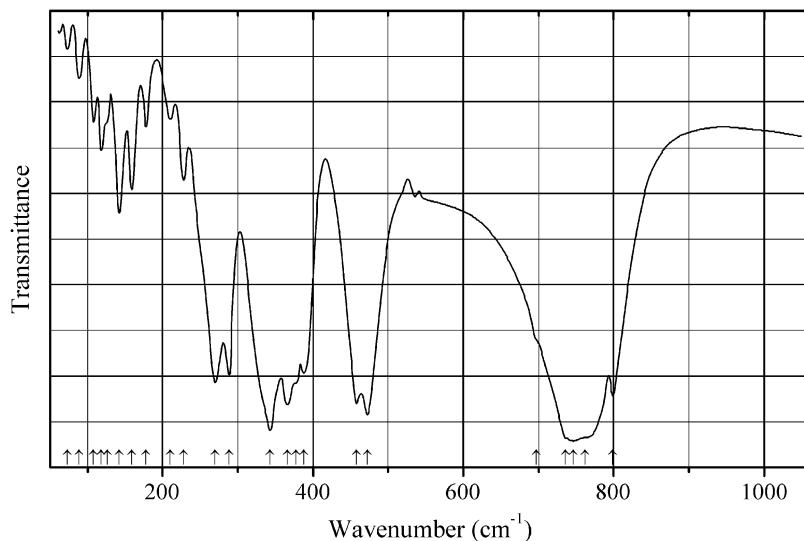
**Source:** Stavrakieva et al. (1988).

**Wavenumbers (cm<sup>-1</sup>):** 725, 681sh, 650s, 585sh, 480w, 415.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.

## 2.19 Iodides, Iodites, and Iodates

### I15 Copper iodate $\alpha\text{-Cu(}(\text{IO}_3)_2$



**Origin:** Synthetic.

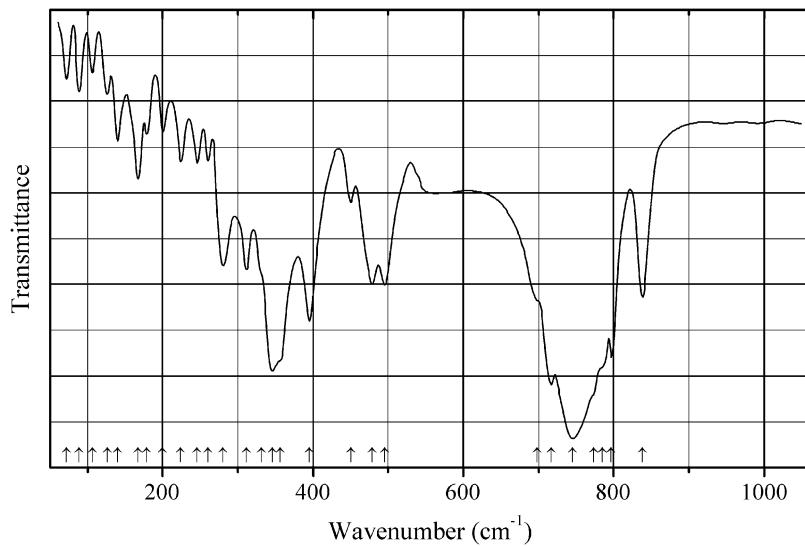
**Description:** Light yellow green crystal clusters and spherulites obtained by heating bellingerite  $\text{Cu(}(\text{IO}_3)_2\cdot 2\text{H}_2\text{O}$  to 110 °C. Characterized by powder X-ray diffraction data. Point group 2. Optically biaxial (+) or (-),  $\alpha = 1.88$ ,  $\beta = 1.94$ ,  $\gamma = 2.00$ ,  $2V$  is medium. Decomposes at 460 °C.

**Kind of sample preparation and/or method of registration of the spectrum:** Fluorolube mull (above 1500  $\text{cm}^{-1}$ ), KBr disc (from 550 to 1500  $\text{cm}^{-1}$ ), and Nujol mull (below 550  $\text{cm}^{-1}$ ). Transmission.

**Source:** Nassau et al. (1973).

**Wavenumbers (cm<sup>-1</sup>):** 799, 762sh, 746s, 736sh, 697, 472s, 458s, 388, 377sh, 366s, 343s, 288, 270s, 228, 210w, 178, 159, 142, 126sh, 118, 108, 89w, 73w.

## I16 Copper iodate $\beta$ -Cu(IO<sub>3</sub>)<sub>2</sub>



**Origin:** Synthetic.

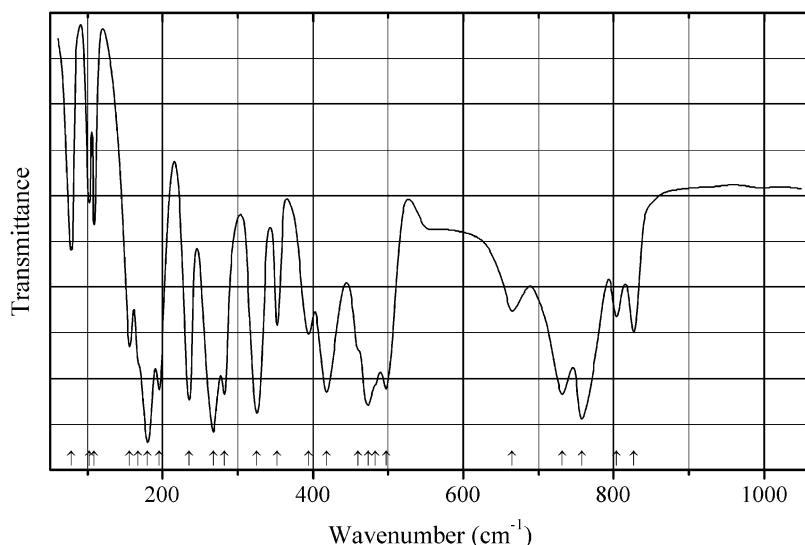
**Description:** Light green crystal clusters and dendrites obtained by a gel growth technique. Characterized by powder X-ray diffraction data. Point group -1. Optically biaxial (-),  $\alpha = 1.90$ ,  $\beta = 1.94$ ,  $\gamma = 1.96$ , 2V is large. Decomposes at 250 °C to form  $\alpha\text{-Cu}(\text{IO}_3)_2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Fluorolube mull (above  $1500\text{ cm}^{-1}$ ), KBr disc (from  $550$  to  $1500\text{ cm}^{-1}$ ), and Nujol mull (below  $550\text{ cm}^{-1}$ ). Transmission.

**Source:** Nassau et al. (1973).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 838, 797, 785sh, 774sh, 745s, 717s, 698sh, 495, 479, 450, 395s, 356sh, 346s, 331sh, 311, 280, 260w, 246w, 224w, 200w, 179w, 167, 140w, 126w, 106w, 89w, 72w.

## I17 Copper iodate $\gamma$ -Cu(IO<sub>3</sub>)<sub>2</sub>



**Origin:** Synthetic.

**Description:** Dark yellow crystals and crystal clusters obtained by a gel growth technique. Characterized by powder X-ray diffraction data. Point group  $2/m$ . Optically biaxial (-),  $\alpha = 1.89$ ,  $\beta = 1.96$ ,  $\gamma = 1.99$ ,  $2V$  is medium. Decomposes at  $460\text{ }^{\circ}\text{C}$  to form CuO.

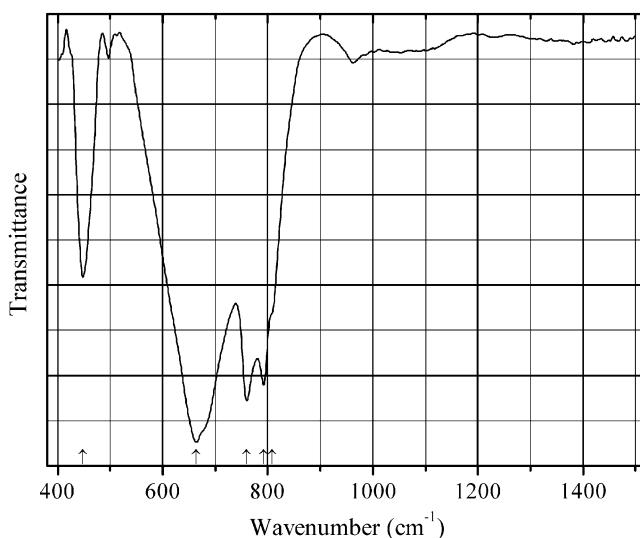
**Kind of sample preparation and/or method of registration of the spectrum:** Fluorolube mull (above  $1500\text{ cm}^{-1}$ ), KBr disc (from  $550$  to  $1500\text{ cm}^{-1}$ ), and Nujol mull (below  $550\text{ cm}^{-1}$ ). Transmission.

**Source:** Nassau et al. (1973).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 827, 804, 758s, 732, 665, 497, 483sh, 473s, 460sh, 418, 394, 352, 325s, 282, 267s, 235, 195, 180s, 167, 156, 109, 102, 78.

**Note:** In the cited paper, the wavenumber  $180\text{ cm}^{-1}$  is erroneously indicated as  $170\text{ cm}^{-1}$ .

### I18 Potassium titanium iodate $\text{K}_2\text{Ti}(\text{IO}_3)_6$



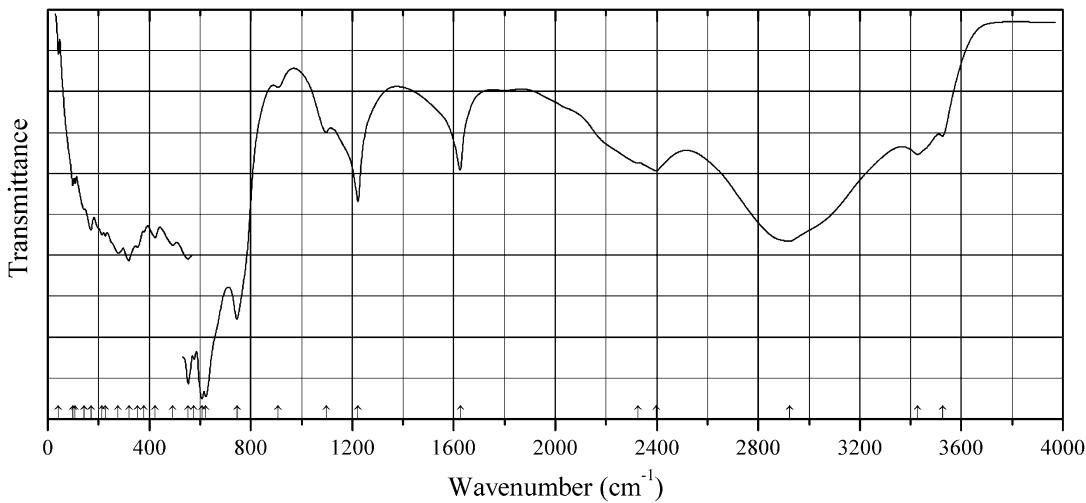
**Origin:** Synthetic.

**Description:** Synthesized hydrothermally from  $\text{K}_2\text{CO}_3$ ,  $\text{TiO}_2$ , and  $\text{HIO}_3$  at  $230\text{ }^{\circ}\text{C}$  for 4 days. Characterized by powder X-ray diffraction data. The crystal structure is solved. Trigonal, space group  $R\bar{3}$ ,  $a = 11.2703(6)$ ,  $c = 11.3514(11)\text{ \AA}$ ,  $V = 1248.68(15)\text{ \AA}^3$ ,  $Z = 3$ .  $D_{\text{calc}} = 4.690\text{ g/cm}^3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Chang et al. (2009).

**Wavenumbers ( $\text{cm}^{-1}$ ):** 808sh, 792s, 760s, 664s, 448.

**I19 Copper acid diperiodate hydrate** Cu(H<sub>4</sub>I<sub>2</sub>O<sub>10</sub>)·6H<sub>2</sub>O

**Origin:** Synthetic.

**Description:** Monoclinic, space group  $P2_1/c$ ,  $Z = 2$ . In the crystal structure, the centrosymmetric  $H_4I_2O_{10}^{2-}$  anions are formed by two edge-sharing crystallographically equivalent  $IO_6$  octahedra.

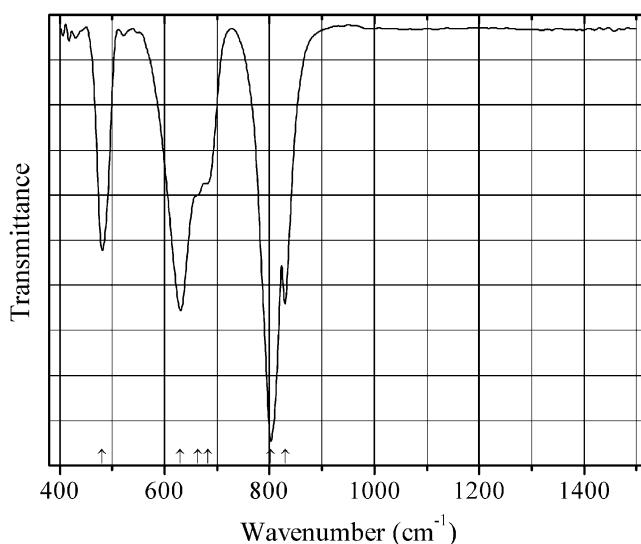
**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection (above  $500\text{ cm}^{-1}$ ). Nujol mull, transmission (below  $500\text{ cm}^{-1}$ ).

**Source:** Jaquet and Haeuseler (2008).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 3526, 3427, 2924s (broad), 2397, 2326, 1626, 1223, 1097, 908, 746s, 623s, 608s, 576s, 553s, 492, 424, 380, 353, 320s, 277, 226, 214, 171, 145sh, 108, 99, 42w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 805s, 756, 746s, 704, 671, 630s, 620s, 443, 413, 396, 356w, 345w, 329, 311.

**I20 Sodium titanium iodate** Na<sub>2</sub>Ti( IO<sub>3</sub>)<sub>6</sub>

**Origin:** Synthetic.

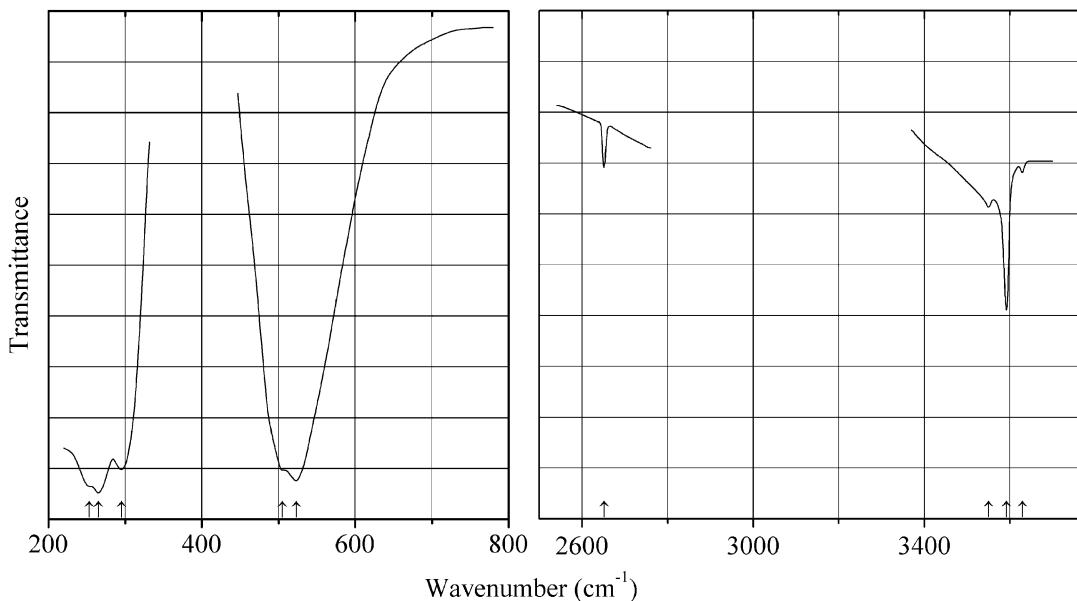
**Description:** Colorless acicular crystals synthesized hydrothermally from  $\text{Na}_2\text{CO}_3$ ,  $\text{TiO}_2$ , and  $\text{HIO}_3$  at  $230^\circ\text{C}$  for 4 days. Characterized by powder X-ray diffraction data. The crystal structure is solved. Hexagonal, space group  $P6_3$ ,  $a = 9.649(3)$  Å,  $c = 5.198(3)$  Å,  $V = 419.1(3)$  Å $^3$ ,  $Z = 1$ .  $D_{\text{calc}} = 4.530$  g/cm $^3$ . The  $\text{Ti}^{4+}$  cation is disordered over two half-occupied sites

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated. Possibly, a procedure of baseline correction has been applied.

**Source:** Chang et al. (2009).

**Wavenumbers (cm $^{-1}$ ):** 830, 803s, 682sh, 663sh, 630, 481.

### I21 Laurionite I-analogue $\text{Pb}(\text{OH})\text{I}$



**Origin:** Synthetic.

**Description:** Characterized by powder X-ray diffraction data and thermoanalytical methods. Isostructural with laurionite.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr or CsI disc, and Nujol or poly(chlorotrifluorethene) mull. Transmission.

**Source:** Lutz et al. (1995).

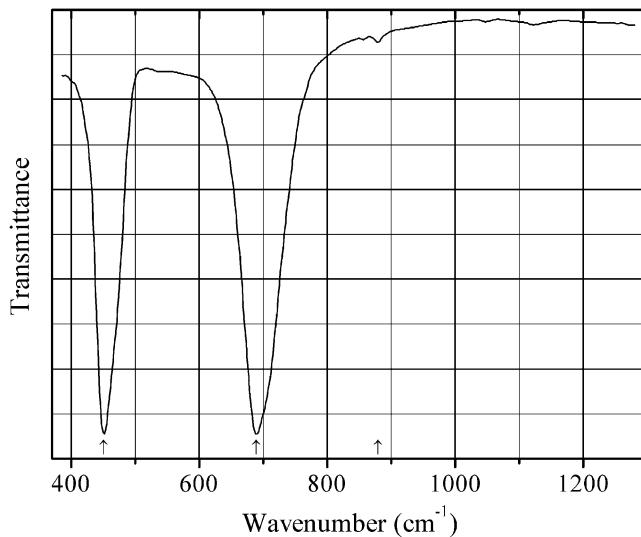
**Wavenumbers (IR, cm $^{-1}$ ):** 3629, 3592, 3550, 523s, 505sh, 295, 265s, 253.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 3496s, 318w, 244w, 172w, 104, 72, 55s, 50s

## 2.20 Xenates

### Xe1 Double perovskite $\text{KBa}(\text{XeNaO}_6)$ $\text{KBa}(\text{XeNaO}_6)$



**Origin:** Synthetic.

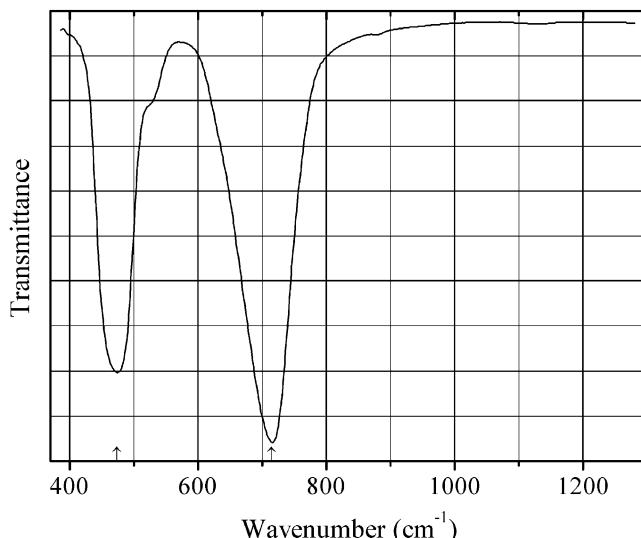
**Description:** Synthesized hydrothermally from KOH, NaOH, Ba(NO<sub>3</sub>)<sub>2</sub>, and Na<sub>4</sub>XeO<sub>6</sub> at 170 °C for 24 h. Characterized by TGA-DSC data, powder X-ray diffraction, and EDX analyses. The crystal structure is solved and refined by the Rietveld method. Cubic, space group *Fm-3m*,  $a = 8.3188(2)$  Å,  $V = 575.67(3)$  Å<sup>3</sup>,  $Z = 4$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Britvin et al. (2015).

**Wavenumbers (cm<sup>-1</sup>):** 1626w, 1434w, 1383w, 1392w, 879w, 689s, 451s.

### Xe2 Double perovskite $\text{KCa}(\text{XeNaO}_6)$ $\text{KCa}(\text{XeNaO}_6)$



**Origin:** Synthetic.

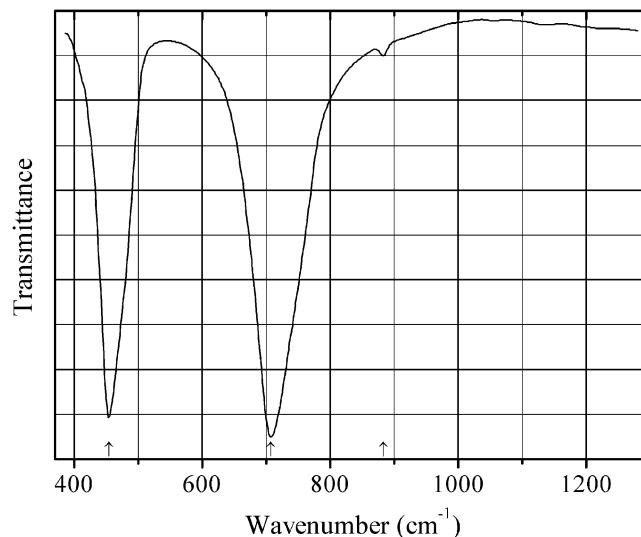
**Description:** Synthesized hydrothermally from KOH, NaOH, Ca(NO<sub>3</sub>)<sub>2</sub>·4H<sub>2</sub>O, and Na<sub>4</sub>XeO<sub>6</sub> at 170 °C for 24 h. Characterized by TGA-DSC data, powder X-ray diffraction, and EDX analyses. The crystal structure is solved and refined by the Rietveld method. Tetragonal, space group *I*4/*m*, *a* = 5.7500(1), *c* = 8.1558(2) Å, *V* = 269.66(1) Å<sup>3</sup>, *Z* = 2.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Britvin et al. (2015).

**Wavenumbers (cm<sup>-1</sup>):** 715s, 474s.

### Xe3 Double perovskite KSr(XeNaO<sub>6</sub>) KSr(XeNaO<sub>6</sub>)



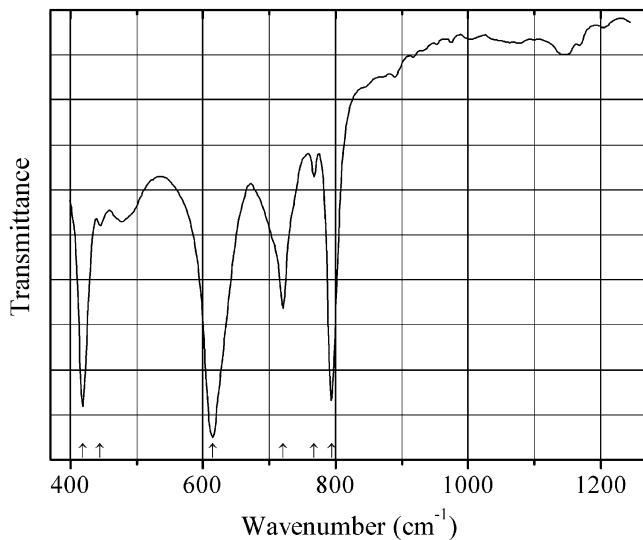
**Origin:** Synthetic.

**Description:** Synthesized hydrothermally from KOH, NaOH, Sr(NO<sub>3</sub>)<sub>2</sub>, and Na<sub>4</sub>XeO<sub>6</sub> at 170 °C for 24 h. Characterized by TGA-DSC data, powder X-ray diffraction, and EDX analyses. The crystal structure is solved and refined by the Rietveld method. Cubic, space group *Fm*-3*m*, *a* = 8.1920(1) Å, *V* = 549.76(2) Å<sup>3</sup>, *Z* = 4.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Britvin et al. (2015).

**Wavenumbers (cm<sup>-1</sup>):** 1634w, 1444w, 1396w, 883w, 707s, 454s.

**Xe4 Layered perovskite  $K_4Xe_3O_{12}$   $K_4Xe_3O_{12}$** 

**Origin:** Synthetic.

**Description:** Aggregate of yellow platelets. Hexagonal. The crystal structure contains three-layer perovskite slabs composed of inner layers of  $[XeO_6]^{4-}$  (perxenate) octahedra, which are sandwiched between the layers of neutral  $XeO_3$  molecules.

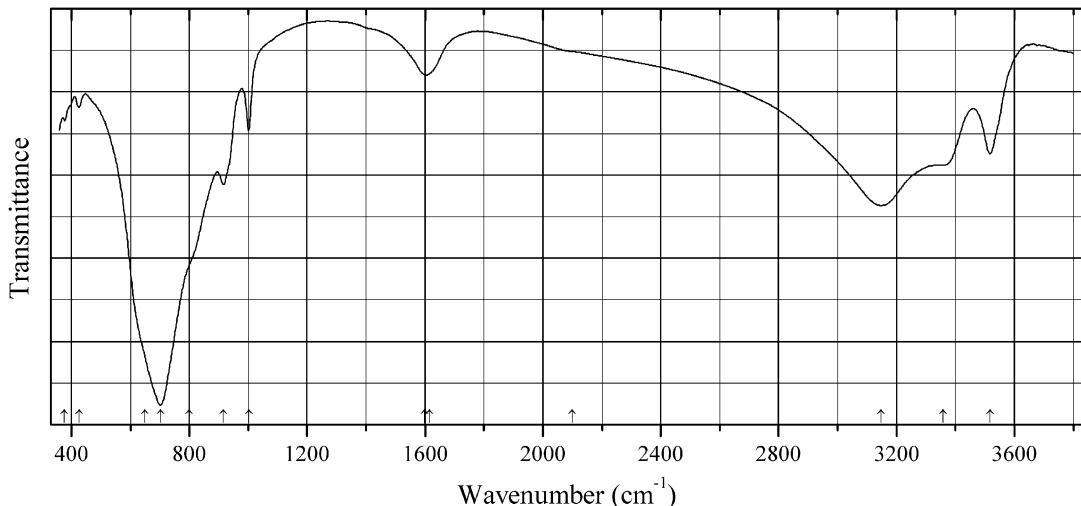
**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull. Transmission.

**Source:** Britvin et al. (2016).

**Wavenumbers (cm⁻¹):** 794s, 768w, 721, 615s, 445w, 419s.

**Note:** The band at 721  $\text{cm}^{-1}$  is due to absorption of Nujol.

## 2.21 Tungstates and W-Bearing Oxides

**W18 Hydrotungstate  $WO_2(OH)_2 \cdot H_2O$** 

**Origin:** Alyaskitovoe Sn-W deposit, eastern Sakha Republic (Yakutia), Siberia, Russia.

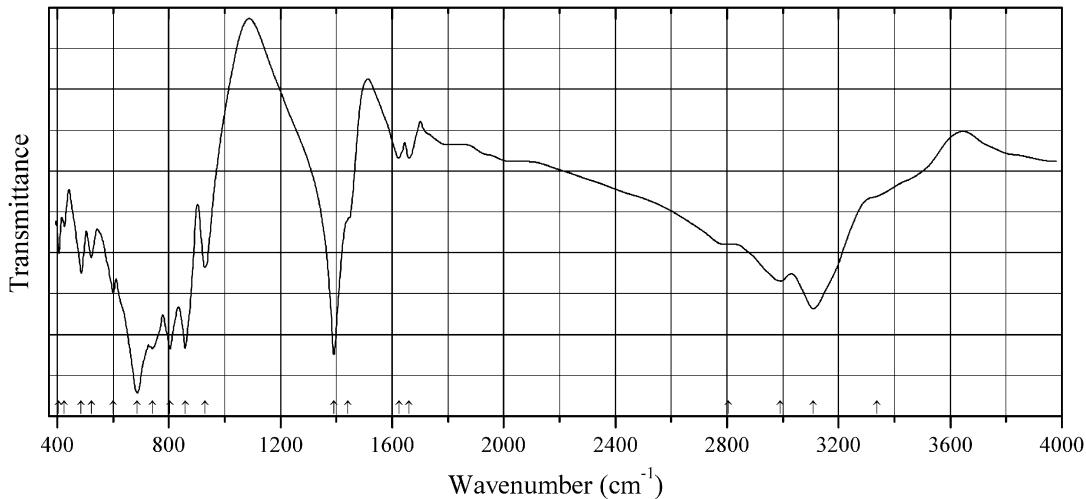
**Description:** Yellow, massive. Investigated by I.V. Pekov. Characterized by qualitative electron microprobe analyses. The strongest lines of the powder X-ray diffraction pattern [ $d$ , Å ( $I$ , %)] are: 6.93 (100), 3.70 (60), 3.44 (30), 3.25 (40), 2.62 (70), 2.54 (50), 1.95 (70).

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Wavenumbers (cm<sup>-1</sup>):** 3518, 3359, 3147, 2100sh, 1615sh, 1599, 1002, 916, 800sh, 702s, 650sh, 426w, (375w).

**Note:** The spectrum was obtained by N.V. Chukanov.

### W19 Ammonium paratungstate tetrahydrate (NH<sub>4</sub>)<sub>10</sub>[H<sub>2</sub>W<sub>12</sub>O<sub>42</sub>]·4H<sub>2</sub>O



**Origin:** Synthetic.

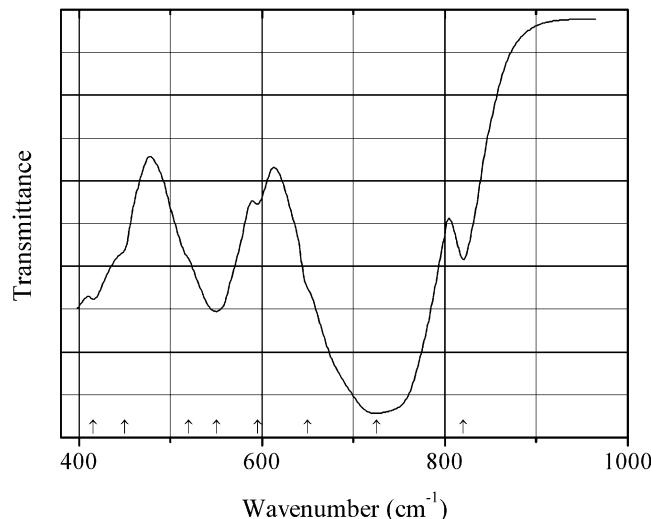
**Description:** Reactant produced by H.C. Starck. Confirmed by elemental analysis. Characterized by powder X-ray diffraction data.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Szilágyi et al. (2004).

**Wavenumbers (cm<sup>-1</sup>):** 3337sh, 3110, 2992, 2805sh, 1661w, 1624w, 1442sh, 1391s, 929, 859s, 805s, 741s, 687s, 601, 522, 486, 426, 406.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum.

**W20 Bismuth tungstate  $\text{Bi}_2\text{WO}_6$** 

**Origin:** Synthetic.

**Description:** Characterized by powder X-ray diffraction data. Orthorhombic, space group  $B2cb$ .

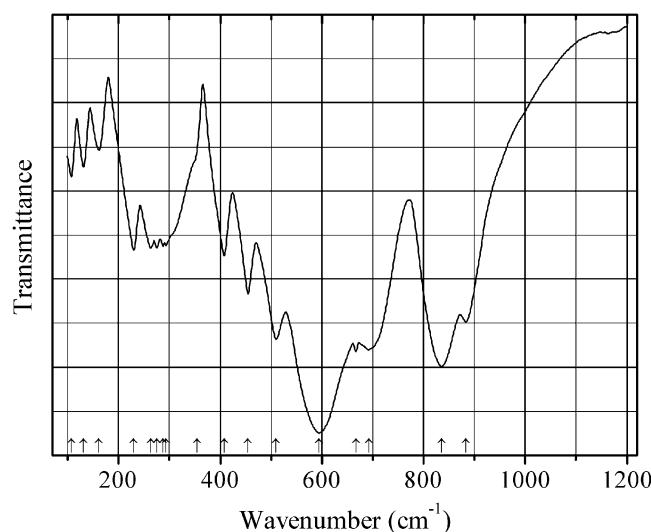
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission.

**Source:** Bode et al. (1973).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 820, 725s, 650sh, 595w, 550s, 520sh, 450sh, 415, 345s, 290, 265, 245, 225.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 820, 800s, 720, 605w, 525w, 460w, 420w, 335, 420w, 310s, 285s, 265, 225, 210.

**W21 Cadmium tungstate  $\text{CdWO}_4$** 

**Origin:** Synthetic.

**Description:** Prepared hydrothermally from corresponding oxides at 473 K for 48 h. Characterized by powder X-ray diffraction data and Rietveld crystal structure refinement. Isostructural with wolframite. Monoclinic, space group  $P2/c$ ,  $a = 5.026(1)$ ,  $b = 5.078(1)$ ,  $c = 5.867(1)$  Å,  $\beta = 91.47(1)^\circ$ ,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr and polyethylene discs. Transmission.

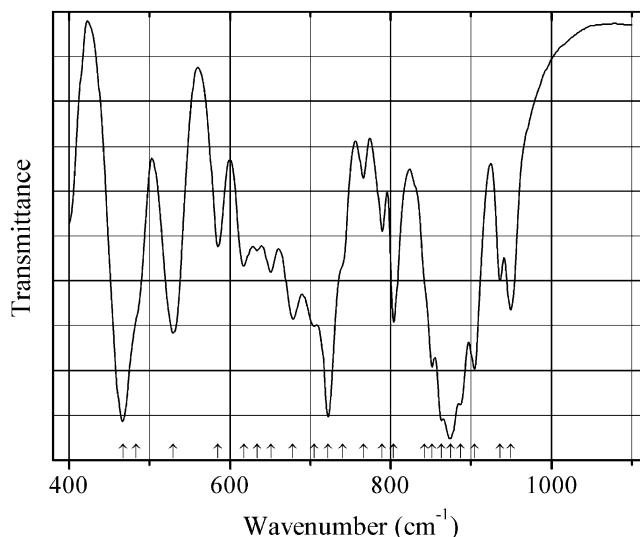
**Source:** Daturi et al. (1997).

**Wavenumbers (IR, cm<sup>-1</sup>):** 884, 835s, 693, 667, 595s, 510, 455, 408, 354sh, 294, 287, 276, 263, 230, 161w, 131w, 107w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 896s, 771, 706, 687, 547, 514, 387, 351, 307s, 269, 248w, 229, 177, 148, 133, 117, 99, 77.

## W22 Cesium uranyl tungstate $\text{Cs}_4[(\text{UO}_2)_4(\text{WO}_5)(\text{W}_2\text{O}_8)\text{O}_2]$ $\text{Cs}_4[(\text{UO}_2)_4(\text{WO}_5)(\text{W}_2\text{O}_8)\text{O}_2]$



**Origin:** Synthetic.

**Description:** Obtained via the high-temperature solid-state method by reacting  $\text{UO}_2(\text{NO}_3)_2$  with  $\text{WO}_3$  and  $\text{CsNO}_3$  (at the molar ratio U:Cs:W = 1:2:3) at 1050 °C for 5 h. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 8.1990(4)$ ,  $b = 32.8343(10)$ ,  $c = 10.7529(6)$  Å,  $\beta = 117.594(4)^\circ$ ,  $V = 2565.5(2)$  Å<sup>3</sup>,  $Z = 4$ .  $D_{\text{calc}} = 6.243$  g/cm<sup>3</sup>.

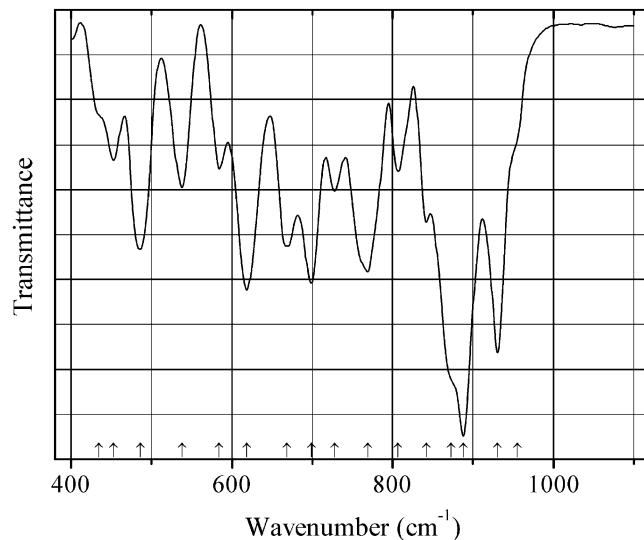
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Xiao et al. (2015).

**Wavenumbers (IR, cm<sup>-1</sup>):** 949, 936, 904, 887, 875s, 863s, 852, 842sh, 804, 789, 766w, 740sh, 722s, 705, 678, 651, 634, 618, 585, 530, 484sh, 467s.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 952, 934, 782s, 765s, 548.

**W23 Cesium uranyl tungstate  $\text{Cs}_4[(\text{UO}_2)_7(\text{WO}_5)_3\text{O}_3]$   $\text{Cs}_4[(\text{UO}_2)_7(\text{WO}_5)_3\text{O}_3]$** 


**Origin:** Synthetic.

**Description:** Obtained via the high-temperature solid-state method by reacting  $\text{UO}_2(\text{NO}_3)_2$  with  $\text{WO}_3$  and  $\text{CsNO}_3$  (at the molar ratio U:Cs:W = 4:4:3) at  $950^\circ\text{C}$  for 15 h. The crystal structure is solved. Monoclinic, space group  $P2_1/c$ ,  $a = 8.6864(4)$ ,  $b = 41.8958(15)$ ,  $c = 10.8213(7)$  Å,  $\beta = 116.467(4)^\circ$ ,  $V = 3525.4(3)$  Å<sup>3</sup>,  $Z = 1$ .  $D_{\text{calc}} = 6.173$  g/cm<sup>3</sup>.

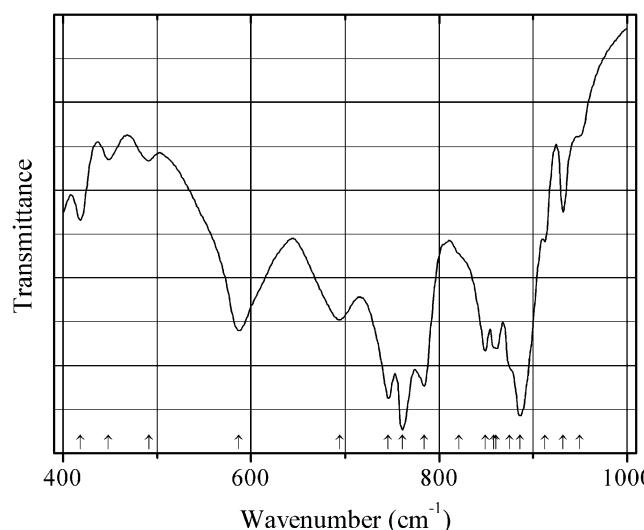
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Xiao et al. (2015).

**Wavenumbers (IR, cm<sup>-1</sup>):** 955sh, 930s, 888s, 873sh, 842, 807, 769, 728, 699, 669, 619, 584, 538, 486, 453, 435sh.

**Note:** The wavenumbers were determined by us based on spectral curve analysis of the published spectrum. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 935, 871, 828, 786s, 766s.

**W24 Cesium uranyl tungstate  $\text{Cs}_8(\text{UO}_2)_4(\text{WO}_4)_4(\text{WO}_5)_2$   $\text{Cs}_8(\text{UO}_2)_4(\text{WO}_4)_4(\text{WO}_5)_2$** 


**Origin:** Synthetic.

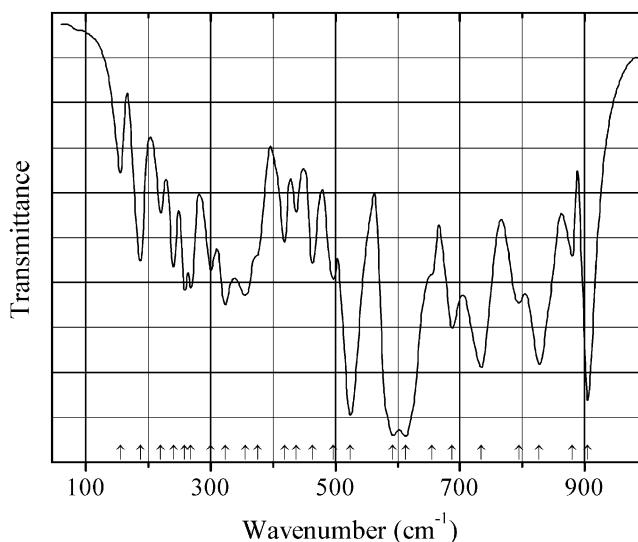
**Description:** Synthesized from a mixture of  $\text{CsNO}_3$ ,  $\text{WO}_3$ , and  $\text{U}_3\text{O}_8$  taken in the ratio  $\text{Cs:U:W} = 4:2:3$  by solid-state reaction in air at  $650^\circ\text{C}$  for 1 week with intermediate grindings. Characterized by powder X-ray diffraction data. The crystal structure is solved. Monoclinic, space group  $P2_1/n$ ,  $a = 11.2460(3)$ ,  $b = 13.8113(3)$ ,  $c = 25.7287(6)$  Å,  $\beta = 90.00^\circ$ ,  $V = 3996.23(17)$  Å $^3$ ,  $Z = 4$ .  $D_{\text{meas}} = 6.079(2)$  g/cm $^3$ ,  $D_{\text{calc}} = 6.087(2)$  g/cm $^3$ . In the structure, the U atoms are in pentagonal bipyramidal coordination, while W atoms are in two different environments, with tetrahedral and square pyramidal coordinations.

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Yagoubi et al. (2007).

**Wavenumbers (cm $^{-1}$ ):** 950w, 932, 913sh, 886s, 875sh, 861, 858, 849, 821sh, 784s, 761s, 746s, 694, 587, 491w, 448w, 418.

### W25 Lithium iron(III) tungstate wolframite-type $\text{LiFe}(\text{WO}_4)_2$



**Origin:** Synthetic.

**Description:** Synthesized from lithium carbonate, iron, and tungsten oxides using a ceramic technique.

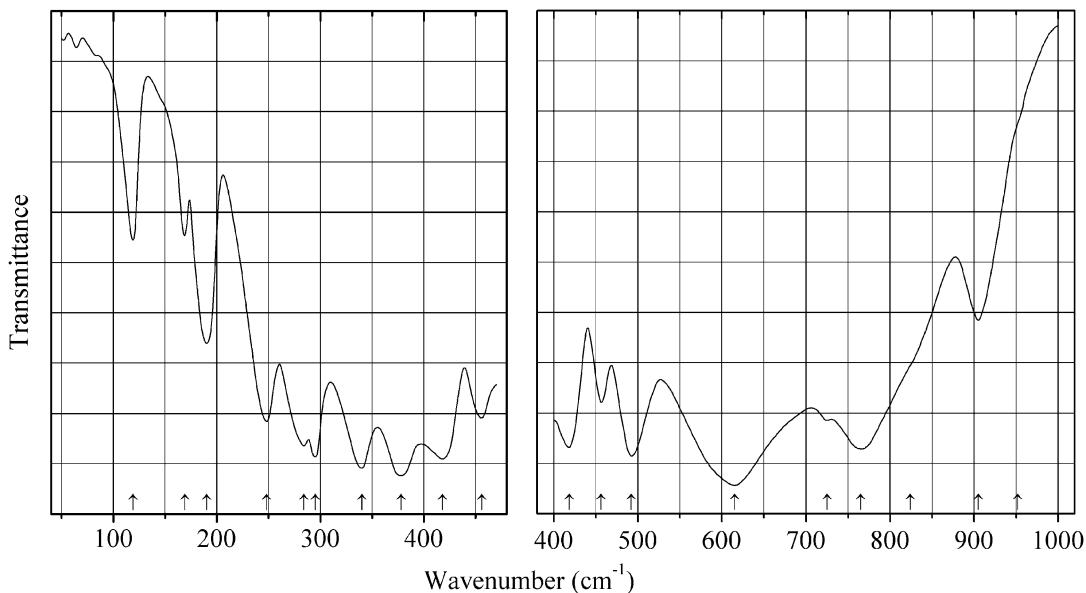
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc and Nujol mull. Transmission.

**Source:** Fomichev and Kondratov (1994).

**Wavenumbers (IR, cm $^{-1}$ ):** 905s, 880, 827, 795, 734, 687, 655, 613s, 592s, 524s, 497, 463, 437, 418, 375sh, 355, 323, 300, 268, 258, 240, 220, 187, 155.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm $^{-1}$ ):** 920s, 875, 786s, 772, 710, 655, 617, 539, 497, 463, 416, 381, 354, 321, 290, 268, 239, 211, 150, 103, 87.

**W26 Lithium copper tungstate  $\text{Li}_2\text{Cu}(\text{WO}_4)_2$** 

**Origin:** Synthetic.

**Description:** Prepared by solid-state reaction from the stoichiometric mixture of  $\text{Li}_2\text{CO}_3$ ,  $\text{WO}_3$ , and  $\text{CuO}$  at 650–700 °C for 146–160 h. Triclinic, space group  $P-1$ ,  $Z = 1$ .

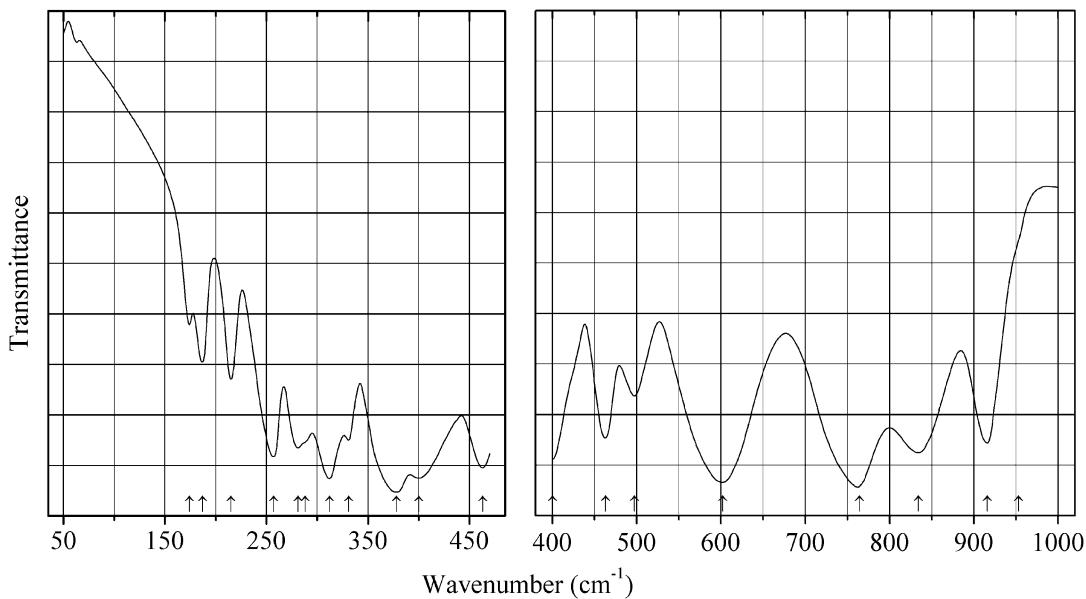
**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull. Absorption.

**Source:** Mączka et al. (2002).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 952sh, 905, 824sh, 765, 615s, 492s, 456, 418, 378s, 340, 295, 284, 248, 190, 169w, 119.

**Note:** A weak band near 720  $\text{cm}^{-1}$  may correspond to Nujol. In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 902s, 769, 726, 636, 553, 470, 398, 363, 307, 256, 211, 174, 127, 112.

**W27 Lithium nickel tungstate  $\text{Li}_2\text{Ni}(\text{WO}_4)_2$** 

**Origin:** Synthetic.

**Description:** Prepared by solid-state reaction from the stoichiometric mixture of  $\text{Li}_2\text{CO}_3$ ,  $\text{WO}_3$ , and  $\text{CuO}$  at 650–700 °C for 146–160 h. Triclinic, space group  $P-1$ ,  $Z = 1$ . Structurally related to wolframite.

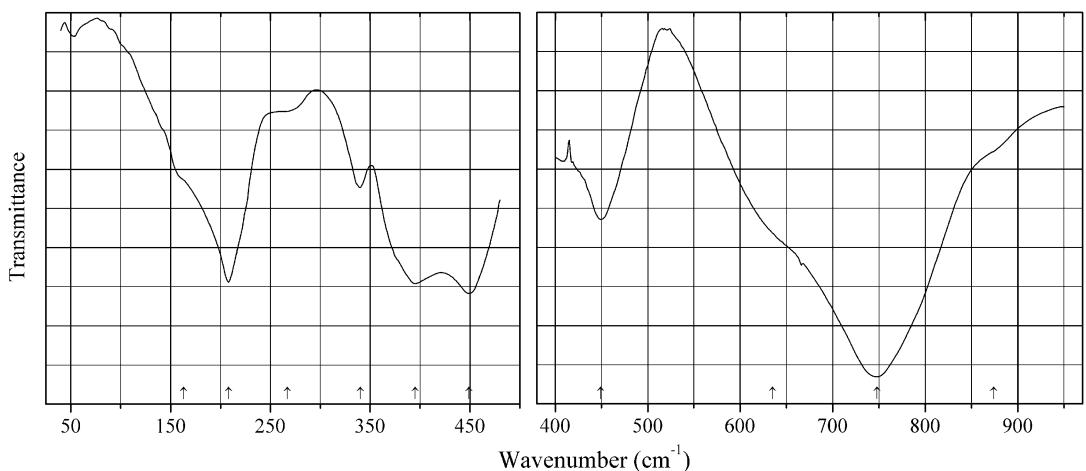
**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull. Absorption.

**Source:** Mączka et al. (2002).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 953sh, 916, 834s, 764s, 602s, 497, 463, 400, 378s, 331, 312, 288sh, 281, 257, 215, 187w, 174w.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 913s, 792, 754, 617w, 553w, 476w, 447w, 418, 387, 353, 311, 282, 266, 222w, 194, 143, 112.

**W28 Potassium antimonate tungstate  $\text{KSbWO}_6$** 

**Origin:** Synthetic.

**Description:** Prepared by the solid-state reaction between  $\text{WO}_3$ ,  $\text{Sb}_2\text{O}_3$ , and  $\text{KNO}_3$  at 973 K. The crystal structure solved by the Rietveld method is related to that of pyrochlore. Cubic, space group  $Fd\bar{3}m$ ,  $a = 10.23671(7)$ ,  $V = 1072.71(1) \text{ \AA}^3$ .  $D_{\text{calc}} = 5.4886 \text{ g/cm}^3$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc and Nujol mull. Absorption.

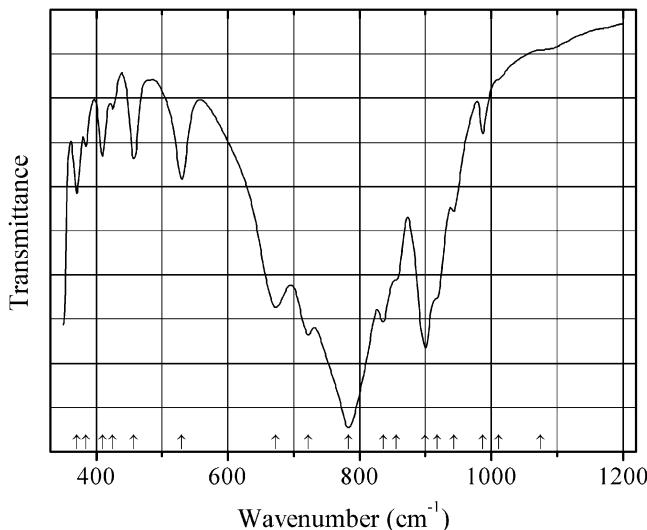
**Source:** Knyazev et al. (2010).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 874sh, 748s, 635sh, 449, 395, 340w, 267sh, 208w, 163sh.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 960, 909, 864, 721s, 654, 506s, 453, 382, 343, 239, 169s.

### W29 Potassium arsenate tungstate $\text{K}(\text{AsW}_2\text{O}_9)$ $\text{K}(\text{AsW}_2\text{O}_9)$



**Origin:** Synthetic.

**Description:** Prepared by the solid-state reaction from  $\text{KNO}_3$ ,  $\text{WO}_3$ , and  $(\text{NH}_4)(\text{H}_2\text{AsO}_4)$  in the molar ratio of 1:2:1, first at 773 K for 24 h, and thereafter (after regrinding) at 1033 K for 24 h. Characterized by powder X-ray diffraction data and EDX analysis. The crystal structure is solved. Orthorhombic, space group  $P2_12_12_1$ ,  $a = 4.9747(3)$ ,  $b = 9.1780(8)$ ,  $c = 16.6817(19) \text{ \AA}$ ,  $V = 761.65(12) \text{ \AA}^3$ ,  $Z = 4$ .  $D_{\text{calc}} = 5.457 \text{ g/cm}^3$ . The structure is based on a 3D framework consisting of corner-sharing  $\text{WO}_6$  octahedra and  $\text{AsO}_4$  tetrahedra.

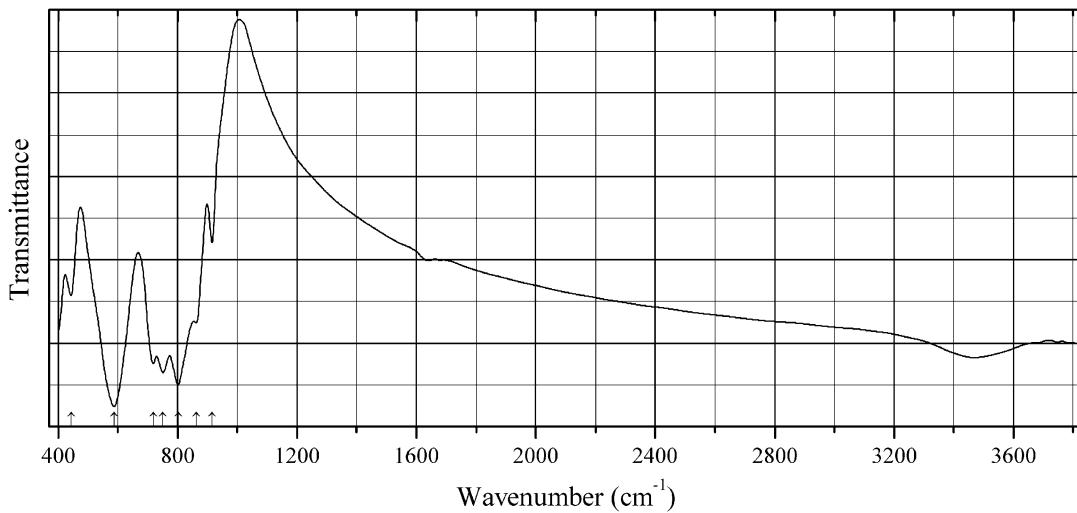
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Absorption.

**Source:** Alekseev et al. (2013).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 1075sh, 1011sh, 987w, 943, 918sh, 900s, 856sh, 836s, 783s, 722s, 672s, 530, 457, 425w, 409, 384w, 370.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The wavenumber  $722 \text{ cm}^{-1}$  is erroneously indicated by Alekseev et al. (2013) as  $772 \text{ cm}^{-1}$ . In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 972s, 893, 805, 710, 654, 273, 246s, 215, 186w, 145s, 134w, 115s, 102w, 83, 69s, 51s, 35s.

**W30 Potassium bismuth(III) tungstate  $\text{KBi}(\text{WO}_4)_2$** 

**Origin:** Synthetic.

**Description:** Crystals grown from the solution in  $\text{K}_2\text{W}_2\text{O}_7$  melt. Monoclinic.  $D_{\text{meas}} = 7.57 \text{ g/cm}^3$ ,  $D_{\text{calc}} = 7.51 \text{ g/cm}^3$ .

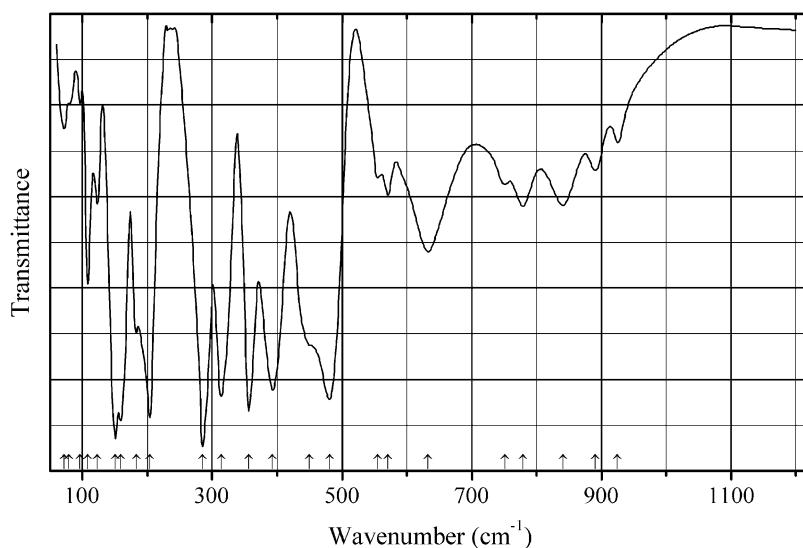
**Kind of sample preparation and/or method of registration of the spectrum:** Transmission. Kind of sample preparation is not indicated.

**Source:** Xie et al. (2007).

**Wavenumbers (IR,  $\text{cm}^{-1}$ ):** 916, 864, 803s, 751s, 719s, 588s, (443), 410.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 922w, 868s, 774, 753s, 709, 693, 637, 517, 430, 395sh, 389w, 363, 330, 302w, 287, 251w, 230w, 218.

**W31 Potassium ytterbium tungstate  $\text{KYb}(\text{WO}_4)_2$** 

**Origin:** Synthetic.

**Description:** Crystal grown from the solution of  $\text{K}_2\text{CO}_3$ ,  $\text{WO}_3$ , and  $\text{Yb}_2\text{O}_3$  by the top-seeded solution growth method using  $\text{K}_2\text{W}_2\text{O}_7$  as the solvent. Characterized by powder X-ray diffraction data. Monoclinic, space group  $C2/c$ ,  $a = 10.590(4)$ ,  $b = 10.290(6)$ ,  $c = 7.478(2)$  Å,  $\beta = 130.70(2)^\circ$ ,  $V = 617.8(5)$  Å<sup>3</sup>,  $Z = 4$ .

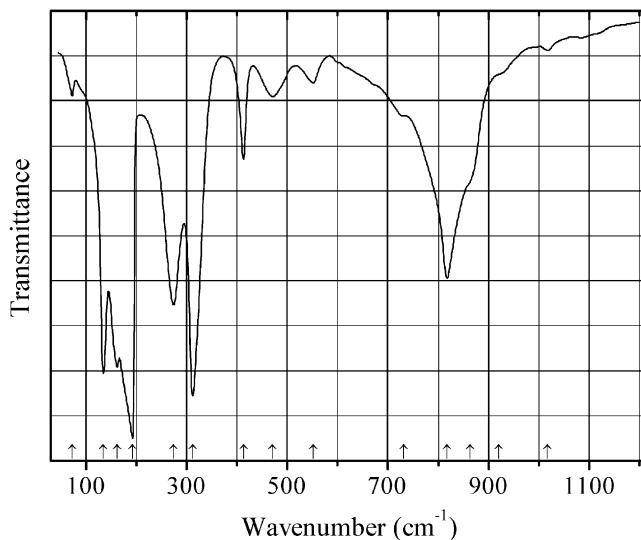
**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission. Conditions of far IR spectrum registration are not characterized.

**Source:** Zhao et al. (2008a).

**Wavenumbers (cm<sup>-1</sup>):** 925, 891, 841, 779, 751, 633, 571, 555, 481s, 450sh, 393s, 356s, 314s, 285s, 204s, 183, 159s, 151s, 123, 108, 96w, 79sh, 72.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, figures of Raman spectra with different scattering configurations are given.

### W32 Strontium tungstate $\text{SrWO}_4$



**Origin:** Synthetic.

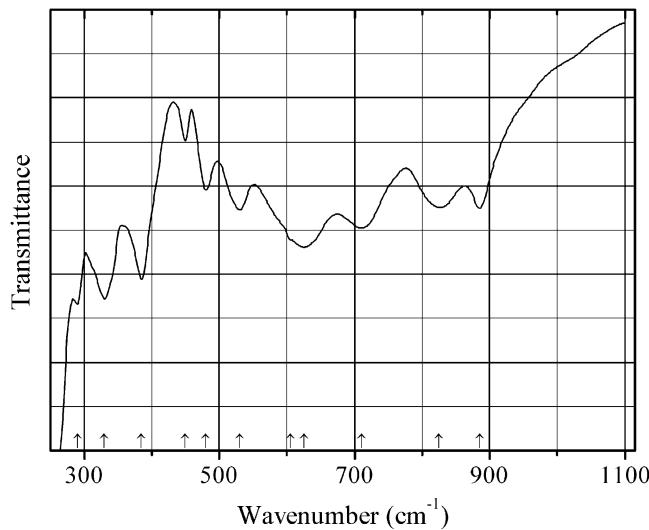
**Description:** Single crystal grown by the Czochralski method. Tetragonal, space group  $I4_1/a$ ,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** Absorption. Kind of sample preparation is not indicated.

**Source:** Ling et al. (2006).

**Wavenumbers (IR, cm<sup>-1</sup>):** 1017w, 921sh, 863sh, 818, 732sh, 552w, 471w, 413, 312s, 274s, 193s, 162s, 135s, 73w.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. In the cited paper, figures of polarized Raman spectra are given.

**W33 Huanzalaite  $MgWO_4$** 

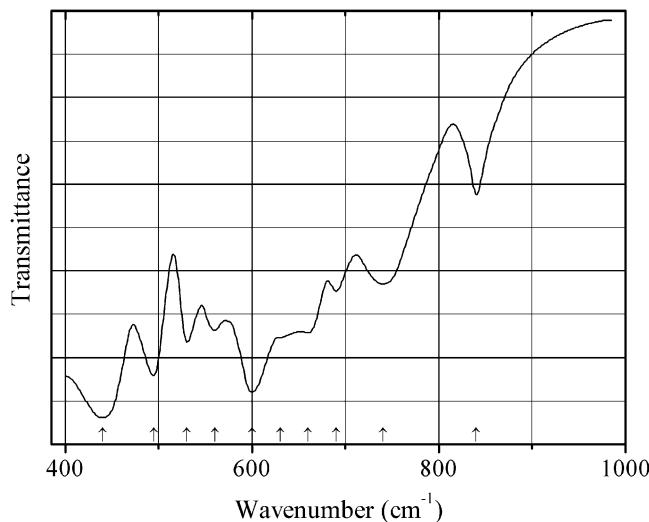
**Origin:** Synthetic.

**Description:** Prepared hydrothermally from sodium tungstate and magnesium nitrate at a temperature above 250 °C for 4 days. Characterized by powder X-ray diffraction data. Monoclinic, space group  $P2/c$ ,  $a = 4.687$ ,  $b = 5.675$ ,  $c = 4.928$  Å,  $\beta = 90.71^\circ$ ,  $Z = 2$ .

**Kind of sample preparation and/or method of registration of the spectrum:** KBr disc. Transmission.

**Source:** Günter and Amberg (1989).

**Wavenumbers (cm⁻¹):** 885, 825, 710, 625s, 605sh, 530, 480, 450w, 385s, 330s, 290.

**W34 Yttrium tungstate  $Y_2WO_6$** 

**Origin:** Synthetic.

**Description:** Characterized by powder X-ray diffraction data. Orthorhombic, space group *B2cb*.

**Kind of sample preparation and/or method of registration of the spectrum:** Transmission.

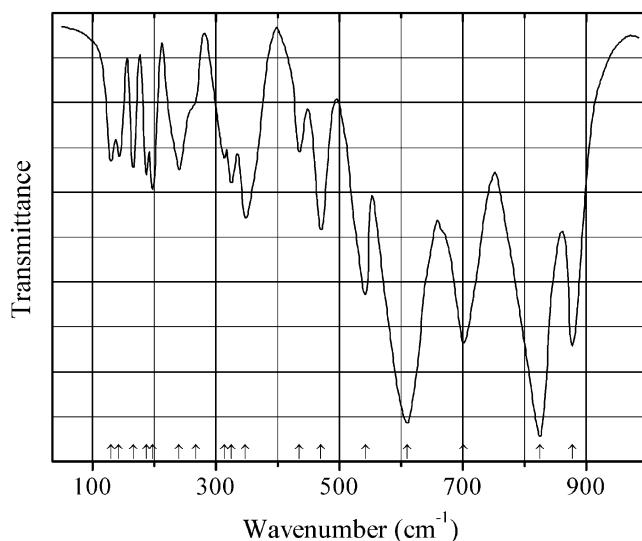
**Source:** Bode et al. (1973).

**Wavenumbers (IR, cm<sup>-1</sup>):** 840w, 740, 690, 660, 630, 600s, 560, 530, 495, 440s, 390, 350, 335, 310, 290, 270, 255, 240, 230, 215.

**Note:** In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman,  $\text{cm}^{-1}$ ):** 935, 835, 710, 695, 675, 625, 600, 555, 525, 505, 450, 430, 400, 370, 345, 315, 290, 275, 260, 240, 225, 200, 185, 145.

## W35 Sanmartinite ZnWO<sub>4</sub>



**Origin:** Synthetic.

**Description:** Synthesized using the ceramic technique. Characterized by powder X-ray diffraction data.

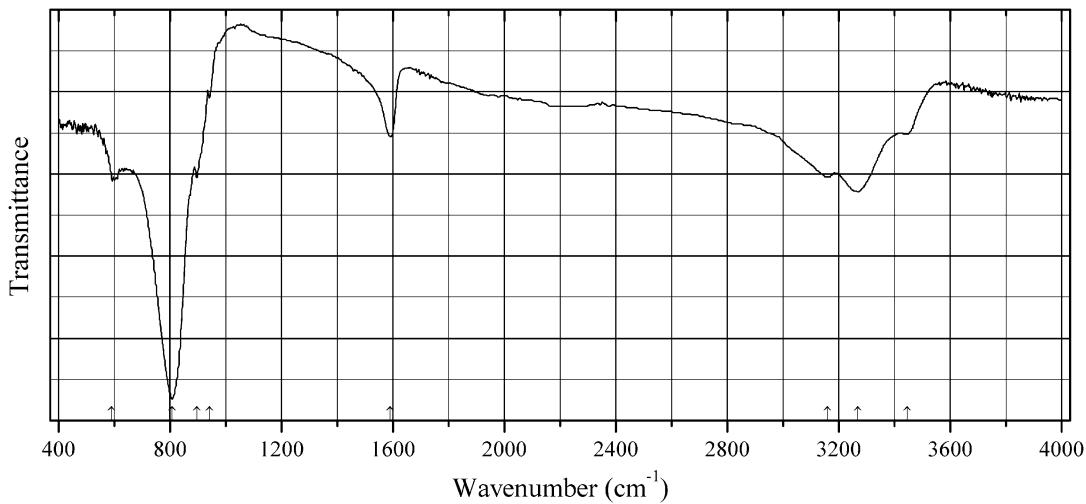
**Kind of sample preparation and/or method of registration of the spectrum:** Nujol mull (?).  
Transmission.

**Source:** Fomichev and Kondratov (1994).

**Wavenumbers (IR, cm<sup>-1</sup>)**: 877s, 825s, 701s, 610s, 542, 470, 435, 348, 325, 314, 267sh, 240, 197, 187, 166, 143, 130.

Note: In the cited paper, Raman spectrum is given.

**Wavenumbers (Raman, cm<sup>-1</sup>):** 910s, 788, 710, 676, 548, 518, 411, 356, 345, 316, 276, 199, 168, 150, 127, 94s, 59

**Re1 Uranyl perrhenate hydrate**  $(\text{UO}_2)_2(\text{ReO}_4)_4 \cdot 3\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Description:** Crystals obtained by evaporation of a solution of equimolar amounts of  $\text{UO}_3$  and  $\text{Re}_2\text{O}_7$ .

Characterized by qualitative energy dispersive analysis. The crystal structure is solved. Triclinic, space group  $P-1$ ,  $a = 5.2771(7)$ ,  $b = 13.100(2)$ ,  $c = 15.476(2)$  Å,  $\alpha = 107.180(2)^\circ$ ,  $\beta = 99.131(3)^\circ$ ,  $\gamma = 94.114(2)^\circ$ ,  $V = 1001.12$  Å<sup>3</sup>,  $Z = 2$ .  $D_{\text{calc}} = 5.291$  g/cm<sup>3</sup>. The structure contains complex chains of uranyl pentagonal bipyramids bridging perrhenate groups via common vertices.

**Kind of sample preparation and/or method of registration of the spectrum:** Attenuated total reflection of a powdered sample.

**Source:** Karimova and Burns (2007).

**Wavenumbers (cm<sup>-1</sup>):** 3446w, 3267, 3159, 1590, 941w, 897, 807s, 590.

**Note:** The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum.



# Some Aspects of the Use of Raman Spectroscopy in Mineralogical Studies

3

## 3.1 General Principles of Raman Spectroscopy

Raman scattering is the process of inelastic light scattering that occurs on fluctuations in the polarizability of molecules which are excited to higher vibrational or rotational energy levels. This phenomenon was discovered in 1928 by C.V. Raman and K.S. Krishnan (for liquids) and L.I. Mandelshtam and G.S. Landsberg (for crystals).

In Raman scattering, a monochromatic line of exciting laser radiation after interaction with a substance is accompanied by an additional set of spectral components. The newly appeared lines are located on the scale of electromagnetic waves symmetrically with respect to the line of exciting radiation and are separated from it by the frequencies of atomic vibrations. The totality of newly emerging spectral components is the Raman spectrum of a substance, which is its diagnostic feature. The phenomenon of Raman scattering is characteristic of substances that are in a gaseous, liquid, or solid state consisting of molecules or molecular complexes with an internal structure, or atoms combined into crystalline structures. Monatomic gas particles that do not interact with each other (for example, inert gases) do not have Raman spectra.

The source of secondary radiation (Raman scattering) is a variable in time electric dipole moment that occurs in the medium as a result of the interaction of particles of a substance with the electric component of external electromagnetic radiation of the visible or close to visible range. The magnitude of the dipole moment depends on the magnitude of the external field and on the polarizability of the substance:

$$\mathbf{p} = \hat{\alpha} \mathbf{E}$$

where  $\mathbf{p}$  is the induced electric dipole moment vector,  $\mathbf{E}$  is the vector of external electric field strength, and  $\hat{\alpha}$  is the polarizability.

The polarizability of the substance depends on the structure of the molecules or crystals forming it, on the types of bonds in the substance, as well as on the nature of the motions of the atoms in the molecules or in the crystals. Polarizability is a variable in time characteristic of the substance, which is modulated by the movements of the particles of the substance itself and the electrical component of the external electromagnetic field, causing the appearance of a variable electric dipole moment in the substance. In accordance with the basic rule of electrodynamics, a system with a variable electric dipole moment in time can

be a source of electromagnetic radiation with a frequency of change in the dipole moment.

In experiments on Raman scattering using monochromatic radiation with a frequency of  $\Omega$ , spectral components with frequencies  $\Omega$ ,  $(\Omega + \omega_i)$  and  $(\Omega - \omega_i)$  are recorded in the spectrum of scattered radiation, where  $\omega_i$  are the frequencies of vibrational and rotational motions of particles of a substance. The spectral region in which the components are located with frequencies greater than the frequency of laser radiation  $(\Omega + \omega_i)$  is commonly called the anti-Stokes region, and the region with lower frequencies  $(\Omega - \omega_i)$  is called the Stokes region.

Under normal conditions, the intensity of the strongest lines in the Stokes region of the Raman spectra is usually  $10^{-6}$ – $10^{-8}$  of the intensity of the exciting line (Reshetnyak and Bukanov 1991). The intensity of the anti-Stokes component is even less by several decimal exponents of magnitude and decreases rapidly with increasing magnitude of the detuning from the laser line. For this reason, the bulk of the experiments are carried out in the Stokes spectral region. As a source of spectral information, mainly vibrational spectra are used.

Polarizability is anisotropic and is described by a second rank tensor, which can be written as a symmetric matrix:

$$\hat{a} = \begin{vmatrix} a_{xx} & a_{xy} & a_{xz} \\ a_{yx} & a_{yy} & a_{yz} \\ a_{zx} & a_{zy} & a_{zz} \end{vmatrix}$$

The component of the polarizability tensor  $a_{ij}$  determines the magnitude of the dipole moment arising in the medium along the  $i$  axis under the action of an electromagnetic field with the direction of the polarization vector of the electric field along the  $j$  axis. This means that for different orientations of the polarization vector of the laser radiation and the polarization vector of the detected scattered radiation in the Raman spectrum, scattering will be recorded on different components of the polarizability tensor. In a general case, Raman scattering occurs at different vibrations, and the recorded scattering lines in the Raman spectra have different frequencies

and intensities. The intensity of the scattering line in the case of nonpolar normal vibrations is determined by the following formula:

$$I \sim \left[ \sum f_i \alpha_{ij} e_j \right]^2, \\ i, j = x, y, z$$

where  $f_i$  and  $e_j$  are components of the unit vectors of the dipole moment polarization and laser radiation, respectively, and  $\alpha_{ij}$  is the change of the polarizability tensor component at a given kind of normal vibrations. Not all types of vibrations can be detected as lines in the Raman spectra. For molecules and crystals with an inversion center, there is an alternative prohibition rule which is very important for experimental practice. According to this rule, for compounds with an inversion center, bands of antisymmetric (with respect to the inversion center) vibrations are forbidden in the Raman spectra, and symmetrical ones are forbidden in the IR spectra. The alternative prohibition rule relates simultaneously to Raman spectroscopy and IR absorption spectroscopy and indicates the complementary nature of these methods of molecular spectroscopy.

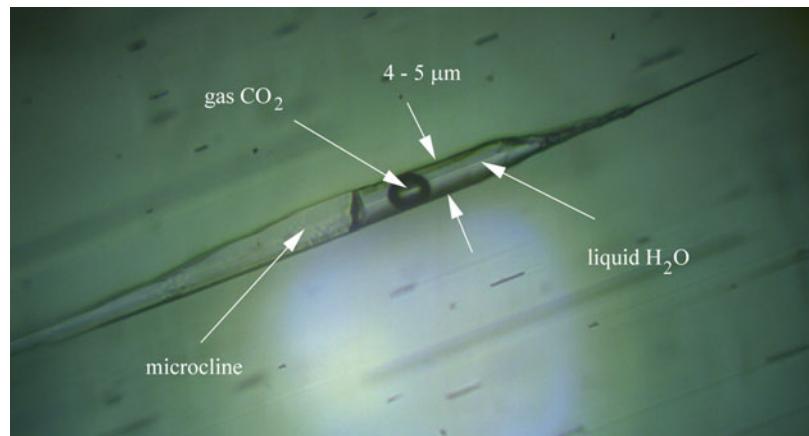
The theory of Raman spectroscopy is described in more detail in numerous publications (Brandmüller and Moser 1962; Anderson 1973; Sushchinsky 1981; Banwell 1983; Zhizhin et al. 1984; Nakamoto 2009).

## 3.2 Specific Features and Possibilities of Raman Spectroscopy: Practical Recommendations

### 3.2.1 Advantages and Disadvantages of the Method

The most important properties of Raman spectroscopy are that this method is nondestructive and local. The ability of laser radiation to penetrate inside transparent minerals makes Raman spectroscopy indispensable for diagnosing mineral phases in inclusions (see, e.g., Figs. 3.1 and 3.2). In this case, the minimum dimensions of the

**Fig. 3.1** A three-phase inclusion in aquamarine. The transverse size of the inclusion is about 4–5  $\mu\text{m}$



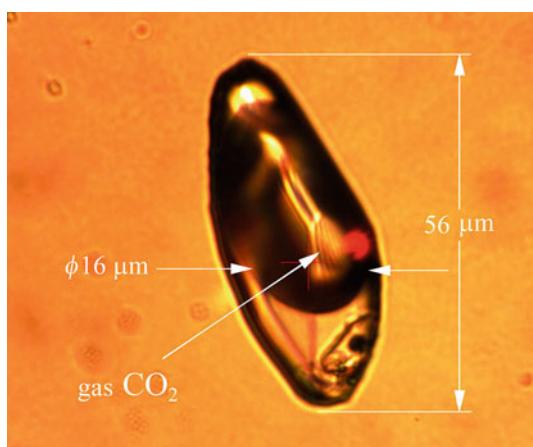
investigated phases are limited by the diameter of the focal spot of laser radiation. When using high-quality optical elements, laser radiation can be focused into a spot with a diameter of up to several microns. In this case, phase diagnostics can be carried out *in situ*, without damage the inclusions and disbalance the phase equilibrium. The highest quality Raman spectra are obtained for solid-state phases because of their high density (Fig. 3.3).

Figure 3.2 illustrates both the large diagnostic capabilities of Raman spectroscopy and the difficulties encountered in the study of inclusions. Laser radiation, before it reaches an inclusion, goes some distance in the host mineral causing Raman scattering in the latter. As a result, the resulting spectrum contains the scattering lines

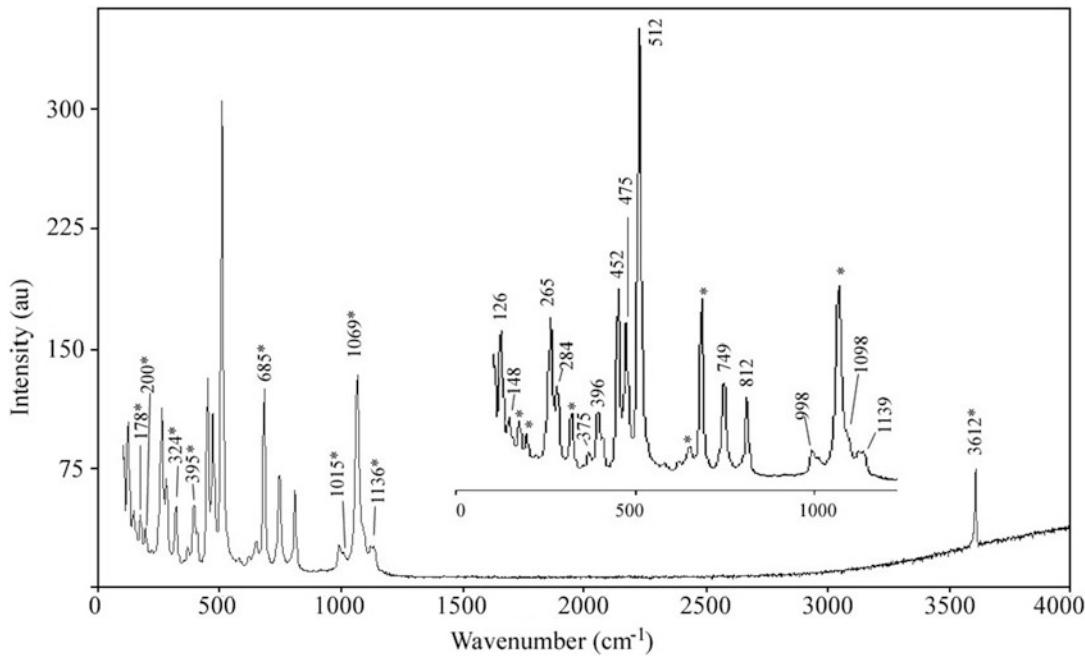
of both the studied inclusion and the host mineral. In the cases when the host mineral spectrum is rich in its own scattering lines, the diagnosis of the substances of microscopic inclusions can be significantly complicated. It should be taken into account that in the spectra of microscopic inclusions usually only most intense scattering lines can be observed, which may have low intensities against the background of the more powerful spectrum of the host mineral. Obtaining spectra of inclusions located as close as possible to the surface of the host mineral reduces the laser beam path through the latter. The depth at which diagnostics of inclusions is possible is limited by the focal length of the lens used.

In some cases, in multiphase inclusions, it is possible to diagnose not only solid, but also liquid (Fig. 3.4) and gaseous (Figs. 3.5 and 3.6) phases.

In the region of stretching vibrations of water, a strong and narrow scattering line with a frequency of  $3610 \text{ cm}^{-1}$  is recorded, which refers to H<sub>2</sub>O molecules located in the channels of the aquamarine structure. Due to the small diameter of the channels (about 0.5 nm), water molecules exist in a constrained state with hydrogen atoms attached to the channel walls and do not form strong hydrogen bonds. This is reflected in the small half-width of the scattering line of about  $4 \text{ cm}^{-1}$ . The broad band at  $3420 \text{ cm}^{-1}$  with a shoulder at  $3250 \text{ cm}^{-1}$  corresponds to O–H-stretching vibrations of water molecules forming rather strong hydrogen bonds and belonging to the liquid phase of the inclusion.

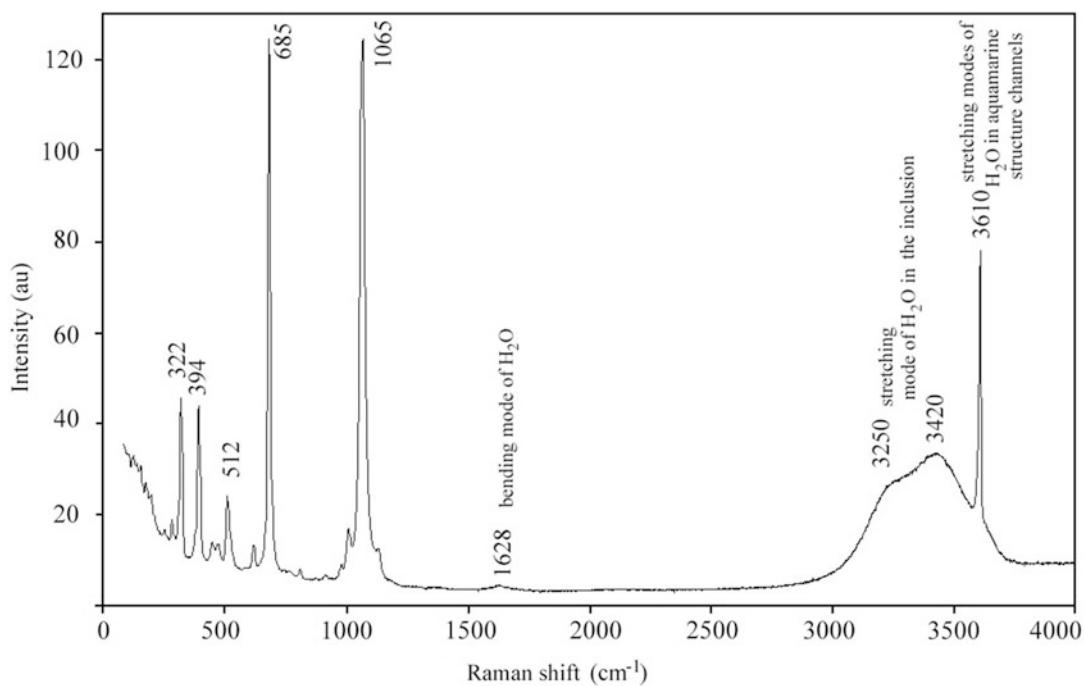


**Fig. 3.2** A multiphase inclusion in topaz



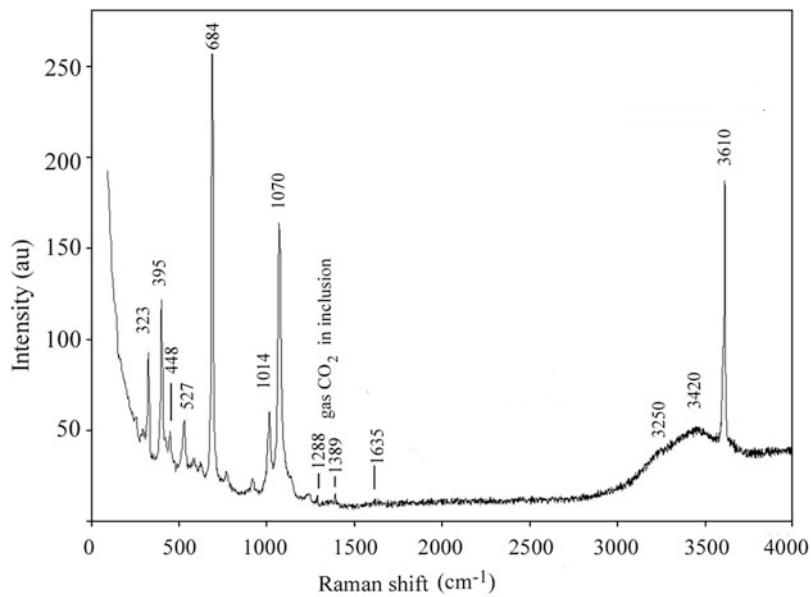
**Fig. 3.3** Raman spectrum of a microscopic inclusion of microcline in aquamarine. Bands marked with an asterisk belong to the aquamarine matrix. The laser emission

wavelength is 532 nm, the spectral resolution is about  $6 \text{ cm}^{-1}$ , and the laser power is 30 mW

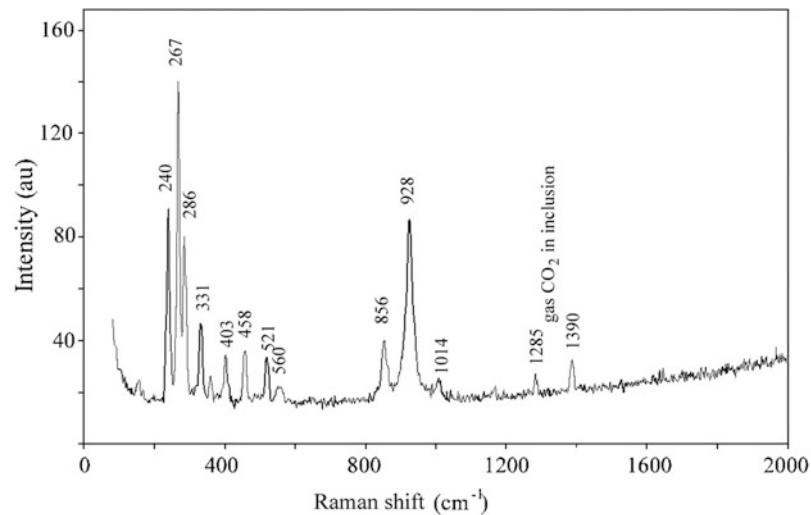


**Fig. 3.4** Raman spectrum of the liquid phase of the inclusion in aquamarine

**Fig. 3.5** Raman spectrum showing weak bands of gaseous CO<sub>2</sub> (gas bubble in the liquid) in the inclusion in aquamarine. All strong narrow bands correspond to aquamarine matrix



**Fig. 3.6** Raman spectrum showing bands of gaseous CO<sub>2</sub> in a multiphase inclusion in topaz (see Fig. 3.2)

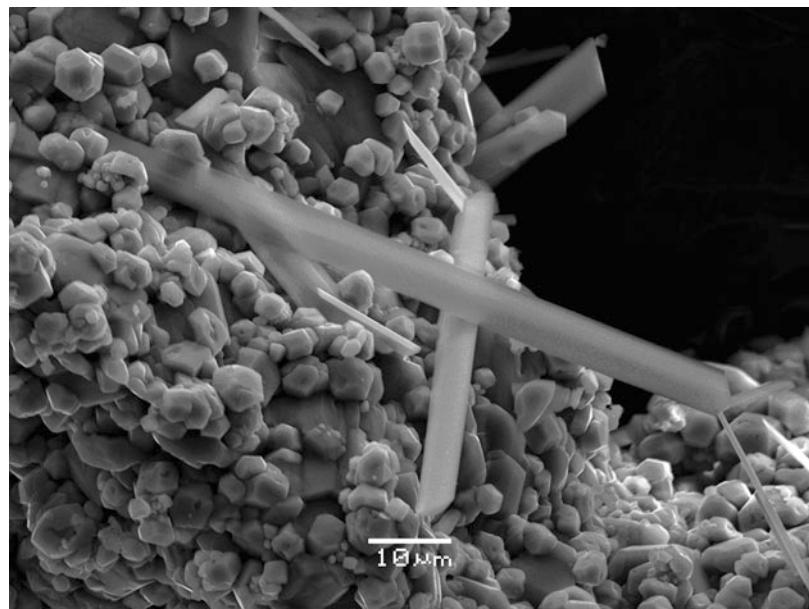


To obtain the maximum possible intensity of the Raman signal, the focal volume of the laser beam must be immersed in the substance of the host mineral and pointed at the object under investigation. In this case, a defocused luminous spot forms on the surface of the host mineral at the entry point of the laser beam, which can cover the working field. In such a situation, it is not possible to determine not only the diameter of the focal spot on the phase being diagnosed, but it is also

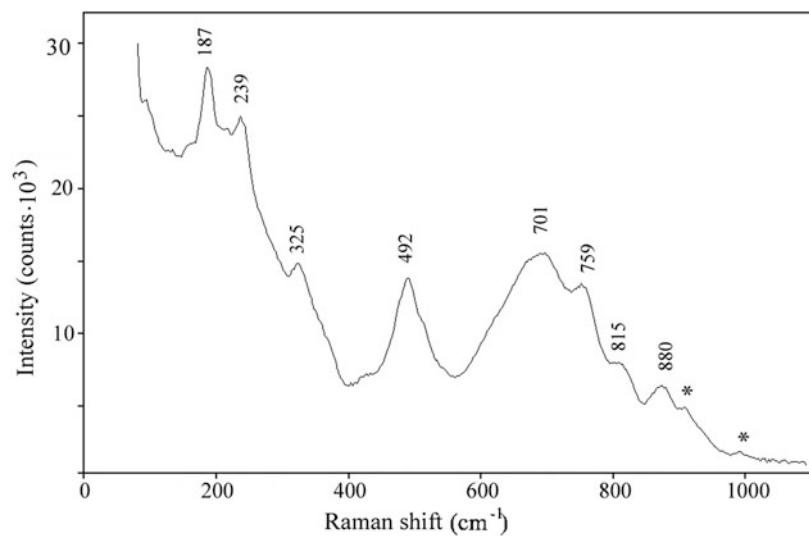
generally difficult to understand whether the laser beam is focused on the inclusion. In this case, one can judge the success of the experiment only from the results of a comparison of the Raman spectra obtained in the pure region of the host mineral and the spectra obtained from inclusions. Reliable confirmation of the result in this situation is the reproducibility of spectral data.

Another difficulty in working with inclusions is a significant loss of laser power when passing

**Fig. 3.7** Sword-like microcrystals of the rare mineral katiarsite  $\text{KTiO}(\text{AsO}_4)$  on arsmirandite crystal crust. SEM image (in secondary electrons)



**Fig. 3.8** Raman spectrum of catiarsite. A weak band near  $1000 \text{ cm}^{-1}$  corresponds to an admixed sulfate. The laser emission wavelength is 532 nm, the spectral resolution is about  $6 \text{ cm}^{-1}$  and the laser power is 30 mW, and the focal spot diameter is  $3 \mu\text{m}$



through the boundary of the inclusion. Uneven boundary can cause strong scattering of the laser beam, reducing the effective exciting power. Moreover, the total internal reflection conditions for a laser beam can be realized on the surface of the inclusion capsule. In this case, the laser beam will not penetrate into the inclusion, and obtaining a Raman spectrum will not be possible.

The “nondestructiveness” and locality of the Raman spectroscopy method were the reason for its widespread use in the study of unique minerals represented by single finds or microscopic monomineral aggregates. If the studied mineral is represented by individual prismatic crystals or thin needles (Fig. 3.7), then to obtain the Raman spectrum (Fig. 3.8), the sample area was chosen

whose linear dimensions are larger than the diameter of the laser beam focal spot. Otherwise, there will be a loss of power of the exciting radiation and the Raman scattering signal.

The intensity of the scattered radiation depends on the number of scattering centers in the focal volume of the laser beam. Therefore, *ceteris paribus*, the best quality of the Raman spectrum will be obtained in the area of the sample where the mineral aggregate has the highest concentration of the substance. For example, with needle-like or finely prismatic microcrystal forms, the Raman spectrum should be recorded at the common base of needle growth. The interpretation of the Raman spectra obtained on the microaggregates of minerals and the identification of the scattering lines related to the mineral of interest require special attention and analysis. When working with microscopic aggregates of minerals, one should take into account the possible presence of mineral impurities, the removal of which is impossible due to the small size.

### 3.2.2 Spectral Band Assignment

Raman spectra primarily reflect the features of the anionic part of the mineral, as well as some polyatomic cations like  $\text{NH}_4^+$  or  $\text{UO}_2^{2-}$ . The

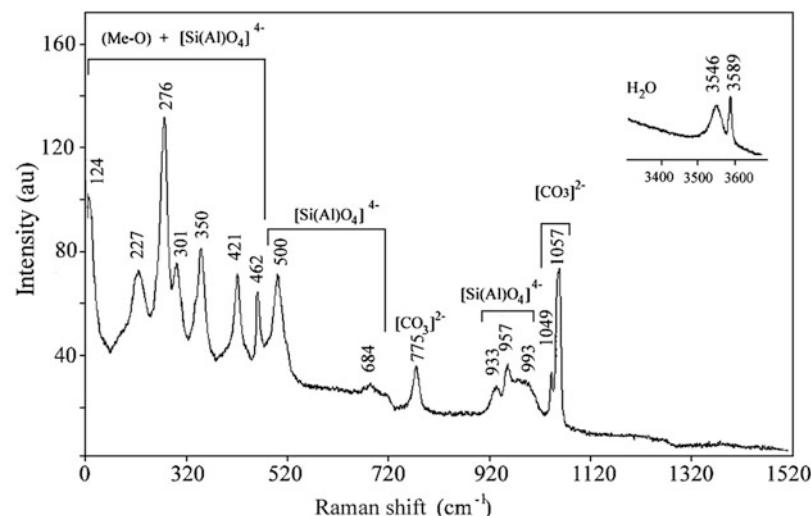
frequencies of symmetric stretching vibrations of some complex anions occurring in the structures of minerals change mainly in the following ranges ( $\text{cm}^{-1}$ ):

|                 |           |                |          |
|-----------------|-----------|----------------|----------|
| Nesosilicates   | 820–980   | Sulfates       | 970–1020 |
| Carbonates      | 1050–1100 | Arsenates      | 800–900  |
| Molybdates      | 780–880   | Tungstates     | 850–920  |
| Orthophosphates | 930–990   | Orthovanadates | 820–880  |

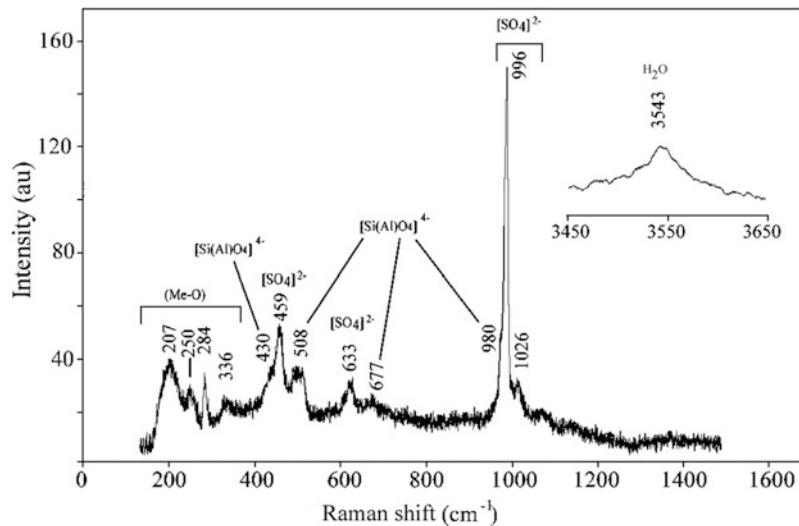
Raman shifts of the stretching vibration bands increase with increasing of polymerization of coordination polyhedra; e.g., for Al-poor framework silicates they are typically in the range 1040–1130  $\text{cm}^{-1}$ .

Thus, scattering lines observed in these ranges can be used for a preliminary assignment of a mineral to one or more class of compounds as a step preceding a more precise specification. When conducting diagnostic studies, it is necessary to take into account that the approximate proportion of the intensities of the Raman lines in the spectra of complex anions is as follows:  $\text{MoO}_4^{2-}$  ( $\approx \text{WO}_4^{2-}$ ):  $\text{SO}_4^{2-}$  :  $\text{PO}_4^{2-}$  :  $\text{CO}_3^{2-}$  :  $\text{SiO}_4^{4-}$  = 10 : 6 : 3 : 1.5 : 1 (for excitation radiation with a wavelength between 488 and 515 nm). This feature can be illustrated by the spectra of cancrinite  $\text{Na}_6\text{Ca}_2[\text{AlSiO}_4]_6(\text{CO}_3)_2 \cdot 2\text{H}_2\text{O}$  (Fig. 3.9) and vishnevite  $\text{Na}_8[\text{AlSiO}_4]_6(\text{SO}_4) \cdot 2\text{H}_2\text{O}$  (Fig. 3.10), structurally related tectosilicates with additional

**Fig. 3.9** Raman spectrum of cancrinite



**Fig. 3.10** Raman spectrum of vishnevite



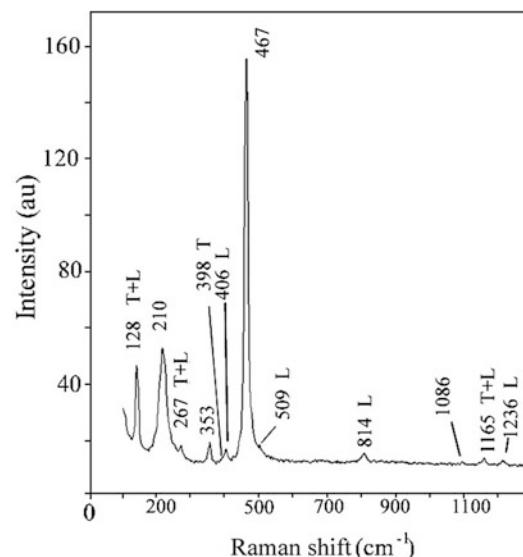
anions. The additional anions  $\text{CO}_3^{2-}$  and  $\text{SiO}_4^{4-}$  play subordinate role in the chemical composition of these minerals. However, the strongest lines in the Raman spectra are the scattering lines corresponding to the internal fully symmetric stretching vibrations of just additional anions. This feature may cause difficulty in determining chemical class of a mineral.

### 3.2.3 Effect of Structural Disorder on Raman Spectra of Minerals

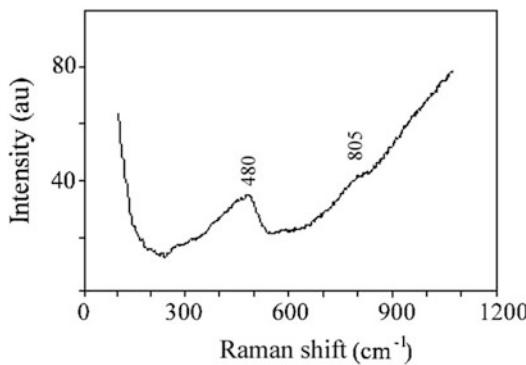
It should be noted that Raman spectroscopy is sensitive to the degree of crystallinity of the substance. This is reflected primarily in the half-widths of the scattering lines. Raman spectra of minerals with perfect crystal structures are distinguished by narrow well-resolved bands (Fig. 3.11). Disturbance or absence of long-range order in the structure of matter, cation disordering and local defects cause broadening and even the disappearance of some scattering lines. This effect is most pronounced in the Raman spectra of metamict minerals, minerals with a colloid-dispersed structure, and glasses (Fig. 3.12).

In the spectrum of quartz, narrow clearly defined scattering lines are recorded that belong to different types of vibrations: “rocking of

tetrahedra” ( $210 \text{ cm}^{-1}$ ), “twisting of tetrahedra” ( $353 \text{ cm}^{-1}$ ), O–Si–O bending ( $467 \text{ cm}^{-1}$ ), and Si–O stretching ( $1086 \text{ cm}^{-1}$ ) (Ranieri et al. 2009). The absence of a long-range order in obsidian, which is a  $\text{SiO}_2$ -rich glass, results in the absence of specific lines corresponding to any symmetry elements. The broad bands at



**Fig. 3.11** Raman spectrum of quartz powder. The laser emission wavelength is  $532 \text{ nm}$ , the spectral resolution is  $6 \text{ cm}^{-1}$ , and the laser power is  $30 \text{ mW}$ . The letters L and T denote components of longitudinal-transverse splitting (see below)



**Fig. 3.12** Raman spectrum of obsidian (volcanic glass). The laser emission wavelength is 532 nm, the spectral resolution is  $6 \text{ cm}^{-1}$ , and the laser power is 30 mW

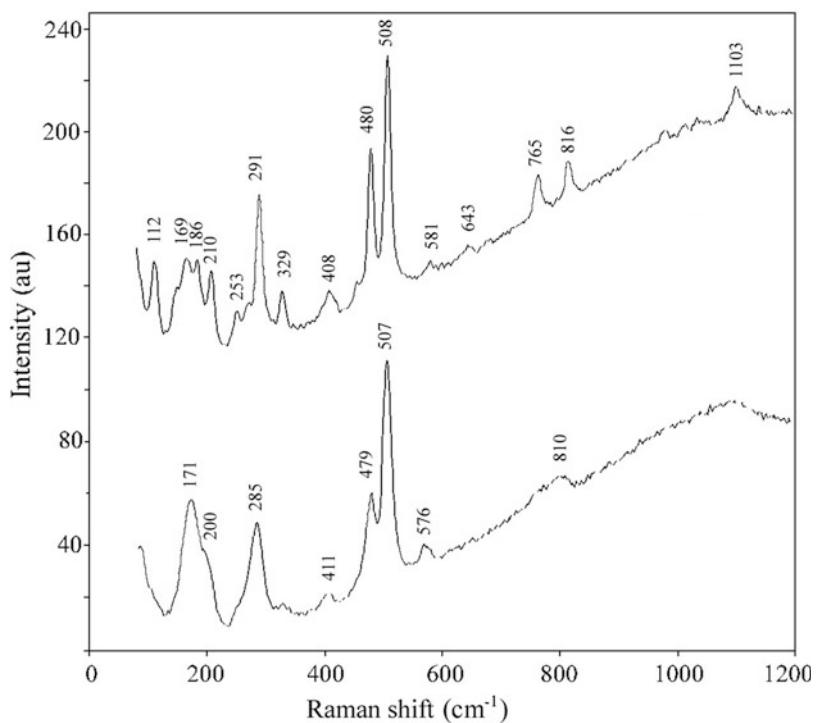
480 and  $805 \text{ cm}^{-1}$  correspond to the totality of vibrations in areas with different local structures.

The sensitivity of Raman scattering to the disordered distribution of atoms between crystallographic positions is clearly reflected in the spectra of feldspars. For example, in the structure of the disordered oligoclase ( $\text{Na,Ca}[\text{AlSi}_3\text{O}_8]$ ), Al atoms are statistically distributed between different

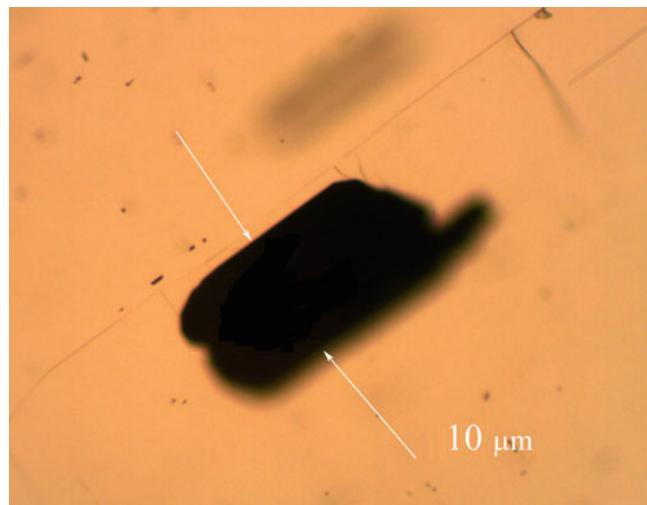
tetrahedral sites, whereas in an ordered variety they are concentrated mainly in only one of independent crystallographic positions. Raman spectra of the two oligoclase varieties differ markedly from each other: in the spectrum of an ordered oligoclase variety, a greater number of scattering lines (Fig. 3.13, upper curve) are recorded, which have a smaller half-width than in the spectrum of a disordered oligoclase (Fig. 3.13, lower curve).

In the study of black microscopic inclusions (Fig. 3.14) in aquamarine, it was found [based on the assignment by Sharma et al. (2001)] that they consist of crystalline graphite, which was diagnosed by the relatively narrow line at  $1574 \text{ cm}^{-1}$ , and X-ray amorphous carbon showing a broad band at  $1336 \text{ cm}^{-1}$  (Fig. 3.15). The Raman spectrum made it possible to suppose that the substance in the inclusion is compressed, since the frequencies of the recorded scattering lines differ from the values of the frequencies characteristic of the same substances under normal conditions (i.e.,  $1360$  and  $1582 \text{ cm}^{-1}$  for amorphous carbon and graphite, respectively).

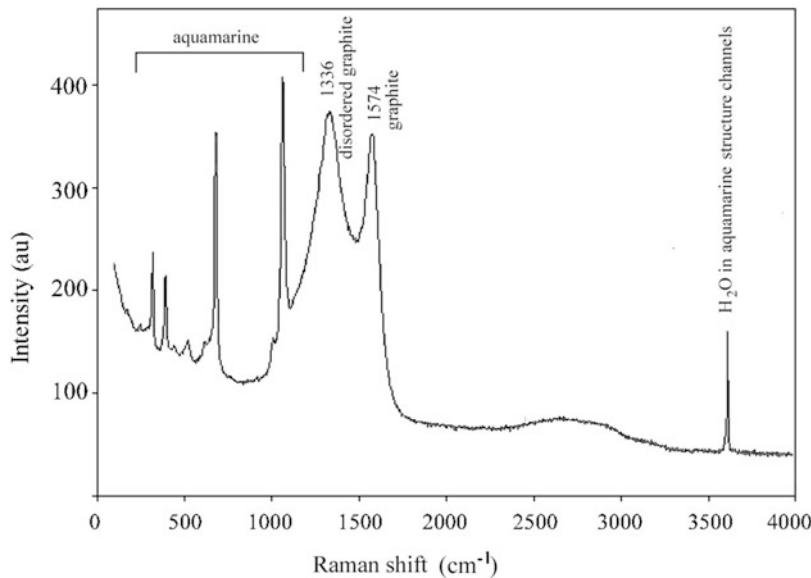
**Fig. 3.13** Raman spectra of the ordered (upper curve) and disordered (lower curve) oligoclase varieties. The laser emission wavelength is 532 nm, the spectral resolution is  $6 \text{ cm}^{-1}$ , and the laser power is 14 mW



**Fig. 3.14** Inclusion of carbonaceous matter in aquamarine



**Fig. 3.15** Raman spectrum of a carbonaceous inclusion in aquamarine. The laser emission wavelength is 532 nm, the spectral resolution is  $6 \text{ cm}^{-1}$ , the laser power is 30 mW, and signal accumulation time is 120 s



### 3.2.4 Selection Rules

The Raman activity of normal modes is determined by changes of polarizability tensor components in corresponding vibrations. The magnitudes of the derivatives of the polarizability tensor components by normal coordinates determine the intensities of these vibrational modes and also form a second-rank symmetric tensor (so-called the Raman tensor) which is defined

for all point symmetry groups (see, e.g., Zhizhin et al. 1984; Kolesov 2018). Nonzero elements of the Raman tensor determine at which relative orientation of the crystallographic axes and the polarizations of the laser and scattered radiation vibrations of a given type of symmetry will be recorded in the Raman spectrum. Based on the Raman tensors, selection rules in Raman scattering for crystals, molecules, molecular groups, and ions are formulated.

For objects with  $C_{2v}$  symmetry, to which  $\text{H}_2\text{O}$  and  $\text{H}_2\text{S}$  molecules belong, vibrations of the symmetry types  $A_1$  (symmetric stretching and bending vibrations) and  $B_1$  (antisymmetric stretching vibrations) are permitted by the selection rules. Corresponding Raman bands of water molecules in the gas phase are observed at 3657, 1595, and  $3756 \text{ cm}^{-1}$ , respectively (Halonen and Carrington Jr 1988).

For isolated undistorted planar trigonal  $AB_3$  ions (symmetry group  $D_{3h}$ ) like  $\text{CO}_3^{2-}$ ,  $\text{NO}_3^-$ , and  $\text{BO}_3^{3-}$ , symmetric stretching vibrations  $\nu_1$  with the symmetry  $A_1'$  as well as stretching ( $\nu_3$ ) and in-plane bending ( $\nu_4$ ) doubly degenerate vibrations of type  $E'$  are permitted in Raman spectra by the selection rules. Out-of-plane bending  $\nu_2$  vibrations with the symmetry  $A_2''$  are prohibited.

For isolated tetrahedral  $AB_4$  ions with the  $T_d$  symmetry ( $\text{MoO}_4^{2-}$ ,  $\text{AsO}_4^{3-}$ ,  $\text{PO}_4^{3-}$ ,  $\text{VO}_4^{3-}$ ,  $\text{SO}_4^{2-}$ ,  $\text{SiO}_4^{4-}$ , etc.) in the Raman spectra the stretching  $\nu_1$  mode (with the  $A_1$  symmetry), bending doubly degenerate  $\nu_2$  mode (with the  $E$  symmetry), and triply degenerate  $\nu_3$  stretching and  $\nu_4$  bending modes (with the  $F_2$  symmetry) are allowed by the selection rules.

In real structures of minerals, the symmetry of tetrahedral ions decreases, sometimes to  $D_{2h}$  (flattened tetrahedron) or even to  $C_s$ , which leads to the removal of degeneracy and splitting of degenerate vibrations into separate components. To identify the scattering lines, one can use the known regularity established by different authors in numerous experimental studies: in most cases, the scattering lines corresponding to fully symmetric stretching vibrations have a smaller width and higher peak intensity than the scattering lines corresponding to degenerate vibrations. This empirical regularity is explained by the greater polarizability of bonds with fully symmetric stretching vibrations (Kolesov 2018).

Symmetry types of the vibrations of isolated complex ions may differ from that in crystals. For example, in calcite  $\text{CaCO}_3$  having  $D_{3d}$  symmetry,  $\text{CO}_3^{2-}$  ions are located in positions on the third-order axis ( $D_3$  positional symmetry) and do not change their symmetry compared to the free state. In this case, the same selection rules are valid as

for an isolated  $\text{CO}_3^{2-}$  ion. On the other hand, in aragonite (orthorhombic  $\text{CaCO}_3$  polymorph with the  $D_{2h}$  symmetry), the crystal structure of which does not have axes of the third order, the positional symmetry of the  $\text{CO}_3^{2-}$  ion decreases to  $C_s$ , and according to the selection rules for the  $D_{2h}$  group, the out-of-plane bending mode ( $\nu_2$ ), which is classified as  $A_g$ , is active in the Raman spectrum of aragonite: corresponding band is observed at  $853 \text{ cm}^{-1}$  (Frech et al. 1980).

In vivianite  $\text{Fe}_3^{2+}[\text{PO}_4]_2 \cdot 8\text{H}_2\text{O}$ , which is monoclinic with the symmetry  $C_{2h}$ , there are no axes of the third order, and the symmetry of the phosphate ion also decreases as compared with isolated  $\text{PO}_4^{3-}$ . As a result, all vibrations are nondegenerate and are classified according to symmetry types as  $A_g$ ,  $A_u$ ,  $B_g$ , and  $B_u$ . In the Raman spectrum of vivianite, only  $A_g$  and  $B_g$  bands appear in accordance with the “alternative prohibition” rule applied to symmetry groups with an inversion center:

| $\text{PO}_4^{3-}$ in aqueous solution<br>(Nakamoto 2009), $\text{cm}^{-1}$ | $\text{PO}_4^{3-}$ in vivianite<br>(Piriou and Poullen 1984), $\text{cm}^{-1}$ |
|---|--|
| $A_1(\nu_1)$ 938  | $A_g(\nu_1)$ 951   |
| $E(\nu_2)$ 420  | $A_g(\nu_2)$ 458; $B_g(\nu_2)$ 425   |
| $F_2(\nu_3)$ 1017   | $A_g(\nu_3)$ 1053, 990; $B_g(\nu_3)$ 1018                                      |
| $F_2(\nu_4)$ 567  | $A_g(\nu_4)$ 572, 539  |

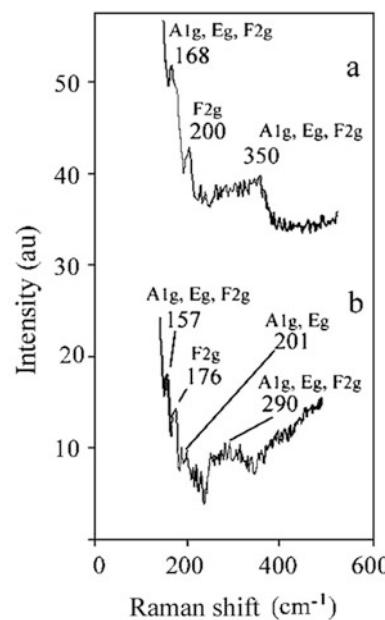
For isolated regular octahedral  $AB_6$  groups,  $\nu_1$  symmetric stretching mode with the symmetry  $A_{1g}$ , doubly degenerate  $\nu_2$  stretching mode with the symmetry  $E_g$  and triply degenerate  $\nu_5$  bending mode with the symmetry  $F_{2g}$  are permitted in the Raman spectra by the selection rules.

In accordance with the “alternative prohibition rule,” in IR spectra of isolated regular octahedral  $AB_6$  groups, only the  $\nu_3$  stretching band and the  $\nu_4$  bending band (both having the  $F_{1u}$  symmetry) are observed. Anionic groups of this type  $[\text{Si}(\text{OH})_6]$ ,  $[\text{Al}(\text{OH})_6]$ ,  $[\text{Fe}^{3+}(\text{OH})_6]$ ,  $[\text{Mn}^{4+}(\text{OH})_6]$ , etc.] occur in the structures of ettringite-group minerals. In ettringite  $\text{Ca}_6[\text{Al}(\text{OH})_6]_2(\text{SO}_4)_3 \cdot 26\text{H}_2\text{O}$ , the symmetry of which is  $C_{3v}$ , with triad axes and reflection planes being the only symmetry elements. As a result, the symmetry of the  $[\text{Al}(\text{OH})_6]^{3-}$  group

is also lowered. The  $\nu_5$  modes which were forbidden in the Raman spectrum according to the “alternative prohibition rule” for the free anion become nondegenerate and active. Vibrational modes of ettringite are classified according to the symmetry types A<sub>1</sub>, A<sub>2</sub>, and E. In accordance with the selection rules, only bands of A<sub>1</sub> and E vibrations appear in the Raman spectra (presumably, the bands at  $\sim 550$  and  $\sim 345$  cm<sup>-1</sup>; see Deb et al. 2003; Renaudin et al. 2007). Vibrations of type A<sub>1</sub> can be separately recorded under the conditions when polarizations of laser and scattered radiation and the C<sub>3</sub> crystallographic axis of a single crystal are parallel to each other.

The C<sub>6</sub> symmetry group of thaumasite Ca<sub>3</sub>[Si(OH)<sub>6</sub>](SO<sub>4</sub>)(CO<sub>3</sub>)·12H<sub>2</sub>O contains axes of the second, third, and sixth orders. In accordance with this set of symmetry elements, the “alternative prohibition rule” becomes inapplicable, and the degeneration is removed from the triple degenerate modes. This leads to an increase in the number of possible scattering lines in the spectrum. In accordance with the table of group characters, in the spectra of structures with such symmetry, the existence of vibrational modes of the A, B, E<sub>1</sub>, and E<sub>2</sub> types is possible. In accordance with the selection rules and Raman scattering tensor, vibrations of symmetry types A, E<sub>1</sub>, and E<sub>2</sub> are active in the Raman spectra. The study of the polarized Raman spectra of a thaumasite single crystal showed that the fully symmetric vibrations of the [Si(OH)<sub>6</sub>]<sup>2-</sup> anion have a frequency of about 660 cm<sup>-1</sup> (Kononov et al. 1990).

An example of the manifestation of the “alternative prohibition rule” is the absence of first-order Raman spectra in some minerals with inversion centers. Such minerals, for example, are halite NaCl and sylvite KCl having a cubic (O<sub>h</sub>) symmetry. All atoms forming the structures of these minerals are located at the centers of inversion, and any displacements from their equilibrium positions violate the symmetry. As a result, the bands corresponding to all kinds of vibrations are forbidden in the first-order Raman spectra. However, with a large signal accumulation time, it is possible to record weak bands of the second order Raman spectra (Fig. 3.16). The selection rules for two-phonon spectra are determined using the tables



**Fig. 3.16** Second-order Raman spectra of halite (a) and sylvite (b). The laser emission wavelength is 532 nm, the spectral resolution is 6 cm<sup>-1</sup>, the laser power is 30 mW, and signal accumulation time is 200 and 25 s, respectively

of the characters of irreducible representations of the point group of the mineral under investigation. Thus, an analysis of the types of symmetry of two-phonon vibrations in crystals with a point group O<sub>h</sub> shows that among the possible combination modes in this point group there are vibrations with symmetry types A<sub>1g</sub>, E<sub>g</sub> and F<sub>2g</sub>, which are allowed in the Raman spectra. Consequently, second order Raman spectra can also be used for diagnostic purposes.

### 3.2.5 The Longitudinal-Transverse Splitting

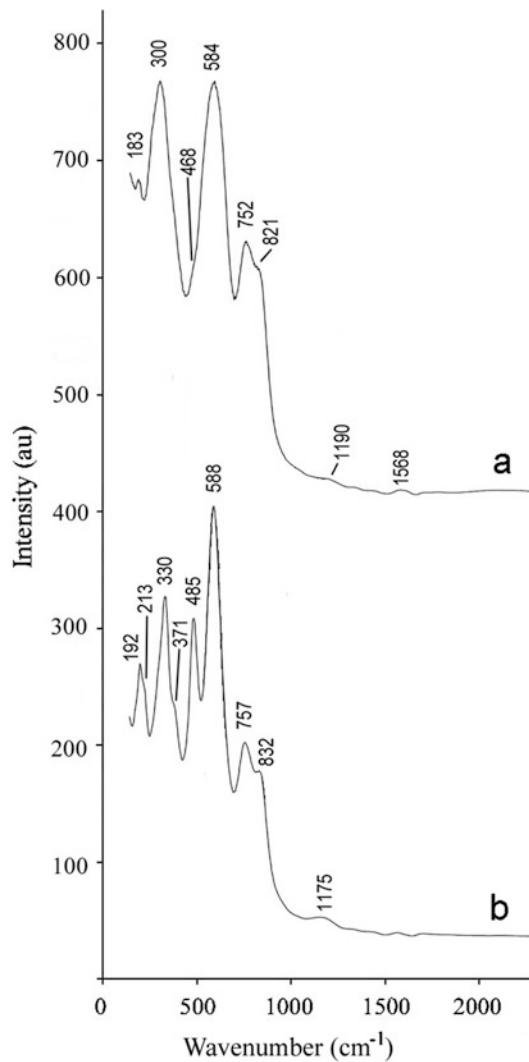
The special feature of the Raman scattering method, which makes it difficult to interpret the spectra, includes the appearance of the longitudinal-transverse (LO-TO) splitting of lines in the spectra in crystals without an inversion center. In such crystals, some vibrations that are active in the Raman spectra are accompanied by changes in the dipole moment. As a result, vibrations of atoms lead to changes in the

macroscopic electric dipole moment in the crystal. The resulting additional electromagnetic field in turn affects the atoms. In the Raman spectra, such an interaction can result in the appearance of additional scattering lines. The *LO-TO* splitting theoretically exists in all cases when scattering occurs on dipole-active vibrations. A weak splitting results in changes of the shapes of some lines and appearance of additional shoulders. However, in crystals with the ionic character of bonds the magnitude of the *LO-TO* splitting can reach considerable values. For example, in the Raman spectrum of LiH, it is almost  $500\text{ cm}^{-1}$ . In Raman spectra of molecular crystals, the splitting value only in some cases reaches  $15\text{ cm}^{-1}$  (Zhizhin et al. 1984), but in most molecular crystals, the *LO-TO* splitting is not observed. The prediction of the *LO-TO* splitting in the spectra of the Raman spectra goes beyond the framework of factor group analysis.

In the case when a mineral without an inversion center has several dipole-active vibrations, several additional scattering lines may appear in the spectrum owing to splitting into *LO-TO* components (see, e.g., Raman spectrum of quartz in Fig. 3.11). As a result, the total number of lines in the spectrum may exceed the number of normal vibrations expected according to group theory. It should be noted that in the infrared absorption spectra, the frequencies of the longitudinal vibrations are not recorded, since only transverse vibrations are excited.

### 3.2.6 Orientation and Polarization Effects; Analysis of Water and OH Groups

A specific feature of Raman scattering is its tensor character. As a result, Raman spectra of single crystals depend on their orientation and the direction of polarization of the vector of the electrical component of the electromagnetic wave of laser radiation. Spectra obtained in different experimental geometries may differ from each other by the number of recorded scattering lines and their intensity (Fig. 3.17).



**Fig. 3.17** Raman spectra of laachite  $(\text{Ca},\text{Mn})_2\text{Zr}_2\text{Nb}_2\text{TiFeO}_{14}$  (monoclinic, point group  $C_{2h}$ ) obtained with the polarization of the laser beam parallel (upper curve) and perpendicular (lower curve) to the  $a$  axis of the crystal. The laser emission wavelength is  $532\text{ nm}$ , the spectral resolution is  $2\text{ cm}^{-1}$ , the laser power is  $6\text{ mW}$ , and the focal spot diameter is about  $15\text{ }\mu\text{m}$

With a random orientation of the single crystal, the scattering line intensities are also random. This uncertainty does not apply to spectra of powdery samples with chaotic orientation of microcrystals. A reproducible total spectrum averaged over all possible spatial orientations of the microcrystals can be obtained only if the size of the microcrystals in the powder is much less

than the diameter of the focal spot of the laser radiation. This mode of spectrum registration is most suitable for diagnostic purposes. In cases where it is impossible to prepare the powder, it is recommended to obtain several spectra at different orientations of the sample in order to select the most representative version of the spectrum.

Raman spectrum of a single crystal, obtained using polarized radiation, makes it possible to draw conclusions regarding the directions of chemical bonds relative to the crystallographic axes. This is especially important for determining the orientation of hydroxyl groups (e.g., in amphiboles, micas, tourmalines). Raman scattering is only possible if the electric field vector of an incident beam is not perpendicular to the O–H bond direction.

To study structural features of minerals, spectra of Raman spectra of single-crystal samples are taken. In such experiments, intensities of scattering lines depend on the mutual orientation of the crystallographic axes and on the directions of the polarization vectors of the incident and scattered radiation. In crystals with a tetragonal, hexagonal/trigonal, and cubic symmetry, it is possible to determine the type of symmetry of the vibrational mode of a group of equivalent coordinates based on polarized Raman spectra. In crystals having lower symmetry, polarization measurements make it possible to obtain information on the orientations of chemical bonds, since in some cases (especially in molecular crystals) polarization of some scattering lines depends on vibrations of single bonds (Kolesov 2018).

The polarizability of a bond in the longitudinal direction is much greater than in the transverse directions. Therefore, the scattering line corresponding to stretching vibrations of this bond is most intense when the polarization of the exciting laser radiation (and in the ideal case of the scattered light) coincides with the direction of this bond. This regularity can be illustrated by the example of micas. In phlogopite  $K(Mg,Fe^{2+})_3[AlSi_3O_{10}](OH,F)_2$  having monoclinic symmetry, OH groups coordinated by divalent octahedral cations are oriented almost parallel to the crystallographic *c* axis, perpendicular to the cleavage plane. The Raman scattering line at

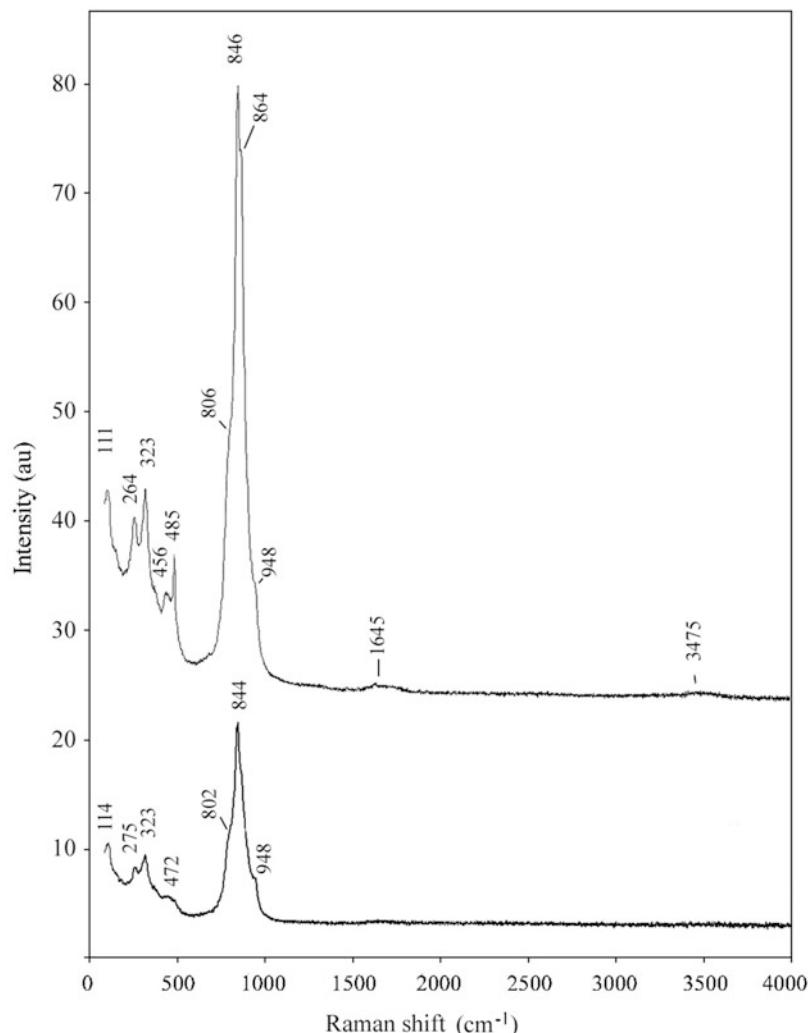
$3709\text{ cm}^{-1}$  corresponding to stretching vibrations of hydroxyl groups has a maximum intensity when the polarization of laser radiation is perpendicular to the cleavage plane of the mineral sample, i.e., parallel to the *c* axis. A weak additional line at about  $3666\text{ cm}^{-1}$  is observed in Raman spectra of phlogopite samples containing trivalent impurity ions,  $Fe^{3+}$  or  $Al^{3+}$ . Since the orientation of hydroxyl groups coordinated by trivalent cations deviates from the direction perpendicular to the cleavage plane, a weak scattering line can be recorded in the Raman spectra with polarization of laser radiation parallel to the cleavage plane. In muscovite  $KAl_2[AlSi_3O_{10}](OH)_2$ , which is a dioctahedral mica, hydroxyl groups are almost parallel to the cleavage plane, and the band of stretching vibrations of OH groups (at  $3628\text{ cm}^{-1}$ ) has a maximum intensity in spectra excited by laser radiation with polarization parallel to the cleavage plane (Tili et al. 1989).

Based on polarized spectra of tourmaline group minerals, it was found that the OH groups are mainly oriented along the threefold *c* crystallographic axis (Gasharova et al. 1997; Berryman et al. 2016). Polarized Raman spectra of the orthorhombic mineral magnesiocarpholite  $MgAl_2Si_2O_6(OH)_4$  revealed the presence of three OH groups, one of which is oriented almost perpendicular to the *c* axis (Fuchs et al. 2001).

In some cases, the orientation of complex anionic groups can be determined from polarized Raman spectra. Based on the data obtained for a columnar thaumasite crystal, Kononov et al. (1990) have confirmed that almost flat  $CO_3^{2-}$  group (Edge and Taylor 1971) is oriented perpendicular to the *C<sub>6</sub>* axis of the crystal.

Raman spectroscopy has a low sensitivity in determination of water in minerals. The  $H_2O$  molecule has a weak polarizability and, as a result, a weak response to excitation radiation. Bands of O–H-stretching vibrations are usually observed in the range from  $3000$  to  $3800\text{ cm}^{-1}$ , but bands of acidic OH groups and very strong hydrogen bonds may have Raman shifts below  $3000\text{ cm}^{-1}$ . In most cases, bands of H–O–H bending vibrations of  $H_2O$  molecules are observed in the range  $1600$ – $1700\text{ cm}^{-1}$ , but with a low water content, these bands are recorded with difficulty and only with a successful selection of

**Fig. 3.18** Raman spectra of martyite  $Zn_3(V_2O_7)(OH)_2 \cdot 2H_2O$  obtained at the laser emission wavelength of 532 nm, the spectral resolution of  $2\text{ cm}^{-1}$ , the laser power of 4 and 13 mW, and the signal accumulation time of 200 and 50 s (for the upper and lower curves, respectively)

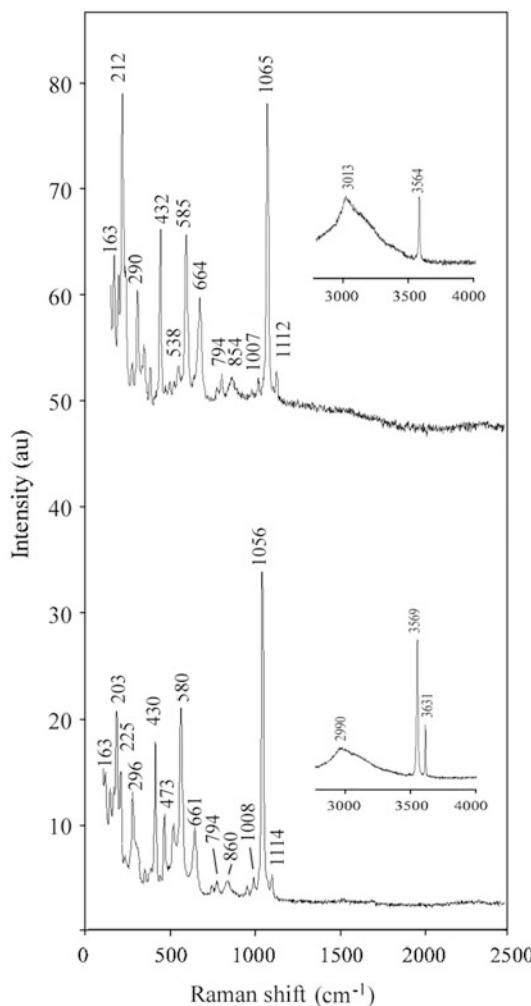


experimental conditions. An increase in the accumulation time at a given laser power or an increase in the laser power may lead to local overheating and dehydration of the sample (see Fig. 3.18).

In the structure of fluorapophyllite-(K), water molecules occupying a single crystallographic position are asymmetric: the positional symmetry of  $H_2O$  decreases to  $C1$ , and the hydrogen atoms belonging to the same molecule are nonequivalent. A significant difference in the interactions of the two hydrogen atoms with their nearest environment leads to the fact that stretching vibrations

of OH bonds in the water molecule are practically independent (Ryskin and Stavitskaya 1990). The broad band with a maximum of about  $3013\text{ cm}^{-1}$  and the narrow band at  $3564\text{ cm}^{-1}$  refer to the stretching vibrations of OH bonds, which form strong and very weak hydrogen bonds, respectively (Fig. 3.19).

In the structure of hydroxylapophyllite-(K), both asymmetric  $H_2O$  molecules and OH groups are present. The broad band at about  $2990\text{ cm}^{-1}$  and the narrow band at  $3569\text{ cm}^{-1}$  correspond to a strong and a weak hydrogen bonds formed by  $H_2O$ , respectively. Another narrow band (with a



**Fig. 3.19** Raman spectra of fluorapophyllite-(K)  $\text{KCa}_4[\text{Si}_8\text{O}_{20}]\text{F}\cdot 8\text{H}_2\text{O}$  (upper curve) and hydroxylapophyllite-(K)  $\text{KCa}_4[\text{Si}_8\text{O}_{20}]\text{OH}\cdot 8\text{H}_2\text{O}$  (lower curve) obtained using 532 nm laser radiation

half-width of about  $3 \text{ cm}^{-1}$ ) is observed at  $3631 \text{ cm}^{-1}$  and corresponds to stretching vibrations of the OH group.

In some cases when the number of hydrogen-containing groups in the mineral is insignificant, the Raman spectroscopy method does not allow one to unambiguously distinguish between water and hydroxyl groups. In such cases, it is more appropriate to use infrared absorption spectroscopy.

### 3.2.7 Effect of Luminescence

Emission of photoluminescence excited by the laser beam is a serious problem of Raman spectroscopy of minerals. Usually, luminescence is observed as broad bands superimposed on the Raman scattering spectrum (Fig. 3.20, upper curve). The intensity of luminescence can be many times (up to  $10^3$ – $10^4$ ) greater than the intensity of the Raman signal, which prevents the registration of a high-quality spectrum or even makes it impossible to obtain Raman spectrum at all.

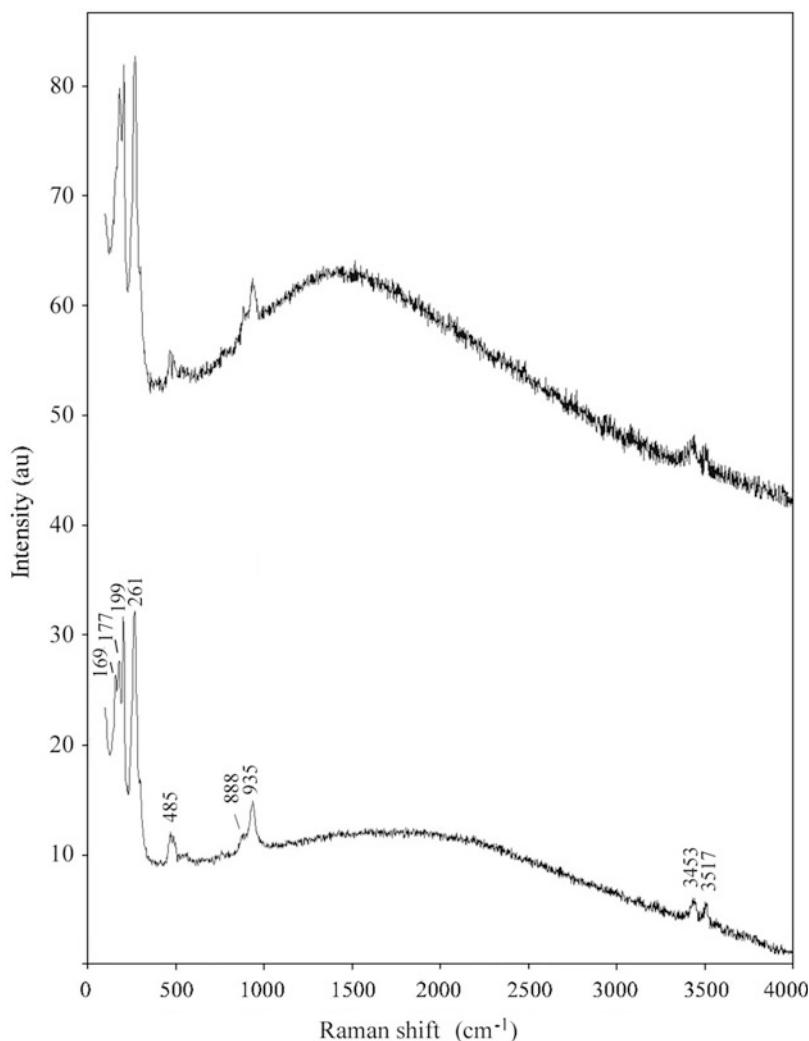
The main cause of luminescence is the coincidence of the frequency of the exciting laser radiation with the frequencies of electronic transitions of the luminescent center in the mineral. The most effective way to eliminate luminescence is the use of laser radiation with a longer wavelength  $\lambda_{\text{exc}}$ , the photon energy of which is insufficient to excite electronic energy levels. Unfortunately, with increasing wavelength of laser radiation, the intensity of the useful Raman signal  $I_R$  decreases significantly according to the law  $I_R \sim \lambda_{\text{exc}}^{-4}$ . In such situations, long-time accumulation of the useful signal leads to an improvement in the signal-to-noise ratio (Fig. 3.20, lower curve).

In cases when it is not possible to eliminate the luminescence, one can resort to recording several spectra using lasers with different wavelengths. For each type of radiation, the spectral luminescence lines appear in a specific spectral range. The bands that will be present with a constant frequency in the spectra obtained at different wavelengths of the exciting radiation should be referred to the lines of Raman scattering.

### 3.2.8 Destructive Effect of Laser Radiation

Local temperature increase due to strong absorption of laser radiation may result in alteration or decomposition of the sample. In the Raman microprobe analysis this problem is especially

**Fig. 3.20** Raman spectra of an unoriented sample of romanorlovite  $K_8Cu_6Cl_{17}(OH)_3$  obtained at the laser emission wavelength of 532 nm, the spectral resolution of  $6\text{ cm}^{-1}$ , the laser power of 3 and 1.5 mW, and the signal accumulation time of 4 and 17 min (for the upper and lower curves, respectively)

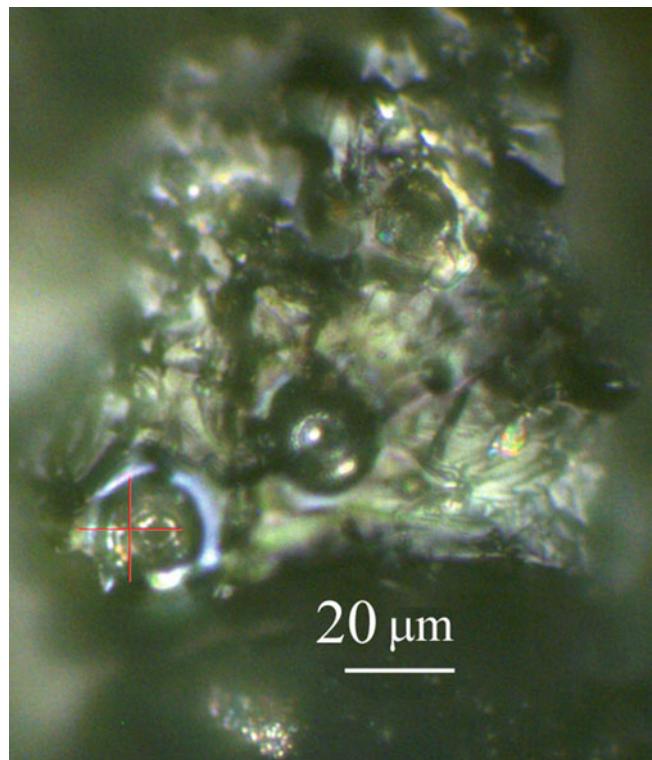


significant. Therefore, the selection of conditions for a nondestructive experiment plays an extremely important role in experiments on Raman scattering.

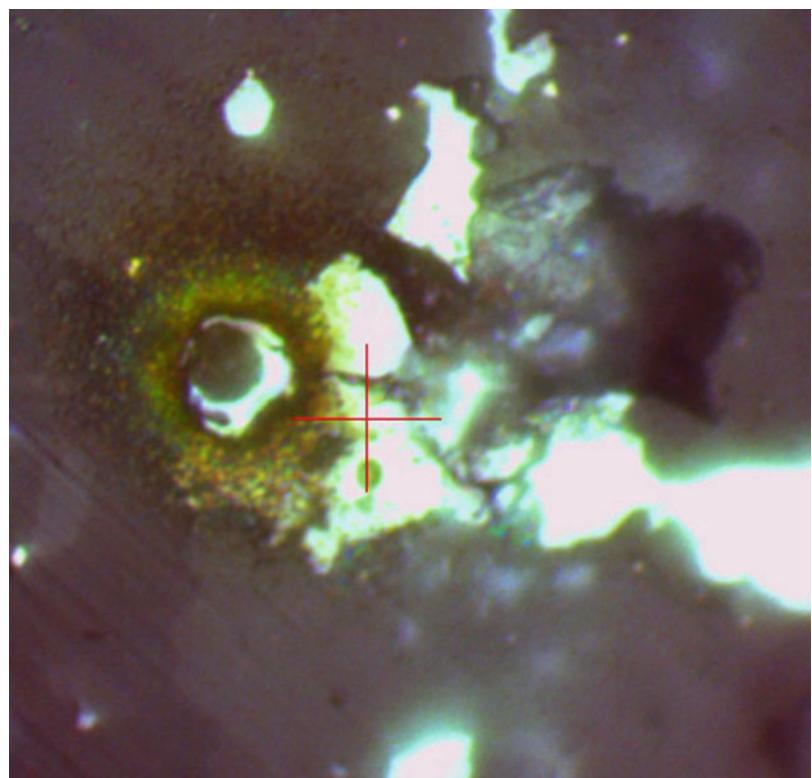
Special attention should be paid to proper selection of laser power when working with highly colored or opaque minerals, which include most sulfides and sulfosalts. Dark coloring of minerals causes a strong absorption of exciting radiation, which results in attenuation of scattered signal. To enhance the intensity of the Raman signal, an increase in the laser pump power is required. However, it should be borne in mind

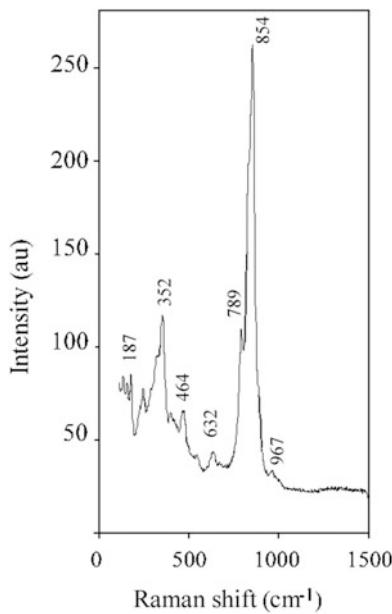
that increasing the power of laser radiation leads to an increase in the energy absorbed by the mineral. Since most minerals have relatively low thermal conductivity, the absorbed energy causes a local increase in temperature in the focal volume of the laser beam. Too high laser power can result in local thermal destruction of the mineral structure, leading to the formation of cavities on the sample surface (Figs. 3.21 and 3.22) or cavities with a destroyed structure inside the sample. However, in most cases optimizing the experimental conditions (reducing the laser excitation power and increasing the signal accumulation

**Fig. 3.21** Caverns formed on the surface of melanarsite at a laser power of 13 mW and laser wavelength of 532 nm, focal spot diameter of  $\sim 15 \mu\text{m}$ , and signal accumulation time of 10 s



**Fig. 3.22** The thermal destruction zone formed on the surface of a crystal of vorontsovite ( $\text{Hg}_5\text{Cu}_4\text{TiAs}_4\text{S}_{12}$ ) at a laser power of 1.5 mW and laser wavelength of 532 nm, focal spot diameter of  $\sim 15 \mu\text{m}$ , and signal accumulation time of 1 h. Field width 100  $\mu\text{m}$ . It was not possible to obtain Raman spectrum of the mineral due to its thermal instability





**Fig. 3.23** Raman spectrum of melanarsite  $\text{K}_3\text{Cu}_7\text{Fe}^{3+}\text{O}_4(\text{AsO}_4)_4$  obtained at the laser emission wavelength of 532 nm, spectral resolution of  $6 \text{ cm}^{-1}$ , laser power of 4 mW, focal spot diameter of  $\sim 15 \mu\text{m}$ , and signal accumulation time of 100 s

time) makes it possible to obtain scattering spectra even on thermally unstable samples (Fig. 3.23).

In some cases, it is possible to reduce the degree of overheating by placing microscopic mineral samples on a metal substrate, which leads to acceleration of the heat sink. The correct sequence of actions when working with an unknown colored opaque or especially valuable sample is the use of low-power laser source at the initial stage of research. A gradual increase in power with constant monitoring of the state of the sample will prevent its damage or destruction. To improve the quality of the Raman spectra at low power of the exciting radiation, an increase in the time of accumulation of the Raman signal may play a positive role.

Additional information on the practical application of Raman spectroscopy can be obtained from numerous books and review articles (Reshetnyak and Bukanov 1991; Nasdala et al. 2004; Larkin 2011; Vandenberghe 2013; Kolesov 2018).



## Raman Spectra of Minerals

4

This chapter provides data on 2104 Raman spectra of minerals and their synthetic counterparts taken from various periodicals. The overwhelming majority of these spectra were obtained on arbitrarily oriented samples. As a result, absolute values band intensities are not very informative. For this reason, we do not show the spectra figures, but only give lists of Raman shifts with indication of the strongest and weakest bands.

Data on the Raman spectra are listed in alphabetical order of mineral names and are accompanied by brief descriptions of the conditions under which the spectra were taken. In most cases, comments are made regarding the quality of the spectrum and/or methods of identification of the reference sample.

### **Abellaite** $\text{NaPb}_2(\text{CO}_3)_2(\text{OH})$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 488 and 568.2 nm laser radiations. The laser radiation power at the sample was 200 and 100 mW, respectively.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3500w, 1750w, 1730w, 1392s, 1350sh, 1068, 1057s, 1052sh, 1036w, 868, 695sh, 681s, 285 (broad), 202, 125w, 98 (broad), 86 (broad), 52s, 37.

**Source:** Brooker et al. (1983).

**Comments:** The band 1036w is a satellite band arising from the isotopic moieties ( $\text{C}^{18}\text{O}^{16}\text{O}_2^{2-}$ ). The sample identification was done and the purity of the substance was proved by powder X-ray diffraction data.

### **Abelsonite** $\text{NiC}_{31}\text{H}_{32}\text{N}_4$

**Origin:** Green River Formation, Utah, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was 90 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** ~1230, ~1170, ~1150, ~1120, ~760.

**Source:** Liu et al. (2015e).

**Comments:** The wave numbers were estimated by us based on spectral curve analysis of the published spectrum. The sample was characterized by powder X-ray diffraction data and chemical analysis.

**Abthurite**  $\text{Sn}^{2+}_{21}\text{O}_6(\text{OH})_{14}\text{Cl}_{16}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on suspension in water using 785.0 nm laser radiation. The laser radiation power at the sample was 200 mW.

**Raman shifts (cm<sup>-1</sup>):** 256, 206s, 170, 156, 147.

**Source:** Chen and Grandbois (2013).

**Comments:** Spectral analysis and Raman shifts calculation were based on semi-quantitative indirect hard modeling (IHM) analysis.

**Acanthite**  $\text{Ag}_2\text{S}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an unoriented crystal using 488.0 nm laser radiation. The laser radiation power is not indicated. The spectrum was measured at 30 K.

**Raman shifts (cm<sup>-1</sup>):** 222s, 200.

**Source:** Milekhin et al. (2011).

**Comments:** For the Raman spectrum of acanthite see also Martina et al. (2012).

**Acetamide solution**  $\text{CH}_3\text{CONH}_2$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on 0.1 M and 0.4 M aqueous solutions of acetamide. The wavelengths of laser excitation lines were 220, 240, 250, 365, and 560 nm. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1662, 1616, 1457, 1404, 1360, 1131, 1005, 871.

**Source:** Dudik et al. (1985).

**Comments:** The line at 871 cm<sup>-1</sup> is strong in experiments with the laser radiation wave lengths of 365 and 560 nm. The lines at 1457, 1616, and 1662 cm<sup>-1</sup> are strong in experiments with the laser radiation wave length of 220 nm. For the Raman spectrum of acetamide solution see also Spinner (1959).

**Actinolite**  $\text{Ca}_2(\text{Mg}_{4.5-2.5}\text{Fe}^{2+}_{0.5-2.5})\text{Si}_8\text{O}_{22}(\text{OH})_2$

**Origin:** Košino, Macedonia.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 and 532.0 nm laser radiations. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1056s, 1026, 954, 926, 899, 744w, 672s, 527, 517w, 477w, 433w, 413w, 391, 368, 346.

**Source:** Jovanovski et al. (2009).

**Comments:** The identification of the sample was done by results of electron microprobe analysis; the purity of the substance was proved by powder X-ray diffraction data. For the Raman spectra of actinolite see also Gopal et al. (2004), Makreski et al. (2006a), Petry et al. (2006), Apopei and Buzgar (2010), Apopei et al. (2011), Andò and Garzanti (2014), and Leissner et al. (2015).

**Actinolite**  $\text{Ca}_2(\text{Mg}_{4.5-2.5}\text{Fe}^{2+}_{0.5-2.5})\text{Si}_8\text{O}_{22}(\text{OH})_2$ **Origin:** Tyrol, Austria.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was 100 mW.**Raman shifts (cm<sup>-1</sup>):** 3675, 3661, 1059, 1027s, 949, 929, 892w, 744, 670s, 577w, 522, 482w, 415, 392s, 369s, 294, 247w, 226s.**Source:** Apopei et al. (2011).**Comments:** No independent analytical data are given for the sample used. For the Raman spectra of actinolite see also Gopal et al. (2004), Makreski et al. (2006a), Petry et al. (2006), Jovanovski et al. (2009), Apopei and Buzgar (2010), Andò and Garzanti (2014), and Leissner et al. (2015).**Adachiite**  $\text{CaFe}^{2+}_3\text{Al}_6(\text{Si}_5\text{AlO}_{18})(\text{BO}_3)_3(\text{OH})_3(\text{OH})$ **Origin:** No data.**Experimental details:** A single crystal was used. The wavelengths of laser excitation lines were 488.0 and 514.5 nm. Laser radiation power at the sample was 14 mW. Polarized spectra were collected in  $y(zz)y$ ,  $y(zx)y$ , and  $y(xx)y$  scattering geometries.**Raman shifts (cm<sup>-1</sup>):** 3679, 3625, 3570, 3565s, 3486.**Source:** Watenphul et al. (2016a).**Comments:** The sample was identified by electron microprobe analysis, and boron was determined by LA-ICP-MS measurement. The Raman shifts are given for the scattering geometry  $y(zz)y$ , in which the Raman intensities are most strong.**Adamite**  $\text{Zn}_2(\text{AsO}_4)(\text{OH})$ **Origin:** Lavrion mining District, Attikí (Attika, Attica) Prefecture, Greece.**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 632.8 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3552s, 890s, 846s, 820, 539, 496, 458, 422, 380, 325.**Source:** Makreski et al. (2013a).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of adamite see also Yang et al. (2001).**Adelite**  $\text{CaMg}(\text{AsO}_4)(\text{OH})$ **Origin:** No data**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3550, 890, 846, 821, 803, 540, 497, 479, 421, 376, 322, 277, 253, 232, 211, 172, 134.**Source:** Martens et al. (2003c).**Comments:** No independent analytical data are given for the sample used. Intensities of Raman bands are not indicated.

**Admontite**  $MgB_6O_{10}\cdot 7H_2O$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powdery sample.

The wavelengths of the laser excitation line and laser radiation power are not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1092w, 963, 881, 637s, 523w, 500w, 428s, 412, 394, 320.**Source:** Derun et al. (2015)**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of admontite see also Kipcak et al. (2014).**Adolfpaterite**  $K(UO_2)(SO_4)(OH)(H_2O)$ **Origin:** Svornost mine, Jáchymov, Krušné Hory (Ore Mts.), Bohemia, Czech Republic (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 780 nm laser radiation. The laser radiation power at the sample was from 4 to 8 mW.**Raman shifts (cm<sup>-1</sup>):** 1169w, 1149w, 1116w, 1063w, 1029w, 993s, 935s, 900s, 843w, 638w, 597w, 456, 442, 399w, 350w, 320, 270, 264, 219, 1198, 169w, 130w, 109w.**Source:** Plášil et al. (2012b).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.**Aegirine**  $NaFe^{3+}Si_2O_6$ **Origin:** Kangerdluarsuk, Greenland (sample 1) and Brewig, Norway (sample 2).**Experimental details:** Raman scattering measurements have been performed on unoriented crystals.

The wavelength of the laser excitation line was 532 nm. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1130w, 1044s, 953s, 866, 758, 678, 544s, 499, 465w, 385, 342s, 309, 294, 273 (sample 1); 1132w, 1041s, 971s, 952, 866, 757, 678, 558, 544s, 496, 466w, 385, 343s, 295, 267 (sample 2).**Source:** Buzatu and Buzgar (2010).**Comments:** No independent analytical data are provided for the samples used. For the Raman spectra of aegirite; see also Andò and Garzanti (2014) and Zhou et al. (2014).**Aegirine Li analogue**  $LiFe^{3+}(Si_2O_6)$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 1064 nm laser radiation. The nominal laser radiation power was 120 mW.**Raman shifts (cm<sup>-1</sup>):** 1084s, 1038s, 1012s, 976, 932, 857, 776w, 684, 575, 553, 519, 493, 387, 363, 347, 325, 313, 294, 284, 263w, 237, 214, 196, 175, 133w, 97.**Source:** Zhang et al. (2002a).**Comments:** The sample used was prepared from a stoichiometric mixture of finely ground  $Li_2CO_3$ ,  $Fe_2O_3$  and  $SiO_2$  by solid-state ceramic sintering techniques at 1223 K and ambient pressure and characterized by neutron powder diffraction and Mössbauer measurements. Monoclinic, space group  $C2/c$ ,  $a = 9.6641(2)$ ,  $b = 8.6612(3)$ ,  $c = 5.2924(2)$  Å,  $\beta = 110.12(1)^\circ$ .

**Aerinite**  $(\text{Ca},\text{Na})_6(\text{Fe}^{3+},\text{Fe}^{2+},\text{Mg},\text{Al})_4(\text{Al},\text{Mg})_6\text{Si}_{12}\text{O}_{36}(\text{OH})_{12}(\text{CO}_3)\cdot 12\text{H}_2\text{O}$ 

**Origin:** Estopiñán dam, Estopiñández Castillo, Huesca, Aragón, Spain.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1236, 1072, 1049, 1013, 974, 933, 909, 885w, 546, 512, 465w, 392, 365s, 331s, 300, 281, 245, 222.

**Source:** Frost et al. (2015y).

**Comments:** The identification of the sample used was done only by means of scanning electron microscopy. In the cited paper, the band at 1236 cm<sup>-1</sup> is assigned to  $\text{CO}_3^{2-}$  asymmetric stretching mode or to a Si–O vibrations. In both cases the position of this band would be anomalous.

**Aeschynite-(Y)**  $(\text{Y},\text{Ln},\text{Ca},\text{Th})(\text{Ti},\text{Nb})_2(\text{O},\text{OH})_6$ 

**Origin:** A granitic pegmatite situated in the Aust-Agder province, southern Norway.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 830, 665, 609, 396, 355, 256, 232, 159, 99.

**Source:** Tomašić et al. (2004).

**Comments:** The identification of the sample was done by powder X-ray diffraction. The chemical composition of the sample was determined by ICP measurement. The Raman spectrum was obtained on a sample which was regained crystal structure after heating up to 1000 °C. The spectrum is of poor quality because the crystallization was not completed.

**Afmite**  $\text{Al}_3(\text{OH})_4(\text{H}_2\text{O})_3(\text{PO}_4)(\text{PO}_3\text{OH})\cdot \text{H}_2\text{O}$ 

**Origin:** Fumade, Tarn, France (type locality).

**Experimental details:** Raman scattering measurements have been performed on an oriented crystal using 514 nm laser radiation. The laser beam was incident on the (001) crystal face. The radiation power on the sample was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** No data: only a figure of the Raman spectrum of afmite is given in the cited paper.

**Source:** Kampf et al. (2011b).

**Comments:** The sample was characterized by electron microprobe analysis and powder X-ray diffraction. The crystal structure is solved. For the Raman spectrum of afmite see also Sanchez-Moral et al. (2011).

**Afwillite**  $\text{Ca}_3[\text{SiO}_4][\text{SiO}_2(\text{OH})_2]\cdot 2\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm laser radiation. The radiation power on the sample was 150 mW.

**Raman shifts (cm<sup>-1</sup>):** 3973, 856s, 819, 785, 550, 410.

**Source:** Stodolski et al. (1985).

**Comments:** The sample was characterized by powder X-ray diffraction.

**Agakhanovite-(Y)**  $\text{YCa}\square\text{KBe}_3\text{Si}_{12}\text{O}_{30}$ 

**Origin:** Heftetjern pegmatite, Tørdal, Southern Norway (type locality).

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 3730w, 3670w, ~3560–3400 (broad), 1120, 1000w, 480s, 360w, 290w, 140.

**Source:** Hawthorne et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved.

**Agardite-(Ce)**  $\text{CeCu}^{2+}_6(\text{AsO}_4)_3(\text{OH})_6 \cdot 3\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power at the sample was 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 885, 868s, 834, 809, 527w, 493w, 475, 461w, 427w, 393w, 319w, 283w, 235, 197w, 170w, 158w, 136w.

**Source:** Frost et al. (2004f).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis, but no analytical data are given in the cited paper.

**Agardite-(La)**  $\text{LaCu}^{2+}_6(\text{AsO}_4)_3(\text{OH})_6 \cdot 3\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power at the sample was 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 888, 867s, 832, 803, 524w, 491w, 473, 470, 425w, 391, 317w, 274w, 234, 196w, 165, 136w.

**Source:** Frost et al. (2004f).

**Comments:** No independent analytical data are given in the cited paper.

**Agardite-(Y)**  $\text{YCu}^{2+}_6(\text{AsO}_4)_3(\text{OH})_6 \cdot 3\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power at the sample was 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 915, 870s, 833, 798w, 557w, 539w, 514w, 486, 468w, 434w, 294w, 267w, 239, 192, 176w, 167w, 142.

**Source:** Frost et al. (2004f).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis, but no independent analytical data are given in the cited paper. For the Raman spectrum of agardite-(Y) see also Morrison et al. (2013).

**Agricolaite**  $K_4(UO_2)(CO_3)_3$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented polycrystalline sample using 514.5 nm  $Ar^+$  laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1569w, 1543w, 1354w, 1320, 1065sh, 1055, 1046sh, 879w, 863w, 806s, 785w, 725, 719w, 693w, 307, 288, 262s, 251w, 249w, 241, 191w, 176sh, 165, 154sh, 132, 123, 119sh, 106, 96w, 91w, 82, 74w, 63, 48w.**Source:** Anderson et al. (1980).**Comments:** The compound was synthesized hydrothermally and characterized by powder X-ray diffraction data.**Ahlfeldite**  $Ni(SeO_3) \cdot 2H_2O$ **Origin:** Pacajake Mine, Bolivia.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3466, 3385s, 3329, 3251, 2185, 2130, 861, 832s, 803s, 751, 719, 595, 532, 508, 430s, 421, 348, 267, 218, 177s, 149s.**Source:** Frost and Keeffe (2009f).**Comments:** No independent analytical data are provided for the sample used.**Ahrensite**  $\gamma\text{-Fe}_2(SiO_4)$ **Origin:** Tissint Martian meteorite (type locality).**Experimental detail:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.3 nm  $Ar^+$  laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 843, 795, 672, 213.**Source:** Ma et al. (2016a).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.**Aikinite**  $CuPbBiS_3$ **Origin:** Karrantza Valley, western area of the Basque Co., Spain.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 633 nm laser radiation with the laser radiation power at the sample of 50 mW and 785 nm laser radiation with the nominal laser radiation power of 150 mW, using filters of 1% and 10%.**Raman shifts (cm<sup>-1</sup>):** 326s, 227s.**Source:** Goienaga et al. (2011).**Comments:** The sample identification was done by means of electron fluorescence analysis.

**Ajoite**  $K_3Cu^{2+}Al_{20}Si_{29}O_{76}(OH)_{16}\cdot 8H_2O$ 

**Origin:** New Cornelia Mine in the Ajo District of Pima County, Arizona, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power at the sample is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3619, 3589, 3574, 3553, 3394, 1155, 1139, 1069, 1048, 1015, 962, 796, 672, 630, 516, 484, 437, 411, 343, 325, 304.

**Source:** Frost and Xi (2012m).

**Comments:** No independent analytical data are given for the sample used.

**Akaganeite**  $(Fe^{3+},Ni^{2+})_8(OH,O)_{16}Cl_{1.25}\cdot nH_2O$ 

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented powdery sample using 636.4 nm laser radiation. The laser radiation power on the sample was 0.34 mW.

**Raman shifts (cm<sup>-1</sup>):** 717, 614w, 537, 415sh, 390s, 311s.

**Source:** Nieuwoudt et al. (2011).

**Comments:** The identification of the sample was done by powder X-ray diffraction data. For the Raman spectra of akaganeite see also Das and Hendry (2011) and Aramendia et al. (2014).

**Åkermanite**  $Ca_2MgSi_2O_7$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented powdered sample in a 90°-scattering geometry using 488 nm laser radiation. The laser radiation power on the sample was from 300 up to 500 mW.

**Raman shifts (cm<sup>-1</sup>):** 1067w, 1012w, 990sh, 948w, 927sh, 906s, 664s, 603, 515, 484, 448, 361sh, 317, 269w, 220, 210, 97.

**Source:** Sharma et al. (1988).

**Comments:** The identification of the sample synthesized from glass was performed by comparison with published Raman data.

**Åkermanite Sr analogue**  $Sr_2Mg(Si_2O_7)$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed using 632.8 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 984sh, 975w, 901s, 838w, 653, 590w, 568w, 475w, 450w, 315.

**Source:** Gabelica-Robert and Tarte (1979).

**Comments:** The sample synthesized by solid-state reaction was characterized by powder X-ray diffraction.

**Akimotoite** MgSiO<sub>3</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented powdered sample using 514.5 nm laser radiation. The nominal laser radiation power was 200 mW.**Raman shifts (cm<sup>-1</sup>):** 802s, 687, 622, 481, 412, 352, 291.**Source:** Okada et al. (2008).**Comments:** The sample was characterized by powder X-ray diffraction data and chemical analysis.

For the Raman spectra of akimotoite see also Ferroir et al. (2008) and Chen and Xie (2015).

**Aklimaite** Ca<sub>4</sub>[Si<sub>2</sub>O<sub>5</sub>(OH)<sub>2</sub>](OH)<sub>4</sub>·5H<sub>2</sub>O**Origin:** Lakargi Mt., Upper Chegem caldera, Kabardino-Balkaria, Northern Caucasus, Russia (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power on the sample was 44 mW.**Raman shifts (cm<sup>-1</sup>):** 3611, 3593, 3549, 3535, 3261, 1666, 1575, 1490, 1380, 1344, 1087w, 999s, 960sh, 924sh, 908s, 838, 680s, 569, 543, 488, 444, 406w, 340s, 254s, 191s, 142.**Source:** Zadov et al. (2013).**Comments:** The wavenumbers are indicated for the maxima of individual bands obtained as a result of the spectral curve analysis. The sample was characterized by powder X-ray diffraction data and chemical analysis. The crystal structure is solved.**Alabandite** MnS**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.4 nm laser radiation. The laser radiation power on the sample was 2 mW.**Raman shifts (cm<sup>-1</sup>):** 580w, 285, 230, 160.**Source:** Avril et al. (2013).**Comments:** The cubic monosulfide alabandite does not have a first-order Raman spectrum due to its ideal rock salt structure. Through local symmetry breaking, the inactive or infrared-active vibrational modes become Raman active. As a result, the Raman peaks are broad and have a very weak intensity. For the Raman spectrum of alabandite see also Ma et al. (2012b).**Alacránite** As<sub>8</sub>S<sub>9</sub>**Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 785 nm laser radiation. The nominal laser radiation power was 3 mW. A non-oriented crystal.**Raman shifts (cm<sup>-1</sup>):** 384, 361, 350sh, 340s, 329, 307, 240sh, 230s.**Source:** Pagliai et al. (2011).**Alamosite** PbSiO<sub>3</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 488 nm laser radiation. A 90°-scattering geometry was employed. The nominal laser radiation power was in the range from 50 to 200 mW.

**Raman shifts (cm<sup>-1</sup>):** 1047w, 1002sh, 987, 955, 946, 924w, 897w, 870w, 780w, 735w, 683w, 647w, 590, 534w, 495w, 469w, 448, 388w, 371w, 355, 324w, 306sh, 272w, 218w, 171w, 146w, 109s, 90, 82, 70, 59s.

**Source:** Furukawa et al. (1979).

**Comments:** The hydrothermally synthesized sample was characterized by powder X-ray diffraction.

### Alarsite Al(AsO<sub>4</sub>)

**Origin:** Synthetic.

**Experimental detail:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 514.5 nm laser radiation. The laser radiation power at the sample was 400 mW.

**Raman shifts (cm<sup>-1</sup>):** 1031w, 1000w, 985s, 939, 930sh, 630w, 613w, 573w, 450sh, 420s, 390, 371w, 347, 319, 311, 260w, 226, 198, 136, 123, 98.

**Source:** Dultz et al. (1975).

**Comments:** No independent analytical data are provided for the sample used.

### Albertiniite Fe<sup>2+</sup>(SO<sub>3</sub>)·3H<sub>2</sub>O

**Origin:** Monte Falò Pb-Zn mine, Coiromonte, Armeno municipality, Verbano Cusio Ossola province, Piedmont, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 473.1 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3350s, 3215s, 1660w, 970s, 950s, 910, 860w, 825w, 660w, 600w, 495sh, 482, 457, 438sh, 324w, 279w, 241w, 197w, 172, 123.

**Source:** Vignola et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### Albite Na(AlSi<sub>3</sub>O<sub>8</sub>)

**Origin:** Alinci, Macedonia.

**Experimental detail:** Raman scattering measurements have been performed on a powdered sample using 532 nm laser radiation. The laser radiation power at the sample was 7 mW.

**Raman shifts (cm<sup>-1</sup>):** 1115w, 100w, 1034w, 1006w, 976w, 816w, 764w, 726w, 646w, 579w, 508s, 479, 458w, 408w, 329w, 291s, 270sh, 251w, 209w, 185w, 171w, 162w, 148w, 113w.

**Source:** Makreski et al. (2009).

**Comments:** The sample was characterized by powder X-ray diffraction. The assignment of Raman bands given in the cited paper is incorrect. For the correct assignment see Többens et al. (2005). For the Raman spectra of albite see also Frezzotti et al. (2012), Karwowski et al. (2013), and McKeown (2005).

### Aleksite PbBi<sub>2</sub>Te<sub>2</sub>S<sub>2</sub>

**Origin:** Panarechensk volcanic-tectonic formation, Kola Peninsula, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 232–235w, 143–147s, 99–103s, (75–79w).

**Source:** Voloshin et al. (2015a).

**Comments:** The samples used were characterized by electron microprobe analyses. For the Raman spectrum of aleksite see also Gehring et al. (2015).

**Alforsite OH-analogue**  $\text{Ba}_5(\text{PO}_4)_3(\text{OH})$

**Origin:** Synthetic.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power at the sample was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 3608, 3583w, 1057w, 1029, 1007w, 934s.

**Source:** Yoder et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data and chemical analysis. It contains 2.95 wt% of a carbonate.

**Allactite**  $\text{Mn}^{2+}{}_7(\text{AsO}_4)_2(\text{OH})_8$

**Origin:** Nordmark, Sweden (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power at the sample is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3561s, 3523, 3489s, 3446, 3395, 3292, 1011, 909, 883s, 859s, 834s, 827s, 808s, 779s, 743, 633, 470, 452, 422, 393, 377, 360s, 350, 331, 323, 298, 288, 271, 241, 197, 158.

**Source:** Frost and Weier (2006).

**Comments:** The sample was characterized by electron microprobe analysis.

**Allanite (Ce)**  $\text{CaCe}(\text{Al}_2\text{Fe}^{2+})[\text{Si}_2\text{O}_7][\text{SiO}_4]\text{O(OH)}$

**Origin:** Brahmaputra River, Bangladesh.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm laser radiation. A nearly 180°-scattering geometry was employed. The laser radiation power on the sample is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1062, 972s, ~900–920sh, 689, ~630, ~550, 457s, 421s, ~380, ~270, ~220, ~180.

**Source:** Andò and Garzanti (2014).

**Comments:** No independent analytical data are given for the sample used.

**Allanite-(Nd)**  $\text{CaNd}(\text{Al}_2\text{Fe}^{2+})[\text{Si}_2\text{O}_7][\text{SiO}_4]\text{O(OH)}$

**Origin:** Kracovice pegmatite, Moldanubian Zone, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 and 633 nm laser radiations. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1052, 995, 964, 926, 897, 873, 841, 691, 632, 595, 573, 571, 493, 457, 442, 428, 385, 354, 321, 294, 279, 256, 221, 199, 160, 126, 107.

**Source:** Čopjaková et al. (2015).

**Comments:** The sample was characterized by ICP and electron microprobe analyses. The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Allanpringite**  $\text{Fe}^{3+}_3(\text{PO}_4)_2(\text{OH})_3 \cdot 5\text{H}_2\text{O}$

**Origin:** Grube Mark, near Essershausen, *ca.* 5 km SE of Weilburg/Lahn, Taunus, Hesse, Germany (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm laser radiation. A 180°-scattering geometry was employed. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~3567, 3412, ~3197, ~3060, ~3052, ~1652, ~1100sh, 1060, 1023, 1009, 987, 590, 555, 516, 491, 470, 424, 355, ~309, 292.

**Source:** Kolitsch et al. (2006).

**Comments:** The sample was characterized by powder X-ray diffraction data and chemical analyses. The crystal structure is solved.

**Allendeite**  $\text{Sc}_4\text{Zr}_3\text{O}_{12}$

**Origin:** Allende meteorite (type locality).

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented crystal using 514.5 nm laser radiation. The laser radiation power on the sample was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** No data: only a figure of the Raman spectrum is given in the cited paper.

**Source:** Ma et al. (2014b).

**Comments:** The sample was characterized by powder X-ray diffraction data and chemical analyses. The strong Raman peaks in the 1300–1000 cm<sup>-1</sup> region may be caused by REE luminescence.

**Allophane**  $\text{Al}_2\text{O}_3(\text{SiO}_2)_{1.3-2.0} \cdot 2.5-3.0\text{H}_2\text{O}$

**Origin:** Reppia, NW Italy.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 and 785 nm laser radiations. The nominal laser radiation power on the sample was 1.4 and 4 mW, respectively.

**Raman shifts (cm<sup>-1</sup>):** 3420s (broad), 2942w, 1638w, 1357w, 1103, 982w, 858–859s.

**Almandine**  $\text{Fe}^{2+}_3\text{Al}_2(\text{SiO}_4)_3$

**Origin:** An unknown locality in Mongolia.

**Experimental details:** Micro-Raman scattering measurements have been performed on a single crystal using 488 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1038s, 930, 916s, 897, 863, 630, 596, 556, 581, 500s, 475, 370s, 342s, 323, 314, 256, 216s, 171s, 166s.

**Source:** Kolesov and Geiger (1998).

**Comments:** Measurements were made perpendicular to the {100} and {110} faces of a single crystal. The sample identification was done by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectra of almandine see also Mingsheng et al. (1994), Makreski et al.

(2005b), Bersani et al. (2009), Ferrari et al. (2009), Jovanovski et al. (2009), Frezzotti et al. (2012), and Andò and Garzanti (2014).

**Almarudite**  $K(\square, Na)_2(Mn, Fe, Mg)_2(Be, Al)_3Si_{12}O_{30}$ 

**Origin:** Bellerberg volcano, Eifel area, Germany (type locality).

**Experimental details:** Micro-Raman scattering measurements have been performed on a single crystal along [0001], using 633 nm He-Ne laser radiation. The nominal laser radiation power was 17 mW.

**Raman shifts (cm<sup>-1</sup>):** 1134s, 1053, 991, 931, 847, 778, 698w, 653, 640, 608, 563, 554, 493s, 460, 382, 346w, 311sh, 290s, 276sh, 236w, 160, 135s, 108sh, 84.

**Source:** Lengauer et al. (2009).

**Comments:** The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

**Alstonite**  $Ba Ca(CO_3)_2$ 

**Origin:** Moore Hill, England.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented polycrystalline sample using 488 and 514.5 nm laser radiations. The nominal laser radiation power at the sample was 200 mW.

**Raman shifts (cm<sup>-1</sup>):** 1489, 1092s, 1067s, 709sh, 693, 284, 252w, 211w, 196, 170, 145s, 130, 102, 79s.

**Source:** Scheetz and White (1977).

**Comments:** No independent analytical data are provided for the sample used.

**Altaite**  $PbTe$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 laser radiation. The laser radiation power at the sample was from 1 to 2 mW.

**Raman shifts (cm<sup>-1</sup>):** Altaite is inactive in Raman due to halite-type structure.

**Source:** Vymazalová et al. (2014).

**Althausite**  $Mg_4(PO_4)_2(OH, O)(F, \square)$ 

**Origin:** Sapucaia pegmatite mine, Minas Gerais, Brazil (?).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3688w, 3653w, 3535, 3523sh, 3511sh, 3500s, 3488, 3472sh, 3455w, 1320br, 1154, 1130s, 1114, 1078w, 1062w, 1049w, 1033s, 993s, 986sh, 964s, 950sh, 917w, 902w, 860w, 668, 638sh, 628sh, 612, 594, 580, 537, 510sh, 499, 488sh, 466, 458, 436sh, 426, 412.

**Source:** Frost et al. (2014p).

**Comments:** The sample identification was made only by SEM. The broad band at 1320 cm<sup>-1</sup> may be due to impurities.

**Alum-(K)**  $\text{KAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ 

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily sample using 488 nm laser radiation. The nominal laser radiation power at the sample was 220 mW. A 90°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3396s, 3072, 1130, 1104w, 989s, 974s, 614, 455, 442w.

**Source:** Barashkov et al. (2004).

**Comments:** For the Raman spectra of alum-(K) see also Makreski et al. (2005a), Brooker and Eysel (1990), and Rao (1941).

**Alum-(K)**  $\text{KAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ 

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 1064 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1086w, 991s, 872w, 841w, 818w, 804w, 757w, 714w, 684w, 603, 517w, 416w, 386w.

**Source:** Makreski et al. (2005a).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of alum-(K) see also Rao (1941), Brooker and Eysel (1990), Barashkov et al. (2004), and Frezzotti et al. (2012).

**Aluminite**  $\text{Al}_2(\text{SO}_4)(\text{OH})_4 \cdot 7\text{H}_2\text{O}$ 

**Origin:** Newhaven, East Sussex, England, UK.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented sample using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not identified

**Raman shifts (cm<sup>-1</sup>):** 3588, 3569, 3439, 3378, 3294, 3157, 2930, 2875, 1136w, 1094, 1069w, 999, 93s, 990, 793w, 680, 642, 631, 607, 575, 490, 440, 333, 317, 285.

**Source:** Frost et al. (2015k).

**Comments:** The sample was characterized only by qualitative EDS analysis.

**Aluminocerite-(Ce)**  $(\text{Ce},\text{REE},\text{Ca})_9(\text{Al},\text{Fe}^{3+})(\text{SiO}_4)_3[\text{SiO}_3(\text{OH})]_4(\text{OH})_3$ 

**Origin:** Ratti quarry, near Baveno, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power at the sample was from 10 to 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 3646w, 1098, 1083, 1010w, 977w, 869, 816, 763, 647w, 579, 507s, 478s, 455, 412, 327, 288, 266, 250w, 205, 181, 168, 147w.

**Source:** Nestola et al. (2009).

**Comments:** The sample was identified by electron microprobe analyses and single-crystal X-ray diffraction.

**Aluminocopiaite**  $(\text{Al},\text{Mg})\text{Fe}^{3+}_4(\text{SO}_4)_6(\text{OH},\text{O})_2 \cdot 20\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532.0 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3566, 3384, 3164, 2428, 1638, 1220, 1123, 1019, 989, 636, 614, 598, 555, 476, 452, 300, 270, 247.**Source:** Kong et al. (2011b).**Comments:** The sample was identified by powder X-ray diffraction data.**Alumohydrocalcite**  $\text{CaAl}_2(\text{CO}_3)_2(\text{OH})_4 \cdot 3\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1091sh, 729, 590.**Source:** Jay et al. (2015).**Comments:** Alumohydrocalcite was identified by the Raman spectrum using data from the RRUFF database as a reference.**Alunite**  $\text{KAl}_3(\text{SO}_4)_2(\text{OH})_6$ **Origin:** Argillic zone hosted by volcanic rocks in Bulgaria.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 1 mW.**Raman shifts (cm<sup>-1</sup>):** 3508s, 3480s, 3068w, 1186, 1151, 1077, 1024s, 653, 560, 508, 484, 381, 345, 234, 161.**Source:** Maubec et al. (2012).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of alunite see also Toumi and Tlili (2008) and Frezzotti et al. (2012).**Alunogen**  $\text{Al}_2(\text{SO}_4)_3(\text{H}_2\text{O})_{12} \cdot 5\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 532 nm laser radiation. The nominal laser radiation power was 9 mW.**Raman shifts (cm<sup>-1</sup>):** 3246br, 3078sh, 1126w, 1086w, 992s, 612, 528w, 470, 339w, 309w.**Source:** Wang and Zhou (2014).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of alunogen see also Buzatu et al. (2016).**Alwilkinsite-(Y)**  $\text{Y}(\text{UO}_2)_3(\text{SO}_4)_2\text{O}(\text{OH})_3(\text{H}_2\text{O})_7 \cdot 7\text{H}_2\text{O}$ **Origin:** Blue Lizard mine, San Juan Co., Utah, USA (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single sample using 780 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1325, 1265s, 1135w, 1080w, 1035, 1015, 990, 900w, 840s, 605, 555, 530, 465w, 455, 380, 320, 288, 268, 240, 200, 170, 145w, 135w, 108w, 90w, 72w, 60.

**Comments:** The broad bands at around 1600 cm<sup>-1</sup> are the result of the fluorescence. The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### Amarantite Fe<sup>3+</sup><sub>2</sub>O(SO<sub>4</sub>)<sub>2</sub>·7H<sub>2</sub>O

**Origin:** Caracoles, Sierra Gorda district, Chile (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3529s, 3480, 3401, 3340, 3227, 3089, 3025, 1648, 1577, 1441, 1233, 1195, 1131, 1098s, 1054, 1039, 1017s, 1006sh, 650w, 622w, 602w, 543w, 491, 451sh, 409, 399sh, 346, 309, 290, 255, 247, 229, 212, 205, 195s, 183sh, 176, 162, 149, 139, 129, 113, 107.

**Source:** Frost et al. (2013a, d).

**Comments:** The sample identification was done only by SEM.

### Amblygonite LiAl(PO<sub>4</sub>)F

**Origin:** Penig, Saxony, Germany.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488.0 nm laser radiation. The nominal laser radiation power at the sample was 200 mW.

**Raman shifts (cm<sup>-1</sup>):** 3348 (broad), 1066, 1043s, 1008s, 645s, 604s, 423, 154.

**Source:** Rondeau et al. (2006).

**Comments:** The sample identification was done by powder X-ray diffraction data and by electron microprobe analysis. For the Raman spectra of amblygonite see also Dias et al. (2011) and Frezzotti et al. (2012).

### Ambrinoite [K,(NH<sub>4</sub>)<sub>2</sub>](As,Sb)<sub>6</sub>(Sb,As)<sub>2</sub>S<sub>13</sub>·H<sub>2</sub>O

**Origin:** Oulx, Susa Valley, Torino, Piedmont, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 628 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3475w, 3150w, 1595w, 1423w, 393s, 371, 364, 352, 341, 324, 294, 216, 207.

**Source:** Biagioni et al. (2011a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved.

### Ameghinite NaB<sub>3</sub>O<sub>3</sub>(OH)<sub>4</sub>

**Origin:** Tincalayu deposit, Salta province, Argentina (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm laser radiation. The laser radiation power is not indicated. The Raman shifts

have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3385, 3343, 3275, 3249, 3230, 3203s, 3191, 1724, 1604, 1531, 1403, 1371, 1320, 1281, 1245, 1213, 1087, 1061, 1027s, 1014, 887, 861, 786, 769, 755, 730, 711, 701, 656, 624, 620s, 615, 574, 530, 503, 464, 405, 367, 352, 224, 197, 145, 135s, 119.

**Source:** Frost and Xi (2012i).

**Comments:** The sample was characterized by powder X-ray diffraction data and chemical analysis.

#### Amesite Mg<sub>2</sub>Al(AlSiO<sub>5</sub>)(OH)<sub>4</sub>

**Origin:** Artificial (a product of hydrothermal alteration of olivine in the presence of AlCl<sub>3</sub>).

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 514 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~1080w, ~1000w, ~845w, ~700s, ~540s, ~495, ~480, ~405s, ~345w, ~273, ~190.

**Source:** Andreani et al. (2013).

**Comments:** The sample was identified as amesite by comparison to the reference spectrum from RUFF database.

#### Ammoniojarosite (NH<sub>4</sub>)Fe<sup>3+</sup><sub>3</sub>(SO<sub>4</sub>)<sub>2</sub>(OH)<sub>6</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm laser radiation. The nominal laser radiation power was less than 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 3485sh, 3434, 3360sh, 3210, 1164, 1092, 1006s, 637sh, 623s, 565, 451, 423s, 342w, 301, 218s, 136.

**Source:** Chio et al. (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of ammoniojarosite see also Sasaki et al. (1998).

#### Grunerite □Fe<sup>2+</sup><sub>2</sub>Fe<sup>2+</sup><sub>5</sub>Si<sub>8</sub>O<sub>22</sub>(OH)<sub>2</sub>

**Origin:** South Africa.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented fibrous aggregate ("amosite") using 632 nm laser radiation. The nominal laser radiation power was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 1093w, 1020s, 968, 904w, 659s, 528, 507w, 423w, 400w, 368w, 348, 307w, 289w, 252w, 216, 182s, 155s.

**Source:** Rinaudo et al. (2004).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

#### Analcime Na(AlSi<sub>2</sub>O<sub>6</sub>)·H<sub>2</sub>O

**Origin:** Aussig, Bohemia, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using Nd-YAG laser radiation. The laser radiation power at the sample was 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 1104, 591w, 483s, 390, 298.

**Source:** Mozgawa (2001).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of analcime see also Frost et al. (2014i).

### Anapaite Ca<sub>2</sub>Fe<sup>2+</sup>(PO<sub>4</sub>)<sub>2</sub>·4H<sub>2</sub>O

**Origin:** Bellver de la Cerdanya, Lérida, Spain.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3248, 3176, 3101, 3022, 2882, 2777, 1658w, 1373w, 1071, 1039, 992w, 965sh, 943s, 808w, 777, 654, 622, 582, 546, 445, 432, 352, 335, 287, 266, 231sh, 281, 202, 186, 170, 155, 149, 136.

**Source:** Frost et al. (2013t).

**Comments:** The sample identification was done only by SEM.

### Anatase TiO<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdery sample using 488 nm laser radiation. The laser radiation power is not indicated. A 90°-scattering geometry was employed. The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 640s, 515, 398, 198w, 147s.

**Source:** Balachandran and Eror (1982).

**Comments:** The sample was characterized by ICP method and electron microprobe analysis. For the Raman spectra of anatase see also Zajzon et al. (2013), Andò and Garzanti (2014), and Martins et al. (2014).

### Anatase TiO<sub>2</sub>

**Origin:** Perkupa, Hungary.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm laser radiation. The nominal laser radiation power at the sample was 13 mW.

**Raman shifts (cm<sup>-1</sup>):** 470, 248s, 226, 182s, 155.

**Source:** Zajzon et al. (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectra of anatase see also Balachandran and Eror (1982), Andò and Garzanti (2014), and Martins et al. (2014).

### Ancylite-(Ce) CeSr(CO<sub>3</sub>)<sub>2</sub>(OH)·H<sub>2</sub>O

**Origin:** Bear Lodge, Wyoming, USA.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1106, 1086s, 1077s, 861w, 744w, 725, 705w, 466, 299, 252s, 223s, 193, 130w, 123w.

**Source:** Chakhmouradian et al. (2017).

**Comments:** The sample was characterized by electron microprobe analyses.

### Andalusite Al<sub>2</sub>SiO<sub>5</sub>

**Origin:** No data.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 1111, 1065, 952, 920s, 834, 719, 606, 553, 453, 361, 323, 293s, 278.

**Source:** Frezzotti et al. (2012).

**Comments:** The data are from the database [www.ens-lyon.fr/LST/Raman](http://www.ens-lyon.fr/LST/Raman). For the Raman spectra of andalusite see also Mernagh and Liu (1991) and Andò and Garzanti (2014).

### Andersonite Na<sub>2</sub>Ca(UO<sub>2</sub>)(CO<sub>3</sub>)<sub>3</sub>·6H<sub>2</sub>O

**Origin:** Grants, New Mexico, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3558, 3510, 2415, 1406, 1370, 1092, 1080, 928, 833, 831, 742, 696, 299, 284, 272, 242, 224, 182, 164.

**Source:** Frost et al. (2004b).

**Comments:** For the Raman spectra of andersonite see also Stefaniak et al. (2009) and Driscoll et al. (2014).

### Andradite Ca<sub>3</sub>Fe<sup>3+</sup><sub>2</sub>(SiO<sub>4</sub>)<sub>3</sub>

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 4480 Å laser radiation. The nominal laser radiation power was 100–150 mW.

**Raman shifts (cm<sup>-1</sup>):** 1000w, 870s, 840w, 816w, 726, 576, 573s, 444, 363s, 366w, 228, 168.

**Source:** Mingsheng et al. (1994).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectra of andradite see also Kolesov and Geiger (1998), Bersani et al. (2009), Katerinopoulou et al. (2009), and Andò and Garzanti (2014).

### Andradite Ca<sub>3</sub>Fe<sup>3+</sup><sub>2</sub>(SiO<sub>4</sub>)<sub>3</sub>

**Origin:** Maronia area, western Thrace, Greece.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm laser radiation. The laser radiation power at the sample was 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 750, 520, 350.

**Source:** Katerinopoulou et al. (2009).

**Comments:** A Cr-, Ti-, and Zr-rich variety was investigated. The empirical formula is (Ca<sub>2.99</sub>Mn<sub>0.03</sub>)(Fe<sup>3+</sup><sub>0.67</sub>Cr<sub>0.54</sub>Al<sub>0.33</sub>Ti<sub>0.29</sub>Zr<sub>0.15</sub>)(Si<sub>2.42</sub>Ti<sub>0.24</sub>Fe<sub>0.18</sub>Al<sub>0.14</sub>)O<sub>12</sub>(OH)<sub>0.11</sub>. The Mössbauer analysis

showed that the total Fe is ferric, preferentially located at the octahedral site. For the Raman spectra of andradite see also Mingsheng et al. (1994), Kolesov and Geiger (1998), Bersani et al. (2009), and Andò and Garzanti (2014).

### Andychristyite $\text{PbCu}^{2+}\text{Te}^{6+}\text{O}_5(\text{H}_2\text{O})$

**Origin:** Otto Mt., near Baker, California, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 780 nm laser radiation. The laser radiation power at the sample was from 4 to 8 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3306w, 870, 708s, 665s, 625s, 552, 461, 402, 316, 291, 242, 214, 181.

**Source:** Kampf et al. (2016b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved.

### Angastonite $\text{CaMgAl}_2(\text{PO}_4)_2(\text{OH})_4 \cdot 7\text{H}_2\text{O}$

**Origin:** Angaston, South Australia (type locality).

**Experimental details:** Raman scattering measurements have been performed using 785 nm laser radiation. The method of sample preparation and the laser radiation power are not indicated.

**Raman shifts ( $\text{cm}^{-1}$ ):** 1159, 988, 630, 539, 502, 415.

**Source:** Mills et al. (2008).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

### Anglesite $\text{Pb}(\text{SO}_4)$

**Origin:** Monte Poni, Sardinia, Italy.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The nominal laser radiation power at the sample was 100 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 1157, 1055w, 978s, 646w, 612, 553w, 450s.

**Source:** Buzgar et al. (2009).

**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. Methods of the identification of the sample are not indicated. For the Raman spectra of anglesite see also Bouchard and Smith (2003), Jehlička et al. (2009b), and Petrov (2014).

### Anhydrite $\text{Ca}(\text{SO}_4)$

**Origin:** Bleiberg, Carinthia, Austria.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm Nd-YAG laser radiation. The nominal laser radiation power at the sample was 100 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 1160, 1129s, 1017s, 678, 630, 503s, 420w, 235w.

**Source:** Buzgar et al. (2009).

**Comments:** For the Raman spectra of anhydrite see also Sarma et al. (1998), Makreski et al. (2005a), White (2009), and Ciobotă et al. (2012).

**Anilite** Cu<sub>7</sub>S<sub>4</sub>**Origin:** Synthetic.**Experimental details:** No data.**Raman shift (cm<sup>-1</sup>):** 470s.**Source:** Palve et al. (2016).**Comments:** The sample was characterized by powder X-ray diffraction data.**Ankerite** Ca(Fe<sup>2+</sup>,Mg)(CO<sub>3</sub>)<sub>2</sub>**Origin:** Brusson, Val d'Ayas, Valle d'Aosta, Italy.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1091, 716, 283.**Source:** Andò and Garzanti (2014).**Comments:** No independent analytical data are provided for the sample used.**Annabergite** Ni<sub>3</sub>(AsO<sub>4</sub>)<sub>2</sub>·8H<sub>2</sub>O**Origin:** 132 North Deposit, Widgiemooltha District, Western Australia.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3419, 3209, 3185, 3010, 941, 854, 800, 676, 466, 442, 401, 350, 321, 286, 260, 242, 225, 203, 175, 160, 155, 119.**Source:** Frost et al. (2003g).**Comments:** No independent analytical data are provided for the sample used.**Annite** KFe<sup>2+</sup><sub>3</sub>(AlSi<sub>3</sub>O<sub>10</sub>)(OH)<sub>2</sub>**Origin:** Sierra los Filahres, Spain.**Experimental details:** Raman scattering measurements have been performed on a partially oriented sample using 488 or 514.5 nm laser radiations. The spectrum was recorded with the electric field polarized either parallel or perpendicular to the cleavage plane. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3654, 1045w, 676s, 272w, 182s.**Source:** Tlili et al. (1989).**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectrum of annite see also Rancourt et al. (2001).**Annite Cl-analogue** KFe<sup>2+</sup><sub>3</sub>(AlSi<sub>3</sub>O<sub>10</sub>)(Cl,OH)<sub>2</sub>**Origin:** Khlebodarovka, Azov Sea region, Ukraine.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal. The wavelength of laser excitation line and the laser radiation power are not indicated.**Raman shifts (cm<sup>-1</sup>):** 3647s, 989s, 811, 660s, 553w, 403, 353.

**Source:** Sharygin et al. (2014).

**Comments:** The Cl-analogue of annite from Khlebodarovka contains up to 7.3 wt% Cl.

### Anorpiment $\text{As}_2\text{S}_3$

**Origin:** Palomo mine, Castrovirreyna province, Huancavelica department, Peru (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 643w, 387sh, 375, 348sh, 334s, 324sh, 234w, 192, 187, 176, 168sh.

**Source:** Kampf et al. (2011a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

### Anorthite $\text{Ca}(\text{Al}_2\text{Si}_2\text{O}_8)$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 488.0 nm laser radiation. The nominal laser radiation power was 600 mW. A 90°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1124w, 1072s, 1044sh, 998sh, 974, 949sh, 908sh, 756w, 741sh, 681, 620w, 590w, 553, 503s, 484sh, 427w, 400w, 369w, 316w, 281, 273, 253, 200sh, 182, 139, 88, 63.

**Source:** Matson et al. (1986).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of anorthite see also Ling et al. (2011).

### Antarcticite $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using 532.2 nm laser radiation. The nominal laser radiation power was 120 mW.

**Raman shifts (cm<sup>-1</sup>):** 3431/3430s, 3410, 3404/3405sh, 3386, 3242.

**Source:** Baumgartner and Bakker (2010).

**Comments:** The Raman spectrum of antarcticite was recorded at -190 °C.

### Antarcticite $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed at -190 °C on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3430s, 3384sh, 3245, 1664, 1647.

**Source:** Uriarte et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Anthophyllite**  $\square\text{Mg}_2\text{Mg}_5\text{Si}_8\text{O}_{22}(\text{OH})_2$ 

**Origin:** Bresimo Mine, near Trento, Trentino Alto Adige, Italy.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented fibers using 632 nm laser radiation. The nominal laser radiation power was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 1044, 928, 699w, 674s, 539, 503w, 433, 410, 387, 342w, 304, 265, 254, 222w, 188.

**Source:** Rinaudo et al. (2004).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectrum of anthophyllite see also Petry et al. (2006), Kloporgge et al. (2001a), and Leissner et al. (2015).

**Anthophyllite**  $\square\text{Mg}_2\text{Mg}_5\text{Si}_8\text{O}_{22}(\text{OH})_2$ 

**Origin:** Origätri, Finland.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented fibers, using 244 nm laser radiation. The laser radiation power at the sample was less than 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 3691s, 3666s, 1052s, 1003sh, 669s, 530s.

**Source:** Petry et al. (2006).

**Comments:** The sample was characterized by electron microprobe analysis. For the Raman spectrum of anthophyllite see also Rinaudo et al. (2004), Kloporgge et al. (2001a), and Leissner et al. (2015).

**Anthraxolite**

**Origin:** Perya, Novaya Zemlya Islands, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 1.2 mW.

**Raman shifts (cm<sup>-1</sup>):** The first-order spectrum: 1180–1200, 1330–1350, ~1500, 1580–1600, 1610–1620sh. The second-order spectrum: 2500, 2700, 2850, 2950, 3230.

**Source:** Golubev et al. (2016).

**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Antigorite**  $\text{Mg}_3\text{Si}_2\text{O}_5(\text{OH})_4$ 

**Origin:** Piedmont Alps, Italy.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 1064 nm laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1044, 683s, 635w, 520w, 375s, 230s.

**Source:** Rinaudo et al. (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Antigorite**  $Mg_3Si_2O_5(OH)_4$ **Origin:** Escambray Massif, Central Cuba.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser output power was from 200 to 600 mW. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 3774, 3760w, 3729s, 3709, 3687, 3658, 3606w, 685s, 377s, 233s.**Source:** Auzende et al. (2004).**Comments:** The Raman shifts are partly indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Antimonselite**  $Sb_2Se_3$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a  $\mu\text{m}$  thick layer using 532 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 252, 189.**Source:** Zhou et al. (2014).**Comments:** The sample was characterized by powder X-ray diffraction data and X-ray photoelectron spectroscopy.**Antimony** Sb**Origin:** Artificial.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm laser radiation. The laser radiation power at the sample was 0.97 mW.**Raman shifts (cm<sup>-1</sup>):** 145s, 105.**Source:** Makreski et al. (2013b).**Comments:** Antimony was obtained as a product of photo-induced decomposition of stibnite  $Sb_2S_3$  and identified due to the resemblance to the spectrum of Sb from Degtyareva et al. (2007). According to Degtyareva et al. (2007) Sb-I (99.999% purity) at ambient pressure is characterized by the Raman shifts of 151s and 114 cm<sup>-1</sup>.**Antlerite**  $Cu^{2+}_3(SO_4)(OH)_4$ **Origin:** Chuquicamata, Chile.**Experimental details:** The method of the sample preparation is not indicated. Raman scattering measurements have been performed using 780 nm laser radiation. The laser radiation power was less than 1 mW.**Raman shifts (cm<sup>-1</sup>):** 3580, 3488, 1905, 1266, 1173, 1148, 1135, 1079s, 990, 985, 902, 786, 759, 651, 629, 606, 600, 485, 469, 440, 415s, 335, 330, 295, 265, 259, 169, 151, 146, 141, 131.**Source:** Martens et al. (2003a).**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The band at 1905 cm<sup>-1</sup> is attributed to the first overtone of symmetric stretching vibrations of  $[SO_4]^{2-}$ . For the Raman spectra of antlerite see also Bouchard and Smith (2003), Frost et al. (2004n), Apopei et al. (2014a), and Coccato et al. (2016).

**Apachite** Cu<sup>2+</sup><sub>9</sub>Si<sub>10</sub>O<sub>29</sub>·11H<sub>2</sub>O

**Origin:** Christmas mine, Christmas area, Banner District, Dripping Spring Mts., Gila Co., Arizona, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3651sh, 3614s, 3579, 3491, 3374, 3215, 2997, 2938, 2894, 2746, 1668, 1610, 1536sh, 1364, 1336, 1287, 1264, 1096, 997, 967s, 939, 898, 837, 777, 673s, 663sh, 529, 512, 479, 449sh, 435s, 402, 349, 335, 314, 305, 289, 253, 238, 221, 207, 195sh, 186, 180sh, 151s, 139sh, 113, 106.

**Source:** Frost and Xi (2012k).

**Comments:** No independent analytical data are provided for the sample used. The very intense sharp Raman band at 3614 cm<sup>-1</sup> is assigned by the authors of the cited article to stretching vibrations of OH groups. The authors suppose that the correct formula of apachite could be Cu<sub>9</sub>Si<sub>10</sub>O<sub>23</sub>(OH)<sub>12</sub>·5H<sub>2</sub>O.

**Aphthitalite** K<sub>3</sub>Na(SO<sub>4</sub>)<sub>2</sub>

**Origin:** Vesuvius volcano, Somma-Vesuvius complex, Naples province, Campania, Italy.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation in a 180°-scattering geometry. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1206–1201, 1084, 996–985s, 626–627, 618–617, 452–451s.

**Source:** Hansteen and Burke (1994).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectrum of aphthitalite see also Jentzsch et al. (2013).

**Apjohnite** Mn<sup>2+</sup>Al<sub>2</sub>(SO<sub>4</sub>)<sub>4</sub>·22H<sub>2</sub>O

**Origin:** Coranda-Hondol ore deposit, Certej, Romania.

**Experimental details:** Method of sample preparation is not indicated. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power at the sample was 22.9 mW.

**Raman shifts (cm<sup>-1</sup>):** 3379, 3299, 3237sh, 3007sh, 1630w, 1227sh, 1141w, 1116w, 1108w, 1086w, 1073sh, 996s, 978sh, 619w, 529w, 469w, 432sh, 311w.

**Source:** Apopei et al. (2014a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. For the Raman spectra of apjohnite see also Reddy et al. (2006) and Locke et al. (2007).

**Apuanite** (Fe<sup>2+</sup>Fe<sup>3+</sup>)<sub>2</sub>(Fe<sup>3+</sup>)<sub>2</sub>Sb<sup>3+</sup><sub>4</sub>)O<sub>12</sub>S

**Origin:** Bucadella Vena, Apuan Alps, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 713sh, 669s, 632sh, 574w, 548, 491, 437sh, 435, 396, 332, 292sh, 274sh, 242sh, 230s, 196, 174, 162sh, 143sh, 121, 106.

**Source:** Bahfenne (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. For the Raman spectrum of apuanite see also Bahfenne et al. (2011a).

#### Aradite BaCa<sub>6</sub>[(SiO<sub>4</sub>)(VO<sub>4</sub>)](VO<sub>4</sub>)<sub>2</sub>F

**Origin:** Hatrurim Complex, Negev desert, Israel (type locality).

**Experimental details:** Experimental details are not identified. The methods used for the investigations are analogous to those reported by Galuskin et al. (2015b).

**Raman shifts (cm<sup>-1</sup>):** 989, 968, 942, 874sh, 859s, 835sh, 449w, 386sh, 366, 293w, 222w.

**Source:** Galuskin et al. (2015e).

**Comments:** The investigated sample has the crystal-chemical formula BaCa<sub>6</sub>[(SiO<sub>4</sub>)<sub>1.2</sub>(VO<sub>4</sub>)<sub>0.5</sub>(PO<sub>4</sub>)<sub>0.1</sub>(SO<sub>4</sub>)<sub>0.2</sub>][(VO<sub>4</sub>)<sub>1.51</sub>(PO<sub>4</sub>)<sub>0.59</sub>]F and is a not an end-member of a complex solid solution. For the Raman spectrum of aradite see also Galuskin et al. (2015b).

#### Aragonite Ca(CO<sub>3</sub>)

**Origin:** No data.

**Experimental details:** Methods of sample preparation are not indicated. Raman scattering measurements have been performed using 1064 nm laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 2905w, 2835w, 1904w, 1574w, 1462w, 1086s, 854w, 717sh, 704w.

**Source:** Edwards et al. (2005).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of aragonite see also Buzgar and Apopei (2009), Behrens et al. (1995), White (2009), Wehrmeister et al. (2010), Frezzotti et al. (2012), Kristova et al. (2014), Shatskiy et al. (2015), and Sánchez-Pastor et al. (2016).

#### Aragonite Ca(CO<sub>3</sub>)

**Origin:** Spania Dolina, Slovakia.

**Experimental details:** Methods of sample preparation are not indicated. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 1050 mW.

**Raman shifts (cm<sup>-1</sup>):** 1573, 1461, 1083s, 701, 250.

**Source:** Buzgar and Apopei (2009).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of aragonite see also Edwards et al. (2005), Behrens et al. (1995), White (2009), Wehrmeister et al. (2010), Frezzotti et al. (2012), Kristova et al. (2014), Shatskiy et al. (2015), and Sánchez-Pastor et al. (2016).

#### Arapovite-related silicate (Ca<sub>0.5</sub>Na<sub>0.5</sub>)<sub>2</sub>NaUSi<sub>8</sub>O<sub>20</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented single crystals using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1139s, 1081, 655, 468, 303, 202w.

**Comments:** The sample was characterized by powder X-ray diffraction data. The crystal structure is solved.

### Aravaipaite Pb<sub>3</sub>AlF<sub>9</sub>·H<sub>2</sub>O

**Origin:** Grand Reef mine, Aravaipa mining district, Arizona, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~3370s, ~3250w, ~2935w, ~1640w, ~620, ~550, ~530, ~400, ~385, ~370, ~330w, ~317w, ~260sh, ~233s, ~175, ~170sh.

**Source:** Kampf et al. (2011c).

**Comments:** The sample identification was done by single-crystal X-ray diffraction. The crystal structure is solved.

### Arcanite K<sub>2</sub>(SO<sub>4</sub>)

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not indicated. Raman scattering measurements have been performed using 532 nm laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1147, 1108, 1094, 985s, 623, 458.

**Source:** Buzgar et al. (2009).

**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. No independent analytical data are provided for the sample used. For the Raman spectrum of arcanite see also Martínez-Arkarazo et al. (2007).

### Archerite H<sub>2</sub>K(PO<sub>4</sub>)

**Origin:** Petrogale cave, Madura, Western Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3235, 3191, 3151, 3089, 3018, 1724sh, 1704, 1660, 1421, 983sh, 917s, 562sh, 533, 477sh, 461sh, 393s, 347, 328sh, 270w, 180, 144.

**Source:** Frost et al. (2012f).

**Comments:** No independent analytical data are provided for the sample used.

### Ardealite Ca<sub>2</sub>(PO<sub>3</sub>OH)(SO<sub>4</sub>)·4H<sub>2</sub>O

**Origin:** Moorba cave, Jurien Bay, Western Australia, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1141, 1102, 1001s, 998sh, 862, 670, 613, 598, 528sh, 505, 448, 421, 363, 230, 198sh, 188, 155, 143.

**Source:** Frost et al. (2011g).

**Comments:** No independent analytical data are provided for the sample used.



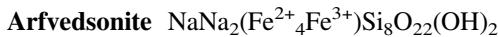
**Origin:** Salm-Château, Vielsalm, Stavelot massif, Luxembourg province, Belgium (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3298, 3211sh, 3149, 3041, 1605s, 1394sh, 1287sh, 1255s, 1218s, 1197s, 947sh, 935, 920sh, 890sh, 877, 865sh, 785sh, 779, 721, 713, 625, 601, 561, 544sh, 519, 471sh, 460, 445, 430, 414, 396, 365sh, 352, 314, 301, 228, 183, 167, 144.

**Source:** Frost et al. (2014s).

**Comments:** No independent analytical data are provided for the sample used. The strong band at 1605 cm<sup>-1</sup> corresponds to an impurity. The spectrum contains broad bands of unknown origin near 2100 cm<sup>-1</sup>.



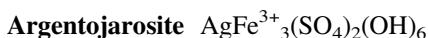
**Origin:** Vodno, Macedonia.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was from 50 to 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1055, 1020w, 974s, 921, 892, 815, 793, 772, 749, 725, 676s, 640w, 610w, 583, 539, 478, 435, 370, 335, 317w, 255sh, 215, 172, 149, 112.

**Source:** Makreski et al. (2006a).

**Comments:** The sample used is an intermediate member between arfvedsonite and magnesioarfvedsonite. The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of arfvedsonite see also Jovanovski et al. (2009) and Leissner et al. (2015).



**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample prepared as a disk 10 mm in diameter with KBr powder. The wavelength of laser excitation line was 514.5 nm. The laser radiation power at the sample was 38 mW.

**Raman shifts (cm<sup>-1</sup>):** 1161w, 1107, 1012, 623, 574w, 449sh, 442s, 363w, 306, 228.

**Source:** Sasaki et al. (1998).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of argentojarosite see also Frost et al. (2006r).



**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample in a 180°-scattering geometry using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 873, 700s, 170w.

**Source:** Madon et al. (1991).

**Comments:** The procedure of verification of the structure of the rutile form GeO<sub>2</sub> has been described by Richet (1990).

**Arisite (Ce)** NaCe<sub>2</sub>(CO<sub>3</sub>)<sub>2</sub>[F<sub>2x</sub>(CO<sub>3</sub>)<sub>1-x</sub>]F

**Origin:** Aris phonolite, Namibia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3449, 3255s, 2642, 2458s, 2068, 1799, 1596, 1455, 1072s, 704s, 396, 187s, 152s.

**Source:** Piilonen et al. (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data, LA-ICP-MS, and electron microprobe analyses. The band at 1596 cm<sup>-1</sup> indicates possible presence of H<sub>2</sub>O molecules.

**Armalcolite** (Mg,Fe<sup>2+</sup>)Ti<sub>2</sub>O<sub>5</sub>

**Origin:** Skallevikshalsen, Lützow-Holm Complex, East Antarctica.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented thin section using 533 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 759, 633s, 393, 201s, 169sh.

**Source:** Kawasaki et al. (2013).

**Comments:** The sample was characterized by electron microprobe analyses.

**Arrojadite-(KFe)** (KNa)Fe<sup>2+</sup>(CaNa<sub>2</sub>)Fe<sup>2+</sup><sub>13</sub>Al(PO<sub>4</sub>)<sub>11</sub>(PO<sub>3</sub>OH)(OH)<sub>2</sub>

**Origin:** Rapid Creek, Richardson Mts., Yukon Territory, Canada.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3574, 3564s, 3553, 3530, 3515, 1714, 1580, 1444, 1187w, 1148w, 1123w, 1092w, 1066, 1024sh, 1005s, 991s, 975s, 951sh, 903, 852, 638, 615, 604sh, 583s, 580, 557s, 548, 540, 513, 479, 463, 449, 424s, 403, 349, 306, 275, 251, 239, 202, 185, 162, 140.

**Source:** Frost et al. (2013ag).

**Comments:** There are discrepancies between some frequencies given in the text and figures. The sample identification was done by XRD and qualitative EDS analysis.

**Arsenbrackebuschite** Pb<sub>2</sub>(Fe<sup>3+</sup>,Zn)(AsO<sub>4</sub>)<sub>2</sub>(OH,H<sub>2</sub>O)

**Origin:** No data.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 972w, 846sh, ~820s, 730, 620, ~464sh, 420, 405sh, ~345, 308, ~240w, ~102–170.

**Source:** Costin et al. (2014).

**Comments:** No independent analytical data are provided for the sample used.

**Arsendescloisite Sr-analogue**  $\text{SrZn}(\text{AsO}_4)(\text{OH})$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 or 473 nm laser radiation. The nominal laser radiation power was 10 or 3 mW.**Raman shifts (cm<sup>-1</sup>):** ~3400sh, 3300, ~3240w, 818s, 804, 790, ~780w, ~450–300w.**Source:** Đorđević et al. (2016).**Comments:** The sample was characterized by single-crystal X-ray diffraction data. The crystal structure is solved.**Arsenolamprite** As**Origin:** Muiane pegmatite, Mozambique.**Experimental details:** Raman scattering measurements have been performed on a melt inclusion in a morganite crystal using 514 or 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 14 mW.**Raman shifts (cm<sup>-1</sup>):** 253s, 225w, 220.**Source:** Thomas and Davidson (2010).**Arseniosiderite**  $\text{Ca}_2\text{Fe}^{3+}{}_{3}\text{O}_2(\text{AsO}_4)_3 \cdot 3\text{H}_2\text{O}$ **Origin:** Romanèche, near Maçon, Saône-et-Loire, France.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 927s, 852s, 828, 772sh, 621, 535, 479w, 441w, 389s, 331w, 298sh, 250s, 227, 197.**Source:** Gomez et al. (2010b).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectrum of arseniosiderite see also Filippi et al. (2007).**Arsenogorceixite**  $\text{BaAl}_3(\text{AsO}_4)(\text{AsO}_3\text{OH})(\text{OH})_6$ **Origin:** Michael mine, Weiler, near Lahr, Schwarzwald (Black Forest), Germany.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power at the sample was 0.01 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3691, 3621, 3473sh, 3301, 2973sh, 2961sh, 2930, 2891, 2863, 2849, 2725, 1597, 1447, 1332, 1307, 1208, 1160, 1148, 1057, 1014, 972s, 873, 818, 814s, 805, 776, 764, 617, 600, 556, 510, 462, 441s, 407, 388, 340s, 318, 264, 244, 189, 167, 137.**Source:** Frost et al. (2012g).**Comments:** No independent analytical data are provided for the sample used. There are discrepancies between the spectrum and its description in the cited paper.**Arsenolite**  $\text{As}_2\text{O}_3$ **Origin:** Cobalt City, Ontario, Canada.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 781, 560, 469, 413w, 368s, 265s, 180.

**Source:** Kloprogge et al. (2006).

**Comments:** The sample was characterized by SEM/EDS. Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. For the Raman spectrum of arsenolite see also Guřka et al. (2012).

### Arsenopyrite FeAsS

**Origin:** Nistru mine, Maramures, Romania.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample in a 180°-scattering geometry using 532 nm laser radiation. The nominal laser radiation power was 210 mW.

**Raman shifts (cm<sup>-1</sup>):** 478, 453, 427, 392, 362, 333, 303, 280s, 253, 231, 217s, 200sh, 187, 180sh, 170, 127, 108sh, 94, 84, 73.

**Source:** Kharbish and András (2014).

**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectrum of arsenopyrite see also Mernagh and Trudu (1993).

### Arsentsumebite Pb<sub>2</sub>Cu(AsO<sub>4</sub>)(SO<sub>4</sub>)(OH)

**Origin:** Tsumeb mine, Tsumeb, Namibia (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3458, 3324, 2925, 2876, 2857, 1446, 1161, 1121w, 1070w, 972s, 906, 853, 814s, 620, 604, 464, 442, 412, 390, 340, 324, 308, 248, 241, 197, 188, 171, 145, 102.

**Source:** Frost et al. (2011n).

**Comments:** No independent analytical data are provided for the sample used. There are discrepancies between the spectrum and its description in the cited paper. Spectroscopic data show possible presence of impurities in the investigated material. For the Raman spectrum of arsentsumebite see also Costin et al. (2014).

### Arsenuranylite Ca(UO<sub>2</sub>)<sub>2</sub>(AsO<sub>4</sub>)<sub>2</sub>(OH)<sub>4</sub>·6H<sub>2</sub>O

**Origin:** Cherkasar deposit, Uzbekistan.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3489, 2929, 2872, 926, 883, 795s, 787s, 561, 558, 494, 493, 462, 422, 388, 344, 298, 259, 213, 170, 150.

**Source:** Frost et al. (2009d).

**Comments:** No independent analytical data are provided for the sample used.

**Arthurite** CuFe<sup>3+</sup><sub>2</sub>(AsO<sub>4</sub>)<sub>2</sub>(OH)<sub>2</sub>·4H<sub>2</sub>O**Origin:** Majuba Hill, Pershing Co., Nevada, USA.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented polished sample. The wavelength of laser excitation line and the laser radiation power are not indicated.**Raman shifts (cm<sup>-1</sup>):** 3496, 3307, 3232, 3162, 1050, 907, 850, 812, 784, 551w, 508s, 450, 426, 368, 343, 288, 259, 245s, 221, 186, 153, 138, 101, 70.**Source:** Jambor et al. (2002).**Comments:** The sample was characterized by electron microprobe analysis. For the Raman spectra of arthurite see also Frost et al. (2003b) and Palmer and Frost (2011).**Artinite** Mg<sub>2</sub>(CO<sub>3</sub>)(OH)<sub>2</sub>·3H<sub>2</sub>O**Origin:** Aichi prefecture, Japan.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3593s, 3589sh, 3573sh, 3229, 3030, 2291, 1673, 1453, 1092s, 1060sh, 913w, 698, 469, 432, 376, 324, 273, 244, 209, 188.**Source:** Frost et al. (2009a).**Comments:** No independent analytical data are provided for the sample used. There are discrepancies between the pattern of the spectrum and its description. For the Raman spectrum of artinite see also Edwards et al. (2005).**Arzakite** Hg<sup>2+</sup><sub>3</sub>S<sub>2</sub>(Br,Cl)<sub>2</sub>**Origin:** No data.**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 or 785 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** ~585, ~480w, ~390, ~270s, ~215s.**Source:** Potgieter-Vermaak et al. (2012).**Asbolane** Mn<sup>4+</sup>(O,OH)<sub>2</sub>(Co,Ni,Mg,Ca)<sub>x</sub>(OH)<sub>2x</sub>·nH<sub>2</sub>O**Origin:** Democratic Republic of Congo.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 3484w, 1206w, 1084w, 950w, 592s, 539s, 489, 376.**Source:** Burlet et al. (2014).**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectra of asbolane see also Burlet and Vanbrabant (2015) and Roqué-Rosell et al. (2010).**Asbolane** Mn<sup>4+</sup>(O,OH)<sub>2</sub>(Co,Ni,Mg,Ca)<sub>x</sub>(OH)<sub>2x</sub>·nH<sub>2</sub>O**Origin:** Democratic Republic of Congo.**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 3484w, 1206w, 1084w, 950w, 592s, 539s, 489, 376.

**Source:** Burlet et al. (2014).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectra of asbolane see also Burlet and Vanbrabant (2015) and Roqué-Rosell et al. (2010).

**Asbolane** Mn<sup>4+</sup>(O,OH)<sub>2</sub>(Co,Ni,Mg,Ca)<sub>x</sub>(OH)<sub>2x</sub>·nH<sub>2</sub>O

**Origin:** A Cu-Co supergene deposit, Ruashi, Katanga, Democratic Republic of Congo.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented polished sample using 532 nm laser radiation. The laser radiation power was 0.2 mW.

**Raman shifts (cm<sup>-1</sup>):** 3455–3475w, 1580–1600w, 1300–900w (a triplet), 627sh, 596s, 553s, 497, 456sh, 374w.

**Source:** Burlet and Vanbrabant (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. For the Raman spectra of asbolane see also Burlet et al. (2014) and Roqué-Rosell et al. (2010).

**Aspedamite** □□<sub>12</sub>(Fe<sup>3+</sup>,Fe<sup>2+</sup>)<sub>3</sub>Nb<sub>4</sub>[Th(Nb,Fe<sup>3+</sup>)<sub>12</sub>O<sub>42</sub>][(H<sub>2</sub>O),(OH)]<sub>12</sub>

**Origin:** Herrebøkasa quarry, Aspedammen, Østfold, southern Norway (type locality).

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 3465w, 3556sh, 1610w, 933, 865sh, 812, 666s, 448w, 359, 234s, 169s, 117.

**Source:** Cooper et al. (2012b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Asselbornite** Pb(UO<sub>2</sub>)<sub>4</sub>(BiO)<sub>3</sub>(AsO<sub>4</sub>)<sub>2</sub>(OH)<sub>7</sub>·4H<sub>2</sub>O

**Origin:** Horní Halže, the Krušnéhory Mountains, Czech Republic (type locality).

**Experimental details:** Methods of sample preparation are not indicated. Raman scattering measurements have been performed using 785 nm laser radiation. The laser radiation power at the sample was 4 mW.

**Raman shifts (cm<sup>-1</sup>):** 1039w, 999w, 962w, 874sh, 842sh, 797s, 673w, 599w, 503, 450w, 395w, 321, 266.

**Source:** Sejkora and Čejka (2007).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Atacamite** Cu<sub>2</sub>Cl(OH)<sub>3</sub>

**Origin:** Atacama, Chile.

**Experimental details:** Raman scattering measurements have been performed on an oriented crystal using 532.8 nm laser radiation. The laser radiation power at the sample was from 0.05 to 1 mW. The spectrum was obtained in the scattering geometry with polarization of the laser beam oriented at 45° with respect to the *c* axis.

**Raman shifts (cm<sup>-1</sup>):** 3433, 3348, 975s, 909s, 846, 819s, 587, 513s, 353w, 177s, 148s, 135, 117, 105s.

**Source:** Bertolotti et al. (2012).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of atacamite see also Frost et al. (2002b), Bouchard and Smith (2003), and Christy et al. (2004).

### Atelstite Bi<sub>2</sub>O(AsO<sub>4</sub>)(OH)

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3095w, 1082w, 887sh, 834s, 802, 782, 767, 623w, 480, 450, 395sh, 370sh, 352, 324, 310, 278s, 219, 200, 173, 118.

**Source:** Frost et al. (2011b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

### Atelisite (Y) Y<sub>4</sub>Si<sub>3</sub>O<sub>8</sub>(OH)<sub>8</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an oriented crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 8 mW. The spectra obtained in the scattering geometries X(ZZ)X, X(YY)X, and Y(YZ)X are similar.

**Raman shifts (cm<sup>-1</sup>):** 3225w, 2964w, 2905w, 885s, 755sh, 709w, 490w.

**Source:** Malcherek et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

### Athabascaite Cu<sub>5</sub>Se<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a nanocrystalline aggregate. The wavelengths of laser radiation and laser radiation power are not indicated.

**Raman shifts (cm<sup>-1</sup>):** 128.

**Source:** Ge and Li (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data and qualitative electron microprobe analysis.

### Atokite Pd<sub>3</sub>Sn

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532.068 nm Nd-YAG laser radiation. The laser radiation power at the sample was between 1 and 2 mW.

**Raman shifts (cm<sup>-1</sup>):** The obtained spectrum does not show characteristic bands.

**Source:** Vymazalová et al. (2014).

**Augelite**  $\text{Al}_2(\text{PO}_4)(\text{OH})_3$ **Origin:** Ehrenfriedersdorf, Saxony, Germany.**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented inclusion in quartz using 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power at the sample was between 100 and 500 mW.**Raman shifts (cm<sup>-1</sup>):** 3537s, 3469s, 3428, 1107, 635s, 367, 252, 227.**Source:** Thomas et al. (1998).**Comments:** The sample was characterized by electron microprobe analysis. For the Raman spectrum of augelite see also Frost and Weier (2004b).**Augite**  $(\text{Ca},\text{Mg},\text{Fe})_2\text{Si}_2\text{O}_6$ **Origin:** Sasa, Macedonia.**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power at the sample was 50 or 100 mW.**Raman shifts (cm<sup>-1</sup>):** 1025sh, 1009s, 907w, 851w, 654s, 549, 523, 510sh, 492w, 372, 336, 301, 229, 186, 178, 146, 122, 116w.**Source:** Makreski et al. (2006b).**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by powder X-ray diffraction data and neutron activation analysis. For the Raman spectra of augite see also Buzatu and Buzgar (2010) and Andò and Garzanti (2014).**Augite**  $(\text{Ca},\text{Mg},\text{Fe})_2\text{Si}_2\text{O}_6$ **Origin:** Techereu area, Apuseni Mts., Romania.**Experimental details:** Methods of sample preparation are not indicated. Raman scattering measurements have been performed using 532 nm laser radiation. The nominal laser radiation power was 100 mW.**Raman shifts (cm<sup>-1</sup>):** 1102sh, 1043sh, 1006s, 928w, 863, 769, 707w, 667s, 555, 533, 392, 355, 327, 299sh, 226w.**Source:** Buzatu and Buzgar (2010).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of augite see also Makreski et al. (2006b) and Andò and Garzanti (2014).**Aurichalcite**  $(\text{Zn},\text{Cu})_5(\text{CO}_3)_2(\text{OH})_6$ **Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm laser radiation. The nominal laser radiation power was 30 mW.**Raman shifts (cm<sup>-1</sup>):** 3331, 1511, 1479, 1074s, 843, 750, 734, 709, 503, 463, 437w, 389, 354w, 234, 211, 175, 141.**Source:** Bouchard and Smith (2003).**Comments:** For the Raman spectra of aurichalcite see also Frost et al. (2007j), Buzgar and Apopei (2009), and Rotondo et al. (2012).

**Aurostibite**  $\text{AuSb}_2$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed at 380 K on an arbitrarily oriented crystal using 514.5, 501.5, 476.5, and 457.9 nm laser radiation. The nominal laser radiation power at the sample was ~200, ~190, ~200, and ~150 mW, respectively. The incident laser light was scattered off a [100] natural cleavage.**Raman shifts (cm<sup>-1</sup>):** 158w, 151s, 122sh, 114s.**Source:** Freund et al. (1977).**Comments:** No independent analytical data are provided for the sample used.**Austinite**  $\text{CaZn}(\text{AsO}_4)(\text{OH})$ **Origin:** Gold Hill Mine, Tooele Co., Utah, USA.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3270, 828s, 814, 802, 779, 418, 403.**Source:** Liu et al. (2015a).**Comments:** The sample used was characterized by powder and single-crystal X-ray diffraction data. IR spectrum shows that the sample contains minor  $\text{SO}_4^{2-}$  substituting arsenate anions. For the Raman spectrum of austinite see also Martens et al. (2003c).**Autunite**  $\text{Ca}(\text{UO}_2)_2(\text{PO}_4)_2 \cdot 10\text{--}12\text{H}_2\text{O}$ **Origin:** Merrivale Quarry, Tavistock, Cornwall, UK.**Experimental details:** Methods of sample preparation are not indicated. Raman scattering measurements have been performed using 785 nm laser radiation. The nominal laser radiation power at the source was ~370 mW.**Raman shifts (cm<sup>-1</sup>):** 1008s, 990, 900sh, ~400, ~270, 210.**Source:** Driscoll et al. (2014).**Comments:** The sample was characterized by electron microprobe analysis. For the Raman spectra of autunite see also Frost (2004d), Frost and Weier (2004c, d).**Avicennite**  $\text{Tl}_2\text{O}_3$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on finely ground powder pressed into pellets using 488 and 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** A spectrum of  $\text{Tl}_2\text{O}_3$ , shows no distinct features above 400 cm<sup>-1</sup> except an absorption edge near 400 cm<sup>-1</sup>.**Source:** White and Keramidas (1972).**Avogadrite**  $\text{KBF}_4$ **Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed in  $\text{N}_2$  atmosphere using 514 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1097, 1043, 775s, 534, 360.

**Source:** Zavorotynska et al. (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of avogadrite see also Bonadeo and Silberman (1970) and Bates and Quist (1974).

### Awaruite Ni<sub>3</sub>Fe

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm laser radiation. The laser radiation power at the sample was 3 mW.

**Raman shifts (cm<sup>-1</sup>):** 701, 566s.

**Source:** Abelló et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Axinite-(Fe) Ca<sub>4</sub>Fe<sup>2+</sup><sub>2</sub>Al<sub>4</sub>[B<sub>2</sub>Si<sub>8</sub>O<sub>30</sub>](OH)<sub>2</sub>

**Origin:** Drum valley, Tulare Co., California, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3368, 1084, 1057, 1005sh, 993sh, 979s, 964s, 959sh, 931, 909, 898, 869, 813, 768, 714s, 678, 645, 619, 590, 574, 562, 547, 512, 485, 445, 422, 418, 390, 344, 319, 275s, 256, 212, 170, 140, 110.

**Source:** Frost et al. (2007b).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of axinite (Fe) see also Andò and Garzanti (2014).

### Azurite Cu<sub>3</sub>(CO<sub>3</sub>)<sub>2</sub>(OH)<sub>2</sub>

**Origin:** Namibia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1579w, 1459w, 1425w, 1098s, 939, 835s, 766, 544, 404s, 339w, 285, 250s.

**Source:** Buzgar and Apopei (2009).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of azurite see also Frost et al. (2002d), Bouchard and Smith (2003), and Frezzotti et al. (2012).

### Backite Pb<sub>2</sub>AlTeO<sub>6</sub>Cl

**Origin:** Grand Central mine, Tombstone Hills, Cochise Co., Arizona, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented grain using 785 nm laser radiation. The laser radiation power at the sample was ~1 mW.

**Raman shifts (cm<sup>-1</sup>):** 967, 733s, 625, 425, 350, 120s.

**Source:** Tait et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The Raman band at  $967\text{ cm}^{-1}$  is assigned to the combination mode  $\sim(350+625)\text{ cm}^{-1}$ .

### Baddeleyite $\text{ZrO}_2$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal in a thin section using  $514.5\text{ nm Ar}^+$  laser radiation. The nominal laser radiation power at the sample was from 30 to  $50\text{ mW}$ . A  $90^\circ$ -scattering geometry was employed.

**Raman shifts ( $\text{cm}^{-1}$ ):**  $757\text{w}, 643, 622, 559, 538, 503, 476, 384\text{s}, 350\text{s}, 308, 264\text{w}, 225, 190\text{s}, 182\text{sh}, 105$ .

**Source:** Galuskina et al. (2013a).

**Comments:** The sample was characterized by SEM/EBSD and electron microprobe analysis. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of baddeleyite see also Zhang et al. (2010a).

### Bafertisite $\text{BaFe}^{2+} \text{Ti}(\text{Si}_2\text{O}_7)\text{O(OH,F)}_2$

**Origin:** Gremyakha-Vyrmes alkaline complex, Kola Peninsula, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using  $632\text{ nm}$  laser radiation. The laser radiation power is not indicated.

**Raman shifts ( $\text{cm}^{-1}$ ):**  $1184\text{w}, 1116, 1027, 988, 966, 917\text{s}, 812\text{s}, 688\text{s (broad)}, 593\text{s}, 478, 418, 355, 336, 264, 230\text{w}, 178, 163, 135$ .

**Source:** Cámara et al. (2016c).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data, electron microprobe analyses, IR, and Mössbauer spectra.

### Baghdadite $\text{Ca}_6\text{Zr}_2(\text{Si}_2\text{O}_7)_2\text{O}_4$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using  $532\text{ nm}$  laser radiation. The nominal laser radiation power at the sample was  $10\text{ mW}$ .

**Raman shifts ( $\text{cm}^{-1}$ ):**  $1034\text{w}, 1011, 975, 958, 944, 921\text{s}, 855, 669\text{s}, 624\text{s}, 568, 542, 521, 476\text{w}, 452, 433, 409, 398, 376, 357\text{s}, 321, 295, 280\text{w}, 262, 245, 214, 198, 171, 148, 127, 122, 106\text{s}, 97, 86$ .

**Source:** Dul et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data. The crystal structure is solved by the Rietveld method.

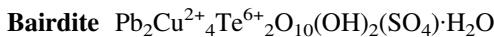
### Bahianite $\text{Al}_5\text{Sb}^{5+} \text{O}_{14}(\text{OH})_2$

**Origin:** Paramirim region, Bahia Province, Brazil (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a  $633\text{ nm He-Ne}$  laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3495, 3462, 3190, 2955, 2718, 2531, 2389, 2273, 2079, 1929, 1808, 1756s, 1489, 1438, 998, 975w, 956w, 952w, 883sh, 856sh, 843sh, 818s, 770, 682, 669sh, 589, 567, 534s, 498, 478s, 471sh, 412s, 405sh, 386, 376, 352, 319, 294, 258s, 220, 199, 165, 158sh, 146sh.

**Source:** Frost and Bahfenne (2010c).



**Origin:** Otto Mt., near Baker, California, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on a partly oriented platelet (from the [100] face of a crystal) using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 977, 721s, 634, 558, 518, 378, 336, 238, 208.

**Source:** Kampf et al. (2013a).

**Comments:** The sample was characterized by powder X-ray diffraction data. The crystal structure is solved. Chemical data are questionable (total sum is 92.97%).



**Origin:** Cerchiara mine, Eastern Liguria, Italy.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal in a 180°-scattering geometry using 632.8 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1136, 973, 888, 868s, 707, 539, 437, 309, 261.

**Source:** Lepore et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved.



**Origin:** Röhrerbühel, near Kitzbühel, Tyrol, Eastern Alps, Austria.

**Experimental details:** Methods of sample preparation are not indicated. Raman scattering measurements have been performed using 515 nm laser radiation. The laser radiation power at the sample was 6 mW.

**Raman shifts (cm<sup>-1</sup>):** 325, 306.

**Source:** Steiner et al. (2010).

**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectrum of balkanite see also Biagioni and Bindi (2016).



**Origin:** Ozernyi district, Salla-Kuolayarvi, Kola Peninsula, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 157, 134s.

**Source:** Voloshin et al. (2015b).

**Comments:** The sample was characterized by electron microprobe analyses.

**Baotite**  $\text{Ba}_4(\text{Ti},\text{Nb},\text{W})_8\text{O}_{16}(\text{SiO}_3)_4\text{Cl}$ 

**Origin:** Bayan Obo REE–Fe–Nb deposit, Inner Mongolia, China (type locality).

**Experimental details:** Methods of sample preparation are not indicated. Raman scattering measurements have been performed using 1064 nm laser radiation. The nominal laser radiation power was from 300 to 380 mW.

**Raman shifts (cm<sup>-1</sup>):** 982, 777, 550, 450, 392, 344, 295, 241, 172.

**Source:** Yuran and Li (1998).

**Comments:** No independent analytical data are provided for the sample used.

**Barahonaite-(Al)**  $(\text{Ca},\text{Cu},\text{Na},\text{Fe}^{3+},\text{Al})_{12}\text{Al}_2(\text{AsO}_4)_8(\text{OH},\text{Cl})_x \cdot n\text{H}_2\text{O}$ 

**Origin:** Sapucaia pegmatite mine, Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3549sh, 3413, 3217, 2993sh, 2702w, 1657w, 1605w, 1450, 1351w, 1304w, 1228w, 1154w, 1072w, 998w, 890sh, 863s, 828s, 802sh, 723w, 529, 506sh, 449, 399, 360, 325, 300, 233, 159.

**Source:** López et al. (2014e).

**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. No independent analytical data are provided for the sample used. For the Raman spectrum of barahonaite-(Al) see also Viñals et al. (2008).

**Barahonaite-(Fe)**  $(\text{Ca},\text{Cu},\text{Na},\text{Fe}^{3+},\text{Al})_{12}\text{Fe}^{3+}_2(\text{AsO}_4)_8(\text{OH},\text{Cl})_x \cdot n\text{H}_2\text{O}$ 

**Origin:** Dolores prospect, near the village of Pastrana, Murcia Province, southeastern Spain (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 908sh, 860s, 828s, 799sh, 517, 508sh, 427, 360w, 325w, 219w, 162, 138, 87w, 65w, 40w.

**Source:** Viñals et al. (2008).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Bararite**  $(\text{NH}_4)_2\text{SiF}_6$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed in 90°-scattering geometry using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was ~1 W.

**Raman shifts (cm<sup>-1</sup>):** (XX)—3236, 1706, 1428, 1406, 650s, 466, 406s, 180; (YY)—1706, 1430, 650, 466, 406s, 180; (ZZ)—3235, 1428, 1406, 650s, 406s.

**Source:** Trefler and Wilkinson (1969).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of bararite see also Jenkins (1986).

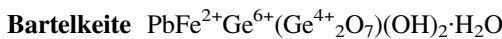
**Barberite**  $(\text{NH}_4)\text{BF}_4$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powdered sample using  $\text{Ar}^+$  laser radiation. The wavelengths of laser excitation line and the laser radiation power are not indicated.**Raman shifts (cm<sup>-1</sup>):** 3400–3300w (broad), 3250s, 767s, 529, 523, 355.**Source:** Schutte and Van Rensburg (1971).**Comments:** No independent analytical data are provided for the sample used.**Barbosalite**  $\text{Fe}^{2+}\text{Fe}^{3+}_2(\text{PO}_4)_2(\text{OH})_2$ **Origin:** Sapucaia mine, Galileia, Minas Gerais (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 2261, 2216, 2090, 1138, 1083sh, 1067, 1044, 1033sh, 1020s, 988w, 968w, 831w, 702, 606, 589, 575sh, 503, 475, 461, 439, 398sh, 381, 361sh, 346s, 312s, 291, 275, 256, 241, 198sh, 187, 179, 166, 151, 145, 133s, 125, 113.**Source:** Frost et al. (2013q).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.**Bariandite Al-free analogue**  $\text{V}_{10}\text{O}_{24}\cdot 9\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powdery sample with crystalline nanoparticles using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power at the sample was 0.2 mW.**Raman shifts (cm<sup>-1</sup>):** 1022, 908s, 518s, 429w, 409w, 270s.**Source:** Menezes et al. (2009).**Comments:** The sample was characterized by powder X-ray diffraction data.**Barićite**  $(\text{Mg},\text{Fe})_3(\text{PO}_4)_2\cdot 8\text{H}_2\text{O}$ **Origin:** Big Fish River, Rapid creek, Richardson Mts., Yukon, Canada (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3480, 3300, 3231, 3121, 3025, 1057, 953s, 859w, 632, 576, 545, 527, 461, 428, 390, 340, 314, 281, 243, 212, 201, 170, 140.**Source:** Frost et al. (2002f).**Comments:** No independent analytical data are provided for the sample used.

**Barioferrite**  $\text{BaFe}^{3+}_{12}\text{O}_{19}$ **Origin:** Synthetic.**Experimental details:** Polarized Raman spectra were collected at temperatures from 10 to 200 K on a single crystal in  $z(xx)-z$  and  $z(yx)-z$  scattering geometries using 610 nm laser radiation. The laser radiation power at the sample was  $\sim 1$  mW.**Raman shifts (cm<sup>-1</sup>):**  $\sim 730\text{sh}$ ,  $\sim 695$ ,  $\sim 627$ ,  $\sim 538$ ,  $\sim 346$  [for the  $z(xx)-z$  configuration at 200 K].**Source:** Chen et al. (2013b).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of barioferrite see also Kreisel et al. (1998a, b, 1999), and Zhao et al. (2008b).**Barioperovskite**  $\text{BaTiO}_3$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powdery sample using 785 nm laser radiation. The nominal laser radiation power was 500 mW.**Raman shifts (cm<sup>-1</sup>):** 719, 517, 292s.**Source:** Cernea (2005).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of barioperovskite see also Ma and Rossman (2008).**Barnesite**  $\text{Na}_2\text{V}^{5+}_6\text{O}_{16}\cdot 3\text{H}_2\text{O}$ **Origin:** Cactus Rat Mine, Thompson district, Grand Co., Utah, USA.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3494, 3435, 3403, 3330, 3253.**Source:** Frost et al. (2004e).**Raman shifts (cm<sup>-1</sup>):** 1010s, 761, 728, 683, 670, 620, 534, 492, 433, 413, 341, 287, 284, 260, 248, 217, 192, 153.**Source:** Frost et al. (2005d).**Comments:** No independent analytical data are provided in the cited papers.**Barringtonite**  $\text{Mg}(\text{CO}_3)\cdot 2\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powdered sample containing other carbonates using 785 nm laser radiation. The nominal laser radiation power was 70 mW.**Raman shifts (cm<sup>-1</sup>):**  $\sim 1095$ .**Source:** Kristova et al. (2014).**Comments:** The sample identification was done by powder X-ray diffraction data.**Barrydawsonite-(Y)**  $\text{Na}_{1.5}\text{Y}_{0.5}\text{CaSi}_3\text{O}_9\text{H}$ **Origin:** Merlot Claim, North Red Wine Pluton, Labrador, Canada (type locality).**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 633 nm laser radiation. The nominal laser radiation power was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 1037s, 1004s, 968, 907, 686, 655s, 524, 506, 463, 445, 416, 362, 312, 272, 244, 207, 148, 107.

**Source:** Mitchell et al. (2015).

**Comments:** Unpolarized and polarized single-crystal spectra showed only minor differences in relative band intensities. The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved.



**Origin:** Tsumeb mine, Tsumeb, Namibia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm laser radiation. The nominal laser radiation power was 200 mW.

**Raman shifts (cm<sup>-1</sup>):** 3490, 3293, 1558, 812, 758s, 549, 492, 393.

**Source:** Origlieri et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved.



**Origin:** Zomba, Malawi.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was 150 mW.

**Experimental details:** Experimental details are not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1014w, 996w, 982w, 958s, 937, 888, 685s, 627, 573w, 542w, 464, 447, 423, 410, 384, 337s, 262w, 234, 202, 191.

**Source:** Yang et al. (2013b).

**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.



**Origin:** Dufton, England.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1167, 1143, 1085, 989s, 648, 619, 461.

**Source:** Buzgar et al. (2009).

**Comments:** No independent analytical data are given for the sample used. For the Raman spectra of baryte see also Jehlička et al. (2009b), White (2009), Ciobotă et al. (2012), and Andò and Garzanti (2014).



**Origin:** No data.

**Experimental details:** Methods of sample preparation are not indicated. Raman scattering measurements have been performed using 785 nm laser radiation. The laser radiation power at source was 320 mW.

**Raman shifts (cm<sup>-1</sup>):** 1166w, 1138w, 1104w, 1084w, 988s, 647w, 617w, 453.

**Source:** Jehlička et al. (2009b).

**Comments:** For the Raman spectra of baryte see also Buzgar et al. (2009), White (2009), Ciobotă et al. (2012), and Andò and Garzanti (2014).

### Barytocalcite $\text{BaCa}(\text{CO}_3)_2$

**Origin:** Alston Moor, England, UK (type locality).

**Experimental details:** Raman scattering measurements have been performed on a powdered sample.

The wavelengths of laser radiation and laser radiation power are not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1510w, 1085s, 715, 700, 688, 314w, 261, 225, 209, 164, 154sh, 127w, 107s, 86w, 70.

**Source:** Scheetz and White (1977).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of barytocalcite see also Frost and Dickfos (2008).

### Bassanite $\text{Ca}(\text{SO}_4) \cdot 0.5\text{H}_2\text{O}$

**Origin:** Artificial (obtained by dehydration at ~338 K of gypsum from an unknown salt core location in India).

**Experimental details:** Raman scattering measurements have been performed in 90°-scattering geometry using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power at the sample was 80 mW.

**Raman shifts (cm<sup>-1</sup>):** 3552, ~1621, 1026w.

**Source:** Sarma et al. (1998).

**Comments:** The new line at 1026 cm<sup>-1</sup> appears in the spectrum of partially dehydrated gypsum. For the Raman spectrum of bassanite see also Apopei et al. (2015).

### Bassoite $\text{SrV}^{4+} \cdot _3\text{O}_7 \cdot 4\text{H}_2\text{O}$

**Origin:** Molinello mine, Val Graveglia, eastern Liguria, Italy (type locality).

**Experimental details:** Methods of sample preparation are not indicated. Raman scattering measurements have been performed using unpolarized 785 nm laser radiation. The nominal laser radiation power at the sample was ~3 mW.

**Raman shifts (cm<sup>-1</sup>):** 3534, 3407, 1645.

**Source:** Bindi et al. (2011a).

**Comments:** Raman spectrum was obtained only in the regions 1250–2000 and 3000–4000 cm<sup>-1</sup>. The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### Bastnäsite-(Ce) $\text{Ce}(\text{CO}_3)\text{F}$

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed using 488 nm laser radiation. The laser radiation power was 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 2621s, 2059, 2009, 1899, 1476s, 1447s, 1345, 1279w, 1098s, 835w, 732w, 670w, 600w, 353, 259.

**Source:** Hong et al. (1999).

**Comments:** For the Raman spectra of bastnäsite-(Ce) see also Yang et al. (2008a) and Frost and Dickfoss (2007a).

**Batiferrite Co-bearing**  $\text{BaFe}_{9.4}\text{Ti}_{1.3}\text{Co}_{1.3}\text{O}_{19}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a platy single crystal oriented perpendicular to the *c*-axis using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 732sh, 694s, 626, 418, 362.

**Source:** Kreisel et al. (1999).

**Comments:** The spectrum was obtained only in the region from 200 to 900 cm<sup>-1</sup>. The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Baumhauerite**  $\text{Pb}_{12}\text{As}_{16}\text{S}_{36}$

**Origin:** Lengenbach, Binntal, Switzerland (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using slightly defocused 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 380, 362, 331, 291s, 254, 222, 192, 161, 137, 114w, 93w, 82.

**Source:** Kharbish (2016).

**Comments:** The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Bavenite**  $\text{Ca}_4\text{Be}_{2+x}\text{Al}_{2-x}\text{Si}_9\text{O}_{26-x}(\text{OH})_{2+x}$  ( $x = 0$  to 1)

**Origin:** An unknown locality in Siberia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 and 785 nm laser radiation. The laser radiation power at the sample was up to 35 mW for the 785 nm laser.

**Raman shifts (cm<sup>-1</sup>):** 945, 674, 544, 505, 448, 401w, 395, 348, 330, 286, 259w, 232, 182w, 173, 140s, 108s.

**Source:** Jehlička et al. (2012).

**Comments:** No independent analytical data are provided for the sample used. The spectrum may correspond to bohseite, a mineral related to bavenite.

**Comments:** For the Raman spectrum of bavenite see also Jehlička and Vandebaele (2015).

**Bayerite**  $\text{Al}(\text{OH})_3$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 25 mW.

**Raman shifts (cm<sup>-1</sup>):** 3425s, 3439, 3449sh, 3546s, 3552, 3654, 904, 868, 547s, 525, 447w, 438, 392, 362w, 325s, 299s, 250, 240, 204w, 147w, 141, 118, 108.

**Source:** Rodgers (1993).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of bayerite see also Rodgers et al. (1989) and Ruan et al. (2001).

**Bayldonite**  $\text{Cu}_3\text{PbO}(\text{AsO}_3\text{OH})_2(\text{OH})_2$

**Origin:** Tsumeb mine, Tsumeb, Namibia.

**Experimental details:** Methods of sample preparation are not indicated. Micro-Raman scattering measurements have been performed using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 0.97 mW.

**Raman shifts (cm<sup>-1</sup>):** 838s, 804, 759w, 495, 428, 397w, 314, 230, 165, 110.

**Source:** Makreski et al. (2015a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. Raman spectrum of bayldonite was also published by Frost et al. (2014d) who neither presented nor assigned the IR bands below 700 cm<sup>-1</sup>: see comment made by Makreski et al. (2015a). The bayldonite formula  $(\text{Cu},\text{Zn})_3\text{Pb}(\text{AsO}_3\text{OH})_2(\text{OH})_2$  given by Frost et al. (2014d) is not charge-balanced. The correct formula should be  $(\text{Cu},\text{Zn})_3\text{Pb}(\text{AsO}_3\text{OH})_2\text{O}_2$  or  $(\text{Cu},\text{Zn})_3\text{Pb}(\text{AsO}_3\text{OH})_2\text{O}(\text{OH})_2$ .

**Bayleyite**  $\text{Mg}_2(\text{UO}_2)(\text{CO}_3)_3 \cdot 18\text{H}_2\text{O}$

**Origin:** Barbora shaft, Jáchymov ore district, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was 3 mW.

**Raman shifts (cm<sup>-1</sup>):** 3560sh, 3425s (broad), 3260, 3150sh, 1642w, 1627w, 1619w, 1608w, 1586w, 1380w, 1067s, 825–832s, 752s, 718sh, 665sh, 253, 234, 191, 166, 114, 59w.

**Source:** Škácha et al. (2014b).

**Baylissite NH<sub>4</sub>-analogue**  $(\text{NH}_4)_2\text{Mg}(\text{CO}_3)_2 \cdot 4\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 3240, 3174, 2885, 1703w, 1440w, 1421w, 1098s, 686, 488.

**Source:** Fischer (2007).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analysis.

**Bazhenovite**  $\text{Ca}_8\text{S}_5(\text{S}_2\text{O}_3)(\text{OH})_{12} \cdot 20\text{H}_2\text{O}$

**Origin:** Chelyabinsk coal basin, South Urals, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 3.5 mW.

**Raman shifts (cm<sup>-1</sup>):** 3473, 3227, 2500, 1620w, 940, 507s, 466s, 218.

**Source:** Bindi et al. (2005).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data. The crystal structure is solved. The Raman line at 2500 cm<sup>-1</sup> is attributed by authors to H<sub>2</sub>S in a condensed form which may be present in the sample.

**Bazirite** BaZrSi<sub>3</sub>O<sub>9</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1148, 1092, 1078, 1067, 1046, 1005, 995, 957s, 948, 937, 639, 579s, 544, 529, 521sh, 507, 480, 464, 448w, 425w, 384s, 369, 356w, 348w, 342, 328, 259, 239, 201s, 184, 173w, 161, 152sh, 143, 133, 117, 109.**Source:** Takahashi et al. (2008).**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.**Bazzite** Be<sub>3</sub>(Sc,Fe<sup>3+</sup>,Mg)<sub>2</sub>Si<sub>6</sub>O<sub>18</sub>Na<sub>0.32·nH<sub>2</sub>O</sub>**Origin:** Furkabasistunnel, Switzerland.**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal using 488 nm laser radiation. The laser radiation power is not indicated. Polarized spectra were collected in 90°-scattering geometry, and the polarization conditions were: (ZZ), (ZY), (XY), and (ZZ+ZX).**Raman shifts (cm<sup>-1</sup>):** (ZZ): 1093, 1060, 672, 570–610 (broad), 392, 315; (ZY): 970, 917, 902sh, 775, 672, 653sh, 603, 556w, 485w, 451, 375, 243, 224, 131; (XY): 1180, 1163, 970, 909, 777, 731, 672, 653sh, 554–601 (broad), 439, 377, 390, 315, 266w; (ZZ+ZX): 3594s, 3535w.**Source:** Hagemann et al. (1990).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.**Beaverite-(Cu)** Pb(Fe<sup>3+</sup><sub>2</sub>Cu)(SO<sub>4</sub>)<sub>2</sub>(OH)<sub>6</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3421, 3380, 3354, 1176, 1164, 1156, 1117, 1103s, 1081, 1076, 1018, 1010s, 999s, 645, 624, 619, 577, 560, 481, 456, 441, 433, 392, 356, 335, 328, 298, 278, 259, 242, 216, 202, 173.**Source:** Frost et al. (2005m).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of beaverite-(Cu) see also Hudson-Edwards et al. (2008).**Becquerelite** Ca(UO<sub>2</sub>)<sub>6</sub>O<sub>4</sub>(OH)<sub>6</sub>·8H<sub>2</sub>O**Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3547, 3429, 3211, 879, 854, 838s, 831, 814, 546, 508, 455, 399, 353, 328, 303, 260, 238, 192, 156, 142, 111.

**Source:** Frost et al. (2007h).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of becquerelite see also Amme et al. (2002).

### Behierite Ta(BO<sub>4</sub>)

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not indicated. Raman scattering measurements have been performed using 488 and 514.5 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1004, 978s, 900, 848, ~700w, 568s, 461s, 284, 204, 191.

**Source:** Heyns et al. (1990).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of behierite see also Ross (1972) and Blasse and van den Heuvel (1973).

### Behoite Be(OH)<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3501, (3489), 3449s, 1133w, 1056, 1031sh, 1000w, 845w, 769, 701, 682, 602, 549w, 459, 446, 400s, 364w, 349s, 280w, 134, 77.

**Source:** Lutz et al. (1998).

**Comments:** No independent analytical data are provided for the sample used.

### Běhounekite U(SO<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>4</sub>

**Origin:** Geschieber vein, Jáchymov (St Joachimsthal), Czech Republic (type locality).

**Experimental details:** Methods of sample preparation are not indicated. Raman scattering measurements have been performed using 480 (in the region of 4000–1900 cm<sup>-1</sup>) and 785 (in the region of 1900–200 cm<sup>-1</sup>) nm laser radiations. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3370s, 3206, 1269, 1251, 1177, 1158, 1102, 1037, 1023s, 994, 638, 619, 598, 451, 438, 417, 268, 250, 198, 178, 125, 116, 98.

**Source:** Plášil et al. (2011b).

**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

### Belakovskiite Na<sub>7</sub>(UO<sub>2</sub>)(SO<sub>4</sub>)<sub>4</sub>(SO<sub>3</sub>OH)(H<sub>2</sub>O)<sub>3</sub>

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not indicated. Raman scattering measurements have been performed using 780 nm laser radiation. The laser radiation power at the sample was from 2 mW to 6 mW.

**Raman shifts (cm<sup>-1</sup>):** 1185, 1070, 1040, 1000, 985w, 903w, 865sh, 840s, 820w, 660, 650, 605, 590sh, 480, 450.

**Source:** Plásil et al. (2015c).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data.

**Bellidoite** Cu<sub>2</sub>Se

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.12 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** No data: Cu<sub>2</sub>Se exhibits very weak Raman features.

**Source:** Izquierdo-Roca et al. (2009).

**Bendadaite** Fe<sup>2+</sup>Fe<sup>3+</sup><sub>2</sub>(AsO<sub>4</sub>)<sub>2</sub>(OH)<sub>2</sub>·4H<sub>2</sub>O

**Origin:** Lavra do Almerindo (Almerindo mine), Linópolis, Divino das Laranjeiras Co., Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 676 nm Kr<sup>+</sup> laser radiation. The nominal laser radiation power is unknown.

**Raman shifts (cm<sup>-1</sup>):** 3385, 3275, 1690w, ~800s.

**Source:** Kolitsch et al. (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Benitoite** BaTiSi<sub>3</sub>O<sub>9</sub>

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not indicated. Raman scattering measurements have been performed using 632.8 nm laser radiation. The nominal laser radiation power was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 1080, 951, 939, 930s, 917, 577s, 539s, 505, 480, 398, 374s, 350, 267s.

**Source:** Choisnet et al. (1975).

**Comments:** No independent analytical data are given for the sample used. For the Raman spectra of benitoite see also Gaft et al. (2004), Ma and Rossman (2008), and Takahashi et al. (2008).

**Benstonite** Ba<sub>6</sub>Ca<sub>6</sub>Mg(CO<sub>3</sub>)<sub>13</sub>

**Origin:** Minerva mine, Cave-in-Rock, Hardin Co., Illinois, USA.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 and 514.5 nm laser radiation. The nominal laser radiation power was 200 mW.

**Raman shifts (cm<sup>-1</sup>):** 1100s, 1096s, 1081s, 1074s, 714, 691, 251, 236, 206w, 171, 136, 96w.

**Source:** Scheetz and White (1977).

**Comments:** No independent analytical data are given for the sample used.

**Beraunite** Fe<sup>2+</sup>Fe<sup>3+</sup><sub>5</sub>(PO<sub>4</sub>)<sub>4</sub>(OH)<sub>5</sub>·6H<sub>2</sub>O

**Origin:** Boca Rica pegmatite, Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of

individual peaks obtained as a result of the spectral curve analysis. The laser radiation power at the sample is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1174, 1155, 1133, 1116, 1098, 1084sh, 1069, 1058, 1051, 1034, 1011s, 990sh, 969sh, 703sh, 687s, 673, 661, 644, 601, 582, 567s, 546, 503, 491, 478, 468, 455, 437, 403, 398, 336, 322, 309sh, 300, 289, 280, 254, 238, 230, 225, 200, 191sh, 153, 1432, 118, 107.

**Source:** Frost et al. (2014al).

**Comments:** No independent analytical data are given for the sample used. In the cited paper incorrect formula of beraunite is given. Brown color of the sample indicates that it is not beraunite, but its oxydation product eleonorite, a mineral isostructural with beraunite.

### Berdesinskiite V<sup>3+</sup><sub>2</sub>TiO<sub>5</sub>

**Origin:** Vihanti, Northern Finland Region, Finland.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm laser radiation. The nominal laser radiation power was 2 or 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 978w, 898w, 768s, 720s, 647, 593, 512w, 485, 445, 411, 388, 341, 311, 257w, 210, 136w, 83.

**Source:** Voloshin et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

### Bergenite Ca<sub>2</sub>Ba<sub>4</sub>(UO<sub>2</sub>)<sub>9</sub>O<sub>6</sub>(PO<sub>4</sub>)<sub>6</sub>·16H<sub>2</sub>O

**Origin:** Mechelgrün, Vogtland, Saxony, Germany.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3607, 3459, 3295, 2944, 1602, 1330, 1152, 1107, 1059, 995s, 991w, 971w, 961, 948, 810, 798sh, 777, 592, 547, 515, 444, 432, 408, 396, 391, 270, 265, 256, 224, 205, 178, 145, 133, 111.

**Source:** Frost et al. (2007e).

**Comments:** The sample was characterized by electron microprobe analysis.

### Berlinite Al(PO<sub>4</sub>)

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample compacted as a pellet using 1064 nm laser radiation. The nominal laser radiation power was 350 mW.

**Raman shifts (cm<sup>-1</sup>):** 1230, 1111s, 1104sh, 1021, 725w, 650, 566, 524, 462s, 439, 418, 379, 335, 306, 258sh, 221, 196, 163, 149sh, 139w, 119, 107, 84.

**Source:** Pînzaru and Onac (2009).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of berlineite see also Thomas and Webster (1999), O'Neill et al. (2006), and Frezzotti et al. (2012).

**Berlinite tetragonal polymorph** Al(PO<sub>4</sub>)**Origin:** Synthetic.**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1124s, 485, 391, 382, 279, 191.**Source:** O'Neill et al. (2006).**Comments:** The sample was characterized by powder X-ray diffraction data.**Bermanite** Mn<sup>2+</sup>Mn<sup>3+</sup><sub>2</sub>(PO<sub>4</sub>)<sub>2</sub>(OH)<sub>2</sub>·4H<sub>2</sub>O**Origin:** El Criollo granitic pegmatite, Cerro Blanco pegmatite group, Córdoba province, Argentina.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3515, 3470, 3425, 3355, 3285, 3202, 3110, 3038, 2961, 1142, 1117, 1071w, 1012sh, 999s, 991s, 978sh, 900, 586, 577, 552sh, 505sh, 489s, 473s, 455, 441, 419, 400, 341, 307, 270, 256, 249sh, 217s, 2009sh, 189, 171, 156sh, 147, 127.**Source:** Frost et al. (2013x).**Comments:** The sample was characterized only by qualitative electron microprobe analysis.**Bernalite** Fe(OH)<sub>3</sub>**Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not indicated. Raman scattering measurements have been performed using 752.6 nm laser radiation. The laser radiation power was from 0.01 to 10 mW.**Raman shifts (cm<sup>-1</sup>):** 398, 299.**Source:** Lepot et al. (2006).**Comments:** No independent analytical data are provided for the sample used.**Berndtite** SnS<sub>2</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power at the sample was 0.4 mW.**Raman shifts (cm<sup>-1</sup>):** 355, 315s, 205, 140w, 44, 25.**Source:** Fontané et al. (2013).**Comments:** For the Raman spectra of berndtite see also Smith et al. (1977), Jiang and Ozin (1997), and Utyuzh et al. (2010).**Berthierite** FeSb<sub>2</sub>S<sub>4</sub>**Origin:** Zlatá Baňa deposit, eastern Slovakia.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample in a 180°-scattering geometry using 632 nm laser radiation. The laser output radiation power was 210 mW.

**Raman shifts (cm<sup>-1</sup>):** 347, 334, 318sh, 297, 277sh, 264s, 251sh, 226, 183, 150sh, 131, 90, 76s, 60.

**Source:** Kharbishi and András (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

### Bertrandite Be<sub>4</sub>Si<sub>2</sub>O<sub>7</sub>(OH)<sub>2</sub>

**Origin:** Albany, Maine, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3587, 3551, 1073w, 990, 947w, 928, 821, 772, 753, 725sh, 711, 694, 579, 538, 487w, 427w, 386w, 358, 352, 330, 301, 241, 231s, 206s, 183s.

**Source:** Hofmeister et al. (1987).

**Comments:** Methods of the sample identification are not indicated. For the Raman spectrum of bertrandite see also Jehlička et al. (2012).

### Beryl Be<sub>3</sub>Al<sub>2</sub>Si<sub>6</sub>O<sub>18</sub>

**Origin:** Čanište, Republic of Macedonia.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3663w, 3595s, 1610w, 1128, 1111, 1070, 1005, 915, 770, 689s, 616, 587, 571, 516s, 400, 326, 286s, 248, 196s, 143.

**Source:** Makreski and Jovanovski (2009).

**Comments:** Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectra of beryl see also Hagemann et al. (1990), Kloprogge and Frost (2000a), Jasinevicius (2009), Jehlička et al. (2012), and Jehlička and Vandenabeele (2015).

### Beryl Be<sub>3</sub>Al<sub>2</sub>Si<sub>6</sub>O<sub>18</sub>

**Origin:** Čanište, Republic of Macedonia.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3663w, 3595s, 1610w, 1128, 1111, 1070, 1005, 915, 770, 689s, 616, 587, 571, 516s, 400, 326, 286s, 248, 196s, 143.

**Source:** Makreski and Jovanovski (2009).

**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectra of beryl see also Hagemann et al. (1990), Kloprogge and Frost (2000a), Jasinevicius (2009), Jehlička et al. (2012), and Jehlička and Vandenabeele (2015).

### Beryl Cs-bearing CsLiBe<sub>2</sub>Al<sub>2</sub>Si<sub>6</sub>O<sub>18</sub>

**Origin:** Piława Górska, Lower Silesia, SW Poland.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1130w, 1100sh, 1069s, 1008, 686s, 531, 400, 323, 245w, 125.

**Source:** Pieczka et al. (2016b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

### Beryllonite NaBe(PO<sub>4</sub>)

**Origin:** Ehrenfriedersdorf complex, Erzgebirge (Ore Mts.), Germany.

**Experimental details:** Micro-Raman scattering measurements have been performed on a microscopic inclusion in quartz using 514 and 488 nm laser radiations. The laser radiation power at the sample was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 1056s, 1012s, 547, 432, 354.

**Source:** Thomas et al. (2011b).

**Comments:** The sample was characterized by ion microprobe analysis.

**Comments:** For the Raman spectra of beryllonite see also Tait et al. (2010) and Frost et al. (2012k).

### Berzeliite (NaCa<sub>2</sub>)Mg<sub>2</sub>(AsO<sub>4</sub>)<sub>3</sub>

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was between 200 and 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 912sh, 891, 841s, 800sh, 506, 473, 461, 431sh, 332, 170, 127, 115.

**Source:** Khorari et al. (1995).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Berzeliite polymorph alluaudite-type (NaCa<sub>2</sub>)Mg<sub>2</sub>(AsO<sub>4</sub>)<sub>3</sub>

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was between 200 and 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 891, 860s, 800sh, 540w, 469, 426, 402sh, 386, 348, 304w, 217sh, 200.

**Source:** Khorari et al. (1995).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Betalomonosovite Na<sub>6</sub>□<sub>4</sub>Ti<sub>4</sub>(Si<sub>2</sub>O<sub>7</sub>)<sub>2</sub>[PO<sub>3</sub>(OH)][PO<sub>2</sub>(OH)<sub>2</sub>]O<sub>2</sub>(OF)

**Origin:** Lovozero alkaline massif, Kola Peninsula, Russia.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed in a 180°-scattering geometry using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1100, 1030, 925s, 862sh, 804, 678, 587, 548, 493, 456, 414.

**Source:** Sokolova et al. (2015a).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analysis. The crystal structure is solved.

**Beudantite**  $PbFe^{3+}_3(AsO_4)(SO_4)(OH)_6$ 

**Origin:** Tsumeb mine, Tsumeb, Namibia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3449, 3391, 3202, 3123, 3005, 1674w, 1319, 1144, 1107, 1081, 998s, 874sh, 851s, 829sh, 807sh, 622, 616, 578w, 560, 476s, 443, 434s, 410sh, 371w, 328, 311, 301sh, 293, 259sh, 248, 216sh, 202s, 143, 137s.

**Source:** Frost et al. (2011i).

**Comments:** No independent analytical data are provided for the sample used.

**Beusite**  $Mn^{2+}Fe^{2+}_2(PO_4)_2$ 

**Origin:** Bull Moose Mine, Custer, South Dakota, USA.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm laser radiation. The laser radiation power at the sample was about 1–5 mW.

**Raman shifts (cm<sup>-1</sup>):** 1080w, 1068, 1012sh, 999, 950s, 628, 589, 573, 442, 409sh, 322, 250w, 237, 200w, 155.

**Source:** Schneider et al. (2013).

**Comments:** The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

**Beyerite**  $CaBi_2O_2(CO_3)_2$ 

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 785 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Source:** Malik et al. (2016).

**Raman shifts (cm<sup>-1</sup>):** 1302, 1069, 674w, 425, 207, 163s.

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Bianchite or Goslarite**  $Zn(SO_4) \cdot 6H_2O$  or  $Zn(SO_4) \cdot 7H_2O$ 

**Origin:** Minei Hill open pit, Baia Sprie deposit, Romania.

**Experimental details:** Raman scattering measurements have been performed on white fine deposition material using 632 nm laser radiation. The laser radiation power at the sample was 53.6 mW.

**Raman shifts (cm<sup>-1</sup>):** 1191, 1080, 1024s, 914, 626, 506, 427, 280, 222.

**Source:** Buzatu et al. (2012).

**Comments:** No independent analytical data are provided for the sample used. The Raman spectrum may correspond to bianchite or goslarite. These two minerals have very similar Raman spectra, which makes the identification difficult.

**Bikitaite**  $\text{LiAlSi}_2\text{O}_6 \cdot \text{H}_2\text{O}$ 

**Origin:** Bikita, Zimbabwe (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample in 90°- and 180°-scattering geometries using 488 and 514.5 nm Ar<sup>+</sup> laser radiations. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3588, 3477, 3411, 1641, 964, 504, 396, 255, 155, 104—the spectrum obtained at 5 K.

**Source:** Kolesov and Geiger (2002).

**Comments:** Raman spectra in the region below 1900 cm<sup>-1</sup> were obtained at 5 K. No independent analytical data are provided for the sample used.

**Billietite**  $\text{Ba}(\text{UO}_2)_6\text{O}_4(\text{OH})_6 \cdot 8\text{H}_2\text{O}$ 

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3568, 3487, 3398, 3238, 1604, 963, 873, 831, 830, 810, 800, 795, 737, 556, 528, 460, 452, 416, 363, 337, 290, 259, 244, 208, 200, 167, 158, 117, 109.

**Source:** Frost et al. (2007h).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of billietite see also Qader (2011).

**Biotite**  $\text{K}(\text{Mg},\text{Fe})_3[(\text{Si},\text{Al})_4\text{O}_{10}](\text{OH})_2$ 

**Origin:** No data.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 3680, 3658, 767, 717, 679s, 549, 178.

**Source:** Frezzotti et al. (2012).

**Biphosphammite**  $(\text{NH}_4,\text{K})\text{H}_2(\text{PO}_4)$ 

**Origin:** Synthetic.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1024sh, 925s, 551w, 479, 340, 179.

**Source:** O'Neill et al. (2006).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of biphosphammite see also Frost et al. (2011r).

**Birnessite**  $(\text{Na},\text{Ca},\text{K})_{0.6}(\text{Mn}^{4+},\text{Mn}^{3+})_2\text{O}_4 \cdot 1.5\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power density was 100 W/cm<sup>2</sup>.

**Raman shifts (cm<sup>-1</sup>):** 730, 656s, 575s, 506, 303, 296.

**Source:** Julien et al. (2004).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of birnessite see also Julien et al. (2003) and Roqué-Rosell et al. (2010).

**Birnessite**  $(\text{Na},\text{Ca},\text{K})_{0.6}(\text{Mn}^{4+},\text{Mn}^{3+})_2\text{O}_4 \cdot 1.5\text{H}_2\text{O}$

**Origin:** Moa Bay lateritic deposits, eastern Cuba.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm laser radiation. The nominal laser radiation power was 30 mW.

**Raman shifts (cm<sup>-1</sup>):** 655s, 573, 491w, 281.

**Source:** Roqué-Rosell et al. (2010).

**Comments:** The spectrum in the region from 200 to 900 cm<sup>-1</sup> was obtained. The sample was characterized by powder X-ray diffraction data and chemical analysis. For the Raman spectra of birnessite see also Julien et al. (2003, 2004).

**Bischofite**  $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG pulsed laser with 45 mJ/pulse total energy, up to 20 Hz lasing frequency, and 8 ns pulse width. 90°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3507, 3350.

**Source:** Garcia et al. (2006).

**Comments:** No independent analytical data are given for the sample used.

**Bismite**  $\text{Bi}_2\text{O}_3$

**Origin:** Synthetic.

**Raman shifts (cm<sup>-1</sup>):** 446, 410w, 314, 282, 210, 184, 151, 139, 118s, 102, 93s, 83s, 67s, 59, 53s.

**Source:** Betsch and White (1978).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of bismite see also Narang et al. (1994) and Prekajski et al. (2010).

**Bismoclite**  $\text{BiOCl}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 568.2 nm laser radiation. The laser radiation power at the sample was 25 mW.

**Raman shifts (cm<sup>-1</sup>):** 400, 202, 146s, 60.

**Source:** Davies (1973).

**Comments:** No independent analytical data are given for the sample used. For the Raman spectrum of bismoclite see also Rulmont (1972).

**Bismuth**  $\text{Bi}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a film with thickness about 0.5–1 μ using 532 nm laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 91, 65s.

**Source:** Russo et al. (2008).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

### Bismuthinite Bi<sub>2</sub>S<sub>3</sub>

**Origin:** Panarechensk volcanic-tectonic formation, Kola Peninsula, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 261s, 236s, 185, 169, 100, 83w, 70, 53s.

**Source:** Voloshin et al. (2015a).

**Comments:** The samples used were characterized by electron microprobe analyses. For the Raman spectra of bismuthinite see also Kharbish et al. (2009) and Efthimiopoulos et al. (2014).

### Bismutite Bi<sub>2</sub>O<sub>2</sub>(CO<sub>3</sub>)

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 514.5 and 647.1 nm laser radiations. The laser radiation power is not indicated. A 90°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1690w, 1392, 1360, 1067s, 688w, 667, 519w, 445w, 410, 351, 312w, 277w, 203, 172, 162, 158s, 118w, 97w, 94w, 70s, 53s, 51s, 41s, 23.

**Source:** Taylor et al. (1984).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Bismutocolumbite BiNbO<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 200 mW.

**Raman shifts (cm<sup>-1</sup>):** 883, 730, 624s, 537, 424, 382, 368, 336, 272s, 255, 220, 199, 153s, 139s, 110, 108, 93, 84s, 60s.

**Source:** Ayyub et al. (1986).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of bismutocolumbite see also Ayyub et al. (1987), Yu et al. (1990), and Lee et al. (2003).

### Bismutoferrite Fe<sup>3+</sup><sub>2</sub>Bi(SiO<sub>4</sub>)<sub>2</sub>(OH)

**Origin:** Jáchymov U deposit, Krušné Hory (Ore Mts.), Western Bohemia, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3541, 1598, 1536, 1475, 1290, 1219, 1160, 1093, 1004, 695, 669, 501, 472, 440, 430s, 417, 386, 348, 333, 323, 306, 280, 273, 244, 223, 217, 196, 165s, 151s, 144s.

**Source:** Frost et al. (2010a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Bismutontantalite**  $\text{BiTaO}_4$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 1084 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was 130 mW.

**Raman shifts (cm<sup>-1</sup>):** 625s, 539, 371, 340, 274, 257s, 222, 201, 157s, 143s, 112, 87, 64.

**Source:** Lee et al. (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Bitikleite**  $\text{Ca}_3(\text{SbSn})(\text{AlO}_4)_3$

**Origin:** Upper Chegem volcanic structure, Kabardino-Balkaria, Northern Caucasus, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation output power was 40–60 mW. A 0°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 832sh, 799, 760, 738sh, 624sh, 600, 500s, 440w, 409w, 356w, 299s, 252, 218w, 190, 161w, 151, 120.

**Source:** Galuskina et al. (2010a).

**Comments:** The sample was characterized by electron micro-diffraction, powder X-ray diffraction data, and electron microprobe analyses.

**Bixbyite**  $\text{Mn}^{3+}_2\text{O}_3$

**Origin:** An unknown locality in Zaire.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was 12.5 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 650sh, 630, 581s, 509.

**Source:** Bernard et al. (1993a).

**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman spectrum of natural bixbyite differs from that of synthetic  $\alpha\text{-Mn}_2\text{O}_3$ : the Raman shifts of the latter are 698, 645, 592, 481, 404, 314, and 192 cm<sup>-1</sup> (Julien et al. 2004). Raman spectrum of presumed bixbyite published by Baioumy et al. (2013) is questionable.

**Blatterite**  $\text{Sb}^{5+}_{3}\text{Mn}^{3+}_{9}\text{Mn}^{2+}_{35}(\text{BO}_3)_{16}\text{O}_{32}$

**Origin:** Bergslagen ore province, south central Sweden.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532.4 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 573s, 214w.

**Source:** Enholm (2016).

**Comments:** The sample was characterized by electron microprobe analyses.

**Blödite**  $\text{Na}_2\text{Mg}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on a powdered sample using 532 nm laser radiation. The laser radiation power at the sample was 2 mW.**Raman shifts (cm<sup>-1</sup>):** ~3300, 1184, 1104, 1058, 995s, 631, 463, 449.**Source:** Jentzsch et al. (2011).**Comments:** No independent analytical data are provided for the sample used.**Bluebellite**  $\text{Cu}_6(\text{IO}_3)(\text{OH})_{10}\text{Cl}$ **Origin:** Shallow D shaft, Blue Bell claims, Central Mojave Desert, California, USA (type locality).**Experimental details:** Raman scattering measurements have been performed on the (001) face of a flat single crystal using 514.3 nm laser radiation. Laser beam was incident approximately perpendicular to the (001) face. The laser radiation power at the sample was 2 mW.**Raman shifts (cm<sup>-1</sup>):** ~3500, 1007, 680s, 641, 544, 502w, 254, 203, 172.**Source:** Mills et al. (2014b).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.**Bluelizardite**  $\text{Na}_7(\text{UO}_2)(\text{SO}_4)_4\text{Cl}(\text{H}_2\text{O})_2$ **Origin:** Blue Lizard mine, San Juan Co., Utah, USA (type locality).**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The nominal laser radiation power was 3 mW.**Raman shifts (cm<sup>-1</sup>):** 3606, 3576, 3475, 3422, 3343, 3219, 1216, 1189, 1156, 1143, 1090, 1061, 1050, 1012, 1003, 998, 986, 951, 854s, 848sh, 651, 641, 620, 619, 607, 592, 260, 252, 237, 208.**Source:** Plášil et al. (2014a).**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. Plášil et al. (2015d) indicate additional bands at 465 and 445 cm<sup>-1</sup>.**Bobcookeite**  $\text{NaAl}(\text{UO}_2)_2(\text{SO}_4)_4 \cdot 18\text{H}_2\text{O}$ **Origin:** Blue Lizard mine, San Juan Co., Utah, USA (type locality).**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 and 780 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3610, 3565, 3500, 3445, 3380, 3315sh, 3270sh, 3195sh, 1640, 1210, 1145, 1110, 1035, 1010s, 990sh, 845s, 630, 600w, 470, 450, 330w, ~210.**Source:** Kampf et al. (2015b).**Comments:** Raman shifts in the range of stretching vibrations of water molecules are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was

characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Bobdownsite**  $\text{Ca}_9\text{Mg}(\text{PO}_3\text{F})(\text{PO}_4)_6$ 

**Origin:** Big Fish River, Yukon, Canada (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1088, 1028w, 989, 966s, 923, 626, 605w, 554, 483w, 433, 406, 282, 158w.

**Source:** Tait et al. (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Bobierrite**  $\text{Mg}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$ 

**Origin:** Zheleznyi mine (Iron mine), Kovdor massif, Kola Peninsula, Russia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3498, 3263, 3212, 3096, 2895, 1072, 998, 951, 909, 842, 787, 717, 693, 668, 631, 583, 557, 542, 468, 435, 420, 364, 318, 290, 282, 262, 233, 215, 182, 170, 149, 136.

**Source:** Frost et al. (2002f).

**Comments:** No independent analytical data are provided for the sample used.

**Bobshannonite**  $\text{Na}_2\text{KBa}(\text{Mn},\text{Na})_8(\text{Nb},\text{Ti})_4(\text{Si}_2\text{O}_7)_4\text{O}_4(\text{OH})_4(\text{O},\text{F})_2$ 

**Origin:** Mont Saint-Hilaire, Québec, Canada (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** ~3655, ~3610, 1038, 970, 901, 716, 680, 608, 580, 510, 410, 341, 310, 240, 207, 143.

**Source:** Sokolova et al. (2015b).

**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Bohdanowiczite**  $\text{AgBiSe}_2$ 

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shift (cm<sup>-1</sup>):** 171, 161.

**Source:** Rajaji et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data. Trigonal,  $a = 8.412$  (6) Å,  $c = 19.63(3)$  Å.

### Böhmite $\gamma\text{-AlO(OH)}$

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power at the sample was 200 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3371, 3220, 3085, 2989, 1072, 732, 674s, 495s, 451, 360s, 228.

**Source:** Ruan et al. (2001).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

### Boleite $\text{KAg}_9\text{Pb}_{26}\text{Cu}_{24}\text{Cl}_{62}(\text{OH})_{48}$

**Origin:** Amelia Mine, Santa Rosalia, Baja, California, Mexico (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3448, 3408, 3371sh, 921, 817, 757, 731, 696, 478, 455, 386, 361, 300, 234, 161s, 146sh, 128sh.

**Source:** Frost et al. (2003j).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of boleite see also Frost and Williams (2004).

### Boltwoodite $(\text{K},\text{Na})(\text{UO}_2)(\text{SiO}_3\text{OH}) \cdot 1.5\text{H}_2\text{O}$

**Origin:** Kladská U deposit, Slavkovský les Mountains, western Bohemia, Czech Republic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 780 nm laser radiation. The laser radiation output power was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 3387w, 3351w, 3313w, 1606w, 1327w, 958, 938, 847sh, 833sh, 804s, 542, 496, 483, 435, 423, 398, 321, 280, 262, 220, 180, 152, 136, 110, 93, 75, 60.

**Source:** Plášil et al. (2016a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectrum of boltwoodite see also Frost et al. (2006e).

### Bonaccordite $\text{Ni}_2\text{Fe}^{3+}\text{O}_2(\text{BO}_3)$

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 20 mW. Polarized spectrum was collected in the (zz) geometry.

**Raman shifts (cm<sup>-1</sup>):** 650s, 582s, 570sh, 544, 526, 495, 473sh, 423, 388w, 357w, 314, 285w, 257w.

**Source:** Leite et al. (2002).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

**Bonattite**  $\text{Cu}(\text{SO}_4) \cdot 3\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1126, 1009s, 620, 587, 481, 429, 386, 250, 160, 123.

**Source:** Fu et al. (2012).

**Comments:** Bands of  $\text{H}_2\text{O}$  stretching vibrations are very weak and poor-resolved. No independent analytical data are provided for the sample used.

**Bonazziite**  $\beta\text{-As}_4\text{S}_4$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 647.1 nm Kr<sup>+</sup> laser radiation. The laser radiation power at the sample was 60 mW.

**Raman shifts (cm<sup>-1</sup>):** 388w, 376w, 362s, 352, 343, 332sh, 217, 211sh, 187s, 164, 144, 62, 56, 42w, 32w.

**Source:** Muniz-Miranda et al. (1996).

**Comments:** The photo-induced transformation from  $\beta\text{-As}_4\text{S}_4$  to pararealgar takes place in the sample under the exposure to a more short-wave radiation.

**Bonazziite**  $\beta\text{-As}_4\text{S}_4$

**Origin:** Khaidarkan deposit, Kyrgyzstan (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 875 nm diode laser radiation. The laser radiation power was 3 mW.

**Raman shifts (cm<sup>-1</sup>):** 362s, 352, 343, 217s, 187s, 164.

**Source:** Bindi et al. (2015b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Boracite**  $\text{Mg}_3\text{B}_7\text{O}_{13}\text{Cl}$

**Origin:** Lüneburg, Lower Saxony, Germany (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3581sh, 3494, 3431sh, 3405s, 3334sh, 3277, 3254w, 2903, 2727sh, 1617, 1583, 1348, 1143, 1136, 1121, 1009s, 671, 660sh, 621, 611sh, 582sh, 536w, 515sh, 494, 473sh, 415, 317, 211s, 182s, 163s, 147, 134s.

**Source:** Frost et al. (2012m).

**Comments:** No independent analytical data are provided for the sample used. The spectrum shows the presence of OH groups.

**Borax**  $\text{Na}_2\text{B}_4\text{O}_5(\text{OH})_4 \cdot 8\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was about 100 mW.**Raman shifts (cm<sup>-1</sup>):** 3575s, 3495s, 3447s, 3400s, 3357s, 3140s, 1640w, 957, 860, 776, 590w, 530, 474, 390, 361, 160, 120, 90, 78.**Source:** Devi et al. (1994).**Comments:** No independent analytical data are provided for the sample used. Polarized spectra of borax single crystals were collected in  $x(yy)z$ ,  $x(yx)z$ ,  $x(zy)z$ , and  $x(zx)z$  scattering geometries too. For the Raman spectra of borax see also Krishnamurti (1955) and Kipcak et al. (2014).**Bornite**  $\text{Cu}_5\text{FeS}_4$ **Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 638 nm laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 784w, 579, 464w, 377, 266s, 201s.**Source:** Lanteigne et al. (2012).**Bosiite**  $\text{NaFe}^{3+}{}_3(\text{Al}_4\text{Mg}_2)(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3\text{O}$ **Origin:** No data.**Experimental details:** Polarized  $-y(zz)y$  Raman scattering measurements have been performed on a single crystal using 488.0 or 514.5 nm  $\text{Ar}^+$  laser radiations. The laser radiation power at the sample was about 14 mW.**Raman shifts (cm<sup>-1</sup>):** No data: only a figure of the Raman spectrum is given in the cited paper.**Source:** Watenphul et al. (2016b).**Comments:** The sample was characterized by electron microprobe analysis.**Botallackite**  $\text{Cu}_2\text{Cl}(\text{OH})_3$ **Origin:** No data.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632.8 and 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation output power was 30 mW at 632.8 nm and is not indicated at 514.5 nm.**Raman shifts (cm<sup>-1</sup>):** 3504, 3420, 897, 857, 678w, 503, 450s, 401s, 324, 279, 251, 175, 155, 115.**Source:** Bouchard and Smith (2003).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.**Botryogen**  $\text{MgFe}^{3+}(\text{SO}_4)_2(\text{OH}) \cdot 7\text{H}_2\text{O}$ **Origin:** Alcaparrosa mine, Antofagasta Province, Chile.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3576, 3441, 3330, 3256, 3107sh, 3186, 1626, 1221, 1202, 1178, 1076, 1041, 1017, 1002s, 607, 563, 499s, 464, 384, 353, 271, 241s, 208, 180, 146.

**Source:** Frost et al. (2011f).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Bottinoite** NiSb<sup>5+</sup><sub>2</sub>(OH)<sub>12</sub>·6H<sub>2</sub>O

**Origin:** Bottino Mine, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3510sh, 3458, 3368, 3291, 3228sh, 3223sh, 1648, 1163w, 1111w, 1080w, 1045w, 735w, 630sh, 618, 599sh, 575sh, 516sh, 501, 316sh, 336, 317, 302, 254, 235, 207, 169, 146, 125, 114.

**Source:** Frost and Bahfenne (2010e).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of bottinoite see also Rintoul et al. (2011) and Bahfenne (2011).

**Boulangierite** Pb<sub>5</sub>Sb<sub>4</sub>S<sub>11</sub>

**Origin:** Zlatá Baňa, Slanské Vrchy Mts., central Slovakia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 632 nm Nd-YAG laser radiation. The laser radiation power radiation density at the sample was  $8.5 \cdot 10^{-3}$  mW/ $\mu\text{m}^2$ . A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 355s, 335, 315, 236, 220, 206, 189, 146, 129sh, 100, 85, 74sh, 62.

**Source:** Kharbish and Jeleň (2016).

**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by electron microprobe analysis.

**Bournonite** CuPbSbS<sub>3</sub>

**Origin:** Felsőbanya, Romania.

**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal with the laser polarization parallel to the *a*-, *b*-, and *c*-axes using 785 nm laser radiation. The laser radiation power at the sample was 1.7 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 339, 324s, 192, 275, 227w, 197, 181, 166.

**Source:** Kharbish et al. (2009).

**Comments:** Slightly varying band positions among polarized spectra are averaged. The sample was characterized by electron microprobe analysis.

**Boussingaultite** (NH<sub>4</sub>)<sub>2</sub>Mg(SO<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O

**Origin:** Larderello, Tuscany, Italy.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm diode laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3380w, 3290w, 3080, 3040, 2918w, 2845w, 1705, 1678, 1460, 1436, 1133w, 1096w, 1063, 983s, 626, 616, 454, 360w, 310w, <222w.

**Source:** Culka et al. (2009).

**Comments:** No independent analytical data are provided for the sample used. Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. For the Raman spectrum of boussingaultite see also Jentzsch et al. (2013).

### Boussingaultite (NH<sub>4</sub>)<sub>2</sub>Mg<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>·6H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 253.7 nm of mercury radiation and exposition of the order of 16 h.

**Raman shifts (cm<sup>-1</sup>):** 3396, 3331, 3281, 3060, 2830, 1469w, 1433, 1141, 1121, 1102, 1091, 1072, 1061, 979s, 622, 455, 265w, 220w, 198, 147, 130, 89w, 54.

**Source:** Shantakumari (1953).

**Comments:** No independent analytical data are provided for the sample used.

### Bowieite Rh<sub>2</sub>S<sub>3</sub>

**Origin:** Svetly Bor complex, Urals, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented grain using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 374, 308s, 287.

**Source:** Zaccarini et al. (2016).

**Comments:** For the Raman spectrum of bowieite see also Singh et al. (2014).

### Braccoite NaMn<sup>2+</sup><sub>5</sub>[Si<sub>5</sub>O<sub>14</sub>(OH)](AsO<sub>3</sub>)(OH)

**Origin:** Valletta mine, Maira Valley, Piedmont, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 632.8 and 532 nm He-Ne and Nd-YAG laser radiations. The nominal laser radiation power was 20 and 80 mW, respectively. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1040sh, 1017s, 932sh, 907s, 829s, 748, 706, 665s, 618, 563w, 525w, 451, 390, 360w, 291, 261w, 226.

**Source:** Cámara et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### Bracewellite CrO(OH)

**Origin:** Artificial.

**Experimental details:** Raman scattering measurements have been performed on a chromium coupon using 647 nm Kr<sup>+</sup> laser radiation. The nominal laser radiation power was 8 mW. A nearly 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** ~825w, ~780w, ~620, ~565s, ~310s.

**Source:** Maslar et al. (2001).

**Comments:** The sample was characterized by X-ray emission spectrum.

**Brackebuschite**  $\text{Pb}_2\text{Mn}^{3+}(\text{VO}_4)_2(\text{OH})$ **Origin:** Sierra de Cordoba, Argentina (type locality).**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 3145w, 859s, 687w, 450w, 334, 158.**Source:** Lafuente and Downs (2016).**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analysis. The crystal structure is solved. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.**Bradleyite**  $\text{Na}_3\text{Mg}(\text{PO}_4)(\text{CO}_3)$ **Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been using 532 nm laser radiation. The nominal laser radiation power was 240 mW.**Raman shifts (cm<sup>-1</sup>):** 1079s, 1067w, 1051, 1033, 971s, 733w, 694w, 627w, 591, 484w, 430, 262, 218, 198, 161.**Source:** Gao et al. (2015).**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.**Braggite** PtS**Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 18,794.59 cm<sup>-1</sup> Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was between 1 and 2 mW.**Raman shifts (cm<sup>-1</sup>):** 378, 360s, 330s, 111.**Source:** Bakker (2014).**Comments:** For the Raman spectra of braggite see also Mernagh and Hoatson (1995), Pikl et al. (1999), and Merkle et al. (1999).**Brandholzite**  $\text{MgSb}_2(\text{OH})_{12}\cdot 6\text{H}_2\text{O}$ **Origin:** Krížnica mine, Pernek deposit, Malé Karpaty Mts., Slovak Republic.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3552, 3483sh, 3466, 3383sh, 3240, 3205sh, 1648w, 1597sh, 1189sh, 1160w, 1093, 1043, 730, 630, 618s, 604, 578sh, 526, 503, 340s, 318s, 303sh, 252w, 232w, 191w, 147w, 115w.**Source:** Frost et al. (2009e).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectra of brandholzite see also Rintoul et al. (2011) and Bahfenne (2011).

**Brannerite**  $\text{UTi}_2\text{O}_6$ 

**Origin:** El Cabril mine, near Cordoba, Sierra Albarrena region, southern Spain.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 759s, 615, 523, 435, 375, 327, 265, 194, 161.

**Source:** Zhang et al. (2013).

**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was preliminarily annealed and characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectra of brannerite see also Frost and Reddy (2011a) and Charalambous et al. (2012).

**Brannockite**  $\text{KSn}_2(\text{Li}_3\text{Si}_{12})\text{O}_{30}$ 

**Origin:** Golden Horn Batholith, Washington, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using 632 nm He-Ne laser radiation. The laser radiation power was 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 1160, 1141, 1042, 992, 947w, 841, 774, 616, 485, 462s, 382, 365w, 343, 282s, 257w, 248w, 204w, 156s, 128, 103s, 93sh, 63.

**Source:** Raschke et al. (2016).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analysis. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Brassite**  $\text{Mg}(\text{AsO}_3\text{OH}) \cdot 4\text{H}_2\text{O}$ 

**Origin:** Jáchymov U deposit, Krušné Hory (Ore Mts.), Western Bohemia, Czech Republic (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3511, 3450, 3387, 3314, 3035, 878sh, 876sh, 862, 809, 739sh, 699, 609, 448, 404, 387sh, 358sh, 298, 274sh, 242, 199, 181, 158sh, 149, 121, 108.

**Source:** Frost et al. (2010h).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Braunite**  $\text{Mn}^{2+}\text{Mn}^{3+}_6\text{O}_8(\text{SiO}_4)$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on microscopic inclusions in in-glaze pigment of the nineteenth-century relief tiles using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 17 mW.

**Raman shifts (cm<sup>-1</sup>):** 958, 686, 617, 513s, 471, 330w, 217, 121.

**Source:** Coutinho et al. (2016).

**Comments:** The sample was characterized by electron microprobe analysis.

**Brazilianite**  $\text{NaAl}_3(\text{PO}_4)_2(\text{OH})_4$ 

**Origin:** Córrego Frio mine, Linópolis, Divino das Laranjeiras, Doce valley, Minas Gerais, Brazil (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3543, 3519, 3472s, 3447, 3417s, 3355, 3291, 3249, 3157, 1579w, 1395, 1150w, 1117, 1074, 1037sh, 1019s, 988s, 973, 953, 723, 660, 636, 615, 599s, 563s, 534, 508sh, 466, 441, 414, 358, 319, 287, 276, 253, 244, 231, 220, 208, 172, 162w, 149, 113, 105.

**Source:** Frost and Xi (2012l).

**Comments:** No independent analytical data are provided for the sample used.

**Bredigite**  $(\text{Ca},\text{Ba})\text{Ca}_{13}\text{Mg}_2(\text{SiO}_4)_8$ 

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 991, 977, 950w, 927w, 907sh, 895sh, 884s, 872s, 857s, 847, 575, 554w, 543w, 526w, 514w, 502w, 424w, 406w, 384w, 375w, 298w, 257w, 240w, 211w, 194w, 149w, 125, 109sh, 68w.

**Source:** Xiong et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Breithauptite** NiSb

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 650.

**Source:** Xie et al. (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Brewsterite-Sr**  $\text{Sr}(\text{Al}_2\text{Si}_6)\text{O}_{16}\cdot 5\text{H}_2\text{O}$ 

**Origin:** Strontian, Agryll, Scotland, UK (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 1.06 μm Nd-YAG laser radiation. The nominal laser radiation power was 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 1136w, 495s, 387, 236, 171.

**Source:** Mozgawa (2001).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Brianyoungite**  $\text{Zn}_3(\text{CO}_3,\text{SO}_4)(\text{OH})_4$ 

**Origin:** Esperanza Mine, Laurion district, Greece.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3669, 3631, 3615, 3564, 3571, 3554, 3531, 3518, 3400, 3297, 3193, 3076, 2973, 2938, 2910, 2880, 2851, 1550, 1457, 1440, 1388, 1367, 1298, 1163, 1127, 1086, 1056s, 1038sh, 984, 973s, 958sh, 736, 704, 638, 609, 528, 507sh, 475, 451, 433, 423, 378, 367, 347, 306, 271, 257w, 277, 216, 160sh, 153sh, 151s, 143s, 132sh, 125, 113, 108.

**Source:** Frost et al. (2015r).

**Comments:** The sample was characterized only by qualitative electron microprobe analysis.

**Briartite**  $\text{Cu}_2\text{FeGeS}_4$ 

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 488.0 or 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 2 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 437, 412w, 396, 378, 342s, 329sh, 304w, 294, 272, 250, 224, 162w, 141, 109.

**Source:** Rincón et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of briartite see also Himmrich and Haeuseler (1991).

**Britvinitie**  $\text{Pb}_{14}\text{Mg}_9(\text{Si}_{10}\text{O}_{28})(\text{BO}_3)_4(\text{CO}_3)_2(\text{OH})_{12}\text{F}_2$ 

**Origin:** Långban deposit, Bergslagen ore region, Filipstad district, Värmland, Sweden (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 633 nm laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3697s, 3543, 1718, 1696w, 1420, 1335, 1230, 1193, 1093, 1041s, 992, 960, 905, 873w, 842, 817, 802, 775, 740w, 717, 690, 667, 593, 489, 412, 303s, 277, 258, 217, 154.

**Source:** Kolitsch et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Brizziite**  $\text{NaSbO}_3$ 

**Origin:** Le Cetine mine, Chiusdino, Siena province, Tuscany, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 830w, 749w, 660s, 617, 508, 315, 307, 230, 204, 158.

**Source:** Frost and Bahfenne (2010a).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of brizziite see also Bittarello et al. (2015).

**Brochantite** Cu<sub>4</sub>(SO<sub>4</sub>)(OH)<sub>6</sub>

**Origin:** Chuquicamata, Chile.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 780 nm Nd-YAG laser radiation. The laser radiation power at the sample was <1 mW.

**Raman shifts (cm<sup>-1</sup>):** 3580s, 3501sh, 3489s, 1906, 1265w, 1173w, 1135w, 1078, 990s, 786, 770, 749, 629, 608, 600, 517, 501, 482, 467, 442, 415, 340, 330, 295, 265, 247, 238, 228, 213, 172, 149, 141, 124.

**Source:** Martens et al. (2003a).

**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by XRD and EDX, but these data are not provided in the cited paper. For the Raman spectra of brochantite see also Makreski et al. (2005a), Schmidt and Lutz (1993), Bouchard and Smith (2003), Frost et al. (2004a), Apopei et al. (2014a), and Coccato et al. (2016).

**Brochantite** Cu<sub>4</sub>(SO<sub>4</sub>)(OH)<sub>6</sub>

**Origin:** Bučim, Macedonia.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3587sh, 3565s, 3536sh, 3508w, 3475, 3388s, 3358, 1160sh, 1134w, 1121sh, 1099sh, 1076, 973s, 904, 871w, 840w, 765w, 710w, 660w, 619, 609sh, 590w, 551w, 510, 480w, 431w, 415w, 394, 363sh, 323w, 292w, 237w, 190, 163w, 141w, 137w, 126w, 116w, 83.

**Source:** Makreski et al. (2005a).

**Comments:** No independent analytical data are provided for the sample used.

**Bromargyrite** AgBr

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a partly oriented crystal, in the  $x(zz)y + x(zx)y$  scattering geometry, using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 262, 176, 82s.

**Source:** Bottger and Damsgard (1971).

**Comments:** The sample was characterized by means of flame emission spectroscopy and mass-spectrometry.

**Bromellite** BeO

**Origin:** Muiane pegmatite, Mozambique.

**Experimental details:** Raman scattering measurements have been performed on inclusions in morganite using 488 and 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 14 mW.

**Raman shifts (cm<sup>-1</sup>):** 1097, 1081, 722, 684s, 678, 388.

**Source:** Thomas and Davidson (2010).

**Comments:** For the Raman spectrum of bromellite see also Devanarayanan et al. (1991).

### Brookite TiO<sub>2</sub>

**Origin:** Magnet Cove, Arkansas.

**Experimental details:** Raman scattering measurements have been performed on oriented crystals using 458, 515 and 633 nm laser radiation. The laser radiation power is not indicated. Polarized spectra were collected in the following scattering geometries: (xx), (yy), and (zz) for the A<sub>1g</sub> Raman mode, (xy) for B<sub>1g</sub>, (xz) for B<sub>2g</sub>, and (yz) for B<sub>3g</sub>.

**Raman shifts (cm<sup>-1</sup>):** A<sub>1g</sub>: 640, 545, 492w, 412w, 324w, 246, 194w, 152s, 125; B<sub>1g</sub>: 622, 449, 381w, 327, 283s, 212, 169; B<sub>2g</sub>: 584, 460s, 391w, 366s, 325, 254w, 160s; B<sub>3g</sub>: 500, 416w, 318s, 212w, 132.

**Source:** Iliev et al. (2013).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of brookite see also Yanqing et al. (2000), Zajzon et al. (2013), and Andò and Garzanti (2014).

### Brownite MnS

**Origin:** Zakłodzie meteorite, Poland (type locality).

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented grain using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 1.5 mW.

**Raman shifts (cm<sup>-1</sup>):** ~620, ~460, ~400sh, ~220w.

**Source:** Ma et al. (2012b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

### Brownleeite MnSi

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal using 532 nm Nd-YAG laser radiation. The laser radiation power density was  $2 \times 10^5$  W/cm<sup>2</sup>. A 180°-scattering geometry was employed. Polarized spectra were collected in the z(yy)-z, z(xx)-z, z(xy)-z, and z(yx)-z scattering geometries. At different scattering geometries the shifts of the Raman lines do not exceed 2 cm<sup>-1</sup>.

**Raman shifts (cm<sup>-1</sup>):** ~310, ~190.

**Source:** Tite et al. (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

### Brownmillerite Ca<sub>2</sub>Fe<sup>3+</sup>AlO<sub>5</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 707s, ~550, ~420, ~380, ~310, ~290, 256s.

**Source:** Dhankhar et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of brownmillerite see also Martínez-Ramírez and Fernández-Carrasco (2011).

### Brucite Mg(OH)<sub>2</sub>

**Origin:** Mariana convergent plate margin, western Pacific Ocean.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal in a polished thin section using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 722, 442s, 276.

**Source:** Sagatowska (2010).

**Comments:** The sample was characterized by electron microprobe analysis. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of brucite see also Lutz et al. (1994).

### Brüggenite Ca(IO<sub>3</sub>)<sub>2</sub>·H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3470, 3376, 832sh, 811, 767, 754sh, 746sh, 382, 343, 333sh, 322sh, 251sh, 229.

**Source:** Alici et al. (1992).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Brugnatellite Mg<sub>6</sub>Fe<sup>3+</sup>(CO<sub>3</sub>)(OH)<sub>13</sub>·4H<sub>2</sub>O

**Origin:** Monte Ramazzo, Genoa, Liguria, Italy.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power at the sample was 5 mW. Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3922, 3696s, 3685s, 3656sh, 2933, 1591w, 1323w, 1102, 1087, 959w, 765w, 698sh, 690s, 664w, 644w, 621.

**Source:** Frost and Bahfenne (2009).

**Comments:** No independent analytical data are given for the sample used. Raman spectrum from Monte Ramazzo given as Supplementary Information does not coincide with the spectrum given in the cited paper.

### Brushite Ca(PO<sub>3</sub>OH)·2H<sub>2</sub>O

**Origin:** Moorba Cave, Jurien Bay, Dandaragan Shire, Western Australia, Australia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632 nm He-Ne laser radiation. The laser radiation power is not detected. Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3533, 3472, 1055, 1000, 985s, 872, 858sh, 576w, 519s, 498, 411s, 276, 209, 140, 109.

**Source:** Frost et al. (2012h).

**Comments:** No independent analytical data are given for the sample used. For the Raman spectrum of brushite see also Xu et al. (1999).

#### Buchwaldite NaCa(PO<sub>4</sub>)

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~1048, ~1026, ~1015, ~966s, ~588s, ~450, ~427.

**Source:** Suchanek et al. (1998).

**Comments:** The sample was characterized by powder X-ray diffraction data.

#### Bukovskýite Fe<sup>3+</sup><sub>2</sub>(AsO<sub>4</sub>)(SO<sub>4</sub>)(OH)·7H<sub>2</sub>O

**Origin:** Kaňk, near Kutná Hora, central Bohemia, Czech Republic (type locality).

**Experimental details:** Raman scattering measurements have been performed on microcrystalline aggregates using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3420w, 3219w, 3102sh, 1652w, 1179, 1131, 1090, 1054, 1010, 984s, 911, 886, 847s, 816s, 613, 552, 511, 464, 428s, 315, 263s, 196, 147.

**Source:** Loun et al. (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectrum of bukovskýite see also Culka et al. (2016).

#### Bunnoite Mn<sup>2+</sup><sub>6</sub>AlSi<sub>6</sub>O<sub>18</sub>(OH)<sub>3</sub>

**Origin:** Kamo Mt., Kochi prefecture, Japan (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 3546sh, 3472, 835, 718, 663, 651, 578, 553, 515s, 490s, 464, 451, 438, 385, 319s, 309s, 267w, 235.

**Source:** Nishio-Hamane et al. (2016a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

#### Bunsenite NiO

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on nano-scaled and slightly agglomerated particles using 532 nm laser radiation. The laser radiation power at the sample was 2.48 mW.

**Raman shifts (cm<sup>-1</sup>):** 1525s, 1093, 497.

**Source:** Thema et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and TEM/EDX. The strong band at 1525 cm<sup>-1</sup> is attributed to the double magnon scattering, but this assignment is questionable.

**Burangaita** NaFe<sup>2+</sup>Al<sub>5</sub>(PO<sub>4</sub>)<sub>4</sub>(OH)<sub>6</sub>·2H<sub>2</sub>O

**Origin:** Hålsjöberg, Sweden.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 150 mW.

**Raman shifts (cm<sup>-1</sup>):** 3618s, 3251s, 1141, 1045s, 1023, 988, 618, 601, 587, 400, 369, 354.

**Source:** Thomas et al. (1998).

**Comments:** No independent analytical data are provided for the sample used.

**Burbankite** (Na,Ca)<sub>3</sub>(Sr,Ba,Ce)<sub>3</sub>(CO<sub>3</sub>)<sub>5</sub>

**Origin:** Kalkfeld carbonatite complex, Namibia.

**Experimental details:** Raman scattering measurements have been performed on microscopic particles in fluid inclusions using a He-Ne laser with the laser radiation power of 1.8 mW or an Ar<sup>+</sup> laser with the power of 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 1078s, ~700w.

**Source:** Bühn et al. (1999).

**Comments:** The sample was characterized by synchrotron powder X-ray diffraction data and electron microprobe analysis. For the Raman spectrum of burbankite see also Bühn et al. (2002) and Chakhmouradian et al. (2017).

**Burbankite** (Na,Ca)<sub>3</sub>(Sr,Ba,Ce)<sub>3</sub>(CO<sub>3</sub>)<sub>5</sub>

**Origin:** Bear Lodge carbonatite, Wyoming, USA.

**Experimental details:** Methods of sample preparation are not described. Micro-Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1085s, 1069w, (970) (broad), 881w, 872w, 738sh, 728sh, 717w, 703w, 286w, 233, 209w, 160, 143.

**Source:** Chakhmouradian et al. (2017).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of burbankite see also Bühn et al. (1999, 2002).

**Burckhardtite** Pb<sub>2</sub>(Fe<sup>3+</sup>Te<sup>6+</sup>)(AlSi<sub>3</sub>O<sub>8</sub>)O<sub>6</sub>

**Origin:** Moctezuma, Sonora, Mexico (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.3 nm cobalt solid-state laser radiation. The laser radiation power at the sample was 0.6 mW.

**Raman shifts (cm<sup>-1</sup>):** 897w, 833w, 690s, 661w, 646s, 619s, 554, 477, ~463sh, 505sh, 391, 322, 295, 202.

**Source:** Christy et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Burgessite** Co<sub>2</sub>(H<sub>2</sub>O)<sub>4</sub>[AsO<sub>3</sub>(OH)]<sub>2</sub>(H<sub>2</sub>O)

**Origin:** Keeley mine, South Larrain Township, Timiskaming District, Ontario, Canada (type locality).

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3591w, 3395, 3328, 3204sh, 3185sh, 852s, 830s, 806s, 740s, 447, 383, 353sh, 322sh, 215, 162.

**Source:** Čejka et al. (2011a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Burkeite** Na<sub>4</sub>(SO<sub>4</sub>)(CO<sub>3</sub>)

**Origin:** Searles Lake, San Bernardino Co., California, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3465w, 3331w, 1244w, 1132, 1102, 1065s, 1008sh, 994s, 981sh, 704, 645, 635sh, 622, 475, 453, 352, 149s, 112.

**Source:** López et al. (2014d).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectra of burkeite see also Korsakov et al. (2009) and Jentzsch et al. (2013).

**Buseckite** (Fe,Zn,Mn)S

**Origin:** Zakłodzie meteorite, Poland (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 1.2 mW.

**Raman shifts (cm<sup>-1</sup>):** 322sh, 296.

**Source:** Ma et al. (2012a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Bustamite** (Ca,Mg,Fe)<sub>2</sub>Si<sub>2</sub>O<sub>6</sub>

**Origin:** Sasa, Macedonia.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 50 or 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1034, 1007, 972s, 869s, 839, 812, 735w, 714w, 644s, 574w, 548w, 511, 489, 446w, 428w, 404, 364s, 350sh, 310, 285sh, 260w, 232, 172, 154w, 138w, 125w, 116.

**Source:** Makreski et al. (2006b).

**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by powder X-ray diffraction data and neutron activation analysis.

**Butlerite** Fe<sup>3+</sup>(SO<sub>4</sub>)(OH)·2H<sub>2</sub>O

**Origin:** Alcaparrosa mine, Cerritos Bayos, Calama, El Loa province, Antofagasta, Chile.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3469sh, 3310w, 3155sh, 3012sh, 1225sh, 1198, 1145sh, 1109s, 1088sh, 1024s, 617sh, 600, 543, 469, 450sh, 408, 374sh, 294sh, 247, 221, 181, 154sh.

**Source:** Čejka et al. (2011b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Buttgenbachite** Cu<sub>36</sub>(NO<sub>3</sub>)<sub>2</sub>Cl<sub>8</sub>(OH)<sub>62</sub>·nH<sub>2</sub>O

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne or 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was  $\leq 30$  mW.

**Raman shifts (cm<sup>-1</sup>):** 1054, 1041, 985, 843, 622, 595, 489, 451, 409s, 349, 314, 259, 236, 193, 184, 164, 145s, 128s.

**Source:** Bouchard and Smith (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Byströmite** MgSb<sup>5+</sup><sub>2</sub>O<sub>6</sub>

**Origin:** Synthetic.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 810w, 749s, 676, 625, 592w, 560w, 570s, 480w, 357, 331, 300, 248w, 231w.

**Source:** Husson et al. (1979).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Cabalzarite** CaMg<sub>2</sub>(AsO<sub>4</sub>)<sub>2</sub>·2H<sub>2</sub>O

**Origin:** No data.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~800, ~750s, ~700sh, ~445.

**Source:** Carey et al. (2015).

**Cabvinitie**  $\text{Th}_2\text{F}_7(\text{OH}) \cdot 3\text{H}_2\text{O}$ 

**Origin:** Su Seinargiu, Sarroch, Cagliari, Sardinia, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** (3407), 3257s, 461, 342, 209s, 113s.

**Source:** Orlandi et al. (2017).

**Comments:** The Raman shifts have been partly determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved.

**Cacoxenite**  $\text{Fe}^{3+}_{24}\text{AlO}_6(\text{PO}_4)_{17}(\text{OH})_{12} \cdot 75\text{H}_2\text{O}$ 

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3599, 3504, 3429, 3251s, 3085, 2947, 2667, 2309, 1231w, 1213w, 1153, 1118, 1081, 1041, 1026, 979, 961, 926w, 619, 606w, 573, 526w, 495w, 433w, 411w, 371w, 307w, 273, 262, 245, 217, 199w, 169w, 155.

**Source:** Frost et al. (2003c).

**Comments:** No independent analytical data are given for the sample used.

**Cadmoindite**  $\text{CdIn}_2\text{S}_4$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 647.1 nm Kr<sup>+</sup> laser radiation. The nominal laser radiation power was <5 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 367s, 360, 315, 301w, 249, 232, 207, 188, 93, 70.

**Source:** Ursaki et al. (2002).

**Comments:** No independent analytical data are given for the sample used. For the Raman spectra of cadmoindite see also Unger et al. (1978), Kulikova et al. (1988), and Syrbu et al. (1996a, b).

**Cadmoselite**  $\text{CdSe}$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 201 for CdSe particles with 2.26 nm in diameter and 205 for CdSe particles with 3.52 nm in diameter.

**Source:** Nien et al. (2008).

**Comments:** The samples were characterized by TEM. Bulk CdSe exhibits a Raman peak at 209 cm<sup>-1</sup> (Widulle et al. 1999).

**Cafarsite**  $\text{Ca}_{5.9}\text{Mn}_{1.7}\text{Fe}_3\text{Ti}_3(\text{AsO}_3)_{12} \cdot 4\text{H}_2\text{O}$ 

**Origin:** Cervandone Mt., Val Devero, Piedmont, Italy.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power at the sample was 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 869, 757, 725, 328, 286, 196s.

**Source:** Frost and Bahfenne (2010d).

**Comments:** No independent analytical data are given for the sample used. For the Raman spectra of cafarsite see also Kloporgg and Frost (1999b) and Bahfenne (2011).

**Cafetite**  $\text{CaTi}_2\text{O}_5 \cdot \text{H}_2\text{O}$ 

**Origin:** Khibiny massif, Kola Peninsula, Russia.

**Experimental details:** Methods of sample preparation are not indicated. Raman scattering measurements have been using 532 nm solid-state laser radiation. The laser radiation output power was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 825, 798, 732w, 602, 482, 449, 419s, 358w, 329, 302, 292, 251s, 203, 190, 177, 152, 126, 110.

**Source:** Martins et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Cahnite**  $\text{Ca}_2\text{B}(\text{AsO}_4)(\text{OH})_4$ 

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 844, 791, 759, 548, 538, 448, 428, 378, 395, 324, 290.

**Source:** Ross (1972).

**Comments:** No independent analytical data are given for the sample used.

**Cairncrossite**  $\text{Sr}_2\text{Ca}_7(\text{Si}_4\text{O}_{10})_4(\text{OH})_2 \cdot 15\text{H}_2\text{O}$ 

**Origin:** Wesselsmine, Kalahari Manganese Field, South Africa (type locality).

**Experimental details:** Methods of sample preparation are not indicated. Raman scattering measurements have been performed using 488 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 8 mW.

**Raman shifts (cm<sup>-1</sup>):** 3670, 3650, 3550s, 1145, 1060, 1030w, 1000sh, 777, 700, 610s, 456, 438, 346w, 280, 183w, 130.

**Source:** Giester et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Calaverite**  $\text{AuTe}_2$ **Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed at 50 K on an oriented crystal using 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was <10 mW. Polarized spectra were collected from the (20-12) face, which is parallel to the  $b$ -axis and makes an angle of  $7^\circ 05'$  with the  $a$ -axis. A  $180^\circ$ -scattering geometry with laser beam polarizations ( $xx$ ) and ( $yy$ ) for  $A_g$ , and ( $xy$ ) for  $B_g$  was employed.

**Raman shifts (cm $^{-1}$ ):**  $A_g(xx)$ : 172, 162, 152, 143w, 128, 119, 101s, 92, 88, 73w, 57w, 47, 42w;  $A_g(yy)$ : 163, 155w, 151, 144w, 134, 127, 119, 109w, 106w, 101w, 97, 72, 57, 47;  $B_g(xy)$ : 162, 154s, 142s, 133, 125s, 118, 108s, 101, 91, 61, 54, 48.

**Source:** van Loosdrecht et al. (1992).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Calciborite**  $\text{CaB}_2\text{O}_4$ **Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm $^{-1}$ ):** 1632, 1525s, ~1450, 1428, 1295, 1231, 1172, 1080, 1002, 811, 788, 738s, 683, 653, 549, 504, 389, 328, 230, 209, 179, 171.

**Source:** Rulmont and Almou (1989).

**Comments:** Raman frequencies are given for a sample with the isotopic composition  $^{40}\text{Ca}^{11}\text{B}_2\text{O}_4$ . The sample was characterized by powder X-ray diffraction data.

**Calcio-olivine**  $\text{Ca}_2(\text{SiO}_4)$ **Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation output power was 0.4 mW.

**Raman shifts (cm $^{-1}$ ):** 924, 885, 857, 838s, 813s, 570w, 558w, 525w, 410, 400, 306, 269, 261, 251, 242, 193, 183, 177, 151, 134w, 125w, 118w.

**Source:** Remy et al. (1997).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of calico-olivine see also Piriou and McMillan (1983).

**Calcioaravaipaite**  $\text{PbCa}_2\text{AlF}_9$ **Origin:** Grand Reef mine, Arizona, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 532 nm solid-state laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm $^{-1}$ ):** 3580s, 3296, 2925w, 2425, 2344, 2203, 2073, 1939w, 1822, 1441w, ~652, 560s, 538s, 417w, 390w, 366w, 323, 277sh, 263, 234, 203, 191, 177, 167.

**Source:** Kampf et al. (2011c).

**Comments:** The sample identification was done by single-crystal X-ray diffraction data. The crystal structure is solved. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

### Calciolangbeinite $K_2Ca_2(SO_4)_3$

**Origin:** Artificial (component of clinker).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514 nm laser radiation. The nominal laser radiation power was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 1203, 1147, 1107, 993, 630.

**Source:** Black and Brooker (2007).

**Comments:** Identification of this phase is tentative and, probably, erroneous. For the Raman spectrum of calciolangbeinite see also Gastaldi et al. (2008).

### Calciolangbeinite $K_2Ca_2(SO_4)_3$

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Micro-Raman scattering measurements have been performed using 632.8 nm laser radiation. The nominal laser radiation power was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 1144w, 1118w, 1025s, 1019s, 1006s, 645, 618, 466, 454.

**Source:** Gastaldi et al. (2008).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of calciolangbeinite see also Black and Brooker (2007).

### Calcioptetersite $CaCu_6(PO_4)_2(PO_3OH)(OH)_6 \cdot 3H_2O$

**Origin:** Domaš, near Olomouc, northern Moravia, Czech Republic (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3494, 3351w, 3301w, 3243w, 2931w, 2882sh, 1606, 1457sh, 1110, 1079, 1042, 947, 873, 577s, 475s, 394, 341, 208, 174, 144, 118.

**Source:** Čejka et al. (2011c).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

### Calcite $Ca(CO_3)$

**Origin:** No data.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 2906w, 2835w, 2707w, 1903w, 1749w, 1436w, 1086s, 713w, 283, 156.

**Source:** Edwards et al. (2005).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of calcite see also Rutt and Nicola (1974), Behrens et al. (1995), Buzgar and Apopei (2009), Wehrmeister et al. (2010), Ciobotă et al. (2012), Frezzotti et al. (2012), Schmid and Dariz (2015), Sánchez-Pastor et al. (2016), and Perrin et al. (2016).

**Calcurmolite**  $(\text{Ca}_{1-x}\text{Na}_x)_2(\text{UO}_2)_3(\text{MoO}_4)_2(\text{OH})_{6-x}\cdot n\text{H}_2\text{O}$

**Origin:** Sokh-Karasu area, Kadzharan Mo Deposit, Kafan District, Armenia (type locality).

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 930, 900sh, 868, 823, 794s, 700, 644, 495, 378, 354sh, 271, 206sh, 144w.

**Source:** Frost et al. (2008c).

**Comments:** No independent analytical data are provided for the sample used. Strong bands in the range from 970 to 1150 cm<sup>-1</sup> in the IR spectrum of calcurmolite given in the cited paper are mainly due to an impurity. The assignment of these bands to MOH bending modes is erroneous. The IR band at 3694 cm<sup>-1</sup> may correspond to the admixture of a clay mineral.

**Calderite**  $\text{Mn}^{2+}_3\text{Fe}^{3+}_2(\text{SiO}_4)_3$

**Experimental details:** Only a calculated Raman spectrum of calderite is given in the cited paper.

**Raman shifts (cm<sup>-1</sup>):** 1017, 897, 887, 884, 871, 840, 597, 580, 552, 493, 486, 450, 373, 355, 349, 344, 300, 293, 284, 217, 211, 186, 169, 158.

**Source:** Arlt et al. (1998).

**Calderónite**  $\text{Pb}_2\text{Fe}^{3+}(\text{VO}_4)_2(\text{OH})$

**Origin:** Karrantza Valley, western area of the Basque Co., Spain.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser (with the laser radiation power at the sample of 20 mW) and 785 nm diode laser radiation (with the radiation output power of 150 mW).

**Raman shifts (cm<sup>-1</sup>):** 977s, 684w, 336, 210w, 159w.

**Source:** Goienaga et al. (2011).

**Comments:** No independent analytical data are given for the sample used.

**Caledonite**  $\text{Cu}_2\text{Pb}_5(\text{SO}_4)_3(\text{CO}_3)(\text{OH})_6$

**Origin:** Hard Luck Claim, near Baker, San Bernardino Co., California, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power at the sample was 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 3439, 3417, 3379, 1674, 1392, 1358, 1124, 1109, 1083, 1053, 977s, 950, 848, 825, 791, 722, 628, 605, 475, 456, 427, 344, 316, 278, 251, 229, 152.

**Source:** Frost et al. (2003e).

**Comments:** No independent analytical data are provided for the sample used.

**Callaghanite** Cu<sub>2</sub>Mg<sub>2</sub>(CO<sub>3</sub>)(OH)<sub>6</sub>·2H<sub>2</sub>O

**Origin:** Gabbs occurrence, Nye Co., Nevada, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power at the sample was 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 3620, 3575, 3564s, 3511, 3502, 3375, 3350, 3040, 2906, 1398s, 1087s, 1013, 961, 944, 871, 840, 749, 707, 688, 517, 499s, 481, 459, 445, 395, 380, 350, 336, 283, 277, 252, 218, 211, 195, 160, 147, 141, 127, 121, 100.

**Source:** Čejka et al. (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Calomel** HgCl

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a single crystal in the (zz) polarization using 514.5 and 632.8 nm He-Ne laser radiations. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 272, 164s, 36s.

**Source:** Radepont (2013).

**Comments:** For the Raman spectrum of calomel see also Markov and Roginskii (2011).

**Calumetite** Cu(OH)<sub>2</sub>·2H<sub>2</sub>O

**Origin:** No data.

**Experimental details:** Methods of sample preparation are not indicated. Raman scattering measurements have been performed using 632.8 nm He-Ne laser radiation. The output laser radiation power was 30 mW.

**Raman shifts (cm<sup>-1</sup>):** 3550, 3450, 1054, 1041s, 985, 843, 622, 595, 489, 451, 409, 347, 314, 259, 236, 193, 184, 164, 145, 139, 128.

**Source:** Bouchard and Smith (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of calumetite see also Bouchard-Abouchakra (2001).

**Camaronesite** Fe<sup>3+</sup><sub>2</sub>(PO<sub>3</sub>OH)<sub>2</sub>(SO<sub>4</sub>)(H<sub>2</sub>O)<sub>4</sub>·1-2H<sub>2</sub>O

**Origin:** Camarones valley, Arica province, Chile (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 3463, 3363, 3140, ~1610, 1080s, 1014s, 937, 526, 305, 254, 227.

**Source:** Kampf et al. (2013d).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved.

**Camerolaite**  $\text{Cu}_6\text{Al}_3(\text{OH})_{18}(\text{H}_2\text{O})_2[\text{Sb}(\text{OH})_6](\text{SO}_4)$ **Origin:** Cap Garonne, France (type locality).**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal with the laser beamorthogonal to the elongation direction of the crystal (*b* axis) using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was from 5 to 30 mW.**Raman shifts (cm<sup>-1</sup>):** 3596, 3558, 3495, 3200–3120, 2330w, 1064, 1050w, 968, 614s, 526s, 447, 347w, 325, 272, 237.**Source:** Mills et al. (2014a).**Comments:** The Raman shifts are given for the holotype sample no. 477.067. The sample was characterized by powder X-ray diffraction data.**Canavesite**  $\text{Mg}_2(\text{HBO}_3)(\text{CO}_3)\cdot 5\text{H}_2\text{O}$ **Origin:** No data.**Experimental details:** Methods of sample preparation are not described. Micro-Raman scattering measurements have been performed using 514.5 nm Ar-Kr laser radiation. The laser radiation power was from 2 to 5 mW.**Raman shifts (cm<sup>-1</sup>):** 3657s, 3484sh, 3392, 3293, 2910, 1458w, 1284, 1105s, 982, 768s, 635w, 548, 174s.**Source:** Grice et al. (1986).**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.**Cancrinite**  $(\text{Na},\text{Ca},\square)_8(\text{Al}_6\text{Si}_6)\text{O}_{24}(\text{CO}_3,\text{SO}_4)_2\cdot 2\text{H}_2\text{O}$ **Origin:** Cava Satom, Cameroon.**Experimental details:** Raman scattering measurements have been performed on a single crystal using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 5 mW.**Raman shifts (cm<sup>-1</sup>):** 3647w, 3536w, 1057s, 1042, 1002, 981, 976, 960, 937, 816, 768, 685, 631, 499, 469, 460, 440, 418, 401, 364, 350, 338, 293s, 277, 231, 161, 115, 108.**Source:** Gatta et al. (2012a).**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. Raman shifts are given for the crystal in two different orientations (crystal rotated by 90°). For the Raman spectra of cancrinite see also Mozgawa (2001) and Lotti (2014).**Cancrinite SO<sub>4</sub>-rich**  $(\text{Na},\text{Ca},\square)_8(\text{Al}_6\text{Si}_6)\text{O}_{24}(\text{CO}_3,\text{SO}_4)_2\cdot 2\text{H}_2\text{O}$ **Origin:** Cinder Lake, Manitoba, Canada.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3591w, 3544, 1060s, 992s, 774w, 720w, 687w, 633w, 515, 465, 441s, 340, 298, 275s, 230, 198, 89s.**Source:** Martins et al. (2016).**Comments:** The sample was characterized by X-ray microdiffraction data and electron microprobe analysis.

**Canfieldite**  $\text{Ag}_8\text{SnS}_6$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514 nm YAG laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 310, 221w, 76s.**Source:** Cheng et al. (2016).**Comments:** The sample was characterized by powder X-ray diffraction data and Hall measurements.**Cannonite**  $\text{Bi}_2\text{O}(\text{SO}_4)(\text{OH})_2$ **Origin:** Alfenza, Crodo, Italy.**Experimental details:** Raman scattering measurements have been performed on an oriented crystal with the polarization of the incident laser beam parallel to *Y* using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3439, 3376, 3190w 1114, 1059, 984s, 621w, 605w, 562, 467, 452s, 438s, 400w, 337, 318s, 279, 222s, 189, 147s, 121s, 101s, 80w, 62.**Source:** Capitani et al. (2013).**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectra of cannonite see also Gama (2000) and Capitani et al. (2014).**Carbocernaite**  $(\text{Sr,Ce,La})(\text{Ca,Na})(\text{CO}_3)_2$ **Origin:** Bear Lodge carbonatite, Wyoming, USA.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm solid-state laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** Ca-Sr-rich variety: 1099s, 1077s, 979s (broad), 864w, 744w, 728sh, 716, 693, 269s, 215, 181, 127. Na-REE-rich variety: 1104s, 1097s, 1079s, 983 (broad) 874w, 860w, 749, 732sh, 724, 716sh, 704w, 677w, 257s, 188, 122.**Source:** Chakhmouradian et al. (2017).**Comments:** The samples were characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The broad bands at ~980 cm<sup>-1</sup> may be due to fluorescence.**Carbonatecyanotrichite**  $\text{Cu}_4\text{Al}_2(\text{CO}_3)(\text{OH})_{12}\cdot 2\text{H}_2\text{O}$ **Origin:** Grandview mine, Coconino Co., Arizona, USA.**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal with the laser beam orthogonal to the elongation direction of the crystal (*b* axis) using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was from 5 to 30 mW.**Raman shifts (cm<sup>-1</sup>):** 3657, 3583, 3400–3300, 2329, 1141w, 977s, 591, 524s, 441, 273w, 233w.**Source:** Mills et al. (2014a).**Comments:** The sample was characterized by powder X-ray diffraction data.

**Carletonite**  $\text{KNa}_4\text{Ca}_4\text{Si}_8\text{O}_{18}(\text{CO}_3)_4(\text{F},\text{OH}) \cdot \text{H}_2\text{O}$ 

**Origin:** Poudrette Quarry, Saint Hilaire Mt., Quebec, Canada (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3595, 3584, 3572, 3570, 3235w, 2905, 2630, 1753w, 1732w, 1662w, 1617w, 1548w, 1481, 1426, 1217, 1086s, 1075s, 1066s, 840, 782, 756w, 735w, 726, 706, 698, 685, 663w, 547, 513, 495, 430, 401, 356, 342, 325w, 316, 289, 235, 217, 194, 174, 157, 142.

**Source:** Frost et al. (2013ai).

**Comments:** No independent analytical data are provided for the sample used.

**Carlfrancisite**  $\text{Mn}^{2+}_3(\text{Mn}^{2+},\text{Mg},\text{Fe}^{3+},\text{Al})_{42}(\text{As}^{3+}\text{O}_3)_2(\text{As}^{5+}\text{O}_4)_4[(\text{Si},\text{As}^{5+})\text{O}_4]_6[(\text{As}^{5+},\text{Si})\text{O}_4]_2(\text{OH})_{42}$ 

**Origin:** Kombat mine, Otavi valley, Namibia (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power at the sample was in the range 5–12.5 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3660w, 3600, 3532, 3463, 1600, 897, 836sh, 819sh, 791s, 732, 616, 514, 400.

**Source:** Hawthorne et al. (2013).

**Comments:** The sample was characterized by powder and single-crystal X-ray diffraction data, and electron microprobe analyses. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Carlfriesite**  $\text{CaTe}^{6+}(\text{Te}^{4+})_2\text{O}_8$ 

**Origin:** Moctezuma mine, New Mexico, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** The IR and Raman spectra of presumed carlfriesite presented in the cited paper are wrong. Actually, spectra of calcite are given. The bands of calcite are erroneously assigned to Te–O-stretching vibrations.

**Source:** Frost et al. (2009g).

**Comments:** No independent analytical data are provided for the sample used.

**Carlinitite**  $\text{Tl}_2\text{S}$ 

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 2.5 mW.

**Raman shifts (cm<sup>-1</sup>):** ~280, ~160 (at room temperature); 280, 192, 171s, 143 (at 12 K).

**Source:** Chia et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Carlosturanite**  $(\text{Mg},\text{Fe}^{2+},\text{Ti})_{21}(\text{Si},\text{Al})_{12}\text{O}_{28}(\text{OH})_{34} \cdot \text{H}_2\text{O}$ 

**Origin:** Val Varaita, Piedmont, northern Italy.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 788sh, 776s, 765sh, 706, 692, 671, 451, 363, 329.

**Source:** Belluso et al. (2007).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Carlsbergite** CrN

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on a powdered single-layer coating on silicon substrate using 633 nm He-Ne laser radiation. The nominal laser radiation power was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 619w, 238w.

**Source:** Barshilia and Rajam (2004).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Carminite**  $\text{PbFe}^{3+}(\text{AsO}_4)_2(\text{OH})_2$ 

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power was <1 mW.

**Raman shifts (cm<sup>-1</sup>):** 3254, 3217, 849, 835, 822, 738, 543, 497, 467, 350, 324, 259, 210.

**Source:** Frost and Kloporgge (2003).

**Comments:** No independent analytical data are provided for the sample used.

**Carnallite**  $\text{KMgCl}_3 \cdot 6\text{H}_2\text{O}$ 

**Origin:** A dolerite sill in eastern Siberia, Russia.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3472sh, 3444s, 3425s, 3401, 1641s, 401, 321w, 217, 202, 126, 97, 71, 59.

**Source:** Grishina et al. (1992).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of carnallite see also Weber et al. (2012).

**Carnegieite** NaAlSiO<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 488 nm Ar<sup>+</sup> laser radiation. The output laser radiation power was 600 mW. A 90°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1072, 982, 964, 949, 803w, 721w, 685, 637w, 487, 444, 433, 404, 379s, 347sh, 340sh, 313sh, 262w, 217, 154, 114.

**Source:** Matson et al. (1986).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Carnotite K<sub>2</sub>(UO<sub>2</sub>)<sub>2</sub>(VO<sub>4</sub>)<sub>2</sub>·3H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 6471 Å Kr laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 975, 825w, 737s, (645w), 585w, 540w, (475w), 410w, 380, 360w, (310w), 275w, 250w, 230w.

**Source:** Baran and Botto (1976).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of carnotite see also Biwer et al. (1990) and Frost et al. (2005c).

### Carpathite C<sub>24</sub>H<sub>12</sub>

**Origin:** Picacho Peak Area, San Benito Co., California, USA.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1627, 1615, 1594, 1449, 1437, 1393w, 1366s, 1350s, 1337, 1289w, 1220, 1044w, 1026, 994w, 949w, 660w, 483s, 450, 369, 304w, 238w.

**Source:** Echigo et al. (2007).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of carpathite see also Zhao et al. (2013b).

### Carpholite Mn<sup>2+</sup>Al<sub>2</sub>Si<sub>2</sub>O<sub>6</sub>(OH)<sub>4</sub>

**Origin:** Vrpsko, Macedonia.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power at the sample was from 50 to 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1087, 1029, 987sh, 958, 919s, 883, 828, 777, 735s, 709, 678, 658, 634, 609, 583sh, 559, 503, 469, 441, 404, 371, 345s, 315, 292, 281, 260, 238, 209, 162sh.

**Source:** Makreski et al. (2006b).

**Comments:** The sample was characterized by powder X-ray diffraction data and neutron activation analysis. For the Raman spectrum of carpholite see also Jovanovski et al. (2009).

### Carrboydite (Ni<sub>1-x</sub>Al<sub>x</sub>)(SO<sub>4</sub>)<sub>x/2</sub>(OH)<sub>2</sub>·nH<sub>2</sub>O (*x* < 0.5, *n* > 3x/2)

**Origin:** Widgiemooltha, Western Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power at the sample was <1 mW.

**Raman shifts (cm<sup>-1</sup>):** 3614, 3445 (broad), 1125, 981s, 631, 613, 563, 552, 499, 457, 403, 318, 248, 227, 205.

**Source:** Frost et al. (2003h).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of carboydite see also Lin et al. (2006).

### Carrollite CuCo<sub>2</sub>S<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 660s, 509, 474.

**Source:** Nie et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

### Caryopilite Mn<sup>2+</sup><sub>3</sub>Si<sub>2</sub>O<sub>5</sub>(OH)<sub>4</sub>

**Origin:** Santa Cruz Formation, Brazil.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** No data: only a figure of the Raman spectrum is given in the cited book.

**Source:** Johnson (2015).

**Comments:** The sample was characterized by electron microprobe analyses.

### Cassiterite SnO<sub>2</sub>

**Origin:** No data.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 633 nm He-Ne laser radiation. The nominal laser radiation power was 30 mW.

**Raman shifts (cm<sup>-1</sup>):** 842, 776, 635s, 475.

**Source:** Bouchard and Smith (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of cassiterite see also Andò and Garzanti (2014) and Evrard et al. (2015).

### Castellaroite Mn<sup>2+</sup><sub>3</sub>(AsO<sub>4</sub>)<sub>2</sub>·4H<sub>2</sub>O

**Origin:** Monte Nero mine, Rocchetta Vara, La Spezia, Liguria, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm Nd-YAG laser radiation. The laser radiation output power was 500 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3942w, 3758w, 3491w, 3241w, 3116w, 2925w, 1663w, 934w, 911sh, 863s, 847sh, 822s, 801s, 578w, 509w, 459sh, 426, 372, 341sh, 275w, 215w, 182w, 150, 143sh, 109.

**Source:** Kampf et al. (2016a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### Caswellsilverite $\text{NaCrS}_2$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal using 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was 50 mW. Polarized spectra were collected in the  $y(xy)z$  and  $y(xx)z$  scattering geometries.

**Raman shifts (cm<sup>-1</sup>):** 317, 252.

**Source:** Unger et al. (1979).

**Comments:** No independent analytical data are provided for the sample used. In the  $y(xy)z$  scattering geometry only a band at 252 cm<sup>-1</sup> is observed.

### Catalanoite $\text{Na}_2(\text{HPO}_4)\cdot 8\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed at 40 °C on an arbitrarily oriented sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was 30 mW.

**Raman shifts (cm<sup>-1</sup>):** 3412s, 3238w, 1089, 987s, 869s, 518, 407w, 388.

**Source:** Ghule et al. (2003).

**Comments:** The sample was characterized by thermogravimetric data.

### Catapleite $\text{Na}_2\text{Zr}(\text{Si}_3\text{O}_9)\cdot 2\text{H}_2\text{O}$

**Origin:** No data.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 1005s, 928, 622, 563.

**Source:** Gaft et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis, but no independent analytical data are provided for the sample used.

### Cattierite $\text{CoS}_2$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a  $\text{CoS}_2$  film using 632.8 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 392s, 316w, 290.

**Source:** Kinner et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Cavansite $\text{Ca}(\text{V}^{4+}\text{O})(\text{Si}_4\text{O}_{10})\cdot 4\text{H}_2\text{O}$

**Origin:** Wagholi Quarry, Maharashtra, India.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3654, 3604, 3577w, 3546, 3504, 3429sh, 1109w, 1088w, 1072w, 1043w, 981s, 973sh, 954sh, 935w, 842w, 823w, 713w, 672, 587sh, 574, 542, 477, 437, 388w, 350, 307sh, 291, 251, 230, 194, 131, 113.

**Source:** Frost and Xi (2012h).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of cavansite see also Prasad and Prasad (2007).

### Cebaite (Ce) Ba<sub>3</sub>Ce<sub>2</sub>(CO<sub>3</sub>)<sub>5</sub>F<sub>2</sub>

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed using 488 nm laser radiation. The nominal laser radiation power was 300 mW.

**Source:** Hong et al. (1999).

**Raman shifts (cm<sup>-1</sup>):** 1088, 911, 1516, 718, 625.

### Čejkaite Na<sub>4</sub>(UO<sub>2</sub>)(CO<sub>3</sub>)<sub>3</sub>

**Origin:** Svornost mine, Jáchymov, Krušné Hory (Ore Mts.), Czech Republic (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1630, 1371sh, 1342, 1327sh, 1074s, 807, 805s, 734, 730, 703, 693, 419, 412, 347, 311s, 291, 281, 262, 194, 165, 143, 122.

**Source:** Čejka et al. (2010b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

### Celadonite KMgFe<sup>3+</sup>Si<sub>4</sub>O<sub>10</sub>(OH)<sub>2</sub>

**Origin:** Akaky River, Cyprus.

**Experimental details:** Raman scattering measurements have been performed on a powdery sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 0.9 mW.

**Raman shifts (cm<sup>-1</sup>):** 3604w, 3583w, 3566s, 3538w, 1597, 1132, 1086, 1056w, 1017sh, 961, 797w, 769w, 701, 551s, 460w, 445w, 393, 318w, 273, 174s.

**Source:** Correia et al. (2007).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of celadonite see also Ospitali et al. (2008).

### Celestine Sr(SO<sub>4</sub>)

**Origin:** Dufton, England.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1160, 1112w, 1003s, 641sh, 623, 461.

**Source:** Buzgar et al. (2009).

**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by EMPA. No independent analytical data are provided for the sample used. For the Raman spectra of celestine see also Kloprogge et al. (2001b), Andò and Garzanti (2014), and Culka et al. (2016a).

### Celsian Ba(Al<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>)

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~1050w, ~990, ~940, ~920sh, ~750w, ~715w, ~695w, ~550w, ~505s, ~470, ~405w, ~365w, ~305, ~250, ~195, ~165.

**Source:** Galuskina et al. (2016b).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of celsian see also Graham et al. (1992) and Colombari et al. (2000).

### Cerianite-(Ce) CeO<sub>2</sub>

**Origin:** Kerimasi volcano, Gregory Rift, northern Tanzania.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 825–820w, 571, 449s, 184.

**Source:** Zaitsev et al. (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectra of cerianite-(Ce) see also Nakajima et al. (1994), Wang et al. (1998b), and Hao (2008).

### Černýite Cu<sub>2</sub>CdSnS<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a thin film. Other experimental details are not described.

**Raman shifts (cm<sup>-1</sup>):** 333, 304, 284.

**Source:** Guo et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the IR spectrum of černýite see also Rincón et al. (2015).

### Ceruleite Cu<sub>2</sub>Al<sub>7</sub>(AsO<sub>4</sub>)<sub>4</sub>(OH)<sub>13</sub>·11.5H<sub>2</sub>O

**Origin:** Emma Louisa gold mine, Guanaco district, Antofagasta, Chile.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3611sh, 3608s, 3597s, 3384, 3222, 3198sh, 3056, 1654w, 1042, 1003w, 951, 932, 903s, 870, 845, 827, 747w, 700w, 662w, 597s, 579sh, 515, 500sh, 464, 451sh, 430sh, 417, 400, 373, 335, 316, 299, 280, 262, 239, 231sh, 208, 195sh, 184sh, 176, 152, 132, 118, 111.

**Source:** Frost et al. (2013b).

**Comments:** No independent analytical data are provided for the sample used.

**Cerussite** Pb(CO<sub>3</sub>)**Origin:** No data.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 633 nm He-Ne laser radiation. The nominal laser radiation power was 30 mW.**Raman shifts (cm<sup>-1</sup>):** 1477, 1370, 1052s, 246, 225, 176, 152.**Source:** Bouchard and Smith (2003).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of cerussite see also Ciomartan et al. (1996), Frost et al. (2003e, f), and Frezzotti et al. (2012).**Cervantite** Sb<sup>3+</sup>Sb<sup>5+</sup>O<sub>4</sub>**Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 402w, 199, 96s.**Source:** Jamal et al. (2013).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of cervantite see also Cody et al. (1979) and Makreski et al. (2013b).**Cesanite** Ca<sub>2</sub>Na<sub>3</sub>(SO<sub>4</sub>)<sub>3</sub>OH**Origin:** No data.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 1104sh, 1004s, 647, 626s, 474, 448s.**Source:** Frezzotti et al. (2012).**Comments:** No independent analytical data are provided for the sample used.**Chabazite-Ca** Ca<sub>2</sub>[Al<sub>4</sub>Si<sub>8</sub>O<sub>24</sub>]·13H<sub>2</sub>O**Origin:** Nidda, Germany.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 300 mW.**Raman shifts (cm<sup>-1</sup>):** 1161w, 1082w, 808w, 697w, 465s, 402w, 357, 264, 204, 128.**Source:** Mozgawa (2001).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of chabazite-Ca see also Pechar and Rykl (1983).**Chalcanthite** Cu(SO<sub>4</sub>)·5H<sub>2</sub>O**Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power at the source was 30 mW.**Raman shifts (cm<sup>-1</sup>):** 3482, 3345, 3206, 1143, 1096, 986s, 612, 465, 426, 332w, 281, 202, 135, 124.**Source:** Bouchard and Smith (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of chalcanthite see also Berger (1976), Christy et al. (2004), Fu et al. (2012), and Bissengaliyeva et al. (2016).

### Chalcoalumite $\text{CuAl}_4(\text{SO}_4)(\text{OH})_{12} \cdot 3\text{H}_2\text{O}$

**Origin:** Červená vein, Jáchymov, Czech Republic.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The output laser radiation power was 2 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3670, 3610, 3450s, 3270sh, 2940w, 2780w, 2650w, 1610w, 1455, 1135, 1110sh, 1005, 981s, 803w, (642sh), 594s, 494, 455, 415w, 220w, 175.

**Source:** Plášil et al. (2014d).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

### Chalcocite $\text{Cu}_2\text{S}$

**Origin:** Synthetic.

**Experimental details:** No data.

**Raman shifts ( $\text{cm}^{-1}$ ):** 465s, 257w.

**Source:** Kumar and Nagarajan (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data and ICP analysis.

### Chalcocyanite $\text{Cu}(\text{SO}_4)$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 1205, 1101, 1045s, 1014s, 671w, 623, 514, 480sh, 448sh, 423, 347, 270, 250sh.

**Source:** Buzgar et al. (2009).

**Comments:** No independent analytical data are provided for the sample used. For the IR spectrum of chalcocyanite see also Fu et al. (2012).

### Chalcomenite $\text{Cu}(\text{Se}^{4+}\text{O}_3) \cdot 2\text{H}_2\text{O}$

**Origin:** El Dragon Mine, Potosí, Bolivia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3506w, 3184w, 2953w, 813s, 720, 690sh, 552, 472, 400w, 367w, 260, 218, 141, 128.

**Source:** Frost and Keeffe (2008b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis, but no analytical data are provided in the cited paper.

**Chalconatronite**  $\text{Na}_2\text{Cu}(\text{CO}_3)_2 \cdot 3\text{H}_2\text{O}$ 

**Origin:** Product of surface alterations of bronze.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1600, 1329, 1073, 1053, 764, 698w, 327s, 261–268.

**Source:** Chiavari et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Chalcophanite**  $\text{ZnMn}^{4+}_3\text{O}_7 \cdot 3\text{H}_2\text{O}$ 

**Origin:** Xiangguang Mn-Ag deposit, northern China.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 651, 606, 502sh, 384w, 273w, 163.

**Source:** Fan et al. (2015).

**Comments:** The sample was characterized by LA-ICP-MS method and electron microprobe analysis. For the Raman spectrum of chalcophanite see also Kim and Stair (2004).

**Chalcophyllite**  $\text{Cu}_{18}\text{Al}_2(\text{AsO}_4)_4(\text{SO}_4)_3(\text{OH})_{24} \cdot 36\text{H}_2\text{O}$ 

**Origin:** Burrus Mine, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3555w, 3390sh, 3129sh, 1636w, 981, 968sh, 867sh, 841s, 814sh, 499, 386, 221sh, 202, 142.

**Source:** Frost et al. (2010g).

**Comments:** No independent analytical data are provided for the sample used. The IR spectrum of presumed chalcophyllite from Burrus Mine given in the cited paper differs substantially from IR spectra of chalcophyllite published elsewhere (Moenke 1962; Chukanov 2014).

**Chalcopyrite**  $\text{CuFeS}_2$ 

**Origin:** Mt. Morgan, Queensland, Australia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was in the range 1–10 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 378, 352, 322, 293s.

**Source:** Mernagh and Trudu (1993).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectra of chalcopyrite see also Sasaki et al. (2009) and White (2009).

**Chalcosiderite** CuFe<sup>3+</sup><sub>6</sub>(PO<sub>4</sub>)<sub>4</sub>(OH)<sub>8</sub>·4H<sub>2</sub>O

**Origin:** Siglo XX mine, Andes Mts., Bustillo province, Bolivia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3543sh, 3514s, 3501sh, 3482sh, 3480sh, 3384sh, 3306, 3200sh, 1194, 1168sh, 1159, 1102, 1062sh, 1042s, 1027sh, 990, 826w, 794sh, 768, 741sh, 636, 598sh, 580, 536, 484, 475sh, 420s, 415sh, 388, 351sh, 333, 293, 272, 264sh, 243sh, 235, 203, 182sh, 176, 153sh, 136s, 125s, 107.

**Source:** Frost et al. (2013af).

**Comments:** The sample was characterized by powder X-ray diffraction data and SEM/EDS, which may correspond to turquoise.

**Chalcostibite** CuSbS<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 329s, 251, 152.

**Source:** Zhang et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectrum of chalcostibite see also Rath et al. (2015).

**Challacolloite** KPb<sub>2</sub>Cl<sub>5</sub>

**Origin:** Artificial (a phase in a fifteenth-century polychrome terracotta relief).

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 785 nm laser radiation. The laser radiation power at the sample was 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 202, 169, 158, 119s, 96, 85, 73.

**Source:** Bezur et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectra of oriented challacolloite crystals see Vtyurin et al. (2004).

**Chambersite** Mn<sub>3</sub>B<sub>7</sub>O<sub>13</sub>Cl

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1684, 1660, 1634sh, 1596m 1548sh, 1426sh, 1412sh, 1399, 1368sh, 1346, 1326sh, 1209, 1169sh, 1146sh, 1129, 1091sh, 1075, 1056, 1045, 1027sh, 989w, 963, 942, 920, 902sh, 871, 853, 836, 797w, 7766, 755w, 721, 705w, 679sh, 660s, 642sh, 617w, 597, 559, 544sh, 523, 508, 402, 393sh, 371sh, 357s, 339sh, 302, 273, 259, 241, 229, 209, 185sh, 177sh, 161s, 143s, 116.

**Source:** Frost et al. (2014f).

**Comments:** No independent analytical data are provided for the sample used.

**Chamosite**  $(\text{Fe}^{2+}, \text{Mg}, \text{Al}, \text{Fe}^{3+})_6(\text{Si}, \text{Al})_4\text{O}_{10}(\text{OH}, \text{O})_8$ **Origin:** Turamdih, India.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented polished section using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power behind the objective was in the range 0.03–0.8 mW. A nearly 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 3644s, 3625s, 3560s, 3434, ~1030, 665s, 615sh, 545s, 518sh, 428w, 361, 198, 127.**Source:** Nasdala et al. (2006).**Comments:** The sample was characterized by electron microprobe analysis.**Changbaiite** PbNb<sub>2</sub>O<sub>6</sub>**Origin:** Synthetic.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 700sh, 676s, 550sh, 529w, 477, 453sh, 423w, 379sh, 361, 323, 3009w, 277, 247, 230w, 202s, 179s, 141s, 119, 89s, 61.**Source:** Repelin et al. (1980).**Comments:** No independent analytical data are provided for the sample used.**Changoite** Na<sub>2</sub>Zn(SO<sub>4</sub>)<sub>2</sub>·4H<sub>2</sub>O**Origin:** Synthetic.**Experimental details:****Raman shifts (cm<sup>-1</sup>):** 3409, 3118, 1189, 1160, 1099, 1064, 985s, 628sh, 612, 473sh, 451.**Source:** Jentzsch et al. (2013).**Chapmanite** Fe<sup>3+</sup><sub>2</sub>Sb<sup>3+</sup>(SiO<sub>4</sub>)<sub>2</sub>(OH)**Origin:** Bořenov, near Mariánské Lázně, western Bohemia, Czech Republic.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3563, 3555, 1590, 1317w, 1120, 1077, 1013, 903, 808, 773, 709, 553, 473w, 436sh, 422, 408, 391, 361sh, 350, 334sh, 313, 293w, 256, 219, 208, 186, 177, 147, 114, 107.**Source:** Frost et al. (2010a).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.**Charoite** (K,Sr,Ba,Mn)<sub>15-16</sub>(Ca,Na)<sub>32</sub>[Si<sub>70</sub>(O,OH)<sub>180</sub>] (OH,F)<sub>4</sub>·nH<sub>2</sub>O**Origin:** Murun massif (Murunskii alkaline complex), Aldan Shield, southwest Yakutia, Siberia, Russia (type locality).**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 2403, 2367, 1135, 1116sh, 1054, 675s, 638, 434w, 242w.

**Source:** Buzatu and Buzgar (2010).

**Comments:** No independent analytical data are provided for the sample used.

**Chegemite** Ca<sub>7</sub>(SiO<sub>4</sub>)<sub>3</sub>(OH)<sub>2</sub>

**Origin:** Upper Chegem volcanic structure, Northern Caucasus, Kabardino-Balkaria, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 20 mW. A 0°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3563s, 3551sh, 3532, 3478s, 924s, 893, 845, 818s, 774, 766, 549, 526s, 403, 389s, 311, 293, 273, 226.

**Source:** Galuskin et al. (2009).

**Comments:** The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved.

**Chekovichite** Bi<sup>3+</sup><sub>2</sub>Te<sup>4+</sup><sub>4</sub>O<sub>11</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power at the sample was 87 mW.

**Raman shifts (cm<sup>-1</sup>):** 761w, 726s, 674sh, 642s, 551w, 419w, 380, 298, 270, 224, 180.

**Source:** Durand (2006).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Chenevixite** Cu(Fe<sup>3+</sup>,Al)(AsO<sub>4</sub>)(OH)<sub>2</sub>

**Origin:** Manto Cuba Mine, San Pedro de Cachiyuyo district, Chañara lprovince, Atacama, Chile.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3501sh, 3405w, 3315sh, 2931w, 2870w, 1688, 1613, 1536, 1238, 1211, 1151, 1130, 883sh, 855s, 836sh, 807s, 495, 450sh, 435s, 408sh, 359, 350, 300.

**Source:** Frost et al. (2015f).

**Comments:** The sample was characterized by qualitative electron microprobe analysis that shows admixture of a silicate. The bands at 1688 and 1613 cm<sup>-1</sup> indicate the presence of H<sub>2</sub>O molecules.

**Cheralite** CaTh(PO<sub>4</sub>)<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline pellet using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 10 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1088w, 982s, 623w, 597w, 573, 537w, 54, 425, 399sh, 289w, 235w.

**Source:** Raison et al. (2008).

**Comments:** The sample was characterized by XRD. For the IR spectrum of cheralite see also Terra et al. (2008).

### Chernikovite (H<sub>3</sub>O)(UO<sub>2</sub>)(PO<sub>4</sub>)·3H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was about 1–4 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3425w, 3215sh, 3078w, 999s, 986, 842s, 458w, 402, 287, 193s, 110.

**Source:** Clavier et al. (2016).

**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by powder X-ray diffraction data and ICP-AES.

### Chernovite-(Y) Y(AsO<sub>4</sub>)

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 888s, 880s, 835s, 395, 255w, 234w, 177w.

**Source:** Pradhan et al. (1987).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Chervetite Pb<sub>2</sub>V<sup>5+</sup><sub>2</sub>O<sub>7</sub>

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 876s, 817s, 751w, 673w, 582, 371, 351s, 324, 258w, 232, 196w, 181w, 140w, 124, 112w, 89, 74.

**Source:** Schwendt and Joniaková (1975).

**Comments:** The sample was characterized by powder X-ray diffraction data and chemical analysis.

### Chiavennite CaMn<sup>2+</sup>(BeOH)<sub>2</sub>Si<sub>5</sub>O<sub>13</sub>·2H<sub>2</sub>O

**Origin:** Prata, Italy.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1068w, 996w, 960w, 919w, 682w, 559, 508, 460s, 428w, 360w, 356w, 352w, 347w, 342w, 299w, 257w, 234w, 324w, 204w, 195w, 148w, 115w, 95w.

**Source:** Jehlička et al. (2012).

**Comments:** No independent analytical data are provided for the sample used.

**Chibaite**  $\text{SiO}_2 \cdot n(\text{CH}_4, \text{C}_2\text{H}_6, \text{C}_3\text{H}_8, \text{C}_4\text{H}_{10})$  ( $n_{\max} = 3/17$ )

**Origin:** Arakawa, Chiba prefecture, Honshu Island, Japan (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3050w, 2960w, 2936, 2908s, 2900, 2866, 989, 873, 805, and a series of bands below 400 cm<sup>-1</sup>.

**Source:** Likhacheva et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of chibaite see also Momma et al. (2011).

**Childrenite**  $\text{Fe}^{2+}\text{Al}(\text{PO}_4)(\text{OH})_2 \cdot \text{H}_2\text{O}$ 

**Origin:** Ponte do Piauí mine, Piauí valley, Itinga, Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3471, 3420sh, 3333, 3199sh, 3043, 1724, 1673, 1573, 1183w, 1142, 1091w, 1011s, 978sh, 969s, 864w, 816w, 608sh, 595s, 562, 466s, 427sh, 405, 347sh, 310, 251, 228, 208, 188sh, 147sh, 138.

**Source:** Frost et al. (2013am).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Chiolite**  $\text{Na}_5\text{Al}_3\text{F}_{14}$ 

**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power at the sample was between 0.5 and 1 W.

**Raman shifts (cm<sup>-1</sup>):**  $A_{1g}$  (xx +yy): 530s, 356, 203, 110s;  $A_{1g}$  (zz): 530s, 414, 356, ~312w, 203w, 110;  $B_{1g}$  (xx -yy): 441w, 320w, ~250w (?);  $B_{2g}$  (xy): 390w, ~250w (?), 223w, 208w;  $E_g$ (xz, yz): 426w, 408, 360w, 248s, 28.

**Source:** Rocquet et al. (1985).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of chiolite see also Carey et al. (2015).

**Chloraluminite**  $\text{AlCl}_3 \cdot 6\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1150, 835, 710w, 615, 572, 530, 430, 315s, 180, 115s, 82w, 57s.

**Source:** Stefov et al. (1992).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Chlorapatite**  $\text{Ca}_5(\text{PO}_4)_3\text{Cl}$ **Origin:** No data.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 1127w, 1039, 963s, 581w, 430w.**Source:** Frezzotti et al. (2012).**Comments:** The methods of the identification of the sample are not indicated. For the Raman spectrum of chlorapatite see also Chen et al. (1995).**Chlorargyrite**  $\text{AgCl}$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 568 nm laser radiation. The nominal laser radiation power was 100 mW.**Raman shifts (cm<sup>-1</sup>):** 386, 240, 149.**Source:** Bottger and Damsgard (1971).**Comments:** Second order Raman spectrum at 300 K is given.**Chloritoid**  $\text{Fe}^{2+}\text{Al}_2\text{O}(\text{SiO}_4)(\text{OH})_2$ **Origin:** Tipam Formation, Bangladesh.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystallin Canada Balsam using 532 nm diode laser radiation. The laser radiation power is not indicated. A nearly 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 880w, 596s, 160.**Source:** Andò and Garzanti (2014).**Comments:** No independent analytical data are provided for the sample used.**Chlorkyuygenite**  $\text{Ca}_{12}\text{Al}_{14}\text{O}_{32}[(\text{H}_2\text{O})_4\text{Cl}_2]$ **Origin:** Upper Chegem caldera, Northern Caucasus, Kabardino-Balkaria, Russia (type locality).**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 652 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** ~3400 (broad), ~3200 (broad), 907sh, 881, 776s, 705s, 511s, 321, 208, 161.**Source:** Galuskin et al. (2015b).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved. No Raman bands of H<sub>2</sub>O molecules are observed in the range from 1500 to 1700 cm<sup>-1</sup>.**Chlormayenite**  $\text{Ca}_{12}\text{Al}_{14}\text{O}_{32}[\square_4\text{Cl}_2]$ **Origin:** Ettringer Bellerberg volcano, near Mayen, Eifel Mts., Germany (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was in the range 30–50 mW. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 3669, 3644sh, 3570sh, 3400, 1094w, 991, 881, 816sh, 772s, 703, 512s, 323.

**Source:** Galuskin et al. (2012c).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved. For the Raman spectrum of chlormayenite see also Ma et al. (2011a).

### **Chlorocalcite** $\text{KCaCl}_3$

**Origin:** A dolerite sill in eastern Siberia, Russia.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 195, 140s, 128sh, 82, 67, 57.

**Source:** Grishina et al. (1992).

**Comments:** No independent analytical data are provided for the sample used.

### **Chloromagnesite** $\text{MgCl}_2$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 243s, 157w.

**Source:** Brambilla et al. (2004).

**Comments:** No independent analytical data are provided for the sample used.

### **Chloroxiphite** $\text{Pb}_3\text{CuO}_2\text{Cl}_2(\text{OH})_2$

**Origin:** Merehead Quarry, Shepton Mallet, Somerset, UK (type locality).

**Experimental details:** Micro-Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power was 0.1 mW.

**Raman shifts (cm<sup>-1</sup>):** 3466, 3437, 3400, 3338, 875, 782, 692, 482, 469, 406, 350, 312, 286, 250, 226, 190, 179, 166, 145, 139s.

**Source:** Frost and Williams (2004).

**Comments:** No independent analytical data are provided for the sample used.

### **Chondrodite** $\text{Mg}_5(\text{SiO}_4)_2\text{F}_2$

**Origin:** Sparta, Sussex Co., New Jersey, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3576, 3570, 3561, 967, 931, 878w, 860s, 845s, 832s, (818w), 786w, 755, 607, 587s, 572, 547s, 430, 390.

**Source:** Frost et al. (2007k).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. Raman shifts are given for chondrodite with the empirical formula

$Mg_{5.04}Fe^{2+}_{0.09}Ti_{0.02}Na_{0.10}(SiO_4)_2F_{1.38}(OH)_x$ . For the Raman spectra of chondrodite see also Mernagh et al. (1999) and Lin et al. (1999).

### Chromatite $CaCr^{6+}O_4$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal. Other experimental details are not described.

**Raman shifts (cm<sup>-1</sup>):** ~900, ~875s.

**Source:** Sánchez-Pastor et al. (2010).

**Comments:** The sample was characterized by electron microprobe analysis.

### Chromite $Fe^{2+}Cr_2O_4$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 647.1 nm Kr<sup>+</sup> laser radiation. The nominal laser radiation power was 0.1 mW.

**Raman shifts (cm<sup>-1</sup>):** 678s, 635sh, 531.

**Source:** Hosterman (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectra of chromite see also Reddy and Frost (2005), Karwowski et al. (2013), Chen et al. (2008a), Sagatowska (2010), Lenaz and Lughí (2013), Andò and Garzanti (2014), and D'Ippolito et al. (2015).

### Chromite $Fe^{2+}Cr_2O_4$

**Origin:** Morasko iron meteorite.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 683s, 642sh, 604w, 513w, 446w.

**Source:** Karwowski et al. (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. Its empirical formula is  $(Mg_{0.34}Mn_{0.04}Zn_{0.07}Al_{0.01}Fe^{2+}_{0.55}Fe_{0.01}Cr_{1.96})O_4$ . For the Raman spectra of chromite see also Hosterman (2011), Reddy and Frost (2005), Chen et al. (2008a), Sagatowska (2010), Lenaz and Lughí (2013), Andò and Garzanti (2014), and D'Ippolito et al. (2015).

### Chrysoberyl $BeAl_2O_4$

**Origin:** Colatine, Esperito Santo, Brazil.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1040w(?), 1020w, 931s, 816, 776, 747, 711, 679, 658, 639s, 567, 546, 518s, 501, 477s, 459, 447, 422, 397, 371w, 242w, 218w.

**Source:** Hofmeister et al. (1987).

**Comments:** No independent analytical data are given for the sample used. For the Raman spectra of chrysoberyl see also Jehlička et al. (2012), Beurlen et al. (2013), and Culka et al. (2016a).

**Chrysocolla**  $(\text{Cu}_{2-x}\text{Al}_x)\text{H}_{2-x}\text{Si}_2\text{O}_5(\text{OH})_4 \cdot n\text{H}_2\text{O}$ 

**Origin:** An unknown locality in Peru.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm diode laser radiation. The laser radiation power at the sample was below 0.5 mW.

**Raman shifts (cm<sup>-1</sup>):** ~1045w, ~945w, ~798w, 676s, ~490sh, 413s, 341, ~210.

**Source:** Bernardino et al. (2016).

**Comments:** No independent analytical data are given for the sample used. For the Raman spectra of chrysocolla see also Frost and Xi (2013a) and Coccato et al. (2016).

**Chrysothallite**  $\text{K}_6\text{Cu}_6\text{Tl}^{3+}\text{Cl}_{17}(\text{OH})_4 \cdot \text{H}_2\text{O}$ 

**Origin:** Second scoria cone of the Northern Breakthrough of the Great Tolbachik Fissure Eruption, Tolbachik volcano, Kamchatka, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm diode laser radiation. The laser radiation power at the sample was ~0.1 mW.

**Raman shifts (cm<sup>-1</sup>):** 3443s, 1580w, 949, 902sh, 465, 320, 295, 275s, 250sh, 206s.

**Source:** Pekov et al. (2015c).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved.

**Chrysotile**  $\text{Mg}_3\text{Si}_2\text{O}_5(\text{OH})_4$ 

**Origin:** Salem, Tamil Nadu, India.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 1064 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1105, 692s, 622, 464, 438w, 390s, 348, 325, 304w, 232s, 180.

**Source:** Anbalagan et al. (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of chrysotile see also Rinaudo et al. (2003), Auzende et al. (2004), and Petry et al. (2006).

**Chukanovite**  $\text{Fe}_2(\text{CO}_3)(\text{OH})_2$ 

**Origin:** Synthetic.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 0.1 mW.

**Raman shifts (cm<sup>-1</sup>):** 3454, 3321, 1510, 1434w, 1070s, 926w, 730, 389, 238w.

**Source:** Saheb et al. (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of chukanovite see also Rémazeilles and Refait (2009).

**Chukhrovite (Ca)**  $\text{Ca}_3\text{Ca}_{1.5}\text{Al}_2(\text{SO}_4)\text{F}_{13} \cdot 12\text{H}_2\text{O}$ 

**Origin:** Val Cavallizza Pb-Zn-(Ag) mine, Cuasso al Monte, Varese province, Italy (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3560, 3470, 3440, 3270, 1632, 1112, 977s, 553, 449, 395w, 345, 281, 211, 181, 140w.

**Source:** Vignola et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

### Churchite-(Nd) (?) Nd(PO<sub>4</sub>)·2H<sub>2</sub>O

**Origin:** Costa Balzi Rossi, Magliolo, Liguria, Italy.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 1316, 1181s, 974, 872w, 805, 742, 677, 633, 532s, 475, 424w, 249, 170w.

**Source:** Bracco et al. (2012).

**Comments:** The sample of presumed churchite-(Nd) was characterized only by electron microprobe analyses. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

### Churchite-(Y) Y(PO<sub>4</sub>)·2H<sub>2</sub>O

**Origin:** Grube Leonie, Auerbach, Oberphalz, Germany.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3327sh, 3205w, 3127w, 3065sh, 1067s, 1029w, 995sh, 984s, 981sh, 707w, 681, 662sh, 649, 565, 497, 369sh, 362, 344sh, 307, 287, 269, 249, 210, 199, 188, 180, 162w, 145, 116sh, 109.

**Source:** Frost et al. (2014g).

**Comments:** No independent analytical data are provided for the sample used.

### Cinnabar α-HgS

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 532 nm laser radiation. The laser radiation power at the sample was from 50 to 520 μW.

**Raman shifts (cm<sup>-1</sup>):** 343w, 282w, 251s, 40s.

**Source:** Radepont (2013).

**Comments:** For the Raman spectra of cinnabar see also Lepot et al. (2006) and Frost et al. (2010c).

### Claringbullite Cu<sup>2+</sup><sub>4</sub>Cl(OH)(OH)<sub>6</sub>

**Origin:** Nchanga Open Pit, Chingola, Zambia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3458sh, 3433s, 3351s, 3331sh, 3211, 970, 906, 815, 579, 511s, 447, 389, 356, 260, 231, 163, 147, 136, 119.

**Source:** Frost et al. (2003i).

**Comments:** No independent analytical data are provided for the sample used.

### Claudetite As<sub>2</sub>O<sub>3</sub>

**Origin:** Jáchymov U deposit, Krušné Hory (Ore Mts.), Western Bohemia, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 814, 632, 626s, 541s, 459s, 356, 354, 284, 284, 259s, 248s, 218, 193, 175.

**Source:** Origlieri et al. (2009).

**Comments:** For the Raman spectrum of claudetite see also Guńka et al. (2012).

### Clausthalite PbSe

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a nanocrystalline aggregate. No other experimental details are described.

**Raman shifts (cm<sup>-1</sup>):** 791, 136s.

**Source:** Ge and Li (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data. The band at 791 cm<sup>-1</sup> may correspond to an impurity.

### Clinoatacamite Cu<sub>2</sub>Cl(OH)<sub>3</sub>

**Origin:** No data.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632.8 nm He-Ne laser radiation. The output laser radiation power was 30 mW.

**Raman shifts (cm<sup>-1</sup>):** 3442, 3355, 3310, 930, 911, 896, 842s, 820s, 804, 590, 511s, 450, 420, 364.

**Source:** Bouchard and Smith (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of clinoatacamite see also Chu et al. (2011), Bertolotti et al. (2012), and Coccato et al. (2016).

### Clinoatacamite Cu<sub>2</sub>Cl(OH)<sub>3</sub>

**Origin:** No data.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was in the range 0.05–1 mW.

**Raman shifts (cm<sup>-1</sup>):** 3434, 3348, 3326, 3308, 971, 927, 893, 818, 581, 511s, 446, 361, 139.

**Source:** Bertolotti et al. (2012).

**Comments:** The sample was characterized by electron microprobe analysis, X-ray photoelectron spectroscopy, and IR spectroscopy. The band at 3326 cm<sup>-1</sup> may be due to an impurity. For the Raman spectra of clinoatacamite see also Bouchard and Smith (2003), Chu et al. (2011), and Coccato et al. (2016).

**Clinobisvanite** Bi(VO<sub>4</sub>)

**Origin:** Londonderry feldspar quarry, Coolgardie area, Western Australia.

**Experimental details:** Micro-Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 828s, 756, 712, 368, 329, 245, 211, 185, 167.

**Source:** Frost et al. (2006i).

**Comments:** No independent analytical data are given for the sample used.

**Clinocervantite** Sb<sup>3+</sup>Sb<sup>5+</sup>O<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on packed powder using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was ~300 mW. A 90°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 754w, 635w, 466, 439w, 405s, 283w, 212s, 195sh, 142, 94, 79s.

**Source:** Cody et al. (1979).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Clinochalcomenite** Cu(Se<sup>4+</sup>O<sub>3</sub>)·2H<sub>2</sub>O

**Origin:** El Dragon Mine, Potosí, Bolivia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3507w, 3193w, 2909w, 967w, 817sh, 811s, 792sh, 749, 700, 552, 489, 378sh, 361, 349sh, 219, 180, 129.

**Source:** Frost and Keeffe (2008b).

**Comments:** Questionable data: the Raman spectrum of presumed clinochalcomenite is very close to that of chalcomenite. No independent analytical data are given for the sample used.

**Clinochlore** Mg<sub>5</sub>Al(AlSi<sub>3</sub>O<sub>10</sub>)(OH)<sub>8</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. A 135°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3679, 3647, 3605, 3477, 679s, 548, 358, 198, 104.

**Source:** Kleppe et al. (2003).

**Comments:** End-member clinochlore, (Mg<sub>5</sub>Al)(Si<sub>3</sub>Al)O<sub>10</sub>(OH)<sub>8</sub>, has been studied. Raman shifts for the range of the OH-stretching vibrations are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Clinoclase** Cu<sub>3</sub>(AsO<sub>4</sub>)(OH)<sub>3</sub>**Origin:** Tin Stope, Majuba Hill mine, Utah, USA.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3559, 3339, 983, 850, 832s, 783, 607, 539, 508, 482, 460, 438, 348, 318, 308, 306, 295, 247, 231, 185, 171, 160, 136.**Source:** Frost et al. (2002e).**Comments:** The sample identification was done by PXRD, by SEM and by EMPA, but corresponding analytical data are not given in the cited paper. For the Raman spectrum of clinoclase see also Martens et al. (2003b).**Clinoenstatite** Mg<sub>2</sub>Si<sub>2</sub>O<sub>6</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was ~50 mW. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 1034s, 1012s, 927w, 848w, 755w, 689s, 666s, 583w, 577w, 523, 480w, 453w, 432, 418, 405, 388w, 371, 344s, 324w, 304w, 279w, 245, 233w, 206, 195, 158, 143.**Source:** Lin (2004).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.**Clinohedrite** CaZn(SiO<sub>4</sub>)·H<sub>2</sub>O**Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 1064 nm Nd-YAG laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 985sh, 951, 857s, 844s, 568sh, 550, 501, 465, 387s, 340, 308, 280w, 235s, 208s.**Source:** Annen and Davis (1993).**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.**Clinometaborite** HBO<sub>2</sub>**Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3130, 2930, 2725w, 1430w, 1400w, 1341w, 1330w, 1264w, 1227w, 1173w, 1135w, 1080w, 980w, 918w, 785s, 765sh, 710w, 680sh, 655, 628, 536, 522, 477, 432, 397, 379, 346sh, 338, 307sh, 293, 277, 226w, 198, 185sh, 178, 147, 131, 119, 108, 94, 77.**Source:** Bertoluzza et al. (1980).**Comments:** The sample was characterized by IR spectrum.

**Clinoptilolite Na**  $\text{Na}_6(\text{Si}_{30}\text{Al}_6)\text{O}_{72} \cdot 20\text{H}_2\text{O}$ 

**Origin:** Dylagówka, Poland.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 1064 nm Nd-YAG laser radiation. The laser radiation power at the sample was 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 1129w, 799w, 514s, 471s, 410s, 182.

**Source:** Mozgawa (2001).

**Comments:** The idealized formula  $(\text{Na},\text{K})_6(\text{Al}_6\text{Si}_{30}\text{O}_{72}) \cdot 20\text{H}_2\text{O}$  is given for the sample described in the cited paper, but no chemical data are presented. The sample was characterized only by powder X-ray diffraction data.

**Clinotobermorite-like mineral**  $\text{Ca}_4\text{Si}_6\text{O}_{17}(\text{H}_2\text{O})_2 \cdot (\text{Ca} \cdot 3\text{H}_2\text{O})(?)$ 

**Origin:** Artificial (an intermediate clinotobermorite-like phase formed during the thermal conversion of tobermorite 11 Å to tobermorite 10 Å).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1077, 1011s, 996, 682s, 619, 523, 484, 445, 410, 360, 302.

**Source:** Biagioni et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Clinzoisite**  $\text{Ca}_2\text{Al}_3[\text{Si}_2\text{O}_7][\text{SiO}_4]\text{O(OH)}$ 

**Origin:** Beura, Verbania, Piemonte, Italy.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 785 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1092, 1050w, 985, 963, 919, 875, 832, 692, 605, 570s, 527, 513, 468sh, 452, 428s, 396, 353w, 328w, 305w, 276, 252, 233, 166w, 138.

**Source:** Andò and Garzanti (2014).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Clintonite**  $\text{CaAlMg}_2(\text{SiAl}_3\text{O}_{10})(\text{OH})_2$ 

**Origin:** Ilmeno-Vishnevogorsky Complex, South Urals, Russia.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 894, 828, 800, 550, 656s, 397, 346, 233, 184, 123.

**Source:** Korinevsky (2015).

**Comments:** The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of clintonite see also Neuville et al. (2002).

**Coalingite**  $Mg_{10}Fe^{3+}_2(CO_3)(OH)_{24}\cdot 2H_2O$ 

**Origin:** Union Carbide mine, San Benito Co., California, USA.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 633 nm He-Ne laser. The laser radiation power at the sample was below 5 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3632, 3596, 3585, 3228, 3030, 2807sh, 2261w, 1768sh, 1655s, 1555sh, 1420, 1093s, 1065sh, 928w, 797w, 702.

**Source:** Frost and Bahfenne (2009).

**Comments:** The spectrum is questionable. No independent analytical data are provided for the sample used. Data in the paper do not coincide with data in supplementary information. IR spectrum of the sample used shows significant admixture of serpentine.

**Cobaltarthurite**  $CoFe^{3+}_2(AsO_4)_2(OH)_2\cdot 4H_2O$ 

**Origin:** Dolores showing, Pastrana, about 10 km east of Mazarrón, the province of Murcia, Spain (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3557, 3250, 3186, 1750–1550w (broad), 1042, 907, 846s, 816, 779, 555w, 509, 458w, 405, 348, 277, 260w, 240s, 231sh, 187, 151, 136, 98, 79, 35.

**Source:** Jambor et al. (2002).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Cobaltaustinite**  $CaCo(AsO_4)(OH)$ 

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3289, 3284, 918sh, 825s, 808, 795, 765, 469, 430, 387, 339, 327, 226, 214, 213, 168.

**Source:** Martens et al. (2003c).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of cobaltaustinite see also Yang et al. (2007a).

**Cobaltkoritnigite**  $Co(AsO_3OH)\cdot H_2O$ 

**Origin:** Richelsdorf District, Hessen, Germany.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3438w, 3165w, 2922, 2862sh, 1687sh, 1611, 1435, 1347, 1291, 1071sh, 1058sh, 1050, 1013sh, 1001s, 985sh, 973sh, 927, 907sh, 838s, 828s, 812sh, 726sh, 681, 637sh, 570w, 554w, 513w, 482, 461w, 430sh, 416sh, 401sh, 386, 367sh, 352sh, 301, 248w, 237sh, 205w, 190w, 166w, 152w, 140sh, 117w, 110w.

**Source:** Frost et al. (2014o).

**Comments:** No independent analytical data are provided for the sample used.

### Cobaltomenite Co(Se<sup>4+</sup>O<sub>3</sub>)·2H<sub>2</sub>O

**Origin:** El Dragon Mine, Potosí, Bolivia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3450sh, 3209, 2962sh, 815sh, 813s, 716, 512, 443, 368w, 280w, 196w.

**Source:** Frost and Keeffe (2008b).

**Comments:** No independent analytical data are provided for the sample used. The Raman spectrum may correspond to Co-rich ahlfeldite.

### Cobaltpentlandite Co<sub>9</sub>S<sub>8</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on nanoparticles using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** ~650.

**Source:** Feng et al. (2015b).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of cobaltpentlandite see also Yin et al. (2008).

### Coccinitite HgI<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an oriented crystal using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated. A 90°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 116, 32, 21.

**Source:** Nakashima et al. (1973).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of coccinitite see also Durig et al. (1969).

### Cochromite CoCr<sub>2</sub>O<sub>4</sub>

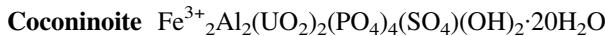
**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an anodized (about 20–25 nm) sample using 632 or 780 nm He-Ne or diode laser radiation. The laser radiation powers are not indicated.

**Raman shifts (cm<sup>-1</sup>):** 684, 603, 514, 449, 195.

**Source:** Zákutná et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.



**Origin:** Jomac mine, White Canyon, San Juan Co., Utah, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1103w, 1085w, 1044sh, 1020s, 998s, 985s, 974sh, 847s, 837s, 826sh, 637w, 620w, 551w, 502sh, 492w, 447w, 409w, 377w, 320w, 229sh, 210sh, 199s, 181s, 147s, 110sh.

**Source:** Frost et al. (2011d).

**Comments:** No independent analytical data are provided for the sample used.



**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using 457.8, 488.0, and 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. A 135°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1164w, 1144w, 1065w, 1036w, 815w, 795w, 661w, 521s, 466, 427, 355, 326, 269s, 204, 176s, 151, 116s, 77s.

**Source:** Hemley (1987a, b).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of coesite see also Yang et al. (2007b), Palmeri et al. (2009), Miyahara et al. (2013), and Perraki and Faryad (2014).



**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample. Kind of laser radiation is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 919s, 906sh, 591, 424.

**Source:** Mesbah et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of coffinite see also Clavier et al. (2014).



**Origin:** Death Valley, Inyo Co., California, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3605s, 3534, 3389sh, 3300, 3182, 3069sh, 1603w, 1527sh, 1323, 1301sh, 1257, 1154, 1084, 1065, 1000sh, 988, 970, 907sh, 892, 876s, 846sh, 813, 788, 745, 709w, 684, 669, 611s, 565, 534, 505, 498, 479w, 455, 436w, 388, 350w, 325sh, 309, 267, 241, 223, 178, 167sh, 149, 129.

**Source:** Frost et al. (2013z).

**Comments:** No quantitative analytical data are provided for the sample used. For the Raman spectrum of colemanite see also Krishnamurti (1955).

### Colimate K<sub>3</sub>VS<sub>4</sub>

**Origin:** Colima volcano, State of Colima, Mexico (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 990, 968, 879, 848, 689, 517, 482, 454, 401s, 387, 367w, 347, 338, 318, 297, 277s, 264s, 245s, 227, 203s, 192s, 180, 168.

**Source:** Ostrooumov et al. (2009).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

### Colinowensite BaCuSi<sub>2</sub>O<sub>6</sub>

**Origin:** Synthetic.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 1060w, 976, 579s, 506s, 454, 372w, 347w, 268, 231w, 173.

**Source:** Finger et al. (1989).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analysis. The crystal structure is solved.

### Coloradoite HgTe

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed at 90 K on a thin oriented sample with a (111) face using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was <100 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 137s, 117, ~106sh.

**Source:** Ingale et al. (1989).

**Comments:** No independent analytical data are provided for the sample used.

### Columbite-(Mg) MgNb<sub>2</sub>O<sub>6</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 647.1 nm Kr<sup>+</sup> laser radiation. The nominal laser radiation power was 400 mW.

**Raman shifts (cm<sup>-1</sup>):** 997, 906s, 850, 721w, 658, 616, 568, 533s, 497, 489, 460w, 451, 411s, 403sh, 389, 379w, 344, 324, 222, 205, 190, 170, 151, 140w, 125sh, 112, 88.

**Source:** Husson et al. (1977a).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Columbite-(Mn)** Mn<sup>2+</sup>Nb<sub>2</sub>O<sub>6</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 647.1 nm Kr<sup>+</sup> laser radiation. The nominal laser radiation power was 400 mW.**Raman shifts (cm<sup>-1</sup>):** 877s, 823, 707w, 634, 624, 606, 531s, 485, 438w, 399, 386w, 361, ~340sh, 314s, 297sh, 287, 274, 263, 248sh, 244s, 214, 206sh, 189sh, 179, 160w, 140s, 127, 113, 89.**Source:** Husson et al. (1977a).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of columbite-(Mn) see also Moreira et al. (2010a).**Comancheite** Hg<sup>2+</sup><sub>55</sub>N<sup>3-</sup><sub>24</sub>(NH<sub>2</sub>,OH)<sub>4</sub>(Cl,Br)<sub>34</sub>**Origin:** Mariposa mine, Terlingua district, Brewster Co., Texas, USA (type locality).**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 785 nm diode laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 633sh, 577s, 545s, 470w, 440w, 315s, 268, 228s, 188s, 174s, ~140s.**Source:** Cooper et al. (2013a).**Comments:** The sample was characterized by single-crystal X-ray diffraction data. The crystal structure is solved.**Combeite** Na<sub>4.5</sub>Ca<sub>3.5</sub>Si<sub>6</sub>O<sub>17.5</sub>(OH)<sub>0.5</sub>**Origin:** Synthetic.**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 22 mW.**Raman shifts (cm<sup>-1</sup>):** 1039w, 986s, 903, 620, 588s, 532, 453w, 423, 346w, 279.**Source:** Lin et al. (2015).**Comments:** The sample was characterized by powder X-ray diffraction data.**Compeignacite** K<sub>2</sub>(UO<sub>2</sub>)<sub>6</sub>O<sub>4</sub>(OH)<sub>6</sub>·7H<sub>2</sub>O**Origin:** West Wheal Owles, St. Just, Cornwall, UK.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 785 nm diode laser radiation. The output laser radiation power was 380 mW.**Raman shifts (cm<sup>-1</sup>):** 834s, 785sh, 549, 460, 402, 329, 204.**Source:** Driscoll et al. (2014).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectrum of compeignacite see also Frost et al. (2008g).**Conichalcite** CaCu(AsO<sub>4</sub>)(OH)**Origin:** Lorena mine, Cloncurry, Queensland, Australia.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of

individual peaks obtained as a result of the spectral curve analysis. The laser radiation power at the sample was 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 3233, 3158, 3086, 962w, 907, 832s, 821sh, 811sh, 781m 750, 534, 463, 446m 430, 389, 358, 335, 328, 303, 286, 274, 206, 180, 161, 121.

**Source:** Martens et al. (2003c).

**Comments:** No independent analytical data are given for the sample used. For the Raman spectra of conichalcite see also Reddy et al. (2005) and Đorđević et al. (2016).

### Connellite Cu<sub>36</sub>(SO<sub>4</sub>)(OH)<sub>62</sub>Cl<sub>8</sub>·6H<sub>2</sub>O

**Origin:** Monte Fucinaia, central Western Italy.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 and 785 nm laser radiations. The laser radiation power at the sample was 4 and 1.4 mW, respectively.

**Raman shifts (cm<sup>-1</sup>):** 3550w, 984s, 585, 524, 446, 404s, 350, 262w, 236w, 192, 184, 132m.

**Source:** Coccato et al. (2016).

**Comments:** The sample identification was done by powder X-ray diffraction. For the Raman spectrum of connellite see also Bouchard and Smith (2003).

### Cooperite PtS

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation output power was 500 mW.

**Raman shifts (cm<sup>-1</sup>):** 328, 325sh (for pure PtS); 454sh, 430, 405sh, 382s, 358, 335, 317 (for a Pd-bearing sample).

**Source:** Pikl et al. (1999).

**Comments:** The samples were characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectrum of cooperite see also Mernagh and Hoatson (1995).

### Copiapite Fe<sup>2+</sup>Fe<sup>3+</sup><sub>4</sub>(SO<sub>4</sub>)<sub>6</sub>(OH)<sub>2</sub>·20H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3527, 3179, 1644, 1224, 1138sh, 1115, 1026, 1005s, 996, 637, 614, 594, 554, 304, 270, 243.

**Source:** Kong et al. (2011b).

**Comments:** The sample was characterized by powder X-ray diffraction data and laser-induced breakdown spectroscopy. For the Raman spectra of copiapite see also Frost (2011c), Sobron and Alpers (2013), Rull et al. (2014), and Apopei et al. (2014a).

### Copiapite Fe<sup>2+</sup>Fe<sup>3+</sup><sub>4</sub>(SO<sub>4</sub>)<sub>6</sub>(OH)<sub>2</sub>·20H<sub>2</sub>O

**Origin:** Coranda-Hondol ore deposit, Certej, Romania.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 7.4 mW.

**Raman shifts (cm<sup>-1</sup>):** 3147, 1651w, 1247, 1143sh, 1113, 1031s, 999s, 748w, 637sh, 609, 558, 477s, 304sh, 274s, 246sh.

**Source:** Apopei et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of copiapite see also Frost (2011c), Kong et al. (2011b), Sobron and Alpers (2013), and Rull et al. (2014).

**Coquandite** Sb<sup>3+</sup><sub>6+x</sub>O<sub>8+x</sub>(SO<sub>4</sub>)(OH)<sub>x</sub>·H<sub>2</sub>O<sub>(1-x)</sub> ( $x = 0.3$ )

**Origin:** Pereta Mine, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3449w, 3318w, 3193w, 3122w, 2961w, 2900w, 2764w, 1588w, 1217sh, 1168w, 1151, 1100, 1072sh, 1020sh, 1007, 990s, 980, 970, 949sh, 787, 751, 600w, 638, 629sh, 610, 600, 508, 459, 429, 417, 375, 359, 317w, 291w, 270sh, 253, 229, 218sh, 216s, 203s, 178, 167s, 149, 129.

**Source:** Frost and Bahfenne (2010f).

**Comments:** No independent analytical data are provided for the sample used.

**Coquimbite** Fe<sup>3+</sup><sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>·9H<sub>2</sub>O

**Origin:** Baia Spriemining area, Romania.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 3388w, 1681w, 1202, 1167w, 1098, 1024, 882w, 604, 503, 457w, 285.

**Source:** Buzatu et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of coquimbite see also Apopei et al. (2012, 2014a), Sobron and Alpers (2013), Rull et al. (2014), and Frost et al. (2014b).

**Corderoite** Hg<sub>3</sub>S<sub>2</sub>Cl<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 288sh, 280s, 132, 115, 63, 50s, 36, 24s.

**Source:** Radepont (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Cordierite** Mg<sub>2</sub>Al<sub>4</sub>Si<sub>5</sub>O<sub>18</sub>

**Origin:** Northern part of the Strangways Metamorphic Complex, central Australia.

**Experimental details:** Raman scattering measurements have been performed on a polished section || (010) of a single crystal using 632.8 nm He-Ne laser radiation. The output laser radiation power was <0.8 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1184, 971, 669, 577, 555, 366, 260s, 127 (for  $E \parallel a$ ); 1010s, 971, 669, 577, 554s, 260 (for  $E \parallel c$ ).

**Source:** Nasdala et al. (2006).

**Comments:** The sample was characterized by electron microprobe analysis. The empirical formula is  $Mg_{1.0}Fe^{2+}_{0.4}Al_4Si_5O_{18}$ . For the Raman spectrum of cordierite see also Majumdar and Mathew (2015). For the Raman spectrum of cordierite (“iolite”) see also Culka et al. (2016a).

### Cordylite (Ce) (Na,Ca,□)BaCe<sub>2</sub>(CO<sub>3</sub>)<sub>4</sub>(F,O)

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed using 488 nm laser radiation. The nominal laser radiation power was 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 1538, 1088, 967, 720, 628.

**Source:** Hong et al. (1999).

### Corkite PbFe<sup>3+</sup><sub>3</sub>(SO<sub>4</sub>)(PO<sub>4</sub>)(OH)<sub>6</sub>

**Origin:** Horn Silver mine, near Frisco, Beacer Co., Utah, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3436, 3347, 3163sh, 1184sh, 1162, 1104s, 1050, 1003s, 996s, 983sh, 857, 821sh, 629sh, 620, 608sh, 572sh, 554, 466sh, 446, 430sh, 381, 274w, 217sh, 201, 144, 131sh, 104.

**Source:** Frost and Palmer (2011a).

**Comments:** No independent analytical data are provided for the sample used.

### Cornetite Cu<sub>3</sub>(PO<sub>4</sub>)(OH)<sub>3</sub>

**Origin:** Banská Bystrica, central Slovakia.

**Experimental details:** Raman scattering measurements have been performed on an oriented crystal, at  $E \parallel b$  and  $E \perp b$ , using 632 nm He-Ne laser radiation. The nominal laser radiation power was 17 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3414, 1137w, 1112w, 1083, 1055, 1016, 971, 945sh, 861, 818, 801w, 750, 703w, 664w, 639w, 606, 539, 515, 477s, 446s, 412, 363, 297, 254w, 241, 214, 209, 174s, 131s, 109s, 86s (for  $E \perp b$ ).

**Source:** Kharbish et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectrum of cornetite see also Frost et al. (2002g).

### Cornubite Cu<sub>5</sub>(AsO<sub>4</sub>)<sub>2</sub>(OH)<sub>4</sub>

**Origin:** Daly mine, Flinders Ranges, South Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power was 1 mW. The Raman shifts have

been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3324, 3042sh, 962w, 815s, 780w, 525w, 496w, 440s, 398, 365w, 327w, 301, 259, 249, 211, 168, 151.

**Source:** Frost et al. (2002e).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of cornubite see also Janeczek et al. (2016).

#### Cornwallite Cu<sub>5</sub>(AsO<sub>4</sub>)<sub>2</sub>(OH)<sub>4</sub>

**Origin:** Penberthy Croft mine, St Hilary, Cornwall, UK.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power was 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3411w, 3350sh, 962w, 877sh, 859s, 806w, 763w, 606, 542, 512w, 454, 449s, 436s, 422, 363sh, 347s, 330sh, 311sh, 275, 279, 246, 203, 169s, 160, 137.

**Source:** Frost et al. (2002e).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of cornwallite see also Ciesielczuk et al. (2016) and Janeczek et al. (2016).

#### Coronadite Pb(Mn<sup>4+</sup><sub>6</sub>Mn<sup>3+</sup><sub>2</sub>)O<sub>16</sub>

**Origin:** Imini, Morocco.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 10 mW. A nearly 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 626s, 585s, 495, 388, 332.

**Source:** Julien et al. (2004).

**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts given by Julien et al. (2004) in Table 5 do not correspond to band positions in Fig. 5 of the cited paper. For the Raman spectrum of coronadite see also Fan et al. (2015).

#### Correianevsite Fe<sup>2+</sup>Mn<sup>2+</sup><sub>2</sub>(PO<sub>4</sub>)<sub>2</sub>·3H<sub>2</sub>O

**Origin:** Cigana mine, Conselheiro Pena, Rio Doce valley, Minas Gerais, Brazil (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** (3462), 3445s, (3400), 3265sh, 1641w, 1587sh, 1572w, 1553sh, 1193w, 1104w, (1093), 1064w, 1007s, 970+963s (unresolved doublet?), (951), 753, 588s, 569sh, (549), 531, 504sh, 482, 458sh, 420, (405), 373, 330w, 286sh, 260, 241w, 223w, 179, 164, 144.

**Source:** Frost et al. (2012j).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. In the cited paper the mineral is described under the name “reddingite.” Our investigations showed that it is correianevsite, a new mineral species of the reddingite group with ordered Fe<sup>2+</sup> and Mn<sup>2+</sup>.

**Corundum**  $\text{Al}_2\text{O}_3$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 780 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 751, 645, 578, 451w, 432, 418s, 378s.**Source:** Jasinevicius (2009).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of corundum see also Shoval et al. (2001) and Andò and Garzanti (2014).**Cosalite**  $\text{Pb}_2\text{Bi}_2\text{S}_5$ **Origin:** An abandoned mine in the Karrantza valley, Basque Co., Spain.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 or 785 nm Ar<sup>+</sup> and diode laser radiation. The laser radiation power at the sample was 20 mW.**Raman shifts (cm<sup>-1</sup>):** 439, 251s, 140s.**Source:** Goienaga et al. (2011).**Comments:** The sample was characterized by energy dispersive X-ray fluorescence. For the Raman spectrum of cosalite see also Fermo and Padeletti (2012).**Cotunnite**  $\text{PbCl}_2$ **Origin:** No data.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632 nm He-Ne laser radiation. The laser radiation output power was 30 mW.**Raman shifts (cm<sup>-1</sup>):** 202, 169, 158.**Source:** Bouchard and Smith (2003).**Comments:** The sample was characterized by powder X-ray diffraction data.**Coulsonite**  $\text{Fe}^{2+}\text{V}^{3+}_2\text{O}_4$ **Origin:** Vihanti deposit, Northern Finland Region, Finland.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm laser radiation. The nominal laser radiation power was 2 or 20 mW.**Raman shifts (cm<sup>-1</sup>):** 1188w, 1144w, 1119w, 1062, 1020w, 994w, 962w, 937w, 908, 873w, 840w, 813w, 772w, 670s, 576, 526, 498, 469, 398w, 351w, 296w, 268w, 236w, 212w, 167, 131, 116.**Source:** Voloshin et al. (2014).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.**Covellite**  $\text{CuS}$ **Origin:** Guinaoang, NW Luzon, Philippines.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was <10 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 471s, 263, 139, 116.

**Source:** Mernagh and Trudu (1993).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Comments:** For the Raman spectra of covellite see also Bouchard and Smith (2003) and Kumar and Nagarajan (2011).

### Crandallite CaAl<sub>3</sub>(PO<sub>4</sub>)(PO<sub>3</sub>OH)(OH)<sub>6</sub>

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 3546sh, 3471, 3305, ~3150, ~1330w, 1228w, 1160, 1108s, 1035s, 982s, 858, 828, 720w, 693, 634, 615, 580, 555sh, 528, 462, 396s, 365, 258s, 223sh, 184s.

**Source:** Breitinger et al. (2006).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of crandallite see also Frost et al. (2011w) and Grey et al. (2011).

### Cranswickite Mg(SO<sub>4</sub>)·4H<sub>2</sub>O

**Origin:** Calingasta, San Juan province, Argentina (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 632 nm He-Ne laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** ~3430, ~3300, 1156, 1120, 1090w, 1002s, 617, 466.

**Source:** Peterson (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data, electron microprobe analysis, and ICP-MS.

### Creaseyite Cu<sub>2</sub>Pb<sub>2</sub>Fe<sup>3+</sup><sub>2</sub>Si<sub>5</sub>O<sub>17</sub>·6H<sub>2</sub>O

**Origin:** St. Anthony Mine, Tiger, Pinal Co., Arizona, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3626s, 3525s, 3470sh, 3162, 2902, 2750sh, 1603, 1543, 1348w, 1071, 998s, 958sh, 920sh, 869s, 802, 712s, 672sh, 603, 511, 481sh, 443, 371, 351, 318, 295, 258sh, 237s, 211sh, 196s, 152sh, 139s, 126.

**Source:** Frost and Xi (2012g).

**Comments:** No independent analytical data are given for the sample used.

### Crednerite CuMnO<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a thin film on quartz substrate using 532 nm diode laser radiation. The nominal laser radiation power was 13 mW.

**Raman shifts (cm<sup>-1</sup>):** 688s, 381w, 314w.

**Source:** Chen et al. (2015b).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Creelite Ca<sub>3</sub>Al<sub>2</sub>(SO<sub>4</sub>)(OH)<sub>2</sub>F<sub>8</sub>·2H<sub>2</sub>O

**Origin:** Santa Eulalia mining district, Chihuahua province, Mexico.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3584, 3524s, 3458, 3382sh, 3349, 3248, 1673w, 1575w, 1503, 1499, 1234w, 1184, 1135, 1084w, 1033w, 1026w, 989sh, 986s, 983sh, 922w, 891, 819w, 765, 663, 629, 601, 596sh, 568w, 548, 483, 457sh, 440, 394, 371w, 348w, 322w, 311w, 286w, 278, 353w, 225, 217sh, 203, 190, 173, 149, 126.

**Source:** Frost et al. (2013al).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

### Cristobalite SiO<sub>2</sub>

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 476.5 nm laser radiation. The nominal laser radiation power was 400 mW.

**Raman shifts (cm<sup>-1</sup>):** 1195, 1089, 1079, 795, 785, 485, 416, 380, 368, 287, 275, 230, 110.

**Source:** Etchepare et al. (1978).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of cristobalite see also Ling et al. (2011), Shoval et al. (2001), Ilieva et al. (2007), Wilson (2014), and Ferrero et al. (2016).

### Cristobalite SiO<sub>2</sub>

**Origin:** Lunar soil.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was in the range from 3 to 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 1075w, 781w, 411s, 229s.

**Source:** Ling et al. (2011).

**Comments:** No independent analytical data are given for the sample used. For the Raman spectra of cristobalite see also Etchepare et al. (1978), Shoval et al. (2001), Ilieva et al. (2007), Wilson (2014), and Ferrero et al. (2016).

### Crocoite Pb(CrO<sub>4</sub>)

**Origin:** Dundas, Tasmania, Australia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sampling lens was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 853sh, 840s, 825sh, 400, 377, 358s, 348, 338, 326, 179w, 135, 118w.

**Source:** Rodgers (1992).

**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample identification was done by XRD, by SEM, and by electron probe analysis. For the Raman spectra of crocoite see also Frost (2004c) and Nasdala et al. (2004).

### Cryptohalite $(\text{NH}_4)_2\text{SiF}_6$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements in the region of N–H-stretching vibrations have been performed using 488 and 514.5 nm  $\text{Ar}^+$  laser radiations. The laser radiation power at the sample was about 100 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3235.

**Source:** Jenkins (1986).

### Cryptomelane $\text{K}(\text{Mn}^{4+})_7\text{Mn}^{3+}\text{O}_{16}$

**Origin:** Synthetic.

**Experimental details:** No data.

**Raman shifts ( $\text{cm}^{-1}$ ):** 743w, 626s, 574s, 508, 470, 386, 257w, 183.

**Source:** Santos et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data and ICP analysis. For the IR spectrum of cryptomelane see also Kim and Stair (2004).

### Cubanite $\text{CuFe}_2\text{S}_3$

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was below 10 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 469s, 374, 328w, 286s.

**Source:** Chandra et al. (2011a, b).

**Comments:** The sample was characterized by powder X-ray diffraction data and Mössbauer spectroscopy. For the Raman spectrum of cubanite see also Petrov (2014).

### Cuboargyrite $\text{AgSbS}_2$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a bulk polycrystalline sample using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power was 50 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 324s, ~311w, 292, 282w, 240sh, 140, 125sh.

**Source:** Gutwirth et al. (2006).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

### Cumengeite $\text{Pb}_{21}\text{Cu}_{20}\text{Cl}_{42}(\text{OH})_{40} \cdot 6\text{H}_2\text{O}$

**Origin:** Beleo, Baja California, Mexico.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts

have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3588sh, 3482s, 3413s, 3366sh, 3180, 1023sh, 984, 891w, 830sh, 797, 715sh, 676s, 500, 465, 376, 347, 307, 271, 243, 192, 154s.

**Source:** Frost et al. (2003j).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of cumengeite see also Bouchard and Smith (2003) and Frost and Williams (2004).

### Cummingtonite $\square\text{Mg}_2\text{Mg}_5\text{Si}_8\text{O}_{22}(\text{OH})_2$

**Origin:** Ca'Mondey, Montescheno, Piemonte, Italy.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514 and 785 nm laser radiations. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3668, 3653, 1038, 671s, 384, 200, 186.

**Source:** Andò and Garzanti (2014).

**Comments:** The methods of the identification of the sample are not indicated. Raman spectrum of presumed cummingtonite was published by Mohanan (1993) and Kloprogge et al. (2001a), but chemical composition of this sample (Mohanan 1993) does not correspond to cummingtonite. For the Raman spectrum of cummingtonite see also Leissner et al. (2015).

### Cuprite Cu<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a crushed sample and a single crystal using 647.1 nm Kr<sup>+</sup> laser radiation. The nominal laser radiation power was 20 mW. A 90°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 640w, 485w, 420w, 300w, 220s, 204, 192, 190, 160w, 150, 125w, 106 (crushed sample); 640, 220, 204, 192, 150 (single crystal).

**Source:** Taylor and Weichman (1971).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of cuprite see also Bouchard and Smith (2003).

### Cuproco piapite Cu<sup>2+</sup>Fe<sup>3+</sup><sub>4</sub>(SO<sub>4</sub>)<sub>6</sub>(OH)<sub>2</sub>·20H<sub>2</sub>O

**Origin:** Rio Tinto Valley near Nerva, Spain.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 997s, 978s, ~620, ~450.

**Source:** Chemtob et al. (2006).

**Comments:** The Raman spectrum is questionable: blue color is very unusual for cuproco piapite. No independent analytical data are provided for the sample used.

### Cuproiridsite CuIr<sub>2</sub>S<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Micro-Raman scattering measurements have been performed in a back-scattering geometry using 514.5 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~402, ~375, ~327, ~300s.

**Source:** Zhang et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of cuproiridsite see also Zhang et al. (2010b).

### Cupromolybdite Cu<sup>2+</sup><sub>3</sub>O(Mo<sup>6+</sup>O<sub>4</sub>)<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a single crystal in different scattering geometries using laser radiation with different wavelengths. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~961, ~934, ~864w, ~842, ~813 [for the 532 nm laser radiation, in the x(y, y +z)-x scattering geometry].

**Source:** Sato et al. (2014).

**Comments:** The sample was characterized by X-ray diffraction.

### Cuprorhodsite CuRh<sub>2</sub>S<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~388, ~358, ~318, ~277s.

**Source:** Ito et al. (2003).

**Comments:** No independent analytical data are provided for the sample used.

### Cuprorivaite CaCuSi<sub>4</sub>O<sub>10</sub>

**Origin:** No data in the cited paper.

**Experimental details:** No data in the cited paper.

**Raman shifts (cm<sup>-1</sup>):** 1086s, 1013, 991, 788, 572, 473, 431s.

**Source:** Boschetti et al. (2008).

**Comments:** Methods of the sample identification are not indicated. For the Raman spectrum of cuprorivaite see also Pagès-Camagna et al. (1999).

### Cuprosklodowskite Cu(UO<sub>2</sub>)<sub>2</sub>(SiO<sub>3</sub>OH)<sub>2</sub>·6H<sub>2</sub>O

**Origin:** Shinkolobwe mine, Shaba province, Democratic Republic of Congo (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3694w, 3571w, 3499, 3435s, 3282s, 2920, 1504, 1297, 1246, 1156, 974, 919w, 917, 901w, 847w, 812sh, 787s, 774w, 759w, 747, 535, 507w, 477w, 411w, 387, 301, 277, 267, 218, 206, 185, 165w, 134w, 114.

**Source:** Frost et al. (2006e).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of cuproskłodowskite see also Driscoll et al. (2014).

### Cuprospinel $\text{Cu}^{2+}\text{Fe}^{3+}_2\text{O}_4$

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Micro-Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The laser radiation output power was 3 mW.

**Raman shifts (cm<sup>-1</sup>):** 632, 656, 549, 462s, 346, 271, 211, 168s (for a sample annealed at 1200°C).

**Source:** Silva et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of cuprospinel see also Li et al. (2015).

### Cuprotungstite $\text{Cu}^{2+}_3(\text{WO}_4)_2(\text{OH})_2$

**Origin:** Cordillera Mine, Peelwood, Australia (?).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 785 nm Nd-YAG laser. The laser radiation power at the sample was 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 926s, 769w, 566, 498w, 415, 353sh, 329, 253, 212, 173w.

**Source:** Frost et al. (2004d).

**Comments:** Questionable data: qualitative electron microprobe analysis given in the cited paper shows a high content of Ca.

### Curienite $\text{Pb}(\text{UO}_2)_2(\text{VO}_4)_2 \cdot 5\text{H}_2\text{O}$

**Origin:** Mounana Mine, Haut Ogoue, Gabon (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 976sh, 959, 860w, 825, 741s, 655w, 569, 534, 465, 410, 374s, 362, 312, 288, 264, 234, 193sh.

**Source:** Frost et al. (2005c).

**Comments:** No independent analytical data are given for the sample used.

### Curite $\text{Pb}_{3+x}[(\text{UO}_2)_4\text{O}_{4+x}(\text{OH})_{3-x}]_2 \cdot 2\text{H}_2\text{O}$

**Origin:** Ranger U Mine, Northern Territory, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3437, 3297, 1530, 886w, 807w, 791, 772, 742w, 650, 561, 503, 415sh, 455, 393, 367, 340, 301sh, 273, 250, 225w, 212, 184, 163sh, 154sh, 144.

**Source:** Frost et al. (2007g).

**Comments:** No independent analytical data are given for the sample used. For the Raman spectrum of curite see also Frost et al. (2007h).

### Cuspidine $\text{Ca}_8(\text{Si}_2\text{O}_7)_2\text{F}_4$

**Origin:** Anakitskii massif, Siberia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal. No other experimental details are described.

**Raman shifts (cm<sup>-1</sup>):** 910s, 654, 361, 300.

**Source:** Sharygin et al. (1996a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectrum of cuspidine see also Sharygin et al. (1996b).

### Cyanochroite $\text{K}_2\text{Cu}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power at the sample was 20 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1159w, 1133w, 1081, 983s, 629, 609, 457, 438, 256, 187, 112, 66.

**Source:** Majzlan et al. (2015)

**Comments:** For the Raman spectrum of cyanochroite see also Jentzsch et al. (2013).

### Cyanotrichite $\text{Cu}_4\text{Al}_2(\text{SO}_4)(\text{OH})_{12}(\text{H}_2\text{O})_2$

**Origin:** Cap Garonne mine, near La Pradet, Var, France.

**Experimental details:** Raman scattering measurements have been performed on a single crystal with the laser beam orthogonal to the elongation direction (*b* axis) using 532 nm Nd-YAG laser radiation. The laser radiation power was below 30 mW.

**Raman shifts (cm<sup>-1</sup>):** 3590, 3300–3400, 2330w, 1142w, 377s, 609w, 592, 525s, 448, 274, 230.

**Source:** Mills et al. (2014a).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Cymrite $\text{Ba}(\text{Si},\text{Al})_4(\text{O},\text{OH})_8 \cdot \text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Unpolarized micro-Raman scattering measurements have been performed on a microcrystalline aggregate using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3567sh, 3500, 1626w, (1555w), 1091w, 953w, 800w, 673w, 470w, 396, 297w, 104s.

**Source:** Graham et al. (1992).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Cyrilovite**  $\text{NaFe}^{3+}_3(\text{PO}_4)_2(\text{OH})_4 \cdot 2\text{H}_2\text{O}$ 

**Origin:** Sapucaia (Proberil) mine, Conselheiro Pena pegmatitedistrict, Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3452, 3328, 3244sh, 3194sh, 1184sh, 1177, 1136, 1105, 1087sh, 1065sh, 1055s, 1038sh, 1013sh, 992s, 974sh, 852, 811, 7762sh, 631s, 612s, 588sh, 541, 498sh, 482, 437, 411, 3065s, 279sh, 261, 216, 197sh, 165, 156, 148, 131sh, 117.

**Source:** Frost et al. (2013u).

**Comments:** No independent analytical data are given for the sample used.

**Czochralskiite**  $\text{Na}_4\text{Ca}_3\text{Mg}(\text{PO}_4)_4$ 

**Origin:** Morasko IAB-MG iron meteorite, Poland (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1119, 1067w, 1053, 1039, 1022, 1011, 986s, 974s, 966s, 606, 585, 578, 441.

**Source:** Karwowski et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Dachiardite Na**  $\text{Na}_4(\text{Si}_{20}\text{Al}_4)\text{O}_{48} \cdot 13\text{H}_2\text{O}$ 

**Origin:** Elba Island, Italy.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 1060 nm Nd-YAG laser radiation. The laser radiation power at the sample was 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 1090w, 714s, 558, 479, 409, 248, 182.

**Source:** Mozgawa (2001).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Danburite**  $\text{CaB}_2\text{Si}_2\text{O}_8$ 

**Origin:** No data.

**Experimental details:** Polarized Raman scattering measurements have been performed on an oriented crystal in different scattering configurations using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):**  $z(xx)y$ —1115, 1018, 983, 957, 925, 917, 783, 635, 619s, 572, 489, 450, 434, 357, 321, 255, 220, 190, 176, 139;  $z(xy)x$ —1185w, 1087w, 1037w, 963w, 885w, 760w, 645w, 619w, 592w, 556w, 472w, 465w, 450w, 344w, 288, 268w, 216w, 201, 150, 136w;  $z(xz)x$ —1160w, 1050w, 1006w, 983, 908, 880w, 783w, 684w, 637, 619, 581w, 471, 450w, 434w, 339, 305, 255, 236, 204, 193, 135, 126;  $z(yz)x$ —1185w, 1037w, 1013w, 980w, 932w, 786w, 725w, 634w, 619w, 562w, 418w, 404w, 315w, 278w, 213, 190w, 162, 148w.

**Source:** Best et al. (1994).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of danburite see also Kimata (1993) and Manara et al. (2009).

**Darapskite**  $\text{Na}_3(\text{SO}_4)(\text{NO}_3)\cdot\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Micro-Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power at the sample was 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 3479sh, 3451w, 1424, 1353, 1171, 1124, 1085, 1060s, 993s, 729, 706, 639, 618, 472w, 455.

**Source:** Jentzsch et al. (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of darapskite see also Jentzsch et al. (2012b) and Linnow et al. (2013).

**Darrellhenryite**  $\text{Na}(\text{Al}_2\text{Li})\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3\text{O}$

**Origin:** No data in the cited paper.

**Experimental details:** Raman scattering measurements have been performed on an oriented crystal in the -y(zz)y scattering geometry using 514.5 or 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 14 mW.

**Raman shifts (cm<sup>-1</sup>):** 3593±4, 3562±4, 3494±8, 3465±11, 1085, 975, 750, 707s, 643, 534sh, 515, 407, 374s, 335w, 315, 268, 249, 223s.

**Source:** Watenphul et al. (2016b).

**Comments:** The sample was characterized by electron microprobe analysis and LA-ICP-MS. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Dashkovaite**  $\text{Mg}(\text{HCOO})_2\cdot 2\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. 90°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1405, 1396, 1385, 1376s, 1367.

**Source:** Stoilova and Koleva (2000).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Datolite**  $\text{CaB}(\text{SiO}_4)(\text{OH})$

**Origin:** Canossa, Réggiонell'Emilia, Italy.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3498s, 2892w, 1355, 1243w, 1202w, 1172, 1154w, 1148, 1077s, 1002sh, 985, 956w, 917, 8872w, 864w, 828w, 765w, 730w, 708sh, 693s, 669, 654, 601sh, 593w, 559w, 491, 466w, 458w, 440w, 424w, 392, 378sh, 362, 332w.

**Source:** Frost et al. (2013ah).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectrum of datolite see also Goryainov et al. (2015).

### **Daubréelite FeCr<sub>2</sub>S<sub>4</sub>**

**Origin:** Bustee, Pesyanoe, and Aubres meteorites.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented samples using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 365s, 290w, 255s, 160.

**Source:** Avril et al. (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectrum of daubréelite see also Lutz et al. (1989).

### **Davidite-(La) La(Y,U)Fe<sub>2</sub>(Ti,Fe,Cr,V)<sub>18</sub>(O,OH,F)<sub>38</sub>**

**Origin:** Billeroo Prospect, South Australia and Radium Hill Mine, Mingary, Olary, South Australia.

**Experimental details:** Raman scattering measurements have been performed on amorphous, metamict samples using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1597w, 1424sh, 1322, 1250w, 1074w, 698sh, 641, 514, 412sh, 394, 293, 206, 169sh, 151s (for the sample from the Billeroo Prospect);

1357sh, 1308, 1255sh, 1065w, 812w, 651s, 609s, 497, 450sh, 408, 380, 297sh, 291s, 223s, 150 (for the sample from the Radium Hill Mine).

**Source:** Frost and Reddy (2011b).

**Comments:** No independent analytical data are provided for the sample used.

### **Davidlloydite Zn<sub>3</sub>(AsO<sub>4</sub>)<sub>2</sub>·4H<sub>2</sub>O**

**Origin:** Tsumeb mine, Tsumeb, Otjikoto (Oshikoto) region, Namibia (type locality).

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 3360, 3295, 3170, 3110, 2950, 865s, 841sh, 550, 504, 454s, 420sh, 394w, 353, 305, 294, 258, 211, 200sh, 182w, 170, 163w, 121w.

**Source:** Hawthorne et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

### **Davisite CaScAlSiO<sub>6</sub>**

**Origin:** Allende meteorite, Chihuahua, Mexico (type locality).

**Experimental details:** Raman scattering measurements have been performed on a grain in polished section using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~855, ~815, ~660, ~540, ~405, ~385, ~330.

**Source:** Ma and Rossman (2009b), Ma et al. (2012c).

### Dawsonite NaAl(CO<sub>3</sub>)(OH)<sub>2</sub>

**Origin:** Poudrette Quarry, Mont Saint-Hilaire, Québec, Canada.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3467w, (3341w), (3295), 3283, 3250, (3218w), 1760w, 1731w, 1691w, 1506s, 1484, 1366w, 1099, 1091s, 1068, 936w, 898, 824, (820w), 747, 731, 590s, 519, 443, 389, (374w), 361, 261, 219, 191s, (188), 152, (141w), 134.

**Source:** Frost et al. (2015h).

**Comments:** The sample was characterized by qualitative electron microprobe analysis. For the Raman spectra of dawsonite see also Serna et al. (1985), Vard and Williams-Jones (1993), Sirbescu and Nabelek (2003), and Frost and Bouzaïd (2007).

### Decrespignyite-(Y) Y<sub>4</sub>Cu(CO<sub>3</sub>)<sub>4</sub>Cl(OH)<sub>5</sub>·2H<sub>2</sub>O

**Origin:** Paratoo copper mine, near Yunta, Olary district, South Australia (type locality).

**Experimental details:** Methods of sample preparation are not described. Micro-Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation output power was 0.3 mW.

**Raman shifts (cm<sup>-1</sup>):** 3463, 3419, 1094s, 1075s, 1062s, 822, 751, 478, 415, 344, 201s.

**Source:** Wallwork et al. (2002).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectrum of decrespignyite-(Y) see also Frost and Palmer (2011g).

### Delafossite Cu<sup>1+</sup>Fe<sup>3+</sup>O<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 692, 351.

**Source:** Pavunny et al. (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data and qualitative electron microprobe analysis. For the Raman spectra of delafossite see also Aktas et al. (2011) and Kučerová et al. (2013).

### Delhayelite K<sub>7</sub>Na<sub>3</sub>Ca<sub>5</sub>Al<sub>2</sub>Si<sub>14</sub>O<sub>38</sub>F<sub>4</sub>Cl<sub>2</sub>

**Origin:** Yukspor Mt., Khibiny massif, Kola Peninsula, Russia.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 50 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3147, 3098, 2980, 2824, 1144, 1081, 998w, 757w, 606s, 581, 495, 407, 353, 307w.

**Source:** Sharygin et al. (2013b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

### Deliensite Fe<sup>2+</sup>(UO<sub>2</sub>)<sub>2</sub>(SO<sub>4</sub>)<sub>2</sub>(OH)<sub>2</sub>·7H<sub>2</sub>O

**Origin:** Schweitzer dump, Jáchymov ore district, Western Bohemia, Czech Republic.

**Experimental details:** Methods of sample preparation are not described. Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was 3 mW.

**Raman shifts (cm<sup>-1</sup>):** ~6300, ~3510, 1637sh, 1625w, 1157w, 1068sh, 1050s, 1024s, 1010sh, 980, 932, 900, 853sh, 838s, 824sh, 747w, 725w, 710w, 653w, 627w, 610w, 573w, 545w, 478, 453, 364, 235, 200, 152sh, 105sh, 90.

**Source:** Plášil et al. (2012a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

### Dellaite Ca<sub>6</sub>(Si<sub>2</sub>O<sub>7</sub>)(SiO<sub>4</sub>)(OH)<sub>2</sub>

**Origin:** Birkhin complex, Eastern Siberia, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was in the range from 30 to 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 3592, 3573, 998, 963, 956sh, 930s, 892, 867s, 821w, 666, 652sh, 551sh, 528, 411, 397, 382sh, 354, 278, 248w, 127w.

**Source:** Armbruster et al. (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

### Delvauxite CaFe<sup>3+</sup><sub>4</sub>(PO<sub>4</sub>)<sub>2</sub>(OH)<sub>8</sub>·4·5H<sub>2</sub>O

**Origin:** Berneau, near Vise, Liège, Belgium (type locality).

**Experimental details:** Raman scattering measurements have been performed on an amorphous SO<sub>4</sub>-rich sample using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3317w, 3193sh, 3029w, 2900w, 1607, 1385sh, 1345, 1085sh, 1006s, 630, 583sh, 485sh, 464s, 439sh, 276, 208, 148sh, 128, 108.

**Source:** Frost et al. (2012d).

**Comments:** No independent analytical data are provided for the sample used. The Raman spectrum of delvauxite is given also by Frost and Palmer (2011d), but bands at 1167, 1095, 799, 780 and 692 cm<sup>-1</sup> in the IR spectrum of this sample correspond to quartz.

**Demartinite**  $K_2SiF_6$ **Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 1064 nm Nd-YAG laser radiation. The nominal laser radiation was in the range 80–200 mW.**Raman shifts (cm<sup>-1</sup>):** 655, 478w, 408.**Source:** Rissom et al. (2008).**Comments:** No independent analytical data are given for the sample used.**Demesmaekerite**  $Pb_2Cu_5(UO_2)_2(Se^{4+}O_3)_6(OH)_6 \cdot 2H_2O$ **Origin:** Musonoi mine, Shaba, Democratic Republic of Congo (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3382, 3319, 1493, 1458sh, 1366, 1095, 1062, 822, 756, 719, 597w, 535, 510, 450sh, 432sh, 351, 295, 269, 215, 178s, 151s, 114sh.**Source:** Frost et al. (2008d).**Comments:** No independent analytical data are given for the sample used.**Demicheleite-(Br)** BiSBr**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 676.4 or 632.8 nm Kr<sup>+</sup> laser radiations with the laser radiation power of 150 mW, as well as a He-Ne laser with the laser radiation power of 40 mW.**Raman shifts (cm<sup>-1</sup>):** 287s, 250, 121, 92, 54, 42sh [x(yx)y, A<sub>g</sub> modes]; 234, 46s [x(zx)y, B<sub>g</sub> modes].**Source:** Furman et al. (1976).**Comments:** No independent analytical data are given for the sample used.**Demicheleite-(Cl)** BiSCl**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 676.4 or 632.8 nm Kr<sup>+</sup> laser radiations with the laser radiation power of 150 mW, as well as a He-Ne laser with the laser radiation power of 40 mW.**Raman shifts (cm<sup>-1</sup>):** 287, 260, 107, 95, 54, 44[x(yx)y, A<sub>g</sub> modes]; 240, 138, 47[x(zx)y, B<sub>g</sub> modes].**Source:** Furman et al. (1976).**Comments:** No independent analytical data are given for the sample used.**Demicheleite-(I)** BiSI**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an oriented crystal in the -y(xy)x geometry using 1064 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 290, 227, 119sh, 108, 85s, 55s, 50, 37s, 30.

**Source:** Teng et al. (1978).

**Comments:** No independent analytical data are given for the sample used. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

**Denningite** CaMn<sup>2+</sup>Te<sup>4+</sup>O<sub>10</sub>

**Origin:** Bambolla mine, Moctezuma, Sonora, Mexico (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 766sh, 734s, 674, 479w, 450w, 381, 349s, 237, 155.

**Source:** Frost et al. (2008h).

**Comments:** No independent analytical data are provided for the sample used.

**Derriksite** Cu<sub>4</sub>(UO<sub>2</sub>)(Se<sup>4+</sup>O<sub>3</sub>)<sub>2</sub>(OH)<sub>6</sub>

**Origin:** Musonoimine, Katanga, Democratic Republic of Congo (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3530, 3407, 3247sh, 2917, 1623w, 1433w, 971s, 943sh, 881, 788s, 282, 257sh, 206, 162w, 137, 117sh.

**Source:** Frost et al. (2014a).

**Comments:** No independent analytical data are provided for the sample used.

**Desautelsite** Mg<sub>6</sub>Mn<sup>3+</sup><sub>2</sub>(CO<sub>3</sub>)(OH)<sub>16</sub>·4H<sub>2</sub>O

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power at the sample was below 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3646, 3608, 3509, 3409, 3325, 2882, 2836w, 2776, 1676w, 1638w, 1610w, 1579w, 1440w, 1407w, 1393, 1372w, 1349, 1342, 1303w, 1110w, 1086, 1062w, 1055, 1016w, 883w, 878w, 873, 560, 535, 506, 455, 436w, 422w, 313w, 281, 254.

**Source:** Frost and Erickson (2005).

**Comments:** No independent analytical data are provided for the sample used.

**Dessauite-(Y)** Sr(Y,U,Mn)Fe<sub>2</sub>(Ti,Fe,Cr,V)<sub>18</sub>(O,OH)<sub>38</sub>

**Origin:** Provence-Alpes-Côte d'Azur, France.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 812, 638s, 604sh, 520, (485w), 430, 360w, 329w, 293, 240.

**Source:** Bittarello et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Destinezite**  $\text{Fe}^{3+}_2(\text{PO}_4)(\text{SO}_4)(\text{OH}) \cdot 6\text{H}_2\text{O}$

**Origin:** Źdanów, Bardzkie Mts. (West Sudetes), Poland.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented thin section of a crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3472, 3224w, 1357w, 1111w, 1048s, 980s, 626, 605sh, 540sh, 460, 268, 200.

**Source:** Koszowska et al. (2005).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. Raman shifts are given for a sample with the highest content of poorly ordered phase. The empirical formula of the sample used is  $\text{Fe}_{2.09}\text{Al}_{0.1}(\text{PO}_4)_{1.08}(\text{SO}_4)_{0.89}(\text{SiO}_4)_{0.13}(\text{OH}) \cdot 4.01\text{H}_2\text{O}$ . For the Raman spectrum of destinezite see also Frost and Palmer (2011f).

**Devilline**  $\text{CaCu}_4(\text{SO}_4)_2(\text{OH})_6 \cdot 3\text{H}_2\text{O}$

**Origin:** Ozernyi district, Salla-Kuolayarvi, Kola Peninsula, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power at the sample was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 3594w, 3563w, 3493w, 1121s, 1041, 992s, 819, 599, 412, 241, 210.

**Source:** Voloshin et al. (2015b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectrum of devilline see also Majzlan et al. (2015).

**Devitoite**  $[\text{Ba}_6(\text{PO}_4)_2(\text{CO}_3)][\text{Fe}^{2+}_7(\text{OH})_4\text{Fe}^{3+}_2\text{O}_2(\text{SiO}_3)_8]$

**Origin:** Esquire #8 claim, Big Creek, Fresno Co., California, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 2.5 mW.

**Raman shifts (cm<sup>-1</sup>):** 1072, 1053, 914s, 700sh, 660s, 463w, 243w.

**Source:** Kampf et al. (2010b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Devitrite**  $\text{Na}_2\text{Ca}_3\text{Si}_6\text{O}_{16}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a single crystal at an angle of 45° between the electric field vector of the exciting laser and the [100] direction. A 633 nm He-Ne laser was used. The laser radiation power at the sample was 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 1126, 1110, 1094, 1079, 1059, 1051, 1010, 1003, 977, 966, 955, 948, 915, 908w, 890w, 836w, 805w, 791, 715, 698, 673s, 659s, 607s, 548, 520, 509, 499, 486, 472, 455, 444, 432, 416, 408, 397, 387, 342, 327, 306, 294, 286, 274, 253, 245, 226, 208, 193, 170, 151, 143, 126, 117, 105.

**Source:** Kahlenberg et al. (2010).

**Comments:** Devitrite is a crystalline impurity phase in industrial soda-lime glasses. The sample was characterized by single-crystal X-ray diffraction data. The crystal structure is solved.

**Dewindtite**  $\text{H}_2\text{Pb}_3(\text{UO}_2)_6\text{O}_4(\text{PO}_4)_4 \cdot 12\text{H}_2\text{O}$

**Origin:** Ranger U mine, Northern Territory, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3524, 3456, 3299, 3297, 1659, 1623, 1117, 1069, 1033, 1021, 994, 978, 8687, 857, 831, 818, 808, 795, 783, 617, 576, 536, 485, 445, 415, 390, 369, 274, 260, 251, 204, 170, 143, 115.

**Source:** Frost et al. (2006c).

**Comments:** The sample was characterized by chemical analysis.

**Diaboleite**  $\text{CuPb}_2\text{Cl}_2(\text{OH})_4$

**Origin:** Mannoth mine, Tiger, Arizona, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3525sh, 3465sh, 3452s, 3436sh, 3405sh, 3340, 978w, 781, 672, 538, 468w, 437w, 365, 294w, 227, 175, 149w, 130w.

**Source:** Frost et al. (2003j).

**Comments:** No independent analytical data are provided for the sample used. In the cited paper, there are differences between Raman shifts given in Fig. 2b and in Table 1. Only Raman shifts from Fig. 2b are listed above. For the Raman spectrum of diaboleite see also Frost and Williams (2004).

**Diadochite**  $\text{Fe}^{3+} \cdot 2(\text{PO}_4)(\text{SO}_4)(\text{OH}) \cdot 6\text{H}_2\text{O}$

**Origin:** Alum Cave Bluff, Great Smoky Mts., Sevier Co., Tennessee, USA.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3533sh, 3428, 3226sh, 2998, 1202sh, 1085, 1045sh, 1005s, 615, 565sh, 487, 448sh, 297sh, 263sh, 220, 142, 109.

**Source:** Frost and Palmer (2011f).

**Comments:** No independent analytical data are provided for the sample used.

**Diamond** C

**Origin:** Kangjinla mining district, Luobusa ophiolite, Southern Tibet.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 1332.6s.

**Source:** Xu et al. (2015b).

**Comments:** For the Raman spectra of diamond see also Knight and White (1989), Hänni et al. (1997), Yang et al. (2007b), Jasinevicius (2009), and Frezzotti et al. (2012).

### Diaspore AlO(OH)

**Origin:** Nevada, USA.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power was 200 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3445, 3363sh, 3226sh, 3119sh, 2936sh, 1186, 1067, 1045, 1018, 956, 918, 837, 812, 790, 705s, 564, 609, 580, 552, 495, 466, 446s, 436, 394, 381, 364, 329, 287, 260s, 216, 207.

**Source:** Ruan et al. (2001).

**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. No independent analytical data are provided for the sample used. For the Raman spectrum of diaspore see also Shoval et al. (2003).

### Dickinsonite-(KMnNa) K(NaMn)CaNa<sub>3</sub>AlMn<sub>13</sub>(PO<sub>4</sub>)<sub>12</sub>(OH)<sub>2</sub>

**Origin:** Branchville, Fairfield Co., Connecticut, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed in the region of O-H-stretching vibrations, on an arbitrarily oriented crystal, using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was in the range from 2 to 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 3557, 3520.

**Source:** Cámara et al. (2006).

**Comments:** The sample was characterized by powder X-ray diffraction data, electron microprobe analysis, and LA-ICP-MS. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

### Dickite Al<sub>2</sub>Si<sub>2</sub>O<sub>5</sub>(OH)<sub>4</sub>

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1190, 1160, 1080, 1025s, 910, 790, 750, 710, 665s, 560, 515, 480, 380, 340, 275, 235s.

**Source:** Frost et al. (1993).

**Comments:** No independent analytical data are given for the sample used. For the Raman spectra of dickite see also Frost (1995), Johnston et al. (1998), and Shoval et al. (2001).

### Digenite Cu<sub>1.8</sub>S

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed at 160 °C using 496.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 2000 mW.

**Raman shifts (cm<sup>-1</sup>):** 469.

**Source:** Liu et al. (2002).

**Comments:** The sample was characterized by powder X-ray diffraction data.

#### Dimorphite As<sub>4</sub>S<sub>3</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 676.4 nm Kr<sup>+</sup> laser radiation. The nominal laser radiation power was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 374sh, 369, 365, 357, 349, 341, 274s, 224, 213, 206, 199, 186, 179, 175, 120w, 54, 51, 44w, 41, 38, 34, 29s, 17.

**Source:** Chattopadhyay et al. (1982).

**Comments:** The sample was characterized by powder X-ray diffraction data.

#### Diomignite Li<sub>2</sub>B<sub>4</sub>O<sub>7</sub>

**Origin:** No data.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 1352w, 1097w, 1028s, 554w, 446w, 390w.

**Source:** Thomas and Davidson (2010).

**Comments:** No independent analytical data are given for the sample used.

#### Diopside CaMgSi<sub>2</sub>O<sub>6</sub>

**Origin:** Zillerthel, Tirol, Austria.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1045, 1010s, 853, 665s, 558w, 531w, 507w, 389, 358, 323, 296sh, 248w, 230w.

**Source:** Buzatu and Buzgar (2010).

**Comments:** No independent analytical data are given for the sample used. For the Raman spectra of diopside see also Richet et al. (1998), Jasinevicius (2009), Frezzotti et al. (2012), and Andò and Garzanti (2014).

#### Dioptase CuSiO<sub>3</sub>H<sub>2</sub>O

**Origin:** No data.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632.8 nm He-Ne laser radiation. The output laser radiation power was 30 mW.

**Raman shifts (cm<sup>-1</sup>):** 3371w, 1025, 1006s, 960, 916, 743, 660s, 525, 452, 431, 400, 357s, 325, 294, 265, 240w, 225, 161, 140, 133.

**Source:** Bouchard and Smith (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of dioptase see also McKeown et al. (1995).

**Dissakisite-(La)** CaLa(Al<sub>2</sub>Mg)[Si<sub>2</sub>O<sub>7</sub>][SiO<sub>4</sub>]O(OH)

**Origin:** Hochwartperidotite, Ultenzone, Alps, Italy.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 514 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3068, 1184, 1063s, 959s, 871s, 684, 566, 455s, 426s, 311, 226, 119.

**Source:** Tumiati et al. (2005).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Dixenite** Cu<sup>1+</sup>Fe<sup>3+</sup>Mn<sup>2+</sup><sub>14</sub>(As<sup>5+</sup>O<sub>4</sub>)(As<sup>3+</sup>O<sub>3</sub>)<sub>5</sub>(SiO<sub>4</sub>)<sub>2</sub>(OH)<sub>6</sub>

**Origin:** Långban deposit, Bergslagen ore region, Filipstad district, Värmland, Sweden (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** See comments below.

**Source:** Bahfenne and Frost (2010d).

**Comments:** No independent analytical data are given for the sample used. The Raman shifts 3644sh, 3582sh, 3449, 3247sh, 1389sh, 1386, 1347s, 1338sh, 1214, 1057s, 1026, 988sh, 944, 861, 751, 688w, 526s, 505sh, 428, 385, 312, 300sh, 282, 212sh, 170sh, and 143 do not correspond to an arsenite. The strongest IR bands of this sample are observed at 1565 and 1361 cm<sup>-1</sup>. This indicates that the investigated sample is not dixenite, but may be a carbonate or an organic compound. The assignment of the band at 1361 cm<sup>-1</sup> to “SiO<sub>4</sub><sup>2-</sup> antisymmetric stretching vibrations” (obviously, the authors meant SiO<sub>4</sub><sup>4-</sup>) is erroneous. Bands of stretching vibrations of SiO<sub>4</sub><sup>4-</sup> groups (in the range from 850 to 930 cm<sup>-1</sup>) are not observed in the IR spectrum of presumed “dixenite.”

**Djerfisherite** K<sub>6</sub>(Fe,Cu,Ni)<sub>25</sub>S<sub>26</sub>Cl

**Origin:** Guli dunite complex, Polar Siberia, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 300.

**Source:** Zaccarini et al. (2007).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Dmisokolovite** K<sub>3</sub>Cu<sub>5</sub>AlO<sub>2</sub>(AsO<sub>4</sub>)<sub>4</sub>

**Origin:** Arsenatnaya fumarole, Tolbachik volcano, Kamchatka, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm diode laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 900sh, 852s, 839s, 819sh, 640, 552sh, 525sh, 500s, 440, 400, 345, 223, 198, 121s, 96.

**Source:** Pekov et al. (2015d).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved.

### Dmisteinbergite Ca(Al<sub>2</sub>Si<sub>2</sub>O<sub>8</sub>)

**Origin:** Carbonaceous chondrite Northwest Africa 2086.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented grain in polished thin section using 532.2 nm Nd-YAG laser radiation. The nominal laser radiation power was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 912s, 893, 801, 504, 442s, 327, 219.

**Source:** Fintor et al. (2013, 2014).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectra of dmisteinbergite see also Nestola et al. (2010).

### Dolomite CaMg(CO<sub>3</sub>)<sub>2</sub>

**Origin:** Azcáratequarry, Eugui, Esteríbar, Spain.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented polished sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1758w, 1443w, 1098s, 882w, 340w, 301, 177.

**Source:** Perrin et al. (2016).

**Comments:** For the Raman spectra of dolomite see also Edwards et al. (2005), Ciobotă et al. (2012), and Frezzotti et al. (2012).

### Domerockite Cu<sub>4</sub>(AsO<sub>4</sub>)(AsO<sub>3</sub>OH)(OH)<sub>3</sub>·H<sub>2</sub>O

**Origin:** Dome Rock mine, South Australia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3420, 3235w, 875sh, 850s, 822s, 808s, 650, 478, 445, 390, 360.

**Source:** Elliott et al. (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### Donnayite-(Y) NaSr<sub>3</sub>CaY(CO<sub>3</sub>)<sub>6</sub>·3H<sub>2</sub>O

**Origin:** Poudrette quarry, Mont Sainte-Hilaire, Québec, Canada (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3760w, 3657sh, 3507sh, 3414, 3297, 3277, 3204sh, 1735w, 1694sh, 1583w, 1520sh, 1382w, 1093sh, 1077s, 1070sh, 1059sh, 728, 716, 694, 669sh, 549, 387, 427, 422, 387, 373, 363sh, 357, 338, 325sh, 287, 239sh, 225, 156s, 143sh.

**Source:** Frost et al. (2016a).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

**Dorallcharite**  $TlFe^{3+}_3(SO_4)_2(OH)_6$

**Origin:** Crven Dol, Allchar, Macedonia (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed in the range 100–1200 cm<sup>-1</sup> using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1165, 1089, 1004s, 621s, 564, 451, 420s, 339w, 300s, 218s, 206, 136s.

**Source:** Makreski et al. (2017).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Dorfmanite**  $Na_2(PO_3OH) \cdot 2H_2O$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed at 65°C on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 30 mW.

**Raman shifts (cm<sup>-1</sup>):** 3391w, 3320w, 3080w, 3028w, 1149, 1072, 950s, 867, 567w, 541w, 513w, 446, 411, 395.

**Source:** Ghule et al. (2003).

**Comments:** The sample was characterized by TG data. For the Raman spectra of dorfmanite see also Ramakrishnan and Aruldas (1987) and Frost et al. (2011).

**Dovyrenite**  $Ca_6Zr(Si_2O_7)_2(OH)_4$

**Origin:** Ioko-Dovyren massif, Northern Baikal region, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed from the natural face (100) of a crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 20 mW. A 0°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3638s, 3632s, 3593sh, 3585s, 3567sh, 1051s, 1002, 948s, 933sh, 836, 814sh, 759, 662s, 595s, 557sh, 518, 463, 437, 416sh, 393w, 372sh, 358, 333, 314, 296, 277, 260, 232.

**Source:** Galuskin et al. (2007b).

**Comments:** The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Downeyite**  $SeO_2$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 435.8 nm radiation (mercury arc). The radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 940w, 909, 889s, 862w, 706, 597s, 524, 364w, 299, 287, 254s, 199, 124.

**Source:** Venkateswaran (1936).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of downeyite see also Gerding (1941) and Stanila et al. (2000).

**Doyleite**  $\text{Al}(\text{OH})_3$

**Origin:** Mont Saint-Hilaire, Rouville RCM (Rouville Co.), Montérégie, Québec, Canada (type locality).

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was 25 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3615sh, 3545, 1080(?), 936, 840(?), 806(?), 580, 392, 305, 279, 229, 208(?), 187(?), 158(?), 124, 117, 107(?).

**Source:** Rodgers (1993).

**Comments:** The sample was characterized by powder X-ray diffraction data. Doubtful bands are marked with a question mark.

**Dravite**  $\text{NaMg}_3\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3(\text{OH})$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an oriented crystal (in the scattering geometry with the electrical field vector of the linearly polarized laser light parallel to the crystallographic *c*-axis) using 488 and 473 nm laser radiations. The nominal laser radiation power was 30 and 12 mW, respectively.

**Raman shifts (cm<sup>-1</sup>):** 3776w, 3740, 3641sh, 3622, 3577, 3549sh, 3513sh, 1060 (broad), 1036, 980sh, 700, 676, 661sh, 635, 550, 493, 400sh, 370s, 313, 215s, 132.

**Source:** Berryman et al. (2016).

**Comments:** In the O–H stretching vibration range Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectra of dravite see also Gasharova et al. (1997), Andò and Garzanti (2014), and Watenphul et al. (2016a, b).

**Dreyerite**  $\text{Bi}(\text{VO}_4)$

**Origin:** Hirschhorn, near Kaisertlautern, Germany (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1164, 1137, 1104, 1082, 987, 836s, 790, 646, 617, 452s, 462sh, 408w, 365, 321sh, 301.

**Source:** Frost et al. (2006i).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Drysdallite**  $\text{MoSe}_2$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an oriented crystal using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 286 ( $E^1_{2g}$ ), 242 ( $A_{1g}$ ), 168 ( $E_{1g}$ ), 25 ( $E^2_{2g}$ ).

**Source:** Sekine et al. (1980).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of drysdallite see also Agnihotri and Sehgal (1972).

### Dufrénoysite Pb<sub>2</sub>As<sub>2</sub>S<sub>5</sub>

**Origin:** Lengenbach, Binntal, Switzerland (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.81 nm He-Ne laser radiation. The laser radiation is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 376, 364s, 327s, 292s, 260s, 221s, 172, 144, 122, 102s, (74w).

**Source:** Kharbishi (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

### Duftite PbCu(AsO<sub>4</sub>)(OH)

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3280sh, 3240, 3192sh, 834s, 813, 792, 769sh, 549, 512, 454, 429, 403, 359, 340, 325, 301, 270, 229.

**Source:** Martens et al. (2003c).

**Comments:** No independent analytical data are provided for the sample used.

### Dumontite Pb<sub>2</sub>(UO<sub>2</sub>)<sub>3</sub>O<sub>2</sub>(PO<sub>4</sub>)<sub>2</sub>·5H<sub>2</sub>O

**Origin:** Shinkolowbe, Congo (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3552sh, 3475, 3352, 3189sh, 1054, 1024, 982, 974sh, 815sh, 800, 780, 571, 551sh, 445sh, 440sh, 293, 271, 246, 175, 149.

**Source:** Frost and Čejka (2009a).

**Comments:** No independent analytical data are provided for the sample used.

### Dumortierite AlAl<sub>6</sub>BSi<sub>3</sub>O<sub>18</sub>

**Origin:** Dehesa, California, USA.

**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal (with the incident laser light perpendicular to the *c*-axis of the crystal) using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 205 mW.

**Raman shifts (cm<sup>-1</sup>):** 1174, 1126w, 1113w, 1099w, 1002, 950s, 905sh, 843w, 808w, 793w, 780w, 750, 705sh, 660sh, 633, 548sh, 510s, 411s, 374, 283s, 228sh, 208s, 163, 147.

**Source:** Goreva et al. (2001).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of dumortierite see also Pieczka et al. (2013).

**Dundasite**  $\text{PbAl}_2(\text{CO}_3)_2(\text{OH})_4 \cdot \text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation output power was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 1090s, 234, 193w, 170, 152w.

**Source:** Goienaga et al. (2011).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

**Durangite**  $\text{NaAl}(\text{AsO}_4)\text{F}$

**Origin:** Barranca Sn mine, Coneto de Comonfort, Durango, Mexico (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 923sh, 912s, 827s, 718w, 610w, 539, 496s, 464, 430, 306w, 267s, 250, 202, 179sh, 160w, 130w.

**Source:** Downs et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

**Dussertite**  $\text{BaFe}^{3+}_3(\text{AsO}_4)(\text{AsO}_3\text{OH})(\text{OH})_6$

**Origin:** Horní Slavkov, Slavkovský les Mts., Bohemia, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3452s, 3439w, 3371s, 3242s, 3015w, 1250, 1220, 1176, 1115w, 902s, 870s, 859, 825w, 754w, 724w, 567, 561, 474s, 429s, 409, 372w, 306w, 275s, 247s, 188.

**Source:** Frost et al. (2011a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Dwornikite**  $\text{Ni}(\text{SO}_4) \cdot \text{H}_2\text{O}$

**Origin:** Artificial (product of Ni corrosion in concentrated sulfuric acid).

**Experimental details:** Raman scattering measurements have been performed on anodic corrosion film using 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was 90 mW.

**Raman shifts (cm<sup>-1</sup>):** 3300 (broad), 1600w, 1190, 1080, 1016s, 890, 596, 418.

**Source:** Melendres and Tani (1986).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Dypingite**  $Mg_5(CO_3)_4(OH)_2 \cdot 5H_2O$ **Origin:** Shinshiro Shi, Aichi Prefecture, Japan.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3648s, 3644, 3519, 3427, 3399sh, 2934w, 2880w, 1767w, 1751w, 1713w, 1601, 1447, 1452, 1366sh, 1122s, 1119s, 1092, 761, 727, 559w, 434w, 311, 249, 227, 203.**Source:** Frost et al. (2009a).**Comments:** Questionable data: no independent analytical data are given for the samples used. The IR spectra of the presumed dypingite sample from Shinshiro Shi correspond to the mixture of serpentine and a carbonate mineral. The IR spectra of presumed dypingite from Clear Creek given in the cited paper are wrong. Actually, they are IR spectra of serpentine with minor admixture of a carbonate other than dypingite. IR bands of serpentine are erroneously assigned to vibrations of dypingite. For Raman spectra of carbonate mixtures containing dypingite see Kristova et al. (2014).**Dzhalindite** In(OH)<sub>3</sub>**Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using Nd-YAG laser radiation. The wavelengths of laser excitation line and laser radiation power are not indicated.**Raman shifts (cm<sup>-1</sup>):** 302, 207.**Source:** Yan et al. (2008).**Comments:** The sample was characterized by powder X-ray diffraction data.**Dzhuluite** Ca<sub>3</sub>(SbSn)(Fe<sup>3+</sup>O<sub>4</sub>)<sub>3</sub>**Origin:** Upper Chegem Caldera, Northern Caucasus, Kabardino-Balkaria, Russia (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was in the range from 30 to 50 mW.**Raman shifts (cm<sup>-1</sup>):** 812sh, 783sh, 756, 726sh, 612sh, 581, 487s, 326sh, 209sh, 285, 264sh, 235, 183, 161, 140, 112w.**Source:** Galuskina et al. (2013b).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Dzierżanowskite** CaCu<sub>2</sub>S<sub>2</sub>**Origin:** Jabel Harmun, Judean Desert, Palestine Autonomy, Israel (type locality).**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented grain using 488 nm solid-state laser radiation. The laser radiation power at the sample was 120 mW.**Raman shifts (cm<sup>-1</sup>):** 300s, 103w, 86w.**Source:** Galuskina et al. (2016a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Eakerite**  $\text{Ca}_2\text{Sn}^{4+}\text{Al}_2\text{Si}_6\text{O}_{18}(\text{OH})_2 \cdot 2\text{H}_2\text{O}$

**Origin:** Foote Mineral Company mine, Kings Mt., North Carolina, USA.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532.0 nm solid-state laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3528, 3405, 3317, 1664, 1085, 1055, 1025, 996w, 974, 948w, 923w, 795, 747, 569s, 548s, 477, 441s, 418s, 393, 350, 337, 276, 234.

**Source:** Uchida et al. (2007).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data. The crystal structure is solved. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Eastonite**  $\text{KAlMg}_2(\text{Si}_2\text{Al}_2)\text{O}_{10}(\text{OH})_2$

**Origin:** Hessdalen, Norway.

**Experimental details:** Raman scattering measurements have been performed on an oriented sample, using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. The spectra were recorded with the electric field polarized perpendicular to the cleavage plane.

**Raman shifts (cm<sup>-1</sup>):** 3700s, 3663s, 1014, 670s, 652s, 400, 361, 274w, 194s, 100.

**Source:** Tlili et al. (1989).

**Comments:** The sample was characterized by electron microprobe analysis. For the Raman spectra of eastonite see also Tlili and Smith (2007) and Wang et al. (2015).

**Eastonite**  $\text{KAlMg}_2(\text{Si}_2\text{Al}_2)\text{O}_{10}(\text{OH})_2$

**Origin:** Easton, Pennsylvania, USA.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample (on either loose grains without preparation or on a pressed pellet of sample powder) using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 13 mW.

**Raman shifts (cm<sup>-1</sup>):** 3718s, 3693, 3678, 1082, 1038, 681s, 456, 427, 391, 351, 279, 192s.

**Source:** Wang et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectra of eastonite see also Tlili and Smith (2007).

**Ecandrewsite**  $\text{ZnTiO}_3$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample compressed into pellet. The wavelengths of laser excitation line and the laser radiation power are not indicated.

**Raman shifts (cm<sup>-1</sup>):** 716s, 624, 490, 474, 395, 350s, 270, 234, 181, 141w.

**Source:** Bernert et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of ecandrewsite see also Beigi et al. (2011).



**Origin:** Harstigen mine, Pajsberg, near Filipstad, Värmland, Sweden.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample, using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power was in the range from 20 to 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 1122s, ~694, 340–310, 154s, 129s.

**Source:** Jonsson (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.



**Origin:** Otto Mt., near Baker, California, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented polished grain using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 2.5 mW.

**Raman shifts (cm<sup>-1</sup>):** 3440, 729s, 692s, 562w, 312w, 274, 260.

**Source:** Kampf et al. (2013b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved. The empirical formula of the sample used is  $\text{Ca}_{0.962}\text{Pb}_{0.073}\text{Cu}^{2+}_{0.971}\text{Mg}_{0.005}\text{Fe}^{3+}_{0.002}\text{Te}^{6+}_{0.986}\text{O}_6\text{H}_{2.052}$ .



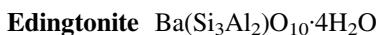
**Origin:** Upper Chegem caldera, Northern Caucasus, Kabardino-Balkaria, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The output laser radiation power was in the range 30–50 mW. A 180°-scattering geometry was employed. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3554, 3547, 3540, 921, 889, 839, 815s, 667w, 556, 527w, 423sh, 406, 394sh, 309, 269, 195w, 172sh, 163, 108w.

**Source:** Galuskin et al. (2012d).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved. The Raman shifts are given for the member of the edgrewite  $\text{Ca}_9(\text{SiO}_4)_4\text{F}_2$ -hydroxyedgrewite  $\text{Ca}_9(\text{SiO}_4)_4(\text{OH})_2$  series with the content of the edgrewite end-member minal more than 50%.



**Origin:** Ice River, near Golden, British Columbia, Canada.

**Experimental details:** Raman scattering measurements have been performed on an oriented sample with the long axis of crystal normal to the polarization direction of the laser beam, using 514.5 nm Ar<sup>+</sup> laser radiation. A 180°-scattering geometry was employed. The laser radiation power at the sample was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 3480s, 1644, 1096s, 1085s, 1077s, 1061s, 1049, 1021, 986s, 722s, 662, 531s, 480, 454s, 447s, 433, 427, 409, 395, 358s, 343s, 337, 330, 323, 311, 302, 284, 272s, 256, 167, 153, 141s.

**Source:** Wopenka et al. (1998).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of edingtonite see also Mozugawa (2001).

**Edoyerite**  $\text{Hg}^{2+}_3(\text{Cr}^{6+}\text{O}_4)\text{S}_2$

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample, using 785 nm Nd-YAG laser radiation. The laser radiation power at the sample was 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 840s, 382, 368, 363, 340, 325, 269s.

**Source:** Frost (2004c).

**Comments:** No independent analytical data are provided for the sample used.

**Effenbergerite**  $\text{BaCuSi}_4\text{O}_{10}$

**Origin:** Artificial.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample, using 514 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 1097s, 986s, 788, 588, 573w, 558w, 517, 454sh, 423s, 380, 339w, 276w.

**Source:** Xia et al. (2014).

**Comments:** No independent analytical data are provided for the sample used.

**Eitelite**  $\text{Na}_2\text{Mg}(\text{CO}_3)_2$

**Origin:** Synthetic.

**Experimental details:** Kind of sample preparation is not indicated. Micro-Raman scattering measurements have been performed in Ar atmosphere using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 1 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1105s, 721w, 263, 208, 91s.

**Source:** Shatskiy et al. (2013).

**Comments:** The sample was characterized by single crystal X-ray diffraction data and energy-dispersive X-ray scan data. For the Raman spectrum of eitelite see also Sharygin et al. (2013c).

**Ekanite**  $\text{Ca}_2\text{ThSi}_8\text{O}_{20}$

**Origin:** Moneragala, Okkampitiya area, Eastern Sri Lanka.

**Experimental details:** Raman scattering measurements have been performed on an annealed metamict sample using 473 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1113s, 1009, 992, 747w, 657, 575, 433s, 395, 368, 350, 274, 189, 157, 133, 113.

**Source:** Nasdala et al. (2016).

**Comments:** The sample was characterized by electron microprobe analysis. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

**Ekplexite**  $(\text{Nb}, \text{Mo})\text{S}_2 \cdot (\text{Mg}_{1-x} \text{Al}_x)(\text{OH})_{2+x}$

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm diode laser radiation. The laser radiation power at the sample was 3 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3530, 3326, 707, 526s, 438, 387sh, 364s, 232sh, 198sh, 161, 120sh.

**Source:** Pekov et al. (2014a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is  $(\text{Nb}_{0.45} \text{Mo}_{0.38} \text{W}_{0.10} \text{V}_{0.04}) \text{S}_2 (\text{Mg}_{0.60} \text{Al}_{0.37} \text{Fe}_{0.02})(\text{OH})_{2.36}$ .

**Elbaite**  $\text{Na}(\text{Al}_{1.5} \text{Li}_{1.5})\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3(\text{OH})$

**Origin:** Granite pegmatite in an unknown locality in Southern California, USA.

**Experimental details:** Raman scattering measurements have been performed on an oriented sample, using 488 and 514.5 nm Ar<sup>+</sup> laser radiations in the range 150–1550 cm<sup>-1</sup>. The laser radiation power is not indicated. A 180°-scattering geometry was employed. Polarized spectra were collected in the z(xx)z, x(yy)x, x(zz)x, z(xy)z and x(zy)x scattering geometries.

**Raman shifts (cm<sup>-1</sup>):** z(xx)z: 1412, 1190, 1077, 760, 731, 693, 641, 407, 373, 222(A<sub>1</sub>), 340(E); x(yy)x: 1412, 1105, 1059, 989, 850, 760, 717, 632, 508, 407, 373, 244, 222(A<sub>1</sub>), 340 (E); x(zz)x: 1442, 1412, 1105, 1059, 989, 860, 760, 717, 637, 508, 407, 373, 244, 222 (A<sub>1</sub>); z(xy)z: 1190, 1077, 731, 373 (E); x(zy)x: 717, 700, 373, 350, 286 (E).

**Source:** Gasharova et al. (1997).

**Comments:** The sample was characterized by powder X-ray diffraction data, electron microprobe analysis, wet chemical analysis for most elements, atom absorption spectroscopy for Li, flame photometry for Na and K, and thermal analysis for OH content. The empirical formula of the sample used is  $(\text{Na}_{0.86} \text{K}_{0.09} \text{Ca}_{0.05})(\text{Li}_{0.99} \text{Mg}_{0.27} \text{Mn}_{0.23} \text{Fe}^{2+}_{0.01} \text{Al}_{1.41})\text{Al}_6 \text{B}_{2.93} \text{Si}_6 \text{O}_{27.26} (\text{OH})_{3.64} \text{F}_{0.10}$ . For the Raman spectra of elbaite see also Natkaniec-Nowak et al. (2009), Hoang et al. (2011), and Fantini et al. (2014).

**Elbaite**  $\text{Na}(\text{Al}_{1.5} \text{Li}_{1.5})\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3(\text{OH})$

**Origin:** Lucyen mines, Vietnam.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample, using 457 nm solid-state laser radiation. The laser radiation power at the sample was 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 3655, 3585, 3560, 3490, 1407w, 1070s, 1033sh, 981, 880w, 836, 808, 733s, 673, 587sh, 551, 517, 476, 447, 404sh, 377s, 335sh.

**Source:** Hoang et al. (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data and energy-dispersive X-ray scan data. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectra of elbaite see also Gasharova et al. (1997), Natkaniec-Nowak et al. (2009), and Fantini et al. (2014).

**Elbrusite**  $\text{Ca}_3(\text{U}^{6+}_{0.5}\text{Zr}_{1.5})(\text{Fe}^{3+}\text{O}_4)_3$ 

**Origin:** Upper Chegem caldera, Kabardino-Balkaria, Northern Caucasus, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal. A  $0^\circ$ -scattering geometry was employed. The wavelength of laser excitation line and the laser radiation power are not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 805sh, 730, 478, 273, 222s.

**Source:** Galuskina et al. (2010b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Eleonorite**  $\text{Fe}^{2+}\text{Fe}^{3+}_5(\text{PO}_4)_4(\text{OH})_5 \cdot 6\text{H}_2\text{O}$ 

**Origin:** Boca Rica pegmatite, Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power at the sample is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1174, 1155, 1133, 1116, 1098, 1084sh, 1069, 1058, 1051, 1034, 1011s, 990sh, 969sh, 703sh, 687s, 673, 661, 644, 601, 582, 567s, 546, 503, 491, 478, 468, 455, 437, 403, 398, 336, 322, 309sh, 300, 289, 280, 254, 238, 230, 225, 200, 191sh, 153, 1432, 118, 107.

**Source:** Frost et al. (2014al).

**Comments:** No independent analytical data are given for the sample used. In the cited paper the mineral is described with the name beraunite, but an incorrect formula of beraunite is given. Brown color of the sample indicates that it is not beraunite, but its oxydation product eleonorite, a mineral isostructural with beraunite (Chukanov et al. 2017a).

**Elpasolite**  $\text{K}_2\text{NaAlF}_6$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 561, 330, 138.

**Source:** Morss (1974).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of elpasolite see also Frezzotti et al. (2012).

**Eltybyuite**  $\text{Ca}_{12}\text{Fe}^{3+}_{10}\text{Si}_4\text{O}_{32}\text{Cl}_6$ 

**Origin:** Upper Chegem caldera, Kabardino-Balkaria, Northern Caucasus, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal, using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation output power was in the range from 30 to 50 mW. A  $180^\circ$ -scattering geometry was employed. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3395w, 936w, 927w, 861, 846, 816s, 784, 699, 558w, 532w, 472sh, 468, 412, 327sh, 309, 260.

**Source:** Galuskin et al. (2013a).

**Comments:** The sample was characterized by single-crystal electron backscatter diffraction data and electron microprobe analyses. The wavenumbers were partly determined by us based on spectral curve analysis of the published spectrum. The empirical formula of the sample used is  $\text{Ca}_{12.12}\text{Mg}_{0.04}\text{Ti}_{0.11}\text{Fe}^{3+}_{9.41}\text{Al}_{1.26}\text{Si}_{2.98}\text{O}_{31.89}\text{Cl}_{5.04}$ . The band positions denoted by Galuskin et al. (2013a) as  $448\text{ cm}^{-1}$  (twice) were determined by us at  $468$  and  $412\text{ cm}^{-1}$ . For the Raman spectrum of eltyubuyite see also Gfeller et al. (2015).

**Emmonsite**  $\text{Fe}^{3+}_2(\text{Te}^{4+}\text{O}_3)_3 \cdot 2\text{H}_2\text{O}$

**Origin:** Moctezuma mine, New Mexico.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a  $633\text{ nm}$  He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts ( $\text{cm}^{-1}$ ):**  $788, 764, 688\text{sh}, 658\text{s}, 440\text{s}, 400\text{s}, 326, 275\text{s}, 227\text{w}, 187\text{s}$ .

**Source:** Frost et al. (2008i).

**Comments:** No independent analytical data are provided for the sample used.

**Enargite**  $\text{Cu}_3\text{AsS}_4$

**Origin:** Butte, Montana, USA.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using  $514.5\text{ nm}$   $\text{Ar}^+$  laser radiation. The laser radiation power at the sample was in the range  $1\text{--}10\text{ mW}$ . A  $180^\circ$ -scattering geometry was employed.

**Raman shifts ( $\text{cm}^{-1}$ ):**  $382\text{s}, 337\text{s}, 298, 269, 170, 151, 133$ .

**Source:** Mernagh and Trudu (1993).

**Comments:** The sample was characterized by electron microprobe analysis. For the Raman spectrum of enargite see also Gow (2015).

**Enargite**  $\text{Cu}_3\text{AsS}_4$

**Origin:** Quirivilca region, Peru.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using  $632.8\text{ nm}$  He-Ne laser radiation. The maximum output laser radiation power was  $100\text{ mW}$ .

**Raman shifts ( $\text{cm}^{-1}$ ):**  $724\text{w}, 679, 384, 338\text{s}, 265$ .

**Source:** Gow (2015).

**Comments:** The sample was characterized with scanning electron microscopy. For the Raman spectrum of enargite see also Mernagh and Trudu (1993).

**Enstatite**  $\text{Mg}_2\text{Si}_2\text{O}_6$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal, using  $488\text{ nm}$   $\text{Ar}^+$  laser radiation. The laser radiation power is not indicated. Polarized spectra were collected in the  $E \parallel (100)$ ,  $E \parallel (010)$  and  $E \parallel (001)$  scattering geometries.

**Raman shifts ( $\text{cm}^{-1}$ ):**  $1035\text{s}, 1013\text{s}, 937, 938, 853, 687\text{s}, 665\text{s}, 581, 554, 541, 527, 446, 423\text{s}, 403\text{s}, 385, 344\text{s}, 303, 239\text{s}, 206, 198\text{s}, 134\text{s}$ .

**Source:** Stalder et al. (2009).

**Comments:** The sample was characterized by electron microprobe analysis. Raman peak positions do not exhibit a significant dependence on scattering geometry. For the Raman spectra of enstatite see also Lin (2004), Frezzotti et al. (2012), and Andò and Garzanti (2014).

### Eosphorite $\text{Mn}^{2+}\text{Al}(\text{PO}_4)(\text{OH})_2\text{H}_2\text{O}$

**Origin:** Roberto mine, Divino das Laranjeiras, Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals, using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3477sh, 3460s, 3313, 3191sh, 3063, 1747, 1651, 1193w, 1142w, 1091w, 1011w, 978sh, 969s, 864sh, 816w, 634sh, 618, 595, 580sh, 560, 473, 462sh, 399, 386sh, 338w, 307, 291, 254, 232, 208, 200, 175, 171, 152, 118.

**Source:** Frost et al. (2013am).

**Comments:** The sample was characterized by electron microprobe analysis. The empirical formula of the sample used is  $(\text{Mn}_{0.72}\text{Fe}_{0.13}\text{Ca}_{0.01})\text{Al}_{1.04}(\text{PO}_4,\text{HPO}_4)_{1.07}(\text{OH}_{1.89}\text{F}_{0.02}) \cdot 0.94\text{H}_2\text{O}$ .

### Epidote $\text{Ca}_2(\text{Al}_2\text{Fe}^{3+})[\text{Si}_2\text{O}_7][\text{SiO}_4]\text{O}(\text{OH})$

**Origin:** Dunje, Macedonia.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample, using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1084, 1040w, 980w, 914s, 885, 864sh, 832w, 599s, 565s, 522w, 508, 452s, 430, 390w, 350, 328w, 314w, 292w, 276, 243, 230, 168, 134.

**Source:** Jovanovski et al. (2009).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectra of epidote see also Jovanovski et al. (2009) and Andò and Garzanti (2014).

### Epistilbite $\text{Ca}_3[\text{Si}_{18}\text{Al}_6\text{O}_{48}] \cdot 16\text{H}_2\text{O}$

**Origin:** Berufjord, Iceland.

**Experimental details:** Kind of sample preparation is not indicated. The measurements have been performed using 1064 nm Nd-YAG laser radiation with the radiation power at the sample of 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 1631sh, 1620, 1117, 801w, 434s, 409s, 255, 179.

**Source:** Mozgawa (2001).

**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

### Epsomite $\text{Mg}(\text{SO}_4) \cdot 7\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 15 mW.

**Raman shifts (cm<sup>-1</sup>):** 3425, 3303, 1672, 1134, 1095, 1061, 984s, 612, 447, 369, 245, 154.

**Source:** Wang et al. (2006a).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of epsomite see also Genceli et al. (2007), Buzgar et al. (2009), Apopei et al. (2012, 2014a), and Jentzsch et al. (2013).

### Epsomite $\text{Mg}(\text{SO}_4) \cdot 7\text{H}_2\text{O}$

**Origin:** Coranda-Hondol ore deposit, Certej, Romania.

**Experimental details:** Kind of sample preparation is not indicated. The measurements have been performed using 532 nm Nd-YAG laser radiation with the power at the sample of 53.6 mW.

**Raman shifts (cm<sup>-1</sup>):** 3285, 3219sh, 1668w, 1136w, 1097w, 1062w, 985s, 615, 449, 371w, 246w.

**Source:** Apopei et al. (2014a).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and scanning electron microscopy. For the Raman spectra of epsomite see also Wang et al. (2006a), Genceli et al. (2007), Buzgar et al. (2009), Apopei et al. (2012), and Jentzsch et al. (2013).

### Ericlaxmanite $\text{Cu}_4\text{O}(\text{AsO}_4)_2$

**Origin:** Arsenatnaya fumarole, Tolbachik volcano, Kamchatka, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample, using 532 nm laser radiation. The laser radiation power at the sample was about 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 889sh, 863sh, 845s, 753, 664, 608, 531sh, 493, 440, 401, 329, 292, 229s, 181, 112.

**Source:** Pekov et al. (2014c).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Cu}_{3.97}\text{Zn}_{0.06}\text{Fe}_{0.02})(\text{As}_{1.94}\text{P}_{0.02}\text{V}_{0.01}\text{S}_{0.01})\text{O}_9$ .

### Erikapohlite $\text{Cu}^{2+}(\text{Zn,Cu,Mg})_4\text{Ca}_2(\text{AsO}_4)_6 \cdot 2\text{H}_2\text{O}$

**Origin:** Tsumeb mine, Tsumeb, Namibia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample, using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 894, 854s, 797s, 582w, 500, 408, 355, 306, 280, 234, 191, 122.

**Source:** Schlüter et al. (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is  $\text{Cu}_3(\text{Zn}_{2.48}\text{Cu}_{0.93}\text{Mg}_{0.77}\text{Fe}_{0.01})\text{Ca}_{2.04}\text{As}_{6.20}\text{O}_{24.71} \cdot 1.29\text{H}_2\text{O}$ . The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

### Eringaite $\text{Ca}_3\text{Sc}_2(\text{SiO}_4)_3$

**Origin:** Wiluy River, Sakha-Yakutia Republic, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power was in the range from 20 to 40 mW.

**Raman shifts (cm<sup>-1</sup>):** 936s, 877s, 815sh, 742, 638, 602, 540sh, 511s, 484sh, 440w, 408, 359s, 336, 309, 255, 220w.

**Source:** Galuskina et al. (2010d).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is  $(\text{Ca}_{3.00}\text{Y}_{0.01})(\text{Sc}_{0.63}\text{Ti}^{4+}_{0.66}\text{Fe}^{3+}_{0.25}\text{Zr}_{0.30}\text{Mg}_{0.08}\text{Cr}^{3+}_{0.06}\text{Fe}^{2+}_{0.01})(\text{Si}_{2.13}\text{Al}_{0.26}\text{Fe}^{3+}_{0.61})\text{O}_{12}$ . The Raman shifts were determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of eringite see also Yun-Fang et al. (2013).

### Eriochalcite CuCl<sub>2</sub>·2H<sub>2</sub>O

**Origin:** Main Lode, Great Australia mine, Cloncurry, Queensland, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3462sh, 3367, 3176w, 1620, 690, 672sh, 405, 390sh, 234, 215s, 117.

**Source:** Frost et al. (2003i).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of eriochalcite see also Christy et al. (2004).

### Erionite-Ca Ca<sub>5</sub>[Si<sub>26</sub>Al<sub>10</sub>O<sub>72</sub>]·30H<sub>2</sub>O

**Origin:** Oregon, USA.

**Experimental details:** Micro-Raman scattering measurements have been performed on an oriented fiber using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 20 mW. Spectra were recorded by placing fiber elongation axis at 0°, 45°, 90°, and 135° with respect to the cross hair of the microscope ocular lens.

**Raman shifts (cm<sup>-1</sup>):** 816w, 790w, 569, 486s, 469sh, 346.

**Source:** Croce et al. (2013).

**Comments:** The Raman shifts are indicated for the fiber orientation with respect to the direction of the laser beam. No independent analytical data are provided for the sample used.

### Erlichmanite OsS<sub>2</sub>

**Origin:** Santa Elena Nappe, Costa Rica.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532.6 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 396w, 342s.

**Source:** Zaccarini et al. (2010).

**Comments:** The sample was characterized by electron microprobe analysis. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of erlichmanite see also Bakker (2014).

### Ernstburkeite Mg(CH<sub>3</sub>SO<sub>3</sub>)<sub>2</sub>·12H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 3021, 2939, 1421, 1055s, 974, 776, 545, 348.

**Source:** Güner et al. (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Erythrite Co<sub>3</sub>(AsO<sub>4</sub>)<sub>2</sub>·8H<sub>2</sub>O

**Origin:** Mt. Cobalt, Queensland, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3337sh, 3200, 3052, 902, 852, 792, 727w, 652w, 467, 457s, 439s, 391, 378, 301, 263, 249s, 234, 223, 209s, 188, 162, 147w, 126.

**Source:** Frost et al. (2003g).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of erythrite see also Frost et al. (2004i) and Kloporgog et al. (2006).

### Erythrosiderite K<sub>2</sub>Fe<sup>3+</sup>Cl<sub>5</sub>·H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an oriented sample. The laser beam was allowed to fall on a crystal face at an angle of 45°. The measurements have been performed using He-Ne laser radiation. The laser radiation power was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 384, 299s, 224, 174, 129.

**Source:** Sharma and Pandya (1974).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of erythrosiderite see also Piszczeck et al. (2003).

### Erythrosiderite K<sub>2</sub>Fe<sup>3+</sup>Cl<sub>5</sub>·H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 1064 nm Nd-YAG laser radiation. The maximum output laser radiation power was about 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1807, 1591, 371, 298, 221, 180, 173, 128.

**Source:** Piszczeck et al. (2003).

**Comments:** The water content in the sample used was established by thermogravimetric analysis. For the Raman spectrum of erythrosiderite see also Sharma and Pandya (1974).

### Eskebornite CuFeSe<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a nanocrystalline sample, using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 471, 348w, 288s.

**Source:** Wang et al. (2009a).

**Comments:** No independent analytical data are provided for the sample used.

**Eskolaite** Cr<sub>2</sub>O<sub>3</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 647.1 nm laser radiation. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 613, 552s, 527, 397w, 350, 300.**Source:** Maslar et al. (2001).**Comments:** No independent analytical data are provided for the reference sample used. For the Raman spectra of eskolaite see also Bouchard and Smith (2003), Hosterman (2011), and Adar (2014).**Esperite** PbCa<sub>2</sub>(ZnSiO<sub>4</sub>)<sub>3</sub>**Origin:** Franklin, New Jersey, USA (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 780 nm solid-state laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 958w, 931w, 900, 846s, 589, 538w, 504, 447s, 409, 368, 335, 297w, 278w, 250, 224, 215w, 200w, 181s, 160, 153.**Source:** Tait et al. (2010).**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is Pb<sub>1.00</sub>(Ca<sub>1.86</sub>Fe<sup>2+</sup><sub>0.07</sub>Mn<sub>0.04</sub>Cr<sup>3+</sup><sub>0.02</sub>)(Zn<sub>1.00</sub>Si<sub>1.00</sub>O<sub>4</sub>)<sub>3</sub>. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.**Ettringite** Ca<sub>6</sub>Al<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>(OH)<sub>12</sub>·26H<sub>2</sub>O**Origin:** Synthetic.**Experimental details:** Kind of sample preparation is not indicated. Raman scattering measurements have been performed in the spectral regions from 200 to 1300 cm<sup>-1</sup> and from 2800 to 4000 cm<sup>-1</sup> using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 15 mW. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 3638, 3440s, 1118w, 1087w, 990s, 615w, 549w, 451, 416w 346w.**Source:** Renaudin et al. (2007).**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectra of ettringite see also Deb et al. (2003) and Frost et al. (2013i).**Euchroite** Cu<sub>2</sub>(AsO<sub>4</sub>)(OH)·3H<sub>2</sub>O**Origin:** L'ubietová-Svätoduška, Banská Bystrica Co., Banská Bystrica region, Slovakia.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3537, 3470, 3278sh, 3116, 2924sh, 1634, 1032w, 976w, 848sh, 836s, 821sh, 768w, 474, 441, 385, 358, 294sh, 246s, 233s, 227sh, 210, 203sh, 171sh, 161s, 144s, 134sh, 112s.**Source:** Frost et al. (2010e).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is  $\text{Cu}_{2.06}[(\text{AsO}_4)_{0.96}(\text{PO}_4)_{0.04}] (\text{OH})_{1.13} \cdot 3\text{H}_2\text{O}$ . For the Raman spectrum of euchroite see also Frost and Bahfenne (2010b).

### Euclase $\text{BeAlSiO}_4(\text{OH})$

**Origin:** An unknown locality in Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 488 nm  $\text{Ar}^+$  laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3587, 3575, 1120, 1059s, 1023, 975, 908s, 880, 806w, 790w, 756w, 747w, 667w, 642w, 602w, 583, 574, 545, 518w, 461sh, 452, 444, 423w, 411w, 397s, 384, 355w, 341sh, 334, 309w, 290s, 276w, 259s, 237, 201, 180, 145.

**Source:** Hofmeister et al. (1987).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of euclase see also Jehlička et al. (2012) and Jehlička and Vandenabeele (2015).

### Eucryptite- $\beta$ $\text{Li}(\text{AlSiO}_4)$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a single crystal at various crystal orientations using 1064 nm Nd-YAG laser radiation. The obtained data were averaged to produce a final spectrum. The nominal laser radiation power was 100 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1099, 1086, 1067(?), 1049, 1032s, 987w, 762w, 711w, 636w, 483s, 466sh, 352, 282, 233w, 187, 157, 142, 108.

**Source:** Zhang et al. (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Kentbrooksite $(\text{Na},\text{REE})_{15}(\text{Ca},\text{REE})_6\text{Mn}^{2+}{}_3\text{Zr}_3\text{Nb}(\text{Si}_{25}\text{O}_{73})\text{OF}_2 \cdot 2\text{H}_2\text{O}$

**Origin:** Sushina Hill Region, Purulia district, West Bengal, India.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample, using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power at the sample was 4 mW.

**Raman shifts (cm<sup>-1</sup>):** 1007s, 991, 975, 727s, 438, 433s, 429w, 354s, 333, 220, 209w, 199, 191s.

**Source:** Chakrabarty et al. (2011).

**Comments:** The sample was characterized by electron microprobe data which correspond to Ca-rich kentbrooksite. In the cited paper the mineral is erroneously described under the name “eudialyte.” The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

### Eugsterite $\text{Na}_4\text{Ca}(\text{SO}_4)_3 \cdot 2\text{H}_2\text{O}$

**Origin:** Efflorescence on the walls of the Manasija Monastery, Serbia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample, using 532 and 780 nm laser radiations.

**Raman shifts (cm<sup>-1</sup>):** 1125, 1084.

**Source:** Matović et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and EDS analysis.

**Eulytine**  $\text{Bi}_4(\text{SiO}_4)_3$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal, using 488 and 514.5 nm  $\text{Ar}^+$  laser radiations. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 991w, 930, 896, 888, 868s, 623w, 547w, 533w, 503w, 491w, 437, 393, 333, 314w, 283w, 276w, 249w, 202, 149, 131, 106, 100sh, 94s, 67.**Source:** Beneventi et al. (1995).**Comments:** No independent analytical data are provided for the sample used.**Euxenite-(Y)**  $(\text{Y}, \text{Ca}, \text{Ce}, \text{U}, \text{Th})(\text{Nb}, \text{Ta}, \text{Ti})_2\text{O}_6$ **Origin:** Billeroo Prospect, South Australia.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 1624sh, 1520w, 1300w, 842, 805sh, 658sh, 624, 493sh, 410, 197sh, 161sh, 152s.**Source:** Frost et al. (2011h).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of euxenite-(Y) see also Gong et al. (1995).**Evansite**  $\text{Al}_3(\text{PO}_4)_6 \cdot 8\text{H}_2\text{O}$ **Origin:** Porto, Northwest Portugal.**Experimental details:** Kind of sample preparation is not indicated. Micro-Raman scattering measurements have been performed with 532 nm laser radiation. The nominal laser radiation power was 6 mW.**Raman shifts (cm<sup>-1</sup>):** 1645, 1364, 1048s, 1008s, 830w, 634, 564, 486, 367.**Source:** Sanchez-Moral et al. (2011).**Comments:** The sample was characterized by powder X-ray diffraction data, electron microprobe analyses, and inductively coupled plasma mass spectrometry.**Eveite**  $\text{Mn}^{2+}_2(\text{AsO}_4)(\text{OH})$ **Origin:** Långban, Filipstad, Värmland, Sweden.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 3564, 870, 827s, 809s, 510, 474w, 439, 222w.**Source:** Yang et al. (2001).**Comments:** The sample was characterized by single-crystal X-ray diffraction data. The crystal structure is solved. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Evenkite**  $C_{23}H_{48}$ **Origin:** Mernek, Slovakia.**Experimental details:** Kind of sample preparation is not indicated. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation with the nominal radiation power of 10 mW and/or 1064 nm Nd-YAG laser radiation with the power of 350 mW. The spectrum was obtained with a beam perpendicular to the (111) crystal face.**Raman shifts (cm<sup>-1</sup>):** 2883s, 2848, 2735, 1464, 1441s, 1420, 1383w, 1370w, 1295, 1265w, 1171, 1133, 1123, 1103w, 1062, 890w, 103w.**Source:** Jehlička et al. (2007a).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of evenkite see also Jehlička et al. (2009a).**Ezcurrite**  $Na_2B_5O_7(OH)_3 \cdot 2H_2O$ **Origin:** Tincalayu Mine, Salardel Hombre Muerto, Salta, Argentina (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3652sh, 3596sh, 3576, 3547, 3509sh, 3431s, 3329sh, 3247sh, 3186, 3098sh, 1691sh, 1641w, 1591sh, 1343, 1333sh, 1318sh, 1193, 1163, 1129sh, 1060, 1048sh, 1037, 1025sh, 1015, 1000, 968, 957sh, 947, 857sh, 842, 803sh, 782sh, 761, 746sh, 726sh, 693w, 590sh, 575s, 550sh, 529, 488, 473sh, 460, 445sh, 385, 350, 317, 286, 273sh, 209sh, 190, 162, 141, 128sh, 115, 108.**Source:** Frost et al. (2014j).**Comments:** The sample was characterized by qualitative electron microprobe analysis which shows Al impurity.**Fabriesite**  $Na_3Al_3Si_3O_{12} \cdot 2H_2O$ **Origin:** Tawmaw, Myanmar.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power at the sample was 5 mW.**Raman shifts (cm<sup>-1</sup>):** 3500, 3200, 1011, 946, 903, 731, 682, 524, 490, 451s, 406, 372, 332, 314, 258w, 228w, 209.**Source:** Ferraris et al. (2014).**Comments:** The sample was characterized by electron microprobe analysis and electron backscatter diffraction. The empirical formula of the sample used is  $(Na_{2.937}Ca_{0.030}K_{0.008}Mg_{0.007}Fe_{0.004}Ba_{0.002}Mn_{0.001})Al_{2.996}Si_{2.999}O_{12} \cdot 2H_{1.993}O$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.**Fairfieldite**  $Ca_2Mn^{2+}(PO_4)_2 \cdot 2H_2O$ **Origin:** Cigana mine, Conselheiro Pena, Rio Doce valley, Minas Gerais, Brazil.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts

have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3271sh, 3139sh, 3040, 2961sh, 1663w, 1632w, 1577w, 1491w, 1466w, 1099s, 1027, 955s, 945sh, 925s, 906, 768, 604s, 584, 552, 442sh, 422s, 369sh, 312, 287, 251, 235, 214, 203sh, 185, 176sh, 136w.

**Source:** Frost et al. (2013ad).

**Comments:** The sample was characterized by electron microprobe data. The empirical formula of the sample used is  $\text{Ca}_2(\text{Mn}_{0.56}\text{Mg}_{0.33}\text{Fe}_{0.11})(\text{PO}_4)_2 \cdot 2\text{H}_2\text{O}$ .

### Falcondoite $\text{Ni}_4\text{Si}_6\text{O}_{15}(\text{OH})_2 \cdot 6\text{H}_2\text{O}$

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 1064 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 823, 705sh, 673s, 640, 386s, 196s.

**Source:** Villanova-de-Benavent et al. (2012).

**Comments:** No independent analytical data are provided for the sample used.

### Falottaite $\text{MnC}_2\text{O}_4 \cdot 3\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Kind of sample preparation is not indicated. The measurements have been performed with using 1064 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1614w, 1478s, 1427, 913, 885, 575, 515, 480w.

**Source:** Mancilla et al. (2009a).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Fangite $\text{Tl}_3\text{AsS}_4$

**Origin:** Allchar deposit, Macedonia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 1.9 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 397, 379s, 367sh, 323, 308, 289sh, 275, 209, 191w, 170, 137, 105.

**Source:** Makreski et al. (2014).

**Comments:** The sample was characterized by energy-dispersive X-ray scan data.

### Farringtonite $\text{Mg}_3(\text{PO}_4)_2$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1151, 1112, 1093w, 1074, 1027s, 981s, 654, 638, 621, 576, 502, 475, 422, 355, 320, 271, 245w, 225w, 189, 177.

**Source:** O'Neill et al. (2006).

**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

**Fassinaite**  $\text{Pb}_2(\text{CO}_3)(\text{S}_2\text{O}_3)$ 

**Origin:** Trentini mine, Mt. Naro, Vicenza province, Veneto, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 0.8 mW.

**Raman shifts (cm<sup>-1</sup>):** 1690w, 1444w, 1322w, 1137w, 1082w, 1061s, 983, 845w, 722w, 661, 637s, 629sh, 602, 549, 520s, 438s, 358, 342, 250w, 203w, 180, 75s.

**Source:** Bindi et al. (2011b).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data, electron microprobe data, and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $\text{Pb}_{2.01}(\text{CO}_3)(\text{S}_{1.82}\text{O}_3)$ .

**Faujasite-Na**  $(\text{Na},\text{Ca},\text{Mg})_2(\text{Si},\text{Al})_{12}\text{O}_{24} \cdot 15\text{H}_2\text{O}$ 

**Origin:** Sasbach, Keiserstuhl, Germany (type locality).

**Experimental details:** Kind of sample preparation is not indicated. Raman scattering measurements have been performed using 1064 nm Nd-YAG laser radiation. The laser radiation power at the sample was 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 1096, 477s, 308, 177.

**Source:** Mozgawa (2001).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Favreauite**  $\text{PbBiCu}_6\text{O}_4(\text{SeO}_3)_4(\text{OH}) \cdot \text{H}_2\text{O}$ 

**Origin:** El Dragón mine, Bolivia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 2.3 mW.

**Raman shifts (cm<sup>-1</sup>):** 3525, 1341w, 1240w, 1065w, 989w, 847s, 795sh, 764w, 542, 493, 392, 320w, 261w, 182.

**Source:** Mills et al. (2014c).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $\text{Pb}_{0.95}\text{Ca}_{0.17}\text{Bi}_{0.90}\text{Cu}_{5.81}\text{Se}_{4.10}\text{O}_{15.96}(\text{OH})_{1.04} \cdot \text{H}_2\text{O}$ .

**Fayalite**  $\text{Fe}^{2+}_2(\text{SiO}_4)$ 

**Origin:** Synthetic.

**Experimental details:** Kind of sample preparation is not indicated. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 940, 838sh, 817s, 724, 643, 588, 508, 384, 315, 293, 197, 173w, 157s, 122.

**Source:** Mouri and Enami (2008).

**Comments:** The Raman shifts were determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of fayalite see also Andò and Garzanti (2014).

**Feitknechtite** Mn<sup>3+</sup>O(OH)**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed in the spectral region from 100 to 1200 cm<sup>-1</sup>, on an arbitrarily oriented sample on the surface of catalyst, using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 0.235 mW.**Raman shifts (cm<sup>-1</sup>):** 635–633, 554–553, 495–492.**Source:** Wang et al. (2014).**Comments:** The sample was characterized by X-ray diffraction and X-ray photoelectron spectroscopy.**Felsőbányaite** Al<sub>4</sub>(SO<sub>4</sub>)(OH)<sub>10</sub>·4H<sub>2</sub>O**Origin:** Recoaro Terme, Vicenza, Italy.**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 532 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3590, 3560w, 1024w, 979s, 883w, 690w, 604, 510w, 451, 388w, 371w, 340w, 313w, 288w, 266w, 254w.**Source:** Boscardin et al. (2009).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.**Ferberite** Fe<sup>2+</sup>(WO<sub>4</sub>)**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm Nd-YAG laser radiation. The laser radiation power at the sample was 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 933, 868, 811, 702, 615, 379, 281, 215.**Source:** Frost et al. (2004d).**Comments:** No independent analytical data are provided for the sample used.**Fergusonite-(Ce)-β** CeNbO<sub>4</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 6 mW. A 180°-scattering geometry was employed. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 801s, 687w, 677w, (654w), 455sh, 397, 390, 347sh, 328sh, 311s, 269, 207, (200), 168, (157), 120sh, 103sh, 96s.**Source:** Siqueira et al. (2010).**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts of 103 and 96 cm<sup>-1</sup> were determined by us based on spectral curve analysis of the published spectrum.

**Fergusonite-(La)- $\beta$**  LaNbO<sub>4</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 6 mW. A 180°-scattering geometry was employed. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 807s, 667, (658), 628, 427, 400, (393), 347sh, 332sh, 327s, 287, 224, 201, 179, 170sh, (137), 126, 115, 110s, 89.**Source:** Siqueira et al. (2010).**Comments:** The sample was characterized by X-ray diffraction data. The Raman shifts of 110 and 89 cm<sup>-1</sup> were determined by us based on spectral curve analysis of the published spectrum.**Fergusonite-(Nd)- $\beta$**  NdNbO<sub>4</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 6 mW. A 180°-scattering geometry was employed. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 808s, 673, 657, 633, 445, 419, 409, 359sh, 335sh, 331s, 303, 230, 212w, 186sh, 182, 130, 123sh, 120.**Source:** Siqueira et al. (2010).**Comments:** The sample was characterized by powder X-ray diffraction data.**Fergusonite-(Y)- $\beta$**  YNbO<sub>4</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented polycrystalline sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 200 mW.**Raman shifts (cm<sup>-1</sup>):** 810s, 677, 660, 627sh, 556, 464, 440w, 420w, 400sh, 344, 330s, 288sh, 237, 200sh, 182sh, 168, 130sh, 117sh, 136, 76, 70w, 55w.**Source:** Pradhan and Choudhary (1987).**Comments:** The sample was characterized by powder X-ray diffraction data.**Fergusonite-(Y)** YNbO<sub>4</sub>**Origin:** No data.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 779, 685w, 401w, 310, 208.**Source:** Tomašić et al. (2008).**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of fergusonite-(Y) see also Gieré et al. (2009).

### Fergusonite-(Y) $\text{YNbO}_4$

**Origin:** A granitic pegmatite situated in the Adamello massif, Italy.

**Experimental details:** Kind of sample preparation is not indicated. Raman scattering measurements have been performed using 488 nm  $\text{Ar}^+$  laser radiation. The laser radiation power behind the objective was 8 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 817s, 698, 665, 444, 423, 379sh, 329s, 289, 230sh, 205sh, 143s.

**Source:** Gieré et al. (2009).

**Comments:** The sample was characterized by electron microprobe analyses. According to powder X-ray diffraction data, the mineral is metamict. It was identified as fergusonite-(Y) on the basis of its Raman spectrum. For the Raman spectrum of fergusonite-(Y) see also Tomašić et al. (2008).

### Fermiïte $\text{Na}_4(\text{UO}_2)(\text{SO}_4)_3 \cdot 3\text{H}_2\text{O}$

**Origin:** Blue Lizard mine, San Juan Co., Utah, USA (type locality).

**Experimental details:** Kind of sample preparation is not indicated. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3540, 3465, 3285, 1606, 1228, 1180, 1120, 1104, 1080, 1013s, 996sh, 992w, 860sh, 830s, 816sh, 638w, 616w, 583w, 506, 443, 384, 188, 163, 153, 132, 110, 55.

**Source:** Kampf et al. (2015c).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $\text{Na}_{3.88}(\text{U}_{1.05}\text{O}_2)(\text{S}_{0.99}\text{O}_4)_3 \cdot 3\text{H}_2\text{O}$ .

### Feroxyhyte $\text{Fe}^{3+}\text{O(OH)}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 0.04 mW. A 180°-scattering geometry was employed. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts ( $\text{cm}^{-1}$ ):** 1442sh, 1330, 713sh, 663, 485sh, 401s, 292s, 222s.

**Source:** Müller et al. (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of feroxyhyte see also Nieuwoudt et al. (2011) and Chen et al. (2014c).

### Ferriallanite-(Ce) $\text{CaCe}(\text{Fe}^{3+}\text{AlFe}^{2+})[\text{Si}_2\text{O}_7][\text{SiO}_4]\text{O(OH)}$ .

**Origin:** Paleokerasia ophiolitic mélange formation, South Othris, Greece.

**Experimental details:** No data.

**Raman shifts ( $\text{cm}^{-1}$ ):** 952w, 887w, 654s, 508s, 478s, 417w, ~377s, 212w, ~188w.

**Source:** Koutsovitis et al. (2013).

**Comments:** No independent analytical data are provided for the sample used.

**Ferricopiaite**  $\text{Fe}^{3+}_{0.67}\text{Fe}^{3+}_4(\text{SO}_4)_6(\text{OH})_2 \cdot 20\text{H}_2\text{O}$ **Origin:** Baia Sprie mining area, Romania.**Experimental details:** Kind of sample preparation is not indicated. Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.**Raman shifts (cm<sup>-1</sup>):** 3135w, 1643, 1226, 1108, 1021s, 992s, 762w, 611, 480, 454sh, 304, 270s.**Source:** Buzatu et al. (2016).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of ferricopiaite see also Ling and Wang (2010), Frost (2011c), Kong et al. (2011b), Apopei et al. (2012, 2014a), Sobron and Alpers (2013), Rull et al. (2014), and Wang and Zhou (2014).**Ferri-eckermannite**  $\text{NaNa}_2\text{Mg}_4\text{Fe}^{3+}\text{Si}_8\text{O}_{22}(\text{OH})_2$ **Experimental details:** Raman scattering measurements have been performed in the spectral region 2600–3800 cm<sup>-1</sup> on an oriented crystal with the polarization of incident light  $E_i$  parallel to the polarization of scattered light  $E_s$  and with the direction of crystal elongation perpendicular to  $E_i$  and parallel to  $E_s$ . 514.5 nm Ar<sup>+</sup> laser radiation was used. The laser radiation power is not indicated. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 3722sh, 3698.**Source:** Leissner et al. (2015).**Comments:** The sample was characterized by electron microprobe analysis and laser ablation inductively coupled-plasma mass spectrometry. The empirical formula of the sample used is  $\text{Na}_{0.51}\text{K}_{0.49}\text{Na}_{2.00}(\text{Mg}_{0.45}\text{Fe}^{3+}_{0.20}\text{Fe}^{2+}_{0.14}\text{Mn}_{0.10}\text{Li}_{0.07}\text{Al}_{0.02}\text{Ti}_{0.02})_5\text{Si}_{8.00}(\text{OH}_{0.58}\text{F}_{0.34}\text{O}_{0.08})_2$ . The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.**Ferrierite-K**  $(\text{K},\text{Na})_5(\text{Si}_{31}\text{Al}_5)\text{O}_{72} \cdot 18\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Kind of sample preparation is not indicated. Raman scattering measurements have been performed in the spectral region from 200 to 1400 cm<sup>-1</sup> using 532 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1163w, 1056, 1029, 833, 797, 576sh, 566, 455s, 432s, 389sh, 370w, 360w, 340, 319, 291sh, 228.**Source:** Suzuki et al. (2009).**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.**Ferrierite-Na**  $(\text{Na},\text{K})_5(\text{Si}_{31}\text{Al}_5)\text{O}_{72} \cdot 18\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Kind of sample preparation is not indicated. Raman scattering measurements have been performed in the spectral region from 200 to 1400 cm<sup>-1</sup> using 532 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1157, 1058, 823, 801, 572, 552, 494sh, 452s, 432s, 342, 316, 220.**Source:** Suzuki et al. (2009).

**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

**Ferrihydrite**  $\text{Fe}^{3+}\text{O}_{10}(\text{OH})_2$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power was 0.04 mW.

**Raman shifts (cm<sup>-1</sup>):** 1377w, 722, 676sh, 513, 358s.

**Source:** Müller et al. (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of ferrihydrite see also Mazzetti and Thistlethwaite (2002) and Das and Hendry (2011).

**Ferrihydrite**  $\text{Fe}^{3+}\text{O}_{10}(\text{OH})_2$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm diode laser radiation. The laser radiation power at the sample was 0.3 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1045s, 707, 508w, 361w.

**Source:** Das and Hendry (2011).

**Comments:** The sample was characterized by X-ray diffraction data. For the Raman spectra of ferrihydrite see also Mazzetti and Thistlethwaite (2002) and Müller et al. (2010).

**Ferri-kaersutite**  $\text{NaCa}_2(\text{Mg}_3\text{Fe}^{3+}\text{Ti})(\text{Si}_6\text{Al}_2)\text{O}_{22}\text{O}_2$

**Experimental details:** Raman scattering measurements have been performed on an oriented crystal with the polarization of incident light  $E_i$  parallel to the polarization of scattered light  $E_s$  and with the direction of crystal elongation perpendicular to  $E_i$  and parallel to  $E_s$ . 514.5 nm Ar<sup>+</sup> laser radiation was used. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3699, 3670sh, 1072sh, 1013, 895, 780sh, 755s, 666, 527, 422, 378, 350sh, 294, 238, 184, 166, 134sh.

**Source:** Leissner et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe data. The empirical formula of the sample used is  $\text{Na}_{0.51}\text{K}_{0.36}\square_{0.13}(\text{Ca}_{0.89}\text{Na}_{0.07}\text{Mg}_{0.04})_2(\text{Mg}_{0.60}\text{Fe}^{3+}_{0.21}\text{Ti}_{0.13}\text{Al}_{0.06})_5(\text{Al}_{0.27}\text{Si}_{0.73})_8(\text{O}_{0.65}\text{OH}_{0.32}\text{F}_{0.03})_2$ . The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

**Ferrilotharmeyerite**  $\text{CaZnFe}^{3+}(\text{AsO}_4)_2(\text{OH})\cdot\text{H}_2\text{O}$

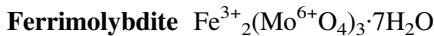
**Origin:** Tsumeb mine, Tsumeb, Namibia (type locality).

**Experimental details:** No data in the cited paper.

**Raman shifts (cm<sup>-1</sup>):** 3440w, 2973sh, 2636sh, 919, 880s, 830s, 814s, 765s, 730, 510, 487sh, 421, 370, 325sh, 230.

**Source:** Frost and Weier (2004e).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.



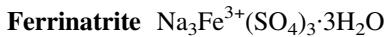
**Origin:** Vrchoslav, Krušné Hory (Ore Mts.), northern Bohemia, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample, using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1882w, 1611w, 991, 968s, 951sh, 935, 836sh, 822, 804sh, 784s, 771sh, 357s, 347, 327sh, 299, 258, 232, 206, 180, 156, 139sh, 115.

**Source:** Sejkora et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The empirical formula of the sample used is  $\text{Fe}_{1.98}[(\text{MoO}_4)_{2.91}(\text{SO}_4)_{0.08}(\text{PO}_4)_{0.03}] \cdot 8\text{H}_2\text{O}$ .



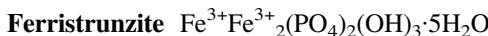
**Origin:** Lignitized wood from La Plaine-Chevrière, Oise, France.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was 2.5 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1614, 1250, 1235, 1220sh, 1202, 1123, 1011, 1002sh, 995s, 965s, 613, 603sh, 533sh, 502sh, 492, 460w, 438w, 267, 247s, 217, 197, 161, 138.

**Source:** Rouchon et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.



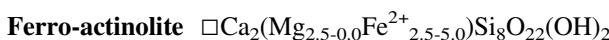
**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample, using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3465, 3367s, 3226, 3042, 1105sh, 1078s, 1022s, 1008sh, 985s, 634sh, 576, 533sh, 503, 454, 394, 354, 321, 302sh, 283s, 259s, 235, 203s, 184, 167s, 147sh.

**Source:** Frost et al. (2002c).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of ferristrunzite see also Frost et al. (2004m).



**Origin:** No data.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** ~1065w, ~740w, ~670s, ~560, ~530, ~380, ~365, ~295w, ~215, ~175.

**Source:** Bersani et al. (2014).

**Comments:** The sample was characterized by electron microprobe analysis. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

**Ferro-glaucophane** Na<sub>2</sub>(Fe<sup>2+</sup>)<sub>3</sub>Al<sub>2</sub>)Si<sub>8</sub>O<sub>22</sub>(OH)<sub>2</sub>

**Origin:** Vernè, Val Varaita, Sampeyre, Cuneo, Piemonte, Italy.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm solid-state laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1101, 1043, 984, 892, 831w, 909, 773, 733w, 667s, 606, 551, 537sh, 486, 765, 444w, 400sh, 385s, 334, 302w, 290w, 253, 207s, 175s, 157, 137w, 118s.

**Source:** Andò and Garzanti (2014).

**Comments:** In the cited paper the mineral is named Fe-glaucophane. No independent analytical data are provided for the sample used. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Ferro-hornblende** (Na,K)<sub>0.1</sub>Ca<sub>2</sub>(Mg,Fe<sup>2+</sup>,Fe<sup>3+</sup>,Al)<sub>5</sub>(Si,Al)<sub>8</sub>O<sub>22</sub>(OH)<sub>2</sub>

**Origin:** Pelagon, Macedonia.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1054w, 1018, 914, 863, 788w, 767w, 665s, 611s, 547, 517sh, 466, 426, 386sh, 330, 319sh, 251s, 226s, 177sh, 159, 115.

**Source:** Makreski et al. (2006a) and Jovanovski et al. (2009).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectrum of hornblende see also Andò and Garzanti (2014).

**Ferrocapholite** Fe<sup>2+</sup>Al<sub>2</sub>Si<sub>2</sub>O<sub>6</sub>(OH)<sub>4</sub>

**Origin:** Cole d'Esischie, Cuneo, Piemonte, Italy.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm solid-state laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1096, 1037, 1017w, 995w, 961, 928, 880, 866, 742s, 711, 664, 610s, 580sh, 562s, 530w, 517w, 498w, 488w, 475, 444, 406s, 350, 310, 282, 261, 238, 211s, 168.

**Source:** Andò and Garzanti (2014).

**Comments:** In the cited paper the mineral is named Fe-capholite. No independent analytical data are provided for the sample used. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Ferroceladonite** KFe<sup>2+</sup>Fe<sup>3+</sup>Si<sub>4</sub>O<sub>10</sub>(OH)<sub>2</sub>

**Origin:** Mont Saint-Hilaire, Rouville RCM (Rouville Co.), Montérégie, Québec, Canada.

**Experimental details:** Kind of sample preparation is not indicated. 514.5 nm Ar<sup>+</sup> laser radiation was used. The laser radiation power was below 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 958, 696, 535, 453, 440, 395, 281, 234sh, 199s, 169sh.

**Source:** Ospitali et al. (2008).

**Comments:** The sample was characterized by electron microprobe analyses.

**Ferrohögbonite** (Fe,Mg,Zn,Al)<sub>3</sub>(Al,Ti,Fe)<sub>8</sub>O<sub>15</sub>(OH) (for the 2N2S polysome)

**Origin:** Aktyuz area, Northern Tien Shan, Kyrgyzstan.

**Experimental details:** Kind of sample preparation is not indicated. 514.5 nm Ar<sup>+</sup> laser radiation was used. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 830, 776, 711, 525, 412, 257.

**Source:** Orozbaev et al. (2011).

**Comments:** Intensities of the Raman bands are not indicated. The sample was characterized by electron microprobe analysis. The empirical formula of the sample used is Mg<sub>1.47</sub>Fe<sup>2+</sup><sub>3.02</sub>Zn<sub>0.04</sub>Fe<sup>3+</sup><sub>1.76</sub>Al<sub>15.13</sub>Ti<sub>0.56</sub>O<sub>30</sub>(OH)<sub>2</sub>. For the Raman spectrum of ferrohögbonite see also Tsunogae and Santosh (2005).

**Ferrokästerite** Cu<sub>2</sub>(Fe,Zn)SnS<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline thin film using 532 nm laser radiation. The laser radiation power was less than 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 378sh, 319s, 284, 256w.

**Source:** Khadka and Kim (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The empirical formula of the sample used is Cu<sub>2</sub>(Fe<sub>77</sub>Zn<sub>23</sub>)SnS<sub>4</sub>. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

**Ferroselite** FeSe<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. Polarized spectra were collected in different scattering geometries.

**Raman shifts (cm<sup>-1</sup>):** 221, 183s.

**Source:** Lutz and Müller (1991).

**Comments** The Raman shifts are given for the scattering geometry *x*(yy)-*x*, in which the Raman intensities are most strong. No independent analytical data are provided for the sample used. For the Raman spectrum of ferroselite see also Wei et al. (2016).

**Ferrosilite** Fe<sup>2+</sup><sub>2</sub>Si<sub>2</sub>O<sub>6</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. Spectra were recorded with the polarization of the laser radiation parallel to the (100) and (001) directions.

**Raman shifts (cm<sup>-1</sup>):** 994s, 951, 888, 660s, 634, 532, 525s, 503, 396s, 349s, 319s, 301s, 247, 168s, 152, 129s.

**Source:** Stalder et al. (2009).

**Comments:** The sample was characterized by electron microprobe analysis. The average Raman shifts are given because the peak positions do not exhibit a significant dependence on orientation.

**Ferrostrunzite**  $\text{Fe}^{2+}\text{Fe}^{3+}_2(\text{PO}_4)_2(\text{OH})_2 \cdot 6\text{H}_2\text{O}$

**Origin:** Arnsberg, Sauerland, Germany.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3492sh, 3405s, 3134, 2943, 1113, 1058s, 1038sh, 1010s, 987sh, 967sh, 634, 568, 531sh, 509sh, 471, 434sh, 408, 396, 328, 297, 249s, 226, 202, 184s, 163s.

**Source:** Frost et al. (2002c).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectrum of ferrostrunzite see also Frost et al. (2004m).

**Ferruccite**  $\text{NaBF}_4$

**Origin:** Synthetic.

**Experimental details:** Raman spectrum was obtained in the spectral region from 150 to 3000 cm<sup>-1</sup> for a sample closed in quartz cell. 514 nm laser radiation was used. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1279w, 1122w, 1060, 1040sh, 784s, 554, 532, 369w, 344.

**Source:** Zavorotynska et al. (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectra of ferruccite see also Bonadeo and Silberman (1970) and Bates et al. (1971).

**Fersmite**  $(\text{Ca,Ce,Na})(\text{Nb,Ta,Ti})_2(\text{O,OH,F})_6$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an oriented single-crystal fiber using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 8 mW. A 180°-scattering geometry was employed. Polarized spectra were collected in the (xx), (xy), (zx), and (zy) scattering geometries.

**Source:** Moreira et al. (2010b).

**Raman shifts (cm<sup>-1</sup>):** (xx): 906, 664, 540, 486, 379, 294s, 289, 242s, 227, 197, 140s, 64; (xy): 850s, 708, 598, 498, 431, 379s, 346, 293s, 262s, 208, 189, 164; (zx): 852, 637, 498s, 457, 380, 315, 2167, 249, 227, 198s, 130s, 111; (zy): 857, 736, 629, 462, 433, 365, 340, 270, 215s, 167, 139s, 65.

**Comments:** The sample was characterized by X-ray diffraction data.

**Feruvite**  $\text{CaFe}^{2+}_3(\text{Al}_5\text{Mg})(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3(\text{OH})$

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample in the spectral regions from 150 to 1600 cm<sup>-1</sup> and from 3000 to 4000 cm<sup>-1</sup> using 457 nm solid-state laser radiation. The laser radiation power at the sample was about 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 3624w, 3550, ~3500sh, 1324, 1095sh, 1054, 1003sh, 808sh, 768, 675sh, 573, 495, 420, 380, 356.

**Source:** Hoang et al. (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

### Fichtelite C<sub>19</sub>H<sub>34</sub>

**Origin:** Třeboň basin, Southern Bohemia, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 1064 nm Nd-YAG and 514.5 nm Ar<sup>+</sup> laser radiations. The nominal laser radiation power was 350 and 10 mW, respectively.

**Raman shifts (cm<sup>-1</sup>):** 2997w, 2987, 2972, 2962w, 2947sh, 2937, 2923s, 2910, 2888, 2864s, 2846sh, 2842sh, 2834sh, 2757w, 2662sh, 1470sh, 1457sh, 1442s, 1381, 1361s, 1335, 1321, 1302, 1293w, 1275, 1264w, 1247s, 1227w, 1213, 1200, 1175, 1155, 1143, 1119w, 1104, 1091w, 1073, 1061sh, 1025, 997, 977, 950sh, 936, 913, 886w, 870, 852, 836, 815, 796, 770, 717s, 579w, 553, 490, 479, 450w, 438w, 399w, 380, 344.

**Source:** Jehlička and Edwards (2008).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of fichtelite see also Jehlička et al. (2005, 2009a).

### Fiedlerite Pb<sub>3</sub>Cl<sub>4</sub>F(OH)·H<sub>2</sub>O

**Origin:** No data.

**Experimental details:** Kind of sample preparation is not indicated. Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 and 514.5 nm laser radiations. The laser radiation power at the source was 30 mW and less than 30 mW, respectively.

**Raman shifts (cm<sup>-1</sup>):** ~737, 600, 331s, 272s, 133s.

**Source:** Bouchard and Smith (2003).

**Comments:** No independent analytical data are provided for the sample used.

### Finnemanite Pb<sub>5</sub>(As<sup>3+</sup>O<sub>3</sub>)<sub>3</sub>Cl

**Origin:** Långban deposit, Filipstad district, Värmland province, Sweden (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 808w, 733s, 726sh, 640, 575, 450w, 372, 354sh, 244, 196sh, 174s, 128s, 113s.

**Source:** Bahfenne et al. (2011c).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of finnemanite see also Bahfenne (2011).

### Flamite Ca<sub>8-x</sub>(Na,K)<sub>x</sub>(SiO<sub>4</sub>)<sub>4-x</sub>(PO<sub>4</sub>)<sub>x</sub>

**Origin:** Hatrurim Basin, Negev Desert, Israel (type locality).

**Experimental details:** Raman scattering measurements have been performed in backscattered geometry, on an arbitrarily oriented sample, using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was up to 17 mW.

**Raman shifts (cm<sup>-1</sup>):** 1003w, 952s, (885sh), 863s, 850s, 714w, 666w, 589sh, 575w, 558sh, 538, 520, 500sh, 439sh, 430w, 396, 294sh, 260, 199sh, 188, 170, 125w, 106w.

**Source:** Sokol et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectrum of flamite see also Gfeller et al. (2015).

### Fliniteite K<sub>2</sub>ZnCl<sub>4</sub>

**Origin:** Tolbachik volcano, Kamchatka, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample in the spectral region from 50 to 4000 cm<sup>-1</sup> using 532 nm diode laser radiation. The laser radiation power at the sample was 13 mW.

**Raman shifts (cm<sup>-1</sup>):** 294s, 192w, 140s, 113sh.

**Source:** Pekov et al. (2015e).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is (K<sub>1.91</sub>Tl<sub>0.09</sub>)<sub>Σ2.00</sub>Zn<sub>1.04</sub>Cl<sub>3.96</sub>.

### Florencite-(La) LaAl<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>(OH)<sub>6</sub>

**Origin:** Igarapé Bahia mine, Serra dos Carajás, Pará, Brazil.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3649, 3440sh, 3158s, 2988sh, 2906sh, 1914s, 1713sh, 1655s, 1479s, 1221w, 1112s, 1064sh, 1021s, 987s, 846w, 783, 766w, 716, 699, 647sh, 614, 680sh, 536s, 524sh, 464, 404, 310, 270s, 255, 202, 194sh, 158w, 130w.

**Source:** Frost et al. (2013an).

**Comments:** The sample was characterized qualitative electron microprobe analysis.

### Fluellite Al<sub>2</sub>(PO<sub>4</sub>)F<sub>2</sub>(OH)·7H<sub>2</sub>O

**Origin:** Krásno, near Horní Slavkov, western Bohemia, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal, using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. Raman spectrum was obtained in the spectral region from 200 to 4000 cm<sup>-1</sup>. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3667, 3396s, 3314, 3124s, 1670w, 1583w, 1122, 1096sh, 1036s, 897w, 835sh, 646, 588, 557, 525s, 513, 459, 410, 342, 311, 295, 279, 251, 220, 208, 199, 191, 173, 151, 139, 123, 116, 108.

**Source:** Čejka et al. (2014a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe data. The empirical formula of the sample used is Al<sub>1.98</sub>(PO<sub>4</sub>)<sub>1.07</sub>F<sub>1.99</sub>(OH)<sub>0.75</sub>·7H<sub>2</sub>O.

**Fluocerite-(Ce)  $\text{CeF}_3$** **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an oriented sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power is not indicated. Polarized spectra were collected in  $x(zx)y$  and  $x(yz)y$  scattering geometries.**Raman shifts ( $\text{cm}^{-1}$ ):** 293s, 290sh, 204, 141.**Source:** Gerlinger and Schaack (1986).**Comments:** The Raman shifts are given for the scattering geometry  $x(zx)y$ , in which the Raman intensities are most strong. The  $z$  axis is taken as the symmetry axis of the crystal and the  $x$  and  $y$  axes are equivalent. No independent analytical data are provided for the sample used. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of fluocerite-(Ce) see also Bauman and Porto (1967).**Fluocerite-(La)  $\text{LaF}_3$** **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented 1% praseodymium-doped  $\text{LaF}_3$  rod using 435.8 nm Hg line as excitation.**Raman shifts ( $\text{cm}^{-1}$ ):** 392, 365, 310, 292, 75.**Source:** Caspers et al. (1964).**Comments:** No independent analytical data are provided. For the Raman spectrum of fluocerite-(La) see also Bauman and Porto (1967).**Fluorapatite  $\text{Ca}_5(\text{PO}_4)_3\text{F}$** **Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on a microcrystalline sample in the spectral region from 140 to 1200  $\text{cm}^{-1}$  using He-Ne laser radiation. The laser radiation power is not indicated.**Raman shifts ( $\text{cm}^{-1}$ ):** 1084w, 1053w, 1041w, 966s, 609, 598, 595, 451w, 434, 268w, 184.**Source:** Griffith (1970).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of fluorapatite see also Adams and Gardner (1974), Harlov et al. (2003), and Frezzotti et al. (2012).**Fluorapatite As-rich  $\text{Ca}_5(\text{PO}_4,\text{AsO}_4)_3\text{F}$** **Origin:** Calvario Mt., Etna, Italy.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 633 and 532 nm laser radiations. The nominal laser radiation power was 20 and 10 mW, respectively.**Raman shifts ( $\text{cm}^{-1}$ ):** 1062sh, 1057sh, 1046, 1034sh, 964s, 877sh, 857s, 827w, 590, 580, 477sh, 430, 392, 372.**Source:** Gianfagna et al. (2014).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The Raman shifts are indicated for the maxima of individual peaks obtained as a result of the spectral curve analysis.

### Fluorapophyllite-(K) $\text{KCa}_4\text{Si}_8\text{O}_{20}\text{F} \cdot 8\text{H}_2\text{O}$

**Origin:** Międzyrzecze Górne, near Bielsko-Biała, Poland.

**Experimental details:** Raman scattering measurements have been performed on an oriented crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was less than 30 mW. Raman measurements were performed in different scattering geometries.

**Raman shifts (cm<sup>-1</sup>):** -z(y'y')z: 3627w, 3559, 3357sh, 3104sh, 3010, 1117w, 1062, 856w, 794w, 665, 584, 542w, 522w, 486w, 433, 401w, 374w, 337w, 298, 231, 209, 166, 133, 123w; -z(x'y')z— 3559w, 3357sh, 3104sh, 3010, 1117w, 1010w, 973w, 840w, 768w, 630w, 463w, 371w, 267w, 226w, 217w, 185, 161, 131; -y'(zz)y': 1063s, 794w, 584, 542, 486, 433, 401, 231, 195, 166; -y'(x'z) y': 1091w, 1011w, 601w, 503w, 487w, 460w, 431w, 342w, 320w, 270w, 216w, 202w, 174w, 139w, 127w.

**Source:** Włodyka and Wrzalik (2004).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is  $(\text{K}_{0.96}\text{Na}_{0.03})\text{Ca}_3.96(\text{Si}_{7.95}\text{Al}_{0.04}\text{P}_{0.03})\text{O}_{19.98}(\text{F}_{0.83}\text{OH}_{0.17}) \cdot 8.02\text{H}_2\text{O}$ . For the Raman spectra of fluorapophyllite-(K) see also Frost and Xi (2012a) and Goryainov et al. (2012).

### Fluor-buergerite $\text{NaFe}^{3+}_3\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3\text{O}_3\text{F}$

**Origin:** Mexiquitic, San Luis Potosí, Mexico.

**Experimental details:** Raman scattering measurements have been performed on an oriented crystal using 514.5 and 457.9 nm Ar<sup>+</sup> laser radiations. The laser radiation power at the sample was about 25 mW. Polarized spectra were collected in (zz) and (xy,z) scattering geometries.

**Raman shifts (cm<sup>-1</sup>):** A<sub>1</sub> (zz): 3530, 1289, 1110w, 1060, 1010, 811w, 753, 706, 638s, 605sh, 541sh, 523, 475w, 406sh, 373s, 300, 260sh, 232s, 154; E (xy,z): 1290, 1260, 1107, 1063, 1012, 982, 957, 757, 733, 707, 656s, 636, 586sh, 550sh, 522w, 475sh, 458, 400s, 375, 328, 300, 275, 265, 233, 212, 154.

**Source:** McKeown (2008).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analysis. The crystal structure is solved. The empirical formula of the sample used is  $\text{NaFe}^{3+}_3\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{O}_{0.92}\text{OH}_{0.08})_{\Sigma 3}\text{F}$ . For the Raman spectra of fluor-buergerite see also Gasharova et al. (1997) and Watenphul et al. (2016a, b).

### Fluorcalciobritholite $(\text{Ca},\text{REE})_5(\text{SiO}_4,\text{PO}_4)_3\text{F}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample. Experimental details are not described.

**Raman shifts (cm<sup>-1</sup>):** 1026sh, 1049w, 958s, 856, 603sh, 580, 557sh, 447sh, 428.

**Source:** Dacheux et al. (2010).

**Comments:** The sample was characterized by X-ray diffraction data and electron microprobe analysis. The empirical formula of the sample used is  $\text{Ca}_9\text{Nd}_{0.5}\text{Th}_{0.5}(\text{PO}_4)_{4.5}(\text{SiO}_4)_{1.5}\text{F}_2$ .

### Fluorcalciomicrolite $(\text{Ca},\text{Na},\square)_2\text{Ta}_2\text{O}_6\text{F}$

**Origin:** Volta Grande pegmatite, Nazareno, Minas Gerais, Brazil (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample 532 nm solid-state laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 891, 792, 664, 530sh, 505s, 417, 331, 292, 239w, 187, 168.

**Source:** Andrade et al. (2013a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Ca}_{1.07}\text{Na}_{0.12}\text{Vac}_{0.12})(\text{Ta}_{1.84}\text{Nb}_{0.14}\text{Sn}_{0.02})[\text{O}_{5.93}(\text{OH})_{0.07}][\text{F}_{0.79}(\text{OH})_{0.21}]$ .

### Fluorcalcioroméite $(\text{Ca},\text{Na})_2\text{Sb}^{5+} \text{O}_6\text{F}$

**Origin:** Starlera mine, Ferrera, Grischun, Switzerland (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm solid-state laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3686, 3630, 827, 790sh, 518s, 468sh, 302w.

**Source:** Atencio et al. (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Ca}_{1.16}\text{Na}_{0.56}\square_{0.22}\text{Fe}^{2+}_{0.03}\text{Mn}^{2+}_{0.03})(\text{Sb}^{5+}_{1.98}\text{Al}_{0.01}\text{W}_{0.01})\text{O}_6[\text{F}_{0.62}(\text{OH})_{0.28}\text{O}_{0.06}\square_{0.04}]$ .

### Fluorcaphite $\text{SrCaCa}_3(\text{PO}_4)_3\text{F}$

**Origin:** Lovozero alkaline complex, Kola Peninsula, Russia.

**Raman shifts (cm<sup>-1</sup>):** See comment below.

**Source:** Chakhmouradian et al. (2005).

**Comments:** Raman microspectroscopy cannot be used to distinguish between fluorcaphite and fluorapatite because their nonpolarized spectra are virtually identical. Polarized spectra in the range 50–350 cm<sup>-1</sup> are sensitive to the local structural environment of A-site cations and can potentially be used for that purpose.

### Fluor-elbaite $\text{Na}(\text{Li}_{1.5}\text{Al}_{1.5})\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3\text{F}$

**Origin:** Paprok mine, Nuristan, Afghanistan.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented cross-section of a single crystal using Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3658, 3594, 3489, 1421, 1064s, 731s, 550, 381, 344, 223.

**Source:** Natkaniec-Nowak et al. (2009).

**Comments:** The sample was characterized by electron microprobe analyses. Raman shifts are given for the central sample zone (zone I) which was identified as fluor-elbaite. The band positions denoted by Natkaniec-Nowak et al. (2009) as 3549 and 224 cm<sup>-1</sup> were determined by us at 3594 and 344 cm<sup>-1</sup>, respectively.

### Fluor-schorl $\text{NaFe}^{2+} \text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3\text{F}$

**Origin:** Steinberg, Zschorlau, Erzgebirge (Saxonian Ore Mountains), Saxony, Germany.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 3563, 1084sh, 1048, 1025sh, 969w, 767s, 694, 665, 632, 537w, 483, 400sh, 364s, 313, 237s, 199.

**Source:** Ertl et al. (2015).

**Comments:** The sample was characterized by X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Na}_{0.82}\text{K}_{0.01}\text{Ca}_{0.01}\square_{0.16})(\text{Fe}^{2+}_{2.30}\text{Al}_{0.38}\text{Mg}_{0.23}\text{Li}_{0.03}\text{Mn}^{2+}_{0.02}\text{Zn}_{0.01})(\text{Al}_{5.80}\text{Fe}^{3+}_{0.10}\text{Ti}_{0.10})(\text{Si}_{5.81}\text{Al}_{0.19}\text{O}_{18})$   $(\text{BO}_3)_3(\text{OH})_3[\text{F}_{0.66}(\text{OH})_{0.34}]$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

### Fluorite $\text{CaF}_2$

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 40 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 322.

**Source:** Gee et al. (1966).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of fluorite see also Tsuda et al. (1993), Dill and Weber (2010), Frezzotti et al. (2012), and Andò and Garzanti (2014).

### Fluorkyuygenite $\text{Ca}_{12}\text{Al}_{14}\text{O}_{32}[(\text{H}_2\text{O})_4\text{F}_2]$

**Origin:** Hatrurim Basin, Negev Desert, Israel (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm solid-state laser radiation. The laser radiation power is not indicated.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3210sh, 3065, 1610w, 940sh, 876sh, 862, 772s, 695, 575, 517s, 392, 344, 320, 234.

**Source:** Galuskin et al. (2015c).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $\text{Ca}_{12.034}(\text{Al}_{13.344}\text{Fe}^{3+}_{0.398}\text{Si}_{0.224})\text{O}_{32}[(\text{H}_2\text{O})_{3.810}\text{F}_{1.894}(\text{OH})_{0.296}]$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

### Fluoramprophyllite $\text{Na}_3(\text{SrNa})\text{Ti}_3(\text{Si}_2\text{O}_7)_2\text{O}_2\text{F}_2$

**Origin:** Poços de Caldas alkaline massif, Morro do Serrote, Minas Gerais, Brazil (type locality)

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm solid-state laser radiation. The laser radiation power is not indicated.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3675w, 1070, 940sh, 893s, 862sh, 825sh, 690, 635w, 590, 462w, 419w, 375w, 346w, 280sh, 230sh, 174w.

**Source:** Andrade et al. (2017).

**Comments:** The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

### Fluormayenite-related garnet

**Origin:** Afrikanda complex, Kola Peninsula, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3630, 1100w, 955w, 863s, 815, 633w, 519, 385sh, 352, 240w.

**Source:** Chakhmouradian et al. (2008).

**Comments:** In the cited paper the mineral is described under the name hibscite. It contains from 4.2 to 6.0 wt% F. The sample was characterized by micro-X-ray diffraction data, electron microprobe analyses, and single-crystal X-ray diffraction. The crystal structure is solved. The compositional range of the sample used may be described as Grs<sub>57–63</sub>Kt<sub>21–27</sub>Fgr<sub>8–11</sub>Adr<sub>0–13</sub>, where Grs, Kt, and Adr are the designations for the grossular, katoite, and andradite, respectively, and Fgr is the hypothetical Ca<sub>3</sub>Al<sub>2</sub>F<sub>12</sub> end-member. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

### Fluormayenite Ca<sub>12</sub>Al<sub>14</sub>O<sub>32</sub>[□<sub>4</sub>F<sub>2</sub>]

**Origin:** Jabel Harmun, Judean Mts., Palestinian Autonomy, Israel (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm solid-state laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3674w, 3572, 918sh, 890, 844, 776s, 709, 619w, 583, 524s, 390, 318s, 276, 250sh, 186.

**Source:** Galuskin et al. (2015c).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is (Ca<sub>11.951</sub>Na<sub>0.037</sub>)<sub>(Al<sub>13.675</sub>Fe<sup>3+</sup><sub>0.270</sub>Mg<sub>0.040</sub>Si<sub>0.009</sub>P<sub>0.005</sub>S<sup>6+</sup><sub>0.013</sub>)O<sub>31.503</sub>(HO)<sub>1.492</sub>[□<sub>4.581</sub>F<sub>1.375</sub>Cl<sub>0.044</sub>]. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.</sub>

### Fluorocronite PbF<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation output power was 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 257.

**Source:** Krishnamurthy and Soots (1970).

**Comments:** No independent analytical data are provided for the sample used.

### Fluoro-edenite NaCa<sub>2</sub>Mg<sub>5</sub>(Si<sub>7</sub>Al)O<sub>22</sub>F<sub>2</sub>

**Origin:** Biancavilla area, Mount Etna, Sicily, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on an oriented sample with the elongation axis at 45° with respect to N-S direction of the cross-hair of the ocular lens using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 20 mW.

**Raman shifts (for the sample no. 3 in Table 1 of the cited paper, cm<sup>-1</sup>):** 1042, 1018, 926, 768, 747, 678s, 586w, 557, 520, 494w, 474w, 436, 408, 381, 365sh, 313, 300sh, 236s, 213w.

**Source:** Fornero et al. (2008).

**Comments:** The sample was characterized by electron microprobe analyses. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Fluorowardite**  $\text{NaAl}_3(\text{PO}_4)_2(\text{OH})_2\text{F}_2 \cdot 2\text{H}_2\text{O}$

**Origin:** Silver Coin mine, Valmy, Nevada, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power at the sample was about 5 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3614w, 3542, 1049s, 1005s, 604s, 489, 431, 384w, 315, 272, 257, 216, 182s, 143.

**Source:** Kampf et al. (2014a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Na}_{0.87}\text{Ca}_{0.13}\text{Mg}_{0.04})(\text{Al}_{2.96}\text{Fe}^{3+}_{0.04})(\text{P}_{1.96}\text{As}_{0.03})\text{O}_{8.12}(\text{OH})_{2.35}\text{F}_{1.53} \cdot 2\text{H}_2\text{O}$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Fluor-uvite**  $\text{CaMg}_3(\text{Al}_5\text{Mg})(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3\text{F}$

**Origin:** No data in the cited paper.

**Experimental details:** Raman scattering measurements have been performed on an oriented crystal in the  $-y(zz)y$  scattering geometry using 514.5 or 488.0 nm  $\text{Ar}^+$  laser radiations. The laser radiation power at the sample was 14 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3770, 3740, 3665, 3642, 3572, 3554sh, 3522sh, 3488sh, 1040, 960w, 798w, 759w, 702, 670, 650, 630, 496, 459, 411, 372s, 316, 243s, 213s, 149w.

**Source:** Watenphul et al. (2016a).

**Comments:** The sample was characterized by electron microprobe analyses and LA-ICP-MS data. The empirical formula of the sample used is  $(\text{Ca}_{0.63}\text{Na}_{0.26}\square_{0.09})(\text{Mg}_{2.92}\text{Ti}_{0.07})(\text{Al}_{5.51}\text{Mg}_{0.49})(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3[\text{F}_{0.55}(\text{OH})_{0.36}\text{O}_{0.09}]$ .

**Fluorwavellite**  $\text{Al}_3(\text{PO}_4)_2(\text{OH})_2\text{F} \cdot 5\text{H}_2\text{O}$

**Origin:** Silver Coin mine, Valmy, Iron Point district, Humboldt Co., Nevada, USA (type locality).

**Experimental details:** Methods of sample preparation are not described. A 785 nm diode laser radiation was used. The laser radiation power is not indicated.

**Raman shifts ( $\text{cm}^{-1}$ ):** 1147w, 1065sh, 1022s, 636, 589sh, 568sh, 550sh, 544s, 410s, 315, 286sh, 277, 224sh, 211.

**Source:** Kampf et al. (2017a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $\text{Al}_{2.96}(\text{PO}_4)_2(\text{OH})_{1.98}\text{F}_{1.02} \cdot 5\text{H}_2\text{O}$  (+0.12H for charge balance). The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Foite**  $\square(\text{Fe}^{2+}_2\text{Al})\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3(\text{OH})$

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an oriented crystal with the crystallographic  $c$  axis parallel to the  $z$  axis using 514.5 and 488.0 nm  $\text{Ar}^+$  laser radiations. The laser radiation power at the sample was 14 mW. Raman spectrum was obtained in the spectral region from 15 to 4000  $\text{cm}^{-1}$ . Polarized spectra were collected in the  $-y(zz)y$ ,  $y(zx)y$ , and  $y(xx)y$  scattering geometries.

**Raman shifts (cm<sup>-1</sup>):** 3726w, 3670w, 3644, 3631, 3570sh, 3551s, 3517, 3484s, 3641, 3630, 3479, 3351, 1054, 1020, 967, 777w, 743w, 696, 677, 630, 493, 459, 401, 367s, 313, 253sh, 236s, 205sh, 192sh, 158w.

**Source:** Watenphul et al. (2016a).

**Comments:** The sample was characterized by electron microprobe and LA-ICP-MS analyses. The Raman shifts are given for the scattering geometry -y(zz)y, in which the Raman intensities are most strong. The empirical formula of the sample used is  $(\square_{0.61}\text{Na}_{0.35}\text{Ca}_{0.03})(\text{Fe}_{1.28}\text{Al}_{1.03}\text{Mn}_{0.41}\text{Li}_{0.18}\text{Mg}_{0.11})\text{Al}_6(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3[(\text{OH})_{0.93}\text{F}_{0.07}]$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

### Foordite $\text{Sn}^{2+}\text{Nb}_2\text{O}_6$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an oriented crystal using 532 nm solid-state laser radiation. The laser radiation power is not indicated. Polarized spectra were collected in the z(xx)-z scattering geometry.

**Raman shifts (cm<sup>-1</sup>):** 794, 665, 575, 432, 372, 348, 303, 257, 249, 224, 201, 185, 161, 135.

**Source:** Noureldine et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of foordite see also Lee et al. (2015).

### Forêtite $\text{Cu}_2\text{Al}_2(\text{AsO}_4)(\text{OH},\text{O},\text{H}_2\text{O})_6$

**Origin:** Cap Garonne mine, France (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample in the spectral region from 50 to 4000 cm<sup>-1</sup> using 532 nm laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3534sh, 3469sh, 3428s, 3343s, 2924, 2889, 2848, 1585, 1458, 848s, 816sh, 495, 446w, 371, 269, 218, 171, 140sh, 114s, 93s.

**Source:** Mills et al. (2012a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is  $\text{Cu}_{1.94}(\text{Al}_{1.96}\text{Fe}_{0.04})(\text{As}_{0.84}\text{S}_{0.09}\text{Si}_{0.04})\text{O}_{10}\text{H}_{5.19}$ .

### Formanite-(Y) $\text{YTaO}_4$

**Origin:** Synthetic.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 825s, 720w, 705, 670, 655w, 480w, 450w, 375w, 345s, 320s, 215s, 120.

**Source:** Blasse (1973).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of formanite-(Y) see also Nazarov (2010).

### Formicaite $\text{Ca}(\text{CHOO})_2$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an oriented crystal using 488.0 nm Ar<sup>+</sup> and 632.8 nm He-Ne laser radiations. The laser radiation power is not indicated.

Polarized spectra were collected in  $x(zz)y$ ,  $x(yx)y$ ,  $x(yx)z$ ,  $x(yz)y$ ,  $x(zy)z$ ,  $x(zx)y$ ,  $x(xz)z$  scattering geometries with 488.8 nm laser excitation, and in  $y(xx)z$ ,  $y(xy)z$ ,  $y(zy)z$ ,  $y(zx)z$  scattering geometries with 632.8 nm laser excitation.

**Raman shifts ( $\text{cm}^{-1}$ ):** 2185w, 2180w, 1406s, 1393s, 801w, 783, 169w, 118, 106, 72s.

**Source:** Krishnan and Ramanujam (1973).

**Comments:** The Raman shifts are given for the scattering geometry  $x(yy)z$  with 488.0 nm  $\text{Ar}^+$  laser radiation, in which the Raman intensities are most strong.

**Fornacite**  $\text{CuPb}_2(\text{CrO}_4)(\text{AsO}_4)(\text{OH})$

**Origin:** Whim Creek Copper mine, Pilbara, Western Australia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm Nd-YAG laser radiation. The laser radiation power at the sample was 1 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 916sh, 890sh, 872sh, 867, 847s, 830s, 790sh, 778sh, 400, 388, 381, 369, 354, 343, 332, 305, 159, 139, 122.

**Source:** Frost (2004c).

**Comments:** No independent analytical data are provided for the sample used.

**Forsterite**  $\text{Mg}_2(\text{SiO}_4)$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample in the spectral region from 100 to 1200  $\text{cm}^{-1}$  using 488 nm  $\text{Ar}^+$  laser radiation. The laser radiation power at the sample was 20 mW. A 135°-scattering geometry was employed.

**Raman shifts ( $\text{cm}^{-1}$ ):** 964, 919, 880sh, 855s, 824s, 608, 589, 544, 434, 374, 337, 329, 314w, 303, 225.

**Source:** Mohanan et al. (1993).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of forsterite see also Piriou and McMillan (1983), Mouri and Enami (2008), Frezzotti et al. (2012), Andò and Garzanti (2014), and Culka et al. (2016a, b).

**Fougèrite**  $\text{Fe}^{2+}{}_4\text{Fe}^{3+}{}_2(\text{OH})_{12}(\text{CO}_3)\cdot 3\text{H}_2\text{O}$

**Origin:** Fougères Forest, Fougères, Ille-et-Vilaine, Brittany, France (type locality).

**Experimental details:** Raman scattering measurements have been performed on a fine-crystalline sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power at the sample was less than 1 mW. A 180°-scattering geometry was employed.

**Raman shifts ( $\text{cm}^{-1}$ ):** 518, 427.

**Source:** Trolard et al. (2007).

**Comments:** The sample was characterized by powder X-ray diffraction data, Mössbauer spectroscopy, and X-ray absorption spectroscopy at the FeK edge. For the Raman spectrum of fougèrite see also Bourrié and Trolard (2010).

**Fraipontite**  $(\text{Zn},\text{Al})_3(\text{Si},\text{Al})_2\text{O}_5(\text{OH})_4$

**Origin:** Blue Bell mine, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts

have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3825w, 3810w, 3781w, 3769w, 3747w, 3737w, 3669w, 3384w, 3367w, (1734), (1408), 1392sh, (1094s), 1089sh, (731), 675, (305), 290sh, (197), 186sh, 157sh, 144s, 115sh, 108.

**Source:** Theiss et al. (2015b).

**Comments:** The sample was characterized by qualitative energy-dispersive X-ray scan data. No independent quantitative analytical data are provided for the sample used. The bands at 1734, 1408, 1094, 731, 305, and 197 cm<sup>-1</sup> correspond to admixed smithsonite.

### Francevillite Ba(UO<sub>2</sub>)<sub>2</sub>(VO<sub>4</sub>)<sub>2</sub>·5H<sub>2</sub>O

**Origin:** Mounana Mine, Haut Ogooué, Gabon (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 977, 965sh, 861, 829, 747s, 609, 526, 485, 470, 405, 370s, 304, 240s, 186, 163sh.

**Source:** Frost et al. (2005c).

**Comments:** No independent analytical data are provided for the sample used.

### Francisite Cu<sub>3</sub>Bi(Se<sup>4+</sup>O<sub>3</sub>)<sub>2</sub>O<sub>2</sub>Cl

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal with laser light polarized in the *xy* plane of the crystal. The laser radiation power and the wavelength of laser radiation are not indicated.

**Raman shifts (cm<sup>-1</sup>):** 583, 538, 484, 324, 173.

**Source:** Miller et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Franckeite Pb<sub>21.7</sub>Sn<sub>9.3</sub>Fe<sub>4.0</sub>Sb<sub>8.1</sub>S<sub>56.9</sub>

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on a pressed powdered sample using 532 nm laser radiation. The nominal laser radiation power was 0.2 mW.

**Raman shifts (cm<sup>-1</sup>):** 650–400sh, 318, 253, 194, 145w, 66s.

**Source:** Molina-Mendoza et al. (2016).

**Comments:** The sample was characterized by selected area electron diffraction data, micro-X-ray photoemission, and scanning tunneling spectroscopy.

### Françoisite-(Nd) Nd(UO<sub>2</sub>)<sub>3</sub>O(OH)(PO<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample in the spectral region from 150 to 2000 cm<sup>-1</sup> using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 998, 934w, 830s, 440–417, 202, 151.

**Source:** Armstrong et al. (2011).

**Comments:** The sample was characterized by elemental and thermal analyses, X-ray diffraction data, and inductively coupled optical emission spectroscopy. The empirical formula of the sample used is Nd<sub>0.92</sub>[ (UO<sub>2</sub>)<sub>3.11</sub>O(OH)(PO<sub>4</sub>)<sub>2.00</sub>] · 5.98H<sub>2</sub>O.

**Franconite** NaNb<sub>2</sub>O<sub>5</sub>(OH) · 3H<sub>2</sub>O

**Origin:** Poudrette (Demix) quarry, Mont Saint-Hilaire, Rouville RCM (Rouville Co.), Montérégie, Québec, Canada (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample in the spectral region from 50 to 4000 cm<sup>-1</sup> using 638 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3416, 924, 879s, 661s, 583, 461, 391, 297, 212.

**Source:** Haring and McDonald (2014b).

**Comments:** It may be that the wavelength of 638 nm is a misprint, and the authors meant 632.8 nm. The sample was characterized by powder X-ray diffraction data, by energy-dispersive X-ray scan data, and by single crystal X-ray diffraction data. The crystal structure is solved. The empirical formula of the sample used is (Na<sub>0.73</sub>Ca<sub>0.13</sub>□<sub>0.14</sub>)<sub>Σ1.00</sub>(Nb<sub>1.96</sub>Ti<sub>0.02</sub>Si<sub>0.02</sub>Al<sub>0.01</sub>)O<sub>5</sub>(OH) · 3H<sub>2</sub>O.

**Frankdicksonite** BaF<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** The Raman spectrum was obtained at 15 K. Other experimental details are not indicated.

**Raman shifts (cm<sup>-1</sup>):** 259sh, 244.

**Source:** Harrington et al. (1971).

**Comments:** No independent analytical data are provided for the sample used. The Raman shift of 259 cm<sup>-1</sup> was determined by us based on spectral curve analysis of the published spectrum.

**Franklinite** ZnFe<sup>3+</sup><sub>2</sub>O<sub>4</sub>

**Origin:** Franklin or Sterling Hill mine, New Jersey, USA.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 1206, 661sh, 597s, 493w, 347.

**Source:** Welsh (2008).

**Comments:** No independent analytical data are provided for the sample used.

**Freboldite** CoSe

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample nucleated after about 50 h milling time using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was less than 5 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 174.

**Source:** Campos et al. (2004a).

**Comments:** The sample was characterized by X-ray diffraction data and electron microprobe analysis.

**Fredrikssonite**  $Mg_2Mn^{3+}O_2(BO_3)$ 

**Origin:** Långban deposit, Bergslagen ore region, Filipstad district, Värmland, Sweden (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** See comment below.

**Source:** Frost (2011b).

**Comments:** All Raman shifts (1750, 1530, 1435, 1086, 712, 282, and 155 cm<sup>-1</sup>) ascribed by Frost (2011b) to fredrikssonite correspond to calcite. The correct Raman shifts of fredrikssonite are (RRUFF ID: R130112; cm<sup>-1</sup>): 933w, 752, 701w, 666, 591s, 520w, 341sh, 317s.

**Fresnoite**  $Ba_2TiO(Si_2O_7)$ 

**Origin:** No data.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 994w, 960w, 928w, 904, 876, 860s, 666, 600, 542w, 477w, 377, 343, 318w, 272, 226, 207w.

**Source:** Gabelica-Robert and Tarte (1981).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of fresnoite see also Mayerhöfer and Dunken (2001) and Ma and Rossman (2008).

**Friedrichbeckite**  $K(\square Na)Mg_2(Be_2Mg)Si_{12}O_{30}$ 

**Origin:** Bellerberg volcano, Eifel paleovolcanic area, Rhineland-Palatinate (Rheinland-Pfalz), Germany (type locality).

**Experimental details:** Raman scattering measurements have been performed on an oriented crystal with direction of the laser beam along [0001] using 633 nm He-Ne laser radiation. The nominal laser radiation power was 17 mW.

**Raman shifts (cm<sup>-1</sup>):** 1132s, 947, 837, ~770, 650, 577, 544, 488s, 461sh, 385, 292s, 162, 128, 69.

**Source:** Lengauer et al. (2009).

**Comments:** The sample was characterized by powder X-ray diffraction data, electron microprobe analyses, and laser-ablation inductively coupled plasma mass spectroscopy data. The crystal structure is solved. The empirical formula of the sample used is  $K_{0.87}Na_{0.86}(Mg_{1.57}Mn_{0.28}Fe_{0.24})(Be_{1.83}Mg_{1.17})[Si_{12}O_{30}]$ . The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

**Frohbergite**  $FeTe_2$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed at 90 K on an oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed. Polarized spectra were collected in y(xx)-y, y(xz)-y, z(xy)-z, x(zy)-x, and y(x,xz)-y scattering geometries.

**Raman shifts (cm<sup>-1</sup>):** 155, 138s, 125.

**Source:** Lutz and Müller (1991).

**Comments:** The Raman shifts are given in the scattering geometry  $y(x,xz)-y$ . The authors note that the origin of the band at  $138\text{ cm}^{-1}$  is not quite clear. No independent analytical data are provided for the sample used.

### Frolovite $\text{Ca}[\text{B}(\text{OH})_4]_2$

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed in the spectral region from 300 to  $1800\text{ cm}^{-1}$  using  $514.5\text{ nm Ar}^+$  laser radiation. The nominal laser radiation power was 300 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 854w, 758s, 547, 390w.

**Source:** Jun et al. (1995).

**Comments:** No independent analytical data are provided for the sample used.

### Frondelite $\text{Mn}^{2+}\text{Fe}^{3+}_4(\text{PO}_4)_3(\text{OH})_5$

**Origin:** Cigana mine, Conselheiro Pena, Rio Doce valley, Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a  $633\text{ nm He-Ne}$  laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3581, 3315, 3144sh, 3029sh, 2886, 2747sh, 1597, 1532, 1416, 1352, 1164sh, 1112, 1071sh, 1027s, 1000, 966sh, 748, 635sh, 612s, 589sh, 572, 481sh, 455, 436sh, 379sh, 329sh, 291, 226s, 207sh, 189, 172sh, 151s, 137sh, 126sh.

**Source:** Frost et al. (2013y).

**Comments:** The sample was characterized by X-ray diffraction data and electron microprobe analysis. The empirical formula of the sample used is  $(\text{Mn}_{0.68}\text{Fe}_{0.32})\text{Fe}^{3+}_{3.72}(\text{PO}_4)_{3.17}(\text{OH})_{4.99}$ . For the Raman spectrum of frondelite see also Faulstich et al. (2013).

### Fulgorite (a high-silicon glass) $\sim(\text{Si},\text{O},\text{Fe})\text{O}_{2-x}$

**Origin:** Greensboro, North Carolina, USA.

**Experimental details:** Raman scattering measurements have been performed using  $514.5\text{ nm Ar}^+$  laser radiation. The laser radiation power at the sample was 1 to 2 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 1188w, 1057, 930w, 796, 603, 488s, 440s.

**Source:** Carter et al. (2010).

**Comments:** The sample was characterized by inductively coupled plasma optical emission spectrometry data. It contains 81.3 wt%  $\text{SiO}_2$ , 8.32 wt%  $\text{Al}_2\text{O}_3$ , 8.48 wt%  $\text{Fe}_2\text{O}_3$ , and minor amounts of other components.

### Gadolinite-(Nd) $\text{Nd}_2\text{Fe}^{2+}\text{Be}_2\text{O}_2(\text{SiO}_4)_2$

**Origin:** Malmkärra mine, ~3.5 km WSW of Norberg, Sweden (type locality).

**Experimental details:** Raman scattering measurements have been performed on a polished section using  $633\text{ nm He-Ne}$  laser radiation. The laser radiation power at the sample was 10 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3525w, 970, 897s, 707w, 677sh, 615w, 550w, 501w, 483w, 428, 411, 383, 363, 339, 306, 292, 279, 265, 225w, 203w, 143w, 104w.

**Source:** Škoda et al. (2017).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### Gahnite $\text{ZnAl}_2\text{O}_4$

**Origin:** Jemaa, Kaduna State, Nigeria.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 473.1 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 661s, 510w, 420.

**Source:** D'Ippolito et al. (2013).

**Comments:** The sample was characterized by single crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Zn}_{0.94}\text{Fe}^{2+}_{0.03}\text{Al}_{0.03})(\text{Al}_{1.96}\text{Fe}^{2+}_{0.03}\text{Fe}^{3+}_{0.01})\text{O}_4$ . For the Raman spectrum of gahnite see also Faulstich et al. (2016).

### Gaidonnayite $\text{Na}_2\text{ZrSi}_3\text{O}_9 \cdot 2\text{H}_2\text{O}$

**Origin:** Toongi rare metal deposit, New South Wales, Australia

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1093sh, 1053, 963s, 926, 704w, 663w, 548s, 526sh, 404, 337sh, 316, 255sh, 199s, 152s.

**Source:** Spandler and Morris (2016).

**Comments:** The sample was characterized by X-ray fluorescence data and laser-ablation inductively coupled plasma mass spectroscopy. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

### Galaxite $\text{Mn}^{2+}\text{Al}_2\text{O}_4$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal in the spectral region from 100 to 900 cm<sup>-1</sup> using 473.1 nm Nd-YAG laser radiation. The laser radiation power at the sample was less than 1 mW. A nearly 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 775, 700w, 644w, 510, 395s, 374sh, 202s.

**Source:** D'Ippolito et al. (2015).

**Comments:** The sample was characterized by electron microprobe analysis.

### Galena PbS

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~450, 205.

**Source:** Sherwin et al. (2005).

**Comments:** No independent analytical data are provided for the sample used. The first-order Raman scattering is forbidden in minerals with the halite structure. However, the peak at  $205\text{ cm}^{-1}$  attributed to forbidden first order spectrum has been registered for galena. For the Raman spectrum of galena see also Frezzotti et al. (2012).

### Galileiite $\text{NaFe}^{2+}_4(\text{PO}_4)_3$

**Origin:** Yanzhuang H6 chondrite, Yanzhuang village, Wenyuan Co., Guangdong province, China.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using  $514.5\text{ nm Ar}^+$  laser radiation. The nominal laser radiation power was  $26.8\text{ mW}$ .

**Raman shifts ( $\text{cm}^{-1}$ ):**  $1129\text{--}1124, 982\text{--}980\text{s}, 599\text{--}596, 558\text{--}554\text{w}, 417\text{--}416, 305\text{--}304\text{w}, 154\text{--}151$ .

**Source:** Xie et al. (2014).

**Comments:** The sample was characterized by electron microprobe analyses. The empirical formula of the sample used is  $(\text{Na}_{0.89}\text{K}_{0.01}\text{Ca}_{0.03}\text{Cr}_{0.05})(\text{Fe}_{3.61}\text{Mn}_{0.29}\text{Mg}_{0.02}\text{Si}_{0.03})\text{P}_{2.99}\text{O}_{12}$ .

### Gallite $\text{CuGaS}_2$

**Origin:** Synthetic.

**Description:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented green-colored crystal with formula closest to pure  $\text{CuGaS}_2$  using  $514.5\text{ nm Ar}^+$  laser radiation. The laser radiation output power was  $30\text{ mW}$ .

**Raman shifts ( $\text{cm}^{-1}$ ):**  $384, 347\text{w}, 309\text{s}, 274\text{w}, 162\text{w}, 112\text{w}, 91\text{w}, 72\text{w}, 32\text{w}$ .

**Source:** Julien et al. (1999).

**Comments:** The sample was characterized by X-ray diffraction data. For the Raman spectrum of gallite see also Cha and Jung (2014).

### Gallium sulfide $\text{Ga}_2\text{S}_3$

**Origin:** Synthetic.

**Description:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using  $514.5\text{ nm Ar}^+$  laser radiation. The laser radiation output power was  $30\text{ mW}$ .

**Raman shifts ( $\text{cm}^{-1}$ ):**  $422, 386\text{w}, 329, 307, 233\text{s}, 147, 140, 114, 86, 72$ .

**Source:** Julien et al. (1999).

**Comments:** The sample was characterized by X-ray diffraction data.

### Galloplumbogummite $\text{Pb}(\text{Ga,Al,Ge})_3(\text{PO}_4)_2(\text{OH})_6$

**Origin:** Tsumeb mine, Tsumeb, Namibia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an oriented sample with three-fold crystallographic axis close to the direction of the polarization of the incident light using  $514.5$  and  $488.0\text{ nm Ar}^+$  laser radiations. The nominal laser radiation power is not indicated. A  $180^\circ$ -scattering geometry was employed.

**Raman shifts ( $\text{cm}^{-1}$ ):**  $3252, 1087\text{s}, 1007\text{s}, 979, 899, 619, 602, 573\text{w}, 566\text{w}, 559\text{w}, 538\text{w}, 492\text{s}, 356, 317, 272, 181, 83, 55$ .

**Source:** Schlüter et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Pb}_{1.04}\text{Ca}_{0.05})(\text{Ga}_{1.41}\text{Al}_{1.35}\text{Ge}_{0.38}\text{Fe}_{0.02})(\text{P}_{1.91}\text{S}_{0.14})\text{O}_{8.44}(\text{OH})_{5.56}$ . The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

### Galuskinite $\text{Ca}_7(\text{SiO}_4)_3(\text{CO}_3)$

**Origin:** Birkhin gabbro massif, Eastern Siberia, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal in the spectral region from 100 to 4000  $\text{cm}^{-1}$  using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation output power was in the range 30–50 mW. A 180°-scattering geometry was employed.

**Raman shifts ( $\text{cm}^{-1}$ ):** 1077s, 1007, 972w, 950, 928, 917, 898w, 889w, 882, 863s, 851s, 843, 704, 661, 570, 555, 525, 439, 404, 392, 367, 315w, 292w, 276, 257, 238, 220, 205, 184, 163, 140w, 124w, 114w.

**Source:** Lazic et al. (2011).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Ca}_{6.936}\text{Na}_{0.086})(\text{Si}_{2.983}\text{P}_{0.018}\text{S}_{0.004})\text{O}_{12}(\text{CO}_3)$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

### Gamagarite $\text{Ba}_2\text{Fe}^{3+}(\text{VO}_4)_2\text{OH}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was 90 mW. A 180°-scattering geometry was employed.

**Raman shifts ( $\text{cm}^{-1}$ ):** 953, 944sh, 918, 904, 874, 853, 846, 827, 799, 728w, 629, ~480sh, ~455sh, 442s, 411sh, 361, 346, 311, 268, 247sh, 229.

**Source:** Sanjeewa et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

### Gananite $\text{BiF}_3$

**Origin:** Synthetic

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 488.0 and 514.5 nm  $\text{Ar}^+$  laser radiations. The nominal laser radiation power was 200 mW. A 90°-scattering geometry was employed.

**Raman shifts ( $\text{cm}^{-1}$ ):** 334sh, 312s, 278sh, 271s, 265sh, 248s, 213, 203, 192, 177sh, 155, 142sh, 127s, 115s, 84, 70sh.

**Source:** Kavun et al. (2010).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Ganomalite**  $\text{Pb}_9\text{Ca}_6(\text{Si}_2\text{O}_7)_4(\text{SiO}_4)\text{O}$ 

**Origin:** Jakobsberg, Bergslagen, Sweden.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 6 mW.

**Raman shifts (cm<sup>-1</sup>):** 1068, 1042, 1000, 902, 886, 848s, 810, 727w, 673w, 564s, 551sh, 520, 486w, 455, 427w, 401w, 373, 354, 291, 242, 208.

**Source:** Kampf et al. (2016c).

**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Ganterite**  $\text{Ba}_{0.5}(\text{Na,K})_{0.5}\text{Al}_2(\text{Si}_{2.5}\text{Al}_{1.5})\text{O}_{10}(\text{OH})_2$ 

**Origin:** Berisal Complex, Simplon Region, Switzerland (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented polished thin section of a single crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 25 mW.

**Raman shifts (cm<sup>-1</sup>):** 1092, 1025, 948, 699s, 595s, 488s, 405sh, 266s.

**Source:** Graeser et al. (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is  $(\text{Ba}_{0.44}\text{K}_{0.28}\text{Na}_{0.27})(\text{Al}_{1.84}\text{Mg}_{0.09}\text{Fe}_{0.04}\text{Ti}_{0.04})[\text{Si}_{2.72}\text{Al}_{1.28}\text{O}_{10}](\text{OH})_{1.89}$ .

**Garavellite**  $\text{FeSbBiS}_4$ 

**Origin:** Malé Karpaty Mts., Western Carpathians, Slovakia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented polished section using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 210 mW. A 180°-scattering geometry was employed. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 364w, 338, 322, 302, 271sh, 249sh, 233sh, 214s, 197sh, 182, 167, 151, 137sh, 120, 99sh, 78s, 61.

**Source:** Kharbish and András (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Garnet**  $\text{Mg}_3(\text{MgSi})\text{Si}_3\text{O}_{12}$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was in the range 5–50 mW.

**Raman shifts (cm<sup>-1</sup>):** 1065, 1034w, 989w, 964sh, 931s, 889, 873sh, 852sh, 802, 724w, 648w, 602s, 559w, 535w, 507w, 498w, 481w, 458, 429w, 398w, 367, 354sh, 336w, 311, 293w, 275w, 261w, 238sh, 226, 205sh, 197, 181, 159, 138w.

**Source:** McMillan et al. (1989).

**Comments:** No independent analytical data are provided for the sample used.

**Gartrellite**  $\text{PbCuFe}^{3+}(\text{AsO}_4)_2(\text{OH})\cdot\text{H}_2\text{O}$ 

**Origin:** Anticline deposit, Ashburton Downs, Western Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3404, 3229, 2999, 1161, 1099, 995, 869s, 842s, 812, 785, 618, 560, 499, 474s, 438s, 357, 331, 304, 238, 201, 164, 140.

**Source:** Frost and Weier (2004e).

**Comments:** No independent analytical data are provided for the sample used. Raman shifts are given for gartrellite with partly isomorphic substitution of arsenate by sulfate. For the Raman spectrum of gartrellite see also López et al. (2014c).

**Garutiite** (Ni,Fe,Ir)

**Origin:** Loma Peguera, Dominican Republic (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532.6 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** The obtained Raman spectrum shows no discernible absorption bands over the range of 150–2000 cm<sup>-1</sup>.

**Source:** McDonald et al. (2010).

**Gaspéite** Ni(CO<sub>3</sub>)

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 488.0 and 514.5 nm Ar<sup>+</sup> laser radiations. The nominal laser radiation power was about 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1731, 1428, 1089, 736, 343, 235.

**Source:** Rutt and Nicola (1974).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Gaudefroyite** Ca<sub>4</sub>Mn<sup>3+</sup><sub>3</sub>(BO<sub>3</sub>)<sub>3</sub>(CO<sub>3</sub>)O<sub>3</sub>

**Origin:** N'Chwaning II mine, Kalahari manganese fields, South Africa.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. Raman spectrum was obtained in the spectral region from 200 to 4000 cm<sup>-1</sup>. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3385, 3249, 3206, 1595w, 1508w, 1491w, 1358sh, 1306sh, 1283, 1263sh, 1227sh, 1210sh, 1194, 1182sh, 1153sh, 1130w, 1112w, 1076, 1070sh, 950sh, 939, 928s, 914sh, 768w, 764w, 748w, 743w, 671s, 649s, 635sh, 584sh, 573, 534, 405w, 389w, 342s, 334sh, 297sh, 287s, 255sh, 244s, 228sh, 211w.

**Source:** Frost et al. (2014ae).

**Comments:** No independent analytical data are provided for the sample used.

**Gaylussite**  $\text{Na}_2\text{Ca}(\text{CO}_3)_2 \cdot 5\text{H}_2\text{O}$ **Origin:** Teels Marsh, Esmeralda Co., Nevada, USA.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3344, 3250sh, 2948sh, 1070s, 719, 698sh, 663w, 518, 258, 222, 158.**Source:** Frost and Dickfos (2007b).**Comments:** No independent analytical data are provided for the sample used.**Gazeevite**  $\text{BaCa}_6(\text{SiO}_4)_2(\text{SO}_4)_2\text{O}$ **Origin:** Jabel Harmun, Judean Mts., Palestinian Autonomy, Israel.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 50 mW.**Raman shifts (cm<sup>-1</sup>):** 1135, 1099, 997s, 963, 865, 638, 555w, 529w, 464, 409, 315w, 266sh, 213, 160w.**Source:** Galuskin et al. (2016a).**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Ba}_{0.85}\text{K}_{0.12}\text{Sr}_{0.02})(\text{Ca}_{5.99}\text{Na}_{0.02})[(\text{SiO}_4)_{1.82}(\text{PO}_4)_{0.14}(\text{AlO}_4)_{0.04}(\text{TiO}_4)_{0.01}][(\text{SO}_4)_{1.85}(\text{PO}_4)_{0.15}]_{\text{O}_{0.84}\text{F}_{0.11}}$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.**Gearksutite**  $\text{CaAlF}_4(\text{OH}) \cdot \text{H}_2\text{O}$ **Origin:** Valedo Ribeira, south of São Paulo and northeast of Paraná, Brazil.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 463, 407, 381, 298w, 226, 209, 169, 147s, 93, 84, 63, 54, 11.**Source:** Ronchi (2003).**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.**Geffroyite**  $(\text{Cu},\text{Fe},\text{Ag})_9\text{Se}_8$ **Origin:** Moroshkovoe lake, Southern Sopchinskoe deposit, Monchegorsk ore district, Kola Peninsula, Russia.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation or 785 nm diode laser radiation. The nominal laser radiation power was 50 mW and 500 mW, respectively.**Raman shifts (cm<sup>-1</sup>):** 445, 365, 264s, 186, 90w, 76.**Source:** Voloshin et al. (2015a).**Comments:** The sample was characterized by electron microprobe analysis. The empirical formula of the sample used is  $(\text{Cu}_{9.20}\text{Ag}_{0.44})(\text{Se}_{4.95}\text{S}_{3.05}\text{Te}_{0.10})$ .

**Gehlenite**  $\text{Ca}_2\text{Al}(\text{SiAl})\text{O}_7$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 488.0 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 500 mW. A 90°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 1005w, 998, 977, 914, 841sh, 796, 655sh, 626s, 528, 459, 425w, 303, 254sh, 240, 218, 180, 150w, 89.**Source:** Sharma et al. (1983).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of gehlenite see also Burshtein et al. (1993) and Bouhifd et al. (2002).**Geikielite**  $\text{MgTiO}_3$ **Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 80 mW.**Raman shifts (cm<sup>-1</sup>):** 714s, 641, 487sh, 485s, 397, 352s, 327s, 306, 281s, 224.**Source:** Okada et al. (2008).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectrum of geikielite see also Reynard and Guyot (1994).**Geminite**  $\text{Cu}^{2+}(\text{AsO}_3\text{OH}) \cdot \text{H}_2\text{O}$ **Origin:** Jáchymov ore district, Krušné Hory (Czech Ore Mts.), western Bohemia, Czech Republic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. Raman spectrum was obtained in the spectral region from 200 to 4000 cm<sup>-1</sup>. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3521w, 3448, 3314, 3152sh, 2814, 2438, 2288, 1299w, 885s, 871sh, 853s, 843sh, 813, 743w, 496, 481sh, 451sh, 421, 345, 333, 310, 284w, 244w, 213, 182sh, 178s, 161s, 136.**Source:** Sejkora et al. (2010).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is  $\text{Cu}_{1.00}[\text{AsO}_3(\text{OH})_{0.96}\text{F}_{0.04}] \cdot \text{H}_2\text{O}$ .**Gerhardtite**  $\text{Cu}_2(\text{NO}_3)(\text{OH})_3$ **Origin:** Great Australia mine, Cloncurry, Queensland, Australia.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3556sh, 3546, 3477, 3417, 3391sh, 1438s, 1417s, 1339, 1324s, 1052, 1048s, 1031, 1024, 887w, 805w, 720w, 711, 668w, 503, 474sh, 458, 437sh, 423sh, 410, 336w, 279, 258, 213, 189s, 165s, 149sh, 132w.

**Source:** Frost et al. (2004h).

**Comments:** No independent quantitative analytical data are provided for the sample used.

**Gerstleyite**  $\text{Na}_2(\text{Sb},\text{As})_8\text{S}_{13}\cdot 2\text{H}_2\text{O}$

**Origin:** Baker mine, Kramer district, Kern Co., California, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 449, 308s, 286s, 251s, 224sh, 188, 144s.

**Source:** Frost et al. (2010c).

**Comments:** No independent analytical data are provided for the sample used.

**Geschieberite**  $\text{K}_2(\text{UO}_2)(\text{SO}_4)_2\cdot 2\text{H}_2\text{O}$

**Origin:** Svornost mine, Jáchymov, Western Bohemia, Czech Republic (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm diode laser radiation. The laser radiation power at the sample was 3 mW.

**Raman shifts (cm<sup>-1</sup>):** 3595, 3506, 3280w, 1216, 1126, 1008s, 992, 984, 832s, 822sh, 652, 606w, 584w, 471, 454w, 386w, 270, 246, 230, 180, 154, 132sh, 100, 80.

**Source:** Plášil et al. (2015c).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{K}_{1.72}\text{Mg}_{0.29}\text{Na}_{0.04}\text{Ca}_{0.01})(\text{U}_{0.98}\text{O}_2)(\text{S}_{0.98}\text{O}_4)_2\cdot 2\text{H}_2\text{O}$ .

**Ghiaraite**  $\text{CaCl}_2\cdot 4\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3511, 3460sh, 3435, 3400, 3364sh, 3242sh, 1657, 1645sh, 1625, 801, 763, 713, 698, 679, 657, 595, 573, 551, 523s, 435s, 405s, 374, 335, 309, 283, 261w, 253w, 232, 212, 204, 184, 173, 163w, 154, 134, 127, 118, 108.

**Source:** Uriarte et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Gibbsite**  $\text{Al}(\text{OH})_3$

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power was 200 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3617s, 3522s, 3433s, 3364s, 1051, 1018, 979, 924, 892, 844, 816, 788, 751, 710, 617w, 602w, 569, 538s, 506, 444, 428, 412, 396s, 380, 371, 322s, 306, 290, 264, 255, 242.

**Source:** Ruan et al. (2001).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of gibbsite see also Rodgers (1992, 1993).

### Gilalite Cu<sub>5</sub>Si<sub>6</sub>O<sub>17</sub>·7H<sub>2</sub>O

**Origin:** São José da Batalha, Brazil.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 633 nm He-Ne laser. The laser radiation power is not indicated. Raman spectrum was obtained in the spectral region from 1200 to 4000 cm<sup>-1</sup>. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3706, 3669s, 3631sh, 3609, 3529, 3478, 3423sh, 3386s, 3347, 3313sh, 3259sh, 3207sh, 3154sh, 3075w, 2999, 2946, 2905sh, 2859sh, 1131sh, 1096sh, 1057sh, 1008, 964sh, 931sh, 898sh, 831, 779, 755sh, 675, 621s, 561, 509sh, 484sh, 443s, 400, 338, 314sh, 250sh, 214s, 150s, 123sh.

**Source:** López et al. (2014b).

**Comments:** The sample was characterized by semiquantitative electron microprobe analysis.

### Gillardite Cu<sub>3</sub>NiCl<sub>2</sub>(OH)<sub>6</sub>

**Origin:** Artificial (a product of Brass corrosion in NaCl solution).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed in the spectral region from 80 to 2000 cm<sup>-1</sup> using 514 nm Ar<sup>+</sup>-Kr<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 941, 900, 566sh, 511s, 458, 418, 371, 145, 127s.

**Source:** Babouri et al. (2015).

**Comments:** The sample was characterized by electron microprobe analysis. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

### Gillespite BaFe<sup>2+</sup>Si<sub>4</sub>O<sub>10</sub>

**Origin:** Minade Las Pozos, Tecate, Baja California, Mexico.

**Experimental details:** Raman scattering measurements have been performed on an oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 170 mW. A 135°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):**  $x-z(yz)z$  (A<sub>1g</sub>): 1018w, 963, 758, 527w, 450, 401, 346, 306, 246, 100s, 41s;  $x-z(yx)z(B_{2g})$ : 992, 971w, 761w, 588w, 491, 379, 307w, 218w, 123s, 64;  $x-z(yy)z$  (B<sub>1g</sub>): 1092s, 1025w, 856w, 789w, 558, 427s, 380, 306, 144, 123, 65w;  $x-z(x+z,y)z$  (E<sub>g</sub>): 1145w, 1018sh, 1017w, 927w, 885, 758, 663w, 558w, 524, 522, 427sh, 378, 341, 331w, 307, 283s, 250, 136sh, 102, 90, 70, 39.

**Source:** McKeown and Bell (1998).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Giniite**  $\text{Fe}^{2+}\text{Fe}^{3+}_4(\text{PO}_4)_4(\text{OH})_2 \cdot 2\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed at 198 K on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3387, 3206, 2918w, 1184sh, 1148sh, 1128, 1040sh, 1023s, 999sh, 948, 766, 627, 618, 584, 487, 461, 446, 396, 346, 327, 234, 202.**Source:** Frost et al. (2007n).**Comments:** The sample was characterized by X-ray diffraction data and qualitative electron microprobe analysis.**Gismondine**  $\text{Ca}_2(\text{Si}_4\text{Al}_4)\text{O}_{16} \cdot 8\text{H}_2\text{O}$ **Origin:** Capo di Bove, Italy.**Raman shifts (cm<sup>-1</sup>):** See comment below.**Source:** Mozgawa (2001).**Comments:** Raman spectrum of presumed gismondine given in the cited paper corresponds to calcite with minor admixture of a silicate.**Glauberite**  $\text{Na}_2\text{Ca}(\text{SO}_4)_2$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 2 mW.**Raman shifts (cm<sup>-1</sup>):** 1167w, 1154, 1138, 1104, 998s, 647, 642, 6321, 621sh, 616, 484w, 469, 452.**Source:** Jentzsch et al. (2012a).**Comments::** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of glauberite see also López et al. (2014f).**Glaucoberinitie**  $(\text{Zn}_{1-x}\text{Al}_x)(\text{SO}_4)_{x/2}(\text{OH})_2 \cdot n\text{H}_2\text{O}$  ( $x < 0.5$ ,  $n > 3x/2$ )**Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3609s, 3520s, 3435sh, 3353s, 3304sh, 1083w, 982, 903, 831w, 712w, 605sh, 559s, 512sh, 437, 384, 319s, 310sh, 243w, 147s, 111.**Source:** Frost et al. (2014ah).**Comments:** No independent analytical data are provided for the sample used.**Glauconite**  $(\text{K},\text{Na})(\text{Fe}^{3+},\text{Al},\text{Mg})_2(\text{Si},\text{Al})_4\text{O}_{10}(\text{OH})_2$ **Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup>, 632.8 He-Ne, and 780.0 diode laser radiations. The laser radiation output power of the He-Ne laser was less than 5 mW.

**Raman shifts (cm<sup>-1</sup>):** ~1100w, ~955w, 697s, 591s, 451sh, 389, 264s, 194s.

**Source:** Ospitali et al. (2008).

**Comments:** The sample was characterized by energy-dispersive X-ray scan data. The Raman shifts are given for Ar<sup>+</sup> laser excitation.

### Glaucomphane $\square\text{Na}_2(\text{Mg}_3\text{Al}_2)(\text{Si}_8\text{O}_{22})(\text{OH})_2$

**Origin:** Sesia-Lanzo zone, Western Alps.

**Experimental details:** Raman scattering measurements have been performed on the oriented samples using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed. Spectra were collected in the scattering geometries with the laser beam perpendicular to (100), (010), and (110) faces of several crystals.

**Raman shifts (cm<sup>-1</sup>):** 3658, 3645, 3630w, 1108w, 1063sh, 1045, 1016, 1010, 1000, 988s, 960sh, 895, 886, 790, 779, 742, 700, 684s, 670s, 611, 560, 525, 490w, 445, 411, 385s, 338, 310w, 256, 231, 210s, 181s, 160, 120.

**Source:** Gillet et al. (1989).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. Raman shifts are given as a sum of spectra in all scattering geometries. For the Raman spectra of glaucomphane see also Makreski et al. (2006a), Jovanovski et al. (2009), Apopei and Buzgar (2010), Andò and Garzanti (2014), and Leissner et al. (2015).

### Glaukophane CuNi(CO<sub>3</sub>)(OH)<sub>2</sub>

**Origin:** Carr Boyd Ni mine, Carr Boyd Rocks, Western Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3481sh, 3382w, 3307w, 1639w, 1522sh, 1496, 1460sh, 1367, 1097, 1087sh, 1065, 751w, 719w, 532w, 432, 352, 272, 222, 189, 157.

**Source:** Frost (2006).

**Comments:** The sample was characterized by X-ray diffraction data and electron microprobe analysis. The empirical formula of the sample used is (Cu<sub>1.1</sub>Ni<sub>0.7</sub>Mg<sub>0.06</sub>)(CO)<sub>3</sub>(OH)<sub>2</sub>.

### Glushinskite Mg(C<sub>2</sub>O<sub>4</sub>)·2H<sub>2</sub>O

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3391, 3367, 3254, 1720w, 1660, 1636, 1612, 1471s, 1454, 915, 861, 657, 585, 527sh, 521s, 310s, 265s, 237s, 226s, 221.

**Source:** Frost (2004d).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of glushinskite see also Frost and Weier (2003), Frost et al. (2004a), and Baran (2014).

**Gmelinite-Na**  $\text{Na}_4(\text{Si}_8\text{Al}_4)\text{O}_{24}\cdot 11\text{H}_2\text{O}$ **Origin:** Nova Scotia, Canada.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 1064 nm Nd-YAG laser radiation. The laser radiation power at the sample was 300 mW.**Raman shifts (cm<sup>-1</sup>):** 1642w, 1118, 464s, 330, 181, 137s.**Source:** Mozgawa (2001).**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.**Goethite**  $\text{FeO}(\text{OH})$ **Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was less than 0.7 mW.**Raman shifts (cm<sup>-1</sup>):** 993w, 685w, 550, 479s, 385s, 299, 243w.**Source:** De Faria et al. (1997).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of goethite see also Kustova et al. (1992), Bouchard and Smith (2003), Lepot et al. (2006), Müller et al. (2010), Nieuwoudt et al. (2011), Roqué-Rosell et al. (2010), Das and Hendry (2011), and Ciobotă et al. (2012).**Goldfieldite**  $\text{Cu}_{10}\text{Te}_4\text{S}_{13}$ **Origin:** Guinaoang, NW Luzon, Philippines.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 10 mW. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 354s, 324sh.**Source:** Mernagh and Trudu (1993).**Comments:** The sample was characterized by electron microprobe analyses.**Goldmanite**  $\text{Ca}_3\text{V}^{3+}_2(\text{SiO}_4)_3$ **Origin:** Pyrrhotite Gorge, Khibiny massif, Kola Peninsula, Russia.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample in the spectral region from 80 to 4000 cm<sup>-1</sup> using 633 nm He-Ne laser radiation. The nominal laser radiation power was 2 or 20 mW.**Raman shifts (cm<sup>-1</sup>):** 989, 932, 880s, 817s, 557s, 527, 495, 374s, 268, 241, 166.**Source:** Voloshin et al. (2014).**Comments:** The sample was characterized by electron microprobe analysis.**Gonnardite**  $(\text{Na,Ca})_2(\text{Si,Al})_5\text{O}_{10}\cdot 3\text{H}_2\text{O}$ **Origin:** Blackhead Quarry, Dunedin, New Zealand.**Experimental details:** Raman scattering measurements have been performed on an oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 120 mW.

A 180°-scattering geometry was employed. Crystal fibers were oriented E–W in a horizontal plane, and perpendicular to the laser beam.

**Raman shifts (cm<sup>-1</sup>):** 3587s, 3455s, 3253s, 1615, 1434, 1328, 1293, 1043w, 1003, 916, 890w, 839, 759w, 742w, 595w, 530s, 496, 441, 362w, 333, 314w, 266w, 232w, 159s.

**Source:** Graham et al. (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The compositional ranges of the sample used correspond to the formula Na<sub>4.78–6.27</sub>Ca<sub>1.31–2.12</sub>(Al<sub>8.41–8.79</sub>Si<sub>11.03–11.84</sub>O<sub>40</sub>). For the Raman spectrum of gonnardite see also Wopenka et al. (1998).

### Goosecreekite Ca(Si<sub>6</sub>Al<sub>2</sub>)O<sub>16</sub>·5H<sub>2</sub>O

**Origin:** No data.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 558w, 550w, 537, 513sh, 497s, 475sh, 450, 419, 414sh, 396sh, 376w.

**Source:** Lewis et al. (2006).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

### Gorceixite BaAl<sub>3</sub>(PO<sub>4</sub>)(PO<sub>3</sub>OH)(OH)<sub>6</sub>

**Origin:** Ilmeny (Il'menskie) Mts., South Urals, Russia.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 1086, 1019, 979s, 906, 816, 601, 496, 456, 341, 243s, 161.

**Source:** Dubinina and Valizer (2011).

**Comments:** The sample was characterized by electron microprobe analyses. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum

### Görgeyite K<sub>2</sub>Ca<sub>5</sub>(SO<sub>4</sub>)<sub>6</sub>·H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample in the spectral region from 200 to 4000 cm<sup>-1</sup> using 633 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3579, 3525s, 1215, 1187, 1175, 1164, 1161, 1137, 1115, 1108, 1085, 1078, 1067, 1013s, 1005s, 711, 661, 654, 631, 602, 595, 480, 457, 440, 433, 281.

**Source:** Kloprogge et al. (2004a).

**Comments:** The sample was characterized by powder X-ray diffraction and qualitative electron microprobe analysis.

### Gormanite Fe<sup>2+</sup><sub>3</sub>Al<sub>4</sub>(PO<sub>4</sub>)<sub>4</sub>(OH)<sub>6</sub>·2H<sub>2</sub>O

**Origin:** Yukon, Canada.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3615w, 3419w, 3404w, 3296w, 2893w, 1478w, 1466w, 1414w, 1382, 1365w, 1342, 1291w, 1247, 1150sh, 1123, 1095s, 1053sh, 996, 969w, 899, 505, 459, 436, 405, 380sh, 364sh, 349, 330w, 314, 195sh, 172w, 151sh.

**Source:** Frost et al. (2003c).

**Comments:** No independent analytical data are provided for the sample used.

### Goryainovite Ca<sub>2</sub>(PO<sub>4</sub>)Cl

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed in the spectral region from 80 to 1400 cm<sup>-1</sup> using 457.9 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 250 mW. A 90°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1120, 1052, 950s, 606, 388.

**Source:** Capobianco et al. (1992).

**Comments:** No independent analytical data are provided for the sample used. Raman shifts are given for a sample doped with MnO<sub>4</sub><sup>3-</sup> (with Mn<sup>5+</sup> concentration of 0.047 wt%). For the Raman spectrum of goryainovite see also Ivanyuk et al. (2017).

### Goslarite Zn(SO<sub>4</sub>)·7H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1492w, 1192, 1084, 1024s, 913w, 671w, 626, 511, 423, 281, 223.

**Source:** Buzgar et al. (2009).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of goslarite see also Coleyshaw et al. (1994) and Buzatu et al. (2012).

### Götzenite NaCa<sub>6</sub>Ti(Si<sub>2</sub>O<sub>7</sub>)<sub>2</sub>OF<sub>3</sub>

**Origin:** Pian di Celle volcano, Umbria, Italy.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 1031, 942, 902, 822s, 774, 664s, 587s, 560sh, 416, 371, 321, 278, 252, 218, 176sh.

**Source:** Sharygin et al. (1996b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

### Goudeyite Cu<sub>6</sub>Al(AsO<sub>4</sub>)<sub>3</sub>(OH)<sub>6</sub>·3H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm Nd-YAG laser radiation. The laser radiation power at the sample was 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3480s, 3393sh, 3361s, 3046, 2921, 2863, 1695w, 1605w, 1434, 13280, 1001, 938, 930, 894sh, 873s, 835s, 814sh, 800, 740, 700, 560, 540, 516sh, 495s, 486sh, 470, 449, 435, 403, 395, 350, 346, 327, 293, 269, 257, 240, 226, 201, 196.

**Source:** Frost et al. (2006n).

**Comments:** The sample was characterized by powder X-ray diffraction data and qualitative EDX analysis.

**Gowerite** Ca[B<sub>5</sub>O<sub>8</sub>(OH)][B(OH)<sub>3</sub>]·3H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 952w, 895s, 862s, 813w, 764s, 482, 391w.

**Source:** Jun et al. (1995).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Goyazite** SrAl<sub>3</sub>(PO<sub>4</sub>)(PO<sub>3</sub>OH)(OH)<sub>6</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power was ~50 mW.

**Raman shifts (cm<sup>-1</sup>):** 3360w, 3150w, 3066, 2910w, 2830w, 1698, 1300w, 1213, 1183w, 1127w, 1102, 1068w, 1046w, 1032s, 986s, 930, ~895sh, 833w, 757, 710, 653, 609, 579, 553, 511, 464, 421, 374s, 321w, ~280sh, 256s, 230sh, 186s.

**Source:** Breitinger et al. (2006).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of goyazite see also López et al. (2013c).

**Graemite** Cu<sup>2+</sup>(Te<sup>4+</sup>O<sub>3</sub>)·H<sub>2</sub>O

**Origin:** Cole Shaft, Arizona, USA.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3450sh, 3268, 2937, 793s, 768sh, 708, 676sh, 648sh, 527sh, 508sh, 507s, 471sh, 438s, 411sh, 380sh, 358sh, 314sh, 291, 257, 184, 146s.

**Source:** Frost and Keeffe (2009b).

**Comments:** No independent analytical data are provided for the sample used.

**Graeserite** Fe<sup>3+</sup><sub>4</sub>Ti<sub>3</sub>As<sup>3+</sup>O<sub>13</sub>(OH)

**Origin:** Monte Leone nappe, Binntal region, Western Alps, Switzerland.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 25 mW.

**Raman shifts (cm<sup>-1</sup>):** 1451.8, 743.3, 591.5, 421.6, 297.5, 163.4.

**Source:** Krzemnicki and Reusser (1998).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is  $(\text{Fe}^{3+}_{2.91}\text{Fe}^{2+}_{0.38}\text{Ti}_{0.54}\text{Pb}_{0.15})\text{Ti}_3(\text{As}^{3+}_{0.94}\text{Sb}^{3+}_{0.07})\text{O}_{13}(\text{OH})$ .

**Graftonite**  $(\text{Fe}^{2+},\text{Mn}^{2+},\text{Ca})_3(\text{PO}_4)_2$

**Origin:** Sowie Góry Mts, SW Poland.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal in the spectral region from 250 to 1300  $\text{cm}^{-1}$  using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1111w, 1018, 966s, 651, 593, 480w, 417, 317w, 285.

**Source:** Łodziński and Sitarz (2009).

**Comments:** The sample was characterized by electron microprobe data. For the Raman spectrum of graftonite see also Schneider et al. (2013).

**Gramaccioliite-(Y)**  $(\text{Pb},\text{Sr})(\text{Y},\text{Mn})\text{Fe}^{3+}_2(\text{Ti},\text{Fe}^{3+})_{18}\text{O}_{38}$

**Origin:** Sambuco, Stura valley, Cuneo province, Italy.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 812, ~710w, 638, 430, 360w, 330w, 293, ~240w.

**Source:** Bittarello et al. (2014).

**Comments:** No independent analytical data are provided for the sample used.

**Grandate**  $\text{Sr}_2\text{Al}(\text{AsO}_4)_2(\text{OH})$

**Origin:** Valletta mine, Maira Valley, Piedmont, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample in the spectral region from 100 to 2500  $\text{cm}^{-1}$  using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 899, 857, 833sh, 790, 547, 526, 512, 499, 425, 418, 386sh, 382, 347, 308, 213, 162, 120.

**Source:** Cámará et al. (2014a).

**Comments:** The sample was characterized by powder and single-crystal X-ray diffraction data and by electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Sr}_{1.41}\text{Ca}_{0.64}\text{Ba}_{0.05}\text{Pb}_{0.01})(\text{Al}_{0.68}\text{Fe}^{3+}_{0.14}\text{Mn}_{0.12}\text{Mg}_{0.13})[(\text{As}_{0.96}\text{V}_{0.01})_{\Sigma 0.97}\text{O}_4]_2(\text{OH})$ .

**Grandidierite**  $\text{MgAl}_3\text{O}_2(\text{BO}_3)(\text{SiO}_4)$

**Origin:** Kolonne area, Sri Lanka.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 1047s, 993s, 982s, 952s, 868s, 717s, 687, 659s, 615w, 551, 492s, 427, 362, 343, 269, 244, 228.

**Source:** Schmetzer et al. (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

## Graphite C

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal and on a microcrystalline sample using 488.0 and 514.5 nm Ar<sup>+</sup> laser radiations. The laser radiation power is not indicated. A 90°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1575s, 1355.

**Source:** Tuinstra and Koenig (1970).

**Comments:** No independent analytical data are provided for the sample used. Different orientations of the graphite single crystal with respect to the incident beam were used, but no changes in the spectrum were detected, and the only Raman line observed occurs at 1575 cm<sup>-1</sup>. Polycrystalline graphite exhibits another band at 1355 cm<sup>-1</sup>, which is attributed to a particle size effect. For the Raman spectra of graphite see also Mishra and Bernhardt (2009), Kaliwoda et al. (2011), and Ogawara and Akai (2014).

## Gratonite Pb<sub>9</sub>As<sub>4</sub>S<sub>15</sub>

**Origin:** Binntal, Switzerland.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed in the spectral region from 50 to 600 cm<sup>-1</sup> using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 370sh, 357s, 333, 312, 237, 186s, 169, 155s, 89sh, 75s.

**Source:** Kharbish (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is (Pb<sub>8.94</sub>Zn<sub>0.04</sub>Cu<sub>0.02</sub>)(As<sub>3.99</sub>Sb<sub>0.01</sub>)S<sub>15</sub>.

## Greenockite CdS

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 785 nm diode laser radiation. The nominal laser radiation power was in the range from 0.6 to 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 598, 560, 425w, 366sh, 345, 305, 252, 232, 210s.

**Source:** Rosi et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectra of greenockite see also Wang et al. (1993) and Chi et al. (2011).

## Gregoryite Na<sub>2</sub>(CO<sub>3</sub>)

**Origin:** Oldoinyo Lengai volcano, northern Tanzania (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-Gd laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1077–1078s, 1003–1005w, 952–954w, 704–710w, 630–635w.

**Source:** Golovin et al. (2017).

**Comments:** For the Raman spectrum of gregoryite see also Zaitsev et al. (2009).

**Greigite**  $\text{Fe}^{2+}\text{Fe}^{3+}_2\text{S}_4$ 

**Origin:** Artificial (from an archaeological artifact).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 0.1 mW.

**Raman shifts (cm<sup>-1</sup>):** 365s, 350s, 250w, 188w, 138w.

**Source:** Rémazeilles et al. (2010).

**Comments:** The sample was characterized by X-ray diffraction data and electron microprobe analysis.

For the Raman spectra of greigite see also Bourdoiseau et al. (2011), Li et al. (2014), and Eder et al. (2014).

**Griceite** LiF

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was 6 mW.

**Raman shifts (cm<sup>-1</sup>):** 191sh, 168s, 142s, 111w, 92.

**Source:** Alharbi et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

**Grimaldiite** CrO(OH)

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1634sh, 1593s, 1537sh, 1504sh, 1179sh, 1153, 981, 889sh, 823s, 630s, 558sh, 452.

**Source:** Yang et al. (2011c).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of grimaldiite see also Maslar et al. (2001).

**Grimaldiite** CrO(OH).

**Origin:** Artificial (a product of Cr corrosion).

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 647.1 nm Kr<sup>+</sup> laser radiation. The laser radiation power at the sample was less than 64 mW. A nearly 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 665sh, 535s, 475, 345w.

**Source:** Maslar et al. (2001).

**Comments:** The sample was characterized by X-ray diffraction data and EDS analysis. For the Raman spectrum of grimaldiite see also Yang et al. (2011c).

**Grimselite**  $K_3Na(UO_2)(CO_3)_3 \cdot H_2O$ **Origin:** No data.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 1063, 812s, 727, 723sh, 692, 686.**Source:** Biswas et al. (2016).**Comments:** The sample was characterized by electron microprobe analysis. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.**Grossite**  $CaAl_4O_7$ **Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The maximum output laser radiation power was 100 mW. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 942, 909s, 837, 807, 793, 756, 714, 686, 660, 630, 568, 457, 412s, 398, 356, 331, 322, 282, 268, 252, 220, 210, 203, 185, 134.**Source:** Hofmeister et al. (2004).**Comments:** The sample was characterized by single-crystal X-ray diffraction data. The crystal structure is solved.**Grossular**  $Ca_3Al_2(SiO_4)_3$ **Origin:** Mengyin, Shandong Province or Gejiu, Yunnan Province, China.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal in the spectral region from 50 to 1200 cm<sup>-1</sup> using 488 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was in the range from 100 to 150 mW.**Raman shifts (cm<sup>-1</sup>):** 1000w, 876s, 821, 777w, 623w, 540, 502w, 405w, 364s, 268, 232, 194w, 172, 135, 108s.**Source:** Mingsheng et al. (1994).**Comments:** The sample was characterized by electron microprobe data. For the Raman spectra of grossular see also Kolesov and Geiger (1998), Bersani et al. (2009), Makreski et al. (2011), and Andò and Garzanti (2014).**Groutite**  $Mn^{3+}O(OH)$ **Origin:** Cuyana Range, Minnesota, USA.**Experimental details:** Raman scattering measurements have been performed on a powdered and pelletised sample in the spectral region from 10 to 1000 cm<sup>-1</sup> using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 10 mW. A ~180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 648w, 615, 552s, 528s, 384s, 352, 278w, 253, 213, 142.**Source:** Julien et al. (2004).**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of groutite see also Bernard et al. (1993a).

**Grumiplucite**  $\text{HgBi}_2\text{S}_4$ 

**Origin:** Rudňany deposit, Slovakia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample in the spectral region from 30 to 3500  $\text{cm}^{-1}$  using 532 nm diode laser radiation. The nominal laser radiation power was 0.5 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 310, 275s, 258, 221s, 162, 144w, 127w, 106w, 92s, 82.

**Source:** Števko et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is  $\text{Hg}_{0.99}\text{Bi}_{1.94}\text{S}_{4.08}$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of grumiplucite see also Lecker (2013).

**Grunerite**  $\square\text{Fe}^{2+}_2\text{Fe}^{2+}_5\text{Si}_8\text{O}_{22}(\text{OH})_2$ 

**Origin:** Schneeberg, Tirol, Austria.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed in the spectral region from 210 to 3400  $\text{cm}^{-1}$  using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 1098, 1027, 999w, 971, 909w, 785w, 761, 747sh, 665s, 566w, 533, 415, 363, 315w, 289, 242w.

**Source:** Apopei and Buzgar (2010).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of grunerite see also Apopei et al. (2011) and Leissner et al. (2015).

**Grunerite**  $\square\text{Fe}^{2+}_2\text{Fe}^{2+}_5\text{Si}_8\text{O}_{22}(\text{OH})_2$ 

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an oriented crystal in the spectral regions from 2600 to 3800  $\text{cm}^{-1}$  using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. Polarized spectra were collected in the parallel-polarized scattering geometries (the polarization of incident light  $E_i$  was parallel to the polarization of scattered light  $E_s$ ) with the crystal-elongation direction parallel to  $E_i \parallel E_s$  and crystal-elongation direction perpendicular to  $E_i \perp E_s$ .

**Raman shifts ( $\text{cm}^{-1}$ ):** 3651, 3635, 3617.

**Source:** Leissner et al. (2015).

**Comments:** The sample was characterized by electron microprobe data. The Raman shifts are given for the scattering geometry with the crystal-elongation direction perpendicular to  $E_i \parallel E_s$ , in which the Raman intensities are most strong. The empirical formula of the sample used is  $(\square_{0.97}\text{Na}_{0.01}\text{Ca}_{0.02})(\text{Fe}_{0.89}\text{Mn}_{0.10}\text{Ca}_{0.01})_2(\text{Fe}_{0.61}\text{Mg}_{0.39})_5\text{Si}_{8.00}\text{OH}_{2.00}$ . For the Raman spectra of grunerite see also Apopei and Buzgar (2010) and Apopei et al. (2011).

**Guanacoite**  $\text{Cu}_2\text{Mg}_3(\text{OH})_4(\text{AsO}_4)_2 \cdot 4\text{H}_2\text{O}$ 

**Origin:** El Guanaco Mine, near Taltal, Chile (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 633 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3561s, 3510w, ~2996sh, 1619w, ~1069w, ~996w, 865s, 837s, 738, ~740sh, ~685sh, 490, 439, 411sh, 390s, ~367sh, 352sh, 315s, ~295sh, 271, 221, 212, 188, 171, 149, 131.

**Source:** Witzke et al. (2006).

**Comments:** The sample was characterized by powder and single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is Cu<sub>2.32</sub>Mg<sub>2.64</sub>(OH)<sub>4.13</sub>(AsO<sub>4</sub>)<sub>1.93</sub>·4.15H<sub>2</sub>O.

### Guanine C<sub>5</sub>H<sub>3</sub>(NH<sub>2</sub>)N<sub>4</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 40 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1675, 1602w, 1551, 1479sh, 1468, 1421, 1390, 1361, 1265, 1234, 1186, 1159w, 937, 879w, 848, 775w, 710w, 693w, 649s, 603w, 562, 547, 495, 397, 357w, 340.

**Source:** Giese and McNaughton (2002).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of guanine see also Mathlouthi et al. (1986).

### Gudmundite FeSbS

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was about 21 mW. A 180°-scattering geometry was employed. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 462w, 362, 352s, 316sh, 305s, 288s, 279sh, 253w, 241, 230sh, 217sh, 210, 201sh, 161sh, 152s, 145sh, 136sh.

**Source:** Kharbish and András (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The empirical formula of the sample used is Fe<sub>1.01</sub>As<sub>0.91</sub>S<sub>1.08</sub>.

### Guilleminite Ba(UO<sub>2</sub>)<sub>3</sub>(Se<sup>4+</sup>O<sub>3</sub>)<sub>2</sub>O<sub>2</sub>·3H<sub>2</sub>O

**Origin:** Musonoi mine, Kolwezi, Katanga (Shaba), Democratic Republic of Congo.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals in the spectral region from 100 to 1700 cm<sup>-1</sup> using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1585w, 1514w, 831sh, 747s, 675sh, 544sh, 478, 419sh, 345sh, 245, 150.

**Source:** Frost et al. (2009c).

**Comments:** No independent analytical data are provided for the sample used.

### Gunningite Zn(SO<sub>4</sub>)·H<sub>2</sub>O

**Origin:** Coranda-Hondolopen pit, Certej Gold-Silver deposit, Certej, Romania.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 7.37 mW.

**Raman shifts (cm<sup>-1</sup>):** 3230w, 1492w, 1192, 1087, 1024s, 884w, 665w, 626, 503, 423, 307sh, 277w, 219w.

**Source:** Apopei et al. (2014a).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of gunningite see also Buzatu et al. (2016).

### Gurimite Ba<sub>3</sub>(VO<sub>4</sub>)<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample. The laser radiation power and wavelength are not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 835s, 777, 414w, 378w, 326s, 169w, 132w, 104w.

**Source:** Azdouz et al. (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data. The crystal structure is solved. For the Raman spectra of gurimite see also Baran et al. (1972), Grzechnik and McMillan (1997), and Galuskina et al. (2016b).

### Gwihabaite (NH<sub>4</sub>)(NO<sub>3</sub>)

**Origin:** Synthetic

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 1458w, 1410w, 1283w, 1040s, 711, 190.

**Source:** Morillas et al. (2016).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of gwihabaite see also Martínez-Arkarazo et al. (2007).

### Gypsum Ca(SO<sub>4</sub>)·2H<sub>2</sub>O

**Origin:** Coranda-Hondol open pit, Certej Au-Agdeposit, Romania.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 14.3 mW.

**Raman shifts (cm<sup>-1</sup>):** 3398, 1136, 1106sh, 1010s, 671w, 623w, 576w, 495w, 416, 312w, 215w.

**Source:** Apopei et al. (2014a).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of gypsum see also Anbalagan et al. (2009), Buzgar et al. (2009), Jehlička et al. (2009b), White (2009), Ciobotă et al. (2012), Capitani et al. (2014), and Wang and Zhou (2014).

### Gyrolite NaCa<sub>16</sub>(Si<sub>23</sub>Al)O<sub>60</sub>(OH)<sub>8</sub>·14H<sub>2</sub>O

**Origin:** No data.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 1057, 1035, 774w, 703w, 628, 598s, 572s, 456, 400, 351, 280s, 207, 169w, 145.

**Source:** De Ferri et al. (2012).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

### Hafnon $\text{Hf}(\text{SiO}_4)$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts ( $\text{cm}^{-1}$ ):** 1021s, 985s, 935, 637w, 548w, 497w, 448, 402, 350, 268w, 213, 166w, 155, 147w.

**Source:** Grüneberger et al. (2016).

**Comments:** The sample was characterized by electron microprobe analysis. The empirical formula of the sample used is  $\text{Hf}_{0.99}\text{Zr}_{0.01}\text{SiO}_4$ . For the Raman spectra of hafnon see also Nicola and Rutt (1974) and Manoun et al. (2006).

### Haidingerite $\text{Ca}(\text{AsO}_3\text{OH}) \cdot \text{H}_2\text{O}$

**Origin:** Jáchymov, Bohemia, Krušné Hory (Czech Ore Mts.), Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3574w, 3455sh, 3412, 2842w, 886sh, 855s, 838sh, 823sh, 745, 739sh, 660w, 433sh, 420, 376sh, 369, 338sh, 323, 299sh, 268w, 220, 180, 145, 123, 115sh.

**Source:** Frost et al. (2010h).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

### Haiweite $\text{Ca}(\text{UO}_2)_2(\text{Si}_5\text{O}_{12})(\text{OH})_2 \cdot 6\text{H}_2\text{O}$

**Origin:** Teófilo Otoni, Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3606sh, 3498, 3375sh, 3273sh, 2923, 2875, 2851, 1170, 1115, 1108, 1087, 1019, 1015sh, 936, 919sh, 887w, 808s, 799s, 756w, 724w, 589, 473, 418w, 375, 317sh, 307, 283w, 264, 260, 236sh, 192s, 148sh, 108.

**Source:** Frost et al. (2006d).

**Comments:** No independent analytical data are provided for the sample used.

### Hakite $\text{Cu}_6[\text{Cu}_4\text{Hg}_2]\text{Sb}_4\text{Se}_{13}$

**Origin:** Příbram uranium and base-metal district, Central Bohemia, Czech Republic.

**Experimental details:** Micro-Raman scattering measurements have been performed on a polished section using 532 nm diode laser radiation. The nominal laser radiation power was 0.5 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 261, 228s, 211sh, 185, 166, 82, 69.

**Source:** Škácha et al. (2017).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

### Halite NaCl

**Origin:** Kłodawa salt mine, Central Poland.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 335.

**Source:** Wesełucha-Birczyńska et al. (2008).

**Comments:** No independent analytical data are provided for the sample used. Possibly, the band at 335 cm<sup>-1</sup> is a combination band of acoustical and optical modes of NaCl.

### Halloysite-10Å Al<sub>2</sub>Si<sub>2</sub>O<sub>5</sub>(OH)<sub>4</sub>·2H<sub>2</sub>O

**Origin:** A Neogene cryptokarst, southern Belgium.

**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3703, 3688, 3642, 3625s, 3598, 3556, 944sh, 910, 826sh, 794, 748, 710, 548sh, 503sh, 465s, 430s, 359sh, 332, 275, 245.

**Source:** Kloprogge and Frost (1999e).

**Comments:** The sample was characterized by powder X-ray diffraction data. Raman shifts are given for an unspecified scattering geometry.

### Halotrichite Fe<sup>2+</sup>Al<sub>2</sub>(SO<sub>4</sub>)<sub>4</sub>·22H<sub>2</sub>O

**Origin:** Corral Hollow, California, USA.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample in the spectral region from 100 to 4000 cm<sup>-1</sup> using 633 nm He-Ne laser radiation. The laser radiation power at the sample was 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3548sh, 3426w, 3270sh, 1147, 1086, 1031w, 985s, 608, 467, 444, 365w, 276sh, 247, 215sh.

**Source:** Locke et al. (2007).

**Comments:** The sample was characterized by X-ray diffraction data and electron microprobe analysis. For the Raman spectrum of halotrichite see also Buzatu et al. (2016).

### Hambergite Be<sub>2</sub>(BO<sub>3</sub>)(OH)

**Origin:** Ehrenfriedersdorf, complex, Erzgebirge (Ore Mts.), Germany.

**Experimental details:** Raman scattering measurements have been performed on a microscopic inclusions in beryl using 488.0 and 514.5 nm Ar<sup>+</sup> laser radiations. The laser radiation power at the sample was about 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 3469, 3403s, 988s, 270, 154s, 147, 123.

**Source:** Thomas et al. (2011b).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of hambergite see also Thomas and Davidson (2010).



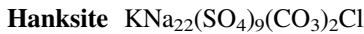
**Origin:** Shiti Ba deposit, Dabashan region, China (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single-crystal thin chip using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3581s, 3540s, 2945, 2250, 1092s, 855w, 699, 405, 265, 193.

**Source:** Liu et al. (2012).

**Comments:** The sample was characterized by powder and single crystal X-ray diffraction data and by electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Ba}_{1.98}\text{Na}_{0.06}\text{K}_{0.01})(\text{Ca}_{0.76}\text{Mg}_{0.12}\text{Y}_{0.06}\text{Sr}_{0.03}\text{La}_{0.01}\text{Nd}_{0.01})(\text{V}_{1.15}\text{Al}_{0.75}\text{Cr}_{0.20}\text{Ti}_{0.12})[(\text{Si}_{2.84}\text{Al}_{1.16})_{\Sigma 4.00}\text{O}_{10}] [(\text{OH})_{1.25}\text{O}_{0.77}] (\text{F}_{0.82}\text{Cl}_{0.01})(\text{CO}_3)_{2.05}$ .



**Origin:** Searles Lake, California, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an oriented sample using 488.0 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. Polarized spectra were collected in the scattering geometries with the laser radiation polarized approximately parallel to the *c* axis, and approximately parallel to the *a* axis.

**Raman shifts (cm<sup>-1</sup>):** 1190w, 1166w, 1156, 1142, 1135, 1124, 1117, 1096w, 1083s, 993s, 979sh, 712w, 634, 625, 620, 474, 470, 459.

**Source:** Palaich et al. (2013).

**Comments:** The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of hanksite see also Morillas et al. (2016).



**Origin:** Lava Cave, near Skipton, Victoria, Australia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3496, 3460, 3384, 3314, 3219, 3185, 3125, 3090sh, 2983sh, 2872, 2649, 2466, 2228, 1947, 1756, 1708, 1661w, 1457w, 1429w, 1227w, 1172w, 1119w, 1070, 1011, 974s, 971s, 882, 802w, 757w, 596w, 556, 522, 513, 436, 415sh, 379, 375, 356, 269, 250, 247, 205, 193w.

**Source:** Frost et al. (2005j).

**Comments:** No independent analytical data are provided for the sample used.



**Origin:** Hannebacher Ley Volcano, Eifel, Germany (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1092–1094, 1005s, 969, 655w, 520, 492, 444, 174.

**Source:** Frost and Keeffe (2009d).

**Comments:** No independent analytical data are provided for the sample used.

### Hansesmarkite Ca<sub>2</sub>Mn<sub>2</sub>Nb<sub>6</sub>O<sub>19</sub>·20H<sub>2</sub>O

**Origin:** Tvedalen, Larvik Plutonic Complex, Vestfold, southern Norway (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 913s, 865, 841sh, 734w, 520w, 473sh, 302, 217.

**Source:** Friis et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is (Ca<sub>1.93</sub>Na<sub>0.02</sub>K<sub>0.01</sub>)(Mn<sub>1.79</sub>Fe<sub>0.11</sub>)Nb<sub>6.00</sub>O<sub>18.84</sub>·20H<sub>2</sub>O.

### Hardystonite Ca<sub>2</sub>ZnSi<sub>2</sub>O<sub>7</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. Polarized spectrum was collected in the ~y(zz)~y scattering geometry.

**Raman shifts (cm<sup>-1</sup>):** 1060, 1020w, 906s, 663s, 614s, 550w, 480, 445, 265, 240sh, 220, 145w, 115w, 100, 60w.

**Source:** Kaminskii et al. (2011).

**Comments:** No independent analytical data are provided for the sample used.

### Harmotome Ba<sub>2</sub>(Si<sub>12</sub>Al<sub>4</sub>)O<sub>32</sub>·12H<sub>2</sub>O

**Origin:** Mannbühl (Giro) quarry, Dannenfels, Kirchheimbolanden, Rhineland-Palatinate, Germany.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 633 He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3615sh, 3526w, (3418w), 3287sh, 1707w, 1648w, 1102, 1020sh, 768w, 728w, 699w, 561w, 546sh, 534w, (515), 491s, 470sh, 428, 358w, 350sh, 335, 319, 289, 199, 183sh, 169sh.

**Source:** Frost et al. (2015q).

**Comments:** The sample was characterized by qualitative electron microprobe analysis. For the Raman spectrum of harmotome see also Mozgawa (2001).

### Harmunite CaFe<sub>2</sub>O<sub>4</sub>

**Origin:** Jabel Harmun, West Bank, Palestinian Autonomy, Israel (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm solid-state laser radiation. The laser radiation power at the sample was 44 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1228, 648s, 585s, 519, 453sh, 4354, 379sh, 364s, 298, 270, 206, 182, 161, 117.  
**Source:** Galuskina et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is Ca<sub>1.013</sub>(Fe<sup>3+</sup><sub>1.957</sub>Al<sub>0.015</sub>Cr<sub>0.011</sub>Ti<sub>0.004</sub>Mg<sub>0.003</sub>)O<sub>4</sub>.

### Harmunite Mn<sup>4+</sup>-bearing Ca<sub>1-x</sub>(Fe<sup>3+</sup>,Mn<sup>4+</sup>)<sub>2</sub>O<sub>4</sub>

**Origin:** Bellerberg volcano, Eifel, Rhineland-Palatinate, Germany.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm solid-state laser radiation. The laser radiation power at the sample was 44 mW.

**Raman shifts (cm<sup>-1</sup>):** 1225, 617sh, 590s, 526, 468, 391w, 327w, 289w, 205w, 161, 115w.

**Source:** Galuskin et al. (2016b).

**Comments:** The sample was characterized electron microprobe data. The empirical formula of the sample used is Ca<sub>0.862</sub>(Fe<sup>3+</sup><sub>1.719</sub>Mn<sup>4+</sup><sub>0.265</sub>Ti<sup>4+</sup><sub>0.012</sub>Mg<sub>0.008</sub>)O<sub>4</sub>.

### Hartite C<sub>20</sub>H<sub>34</sub>

**Origin:** Castelnuovo di Valdarno, Italy.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed in the spectral region from 100 to 3500 cm<sup>-1</sup> using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power was 350 mW.

**Raman shifts (cm<sup>-1</sup>):** 3000, 2978, 2962, 2942s, 2921s, 2907sh, 2886sh, 2866, 2851, 2768w, 2733w, 1480, 1468sh, 1440s, 1387, 1370w, 1356, 1341, 1320w, 1310, 1287, 1264, 1249w, 1230, 1217sh, 1208s, 1180, 1154sh, 1144, 1114(?), 1096s, 1085w, 1075w, 1063, 1041, 1027w, 1013, 996, 976, 963sh, 946, 936, 926(?), 916w, 892, 879, 845, 814, 792s, 770, 745w, 729s, 693, 639, 598w, 558, 543, 526, 489, 452, 403, 389w, 345, 326w, 305.

**Source:** Jehlička and Edwards (2008).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of hartite see also Jehlička et al. (2005).

### Hashemite Ba(CrO<sub>4</sub>)

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample prepared as a pellet using 488 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 200 mW.

**Raman shifts (cm<sup>-1</sup>):** 907, 900, 885w, 873, 864s, 429w, 412w, 404w, 396w, 361, 351, 135w, 112w, 66w.

**Source:** Scheuermann and Schutte (1973a).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Hatchetine A paraffin wax related to evenkite.

**Origin:** Zastávka, near Brno, Bohemian Massif, Czech republic.

**Experimental details:** Raman scattering measurements have been performed on a compacted powder of amorphous sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 2883s, 2847, 2725, 1463s, 1440s, 1418, 1389w, 1371w, 1347, 1295s, 1171.

**Source:** Jehlička et al. (2007a).

**Comments:** No independent analytical data are provided for the sample used.

### Hatrurite Ca<sub>3</sub>SiO<sub>5</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 363.8 nm laser radiation. The nominal laser radiation power was 150 mW.

**Raman shifts (cm<sup>-1</sup>):** 953sh, 929sh, 914, 893, 880, 847s, 812, 741, 540, 521sh, 392, 352, 326, 317sh, 267, 240, 224, 180, 126, 103, 80, 56.

**Source:** Fujimori et al. (2005).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

### Hauerite MnS<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a single crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed. Raman spectrum was collected in the scattering geometry with the laser radiation direction normal to the (111) plane of the crystal.

**Raman shifts (cm<sup>-1</sup>):** 743w, 655, 486s, 246, 223.

**Source:** Verble and Humphrey (1974).

**Comments:** No independent analytical data are provided for the sample used.

### Hausmannite Mn<sup>2+</sup>Mn<sup>3+</sup>O<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample prepared as a pellet using 514.5 nm Ar<sup>+</sup> and 647.1 nm Kr<sup>+</sup> laser radiations. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 668s, 479w, 371, 328, 298.

**Source:** Lutz et al. (1991).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of hausmannite see also Bernard et al. (1993a), Julien et al. (2004), and Mironova-Ulmane et al. (2009).

### Hausmannite Mn<sup>2+</sup>Mn<sup>3+</sup>O<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 10 mW. A nearly 180°-scattering geometry was employed. Raman spectrum was obtained in the spectral region from 10 to 1200 cm<sup>-1</sup>.

**Raman shifts (cm<sup>-1</sup>):** 653s, 579w, 485w, 357, 310.

**Source:** Julien et al. (2004).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of hausmannite see also Lutz et al. (1991), Bernard et al. (1993a), and Mironova-Ulmane et al. (2009).

### Haüyne $\text{Na}_3\text{Ca}(\text{Si}_3\text{Al}_3)\text{O}_{12}(\text{SO})_4$

**Origin:** Sacrofano, Latium, Italy.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was 300 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 1152, 1090, 1027sh, 998sh, 986s, 977s, 643, 610, 545w, 433s.

**Source:** Ballirano (2012).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analysis. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Na}_{4.4}\text{K}_{1.1}\text{Ca}_{2.1})[\text{Si}_6\text{Al}_6\text{O}_{24}](\text{SO}_4)_{1.6}(\text{S}_3)_{0.3}(\text{CO}_2)_{0.1}$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of haüyne see also Caggiani et al. (2014).

### Hawleyite $\text{CdS}$

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was in the range 0.3–5 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 902, 633sh, 598, 295, 254sh.

**Source:** Rosi et al. (2016).

**Comments:** The Raman shifts were determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of hawleyite see also Wang et al. (1993).

### Hawthorneite $\text{BaMgTi}_3\text{Cr}_4\text{Fe}^{2+}_2\text{Fe}^{3+}_2\text{O}_{19}$

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632 nm He-Ne laser radiation. The nominal laser radiation power was in the range 4–8 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 680s, 516, 459sh, 352, 285w.

**Source:** Konzett et al. (2005).

**Comments:** The sample was characterized by electron microprobe analysis.

### Haynesite $(\text{UO}_2)_3(\text{Se}^{4+}\text{O}_3)_2(\text{OH})_2 \cdot 5\text{H}_2\text{O}$

**Origin:** Repete Mine, Blanding, San Juan Co., Utah, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3476w, 862w, 812s, 800s, 741, 582w, 472, 437sh, 419s, 367, 342, 278, 257sh, 219, 157sh, 142.

**Source:** Frost et al. (2006q).

**Comments:** No independent analytical data are provided for the sample used.

**Hazenite**  $\text{KNaMg}_2(\text{PO}_4)_2 \cdot 14\text{H}_2\text{O}$ **Origin:** Mono Lake, California, USA.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm solid-state laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3900–2500, 2380, 1620w, 1100–988sh, 932s, 685w, 559, 430, 290, 234.**Source:** Yang et al. (2011b).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved. The empirical formula of the sample used is  $\text{K}_{0.97}(\text{Na}_{0.96}\text{Ca}_{0.02})\text{Mg}_{2.07}[(\text{P}_{0.98}\text{S}_{0.02})\text{O}_4]_2 \cdot 13.90\text{H}_2\text{O}$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.**Heazlewoodite**  $\text{Ni}_3\text{S}_2$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a sample prepared as a pellet using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 40 mW.**Raman shifts (cm<sup>-1</sup>):** 351s, 324w, 305, 223, 201, 190.**Source:** Cheng and Liu (2007).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectrum of heazlewoodite see also Lanteigne et al. (2012).**Hectorite**  $\text{Na}_{0.3}(\text{Mg},\text{Li})_3\text{Si}_4\text{O}_{10}(\text{F},\text{OH})_2 \cdot n\text{H}_2\text{O}$ **Origin:** No data.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 1082, 944w, 892, 783, 683s, 560, 516w, 461, 379sh, 333, 282, 206sh, 184s.**Source:** Wang et al. (1998a).**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.**Hedenbergite**  $\text{CaFe}^{2+}\text{Si}_2\text{O}_6$ **Origin:** Sasa, Macedonia.**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1030sh, 1010s, 904w, 850w, 655s, 549, 523, 494w, 370, 330, 300, 230w, 182, 145, 121, 115.**Source:** Jovanovski et al. (2009).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectra of hedenbergite see also Huang et al. (2000), Buzatu and Buzgar (2010), and Andò and Garzanti (2014).**Hedenbergite**  $\text{CaFe}^{2+}\text{Si}_2\text{O}_6$ **Origin:** Nordmarken, Sweden.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal. Experimental details are not described.

**Raman shifts (cm<sup>-1</sup>):** 1012s, 894w, 852, 663s, 553w, 524, 499sh, 381, 346w, 315, 231w.

**Source:** Buzatu and Buzgar (2010).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of hedenbergite see also Huang et al. (2000), Jovanovski et al. (2009), and Andò and Garzanti (2014).

### Hedyphane Ca<sub>2</sub>Pb<sub>3</sub>(AsO<sub>4</sub>)<sub>3</sub>Cl

**Origin:** Puttapa mine, Beltana, Flinders Ranges, South Australia, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3659sh, 3563sh, 3458sh, 3409, 3389, 3352sh, 3304sh, 3258, 3235, 848sh, 834sh, 819s, 811sh, 787s, 770, 452, 432sh, 394, 372sh, 349, 334sh, 319s, 201sh, 192sh, 177sh, 162, 151sh, 141sh.

**Source:** Frost et al. (2007c).

**Comments:** No independent analytical data are provided for the sample used. Raman shifts in the OH stretching region indicate that there is isomorphic replacement of Cl for OH.

### Heisenbergite (UO<sub>2</sub>)(OH)<sub>2</sub>·H<sub>2</sub>O

**Origin:** Menzenschwand, Schwarzwald (Black Forest), Germany (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample in the spectral region from 150 to 4000 cm<sup>-1</sup> using 638 nm laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1005w, 923w, 829s, 799sh, 742s, 538, 438, 389sh, 338w, 247w, 190w.

**Source:** Walenta and Theye (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is U<sub>1.044</sub>Pb<sub>0.020</sub>Ba<sub>0.004</sub>Ca<sub>0.008</sub>H<sub>3.672</sub>O<sub>5</sub>.

### Heliophyllite Pb<sub>6</sub>As<sub>2</sub>O<sub>7</sub>Cl<sub>4</sub>

**Origin:** Karrantza valley, Basque Co., Spain.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> and 785 nm diode laser radiations. The laser radiation power at the sample was 20 mW with Ar<sup>+</sup> excitation, and the nominal laser radiation power was 150 mW with diode excitation.

**Raman shifts (cm<sup>-1</sup>):** 808, 746, 718, 160s.

**Source:** Goienaga et al. (2011).

**Comments:** No independent analytical data are provided for the sample used.

### Hellyerite Ni(CO<sub>3</sub>)·6H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1397, 1092s, 721w, 409w, 293, 257, 224sh, 157s.

**Source:** Bette et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data. The crystal structure is solved.

### Hematite Fe<sub>2</sub>O<sub>3</sub>

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was below 0.7 mW.

**Raman shifts (cm<sup>-1</sup>):** 1320, 612, 497w, 411s, 299sh, 293, 246w, 227.

**Source:** De Faria et al. (1997).

**Comments:** The sample was characterized by X-ray diffraction data. For the Raman spectra of hematite see also Bouchard and Smith (2003), Lepot et al. (2006), Müller et al. (2010), Sagatowska (2010), Das and Hendry (2011), Hosterman (2011), Nieuwoudt et al. (2011), Ciobotă et al. (2012), Andò and Garzanti (2014), and Apopei et al. (2014a).

### Hematite Fe<sub>2</sub>O<sub>3</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was below 0.4 mW.

**Raman shifts (cm<sup>-1</sup>):** 1300, 1046, 824w, 657, 610, 494, 408, 292s, 243w, 223s.

**Source:** Müller et al. (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of hematite see also De Faria et al. (1997), Bouchard and Smith (2003), Lepot et al. (2006), Sagatowska (2010), Das and Hendry (2011), Hosterman (2011), Nieuwoudt et al. (2011), Ciobotă et al. (2012), Andò and Garzanti (2014), and Apopei et al. (2014a).

### Hemihedrite ZnPb<sub>10</sub>(CrO<sub>4</sub>)<sub>6</sub>(SiO<sub>4</sub>)<sub>2</sub>F<sub>2</sub>

**Origin:** Florence Pb-Ag mine, Pinal Co., Arizona, USA.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm solid-state laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3389w, 858s, 841s, 825, 784, 370sh, 340.

**Source:** Lafuente et al. (2016).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is Pb<sub>10.21</sub>(Cu<sub>0.65</sub>Zn<sub>0.34</sub>)(Cr<sub>5.93</sub>P<sub>0.07</sub>S<sub>0.04</sub>)(Si<sub>1.83</sub>As<sub>0.10</sub>)O<sub>34</sub>H<sub>1.62</sub>. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of hemihedrite see also Frost (2004c).

### Hemimorphite Zn<sub>4</sub>(Si<sub>2</sub>O<sub>7</sub>)(OH)<sub>2</sub>·H<sub>2</sub>O

**Origin:** Sasa, Macedonia.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample in the spectral region from 100 to 1300 cm<sup>-1</sup> using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 980w, 930s, 678, 559w, 516w, 452, 402, 332, 304w, 282w, 218w, 169, 132s.  
**Source:** Makreski et al. (2007).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectrum of hemimorphite see also Jovanovski et al. (2009).

### Hemleyite FeSiO<sub>3</sub>

**Origin:** Suizhou L6 chondrite (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample. Experimental details are not described.

**Raman shifts (cm<sup>-1</sup>):** 795s, 673, 611, 476, 403, 342.

**Source:** Bindi et al. (2017).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Fe}^{2+}_{0.48}\text{Mg}_{0.37}\text{Ca}_{0.04}\text{Na}_{0.04}\text{Mn}^{2+}_{0.03}\text{Al}_{0.03}\text{Cr}^{3+}_{0.01})\text{Si}_{1.00}\text{O}_3$ .

### Hemusite Cu<sup>1+</sup><sub>4</sub>Cu<sup>2+</sup><sub>2</sub>SnMoS<sub>8</sub>

**Origin:** Zijin Cu-Au mine, China.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 826, 658, 413, 348, 294, 262.

**Source:** Liu et al. (2012).

**Comments:** The empirical formula of the sample used is Cu<sub>6.03</sub>Sn<sub>0.95</sub>Fe<sub>0.14</sub>Mo<sub>0.97</sub>S<sub>8.0</sub>.

### Hendricksite KZn<sub>3</sub>(Si<sub>3</sub>Al)O<sub>10</sub>(OH)<sub>2</sub>

**Origin:** Franklin Furnace, New Jersey, USA.

**Experimental details:** Raman scattering measurements have been performed on an oriented sample using 514.5 and 488 nm Ar<sup>+</sup> laser radiations. The laser radiation power is not indicated. Spectra were collected in scattering geometries with incident laser polarization parallel and perpendicular to the cleavage plane.

**Source:** Tlili et al. (1989).

**Raman shifts (cm<sup>-1</sup>):** 1028, 677s, 644, 321w, 317w, 278w, 189s, 94w.

**Comments:** The sample was characterized by electron microprobe analyses. The Raman shifts are given as the sum of the both scattering geometries.

### Henmilite Ca<sub>2</sub>Cu[B(OH)<sub>4</sub>]<sub>2</sub>(OH)<sub>4</sub>

**Origin:** Fuka mine, Okayama prefecture, Honshu Island, Japan (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3609s, 3593sh, 3559s, 3501, 3457sh, 3424s, 3396sh, 3328s, 3269s, 3195sh, 3101sh, 1270w, 1208w, 984w, 969sh, 951w, 922w, 902sh, 834w, 823w, 758s, 752sh, 745sh, 697sh, 598w, 562w, 547w, 534sh, 479sh, 469, 415w, 403w,m 365, 353sh, 335w, 290, 267sh, 255, 240, 225, 217sh, 197, 181sh, 172, 162, 148, 128.

**Source:** Frost and Xi (2013e).

**Comments:** No independent analytical data are provided for the sample used.

**Henrictmierite**  $\text{Ca}_3\text{Mn}^{3+}_2(\text{SiO}_4)_2(\text{OH})_4$

**Origin:** N'Chwaning II mine, Kalahari Manganese Fields, South Africa.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 200 mW.

**Raman shifts (cm<sup>-1</sup>):** 3428, 989w, 921, 882, 834w, 567s, 547w, 500s, 469w, 435, 373, 337, 322sh, 278, 257sh, 248, 168, 151.

**Source:** Friedrich et al. (2015).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Ca}_{2.98}\text{Na}_{0.01}\text{Mg}_{0.01})(\text{Mn}_{1.95}\text{Fe}_{0.01}\text{Al}_{0.04})[\text{SiO}_4]_{2.07}[\text{O}_4\text{H}_4]_{0.93}$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Henryite**  $\text{Cu}_4\text{Ag}_3\text{Te}_4$

**Origin:** Pyrrhotite gorge, Lovchorsk Mt., Khibiny massif, Kola Peninsula, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> or 785 nm diode laser radiation. The nominal laser radiation power was 50 mW or 500 mW, respectively.

**Raman shifts (cm<sup>-1</sup>):** 148s, 118s, 91w.

**Source:** Voloshin et al. (2015a).

**Comments:** The sample was characterized by electron microprobe analyses. The empirical formula of the sample used is  $\text{Cu}_{3.89}(\text{Ag}_{2.75}\text{Au}_{0.03})\text{Te}_{4.00}$ .

**Herbertsmithite**  $\text{Cu}_3\text{Zn}(\text{OH})_6\text{Cl}_2$

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an oriented sample with the laser beam direction normal to the *xy* plane of a crystal using 532 nm laser radiation. The nominal laser radiation power was 1 mW. A nearly 180°-scattering geometry was employed. Polarized spectra were collected during rotation of the sample within the crystallographic *xy* plane with the axis of rotation along of the incident light.

**Raman shifts (cm<sup>-1</sup>):** 943, 702, 501s, 402, 365, 230w, 148, 123s [for the (xx) scattering geometry].

**Source:** Wulferding et al. (2010).

**Comments:** The empirical formula of the sample used is  $\text{Zn}_{0.8}\text{Cu}_{3.2}(\text{OH})_6\text{Cl}_2$ . For the Raman spectrum of herbertsmithite see also Chu et al. (2011).

**Hercynite**  $\text{Fe}^{2+}\text{Al}_2\text{O}_4$

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 632.8 nm He-Ne laser radiation. The laser radiation power was less than 1 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 748s, 699w, 617, 504, 400, 366sh, 189s.

**Source:** D'Ippolito et al. (2015).

**Comments:** The sample was characterized by electron microprobe analysis.

### Herderite CaBe(PO<sub>4</sub>)F

**Origin:** Ehrenfriedersdorf complex, Erzgebirge (Ore Mts.), Germany.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented microscopic inclusion in quartz using 488 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 450 mW.

**Raman shifts (cm<sup>-1</sup>):** 1005, 983s, 595, 584.

**Source:** Rickers et al. (2006).

**Comments:** No independent analytical data are provided for the sample used.

### Herzenbergite SnS

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power at the sample was less than 0.4 mW.

**Raman shifts (cm<sup>-1</sup>):** 220, 192s, 165, 95, 67w, 48, 39s.

**Source:** Fontané et al. (2013).

**Comments:** The sample was characterized by X-ray diffraction data. For the Raman spectrum of herzenbergite see also Chandrasekhar et al. (1977).

### Hessite Ag<sub>2</sub>Te

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 488, 515, and 633 nm laser radiations. The nominal laser radiation power was 0.3 mW.

**Raman shifts (cm<sup>-1</sup>):** 138, 110, 80.

**Source:** Milenov et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

### Hetaerolite ZnMn<sup>3+</sup><sub>2</sub>O<sub>4</sub>

**Origin:** Madjarovo deposit, Eastern Rhodopes, Bulgaria.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 38 mW.

**Raman shifts (cm<sup>-1</sup>):** 684s, 637, 595sh, 574, 515w, 487w, 388s, 374sh, 329, 309sh.

**Source:** Vassileva et al. (2005).

**Comments:** The sample was characterized by X-ray diffraction data and electron microprobe analyses. For the Raman spectrum of hetaerolite see also Javed et al. (2013).

**Heterogenite**  $\text{Co}^{3+}\text{O(OH)}$ 

**Origin:** Mindigi mine, Katanga copperbelt, Katanga province, Democratic Republic of Congo.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was 2 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1202w, 1133w, 670, 626, 572, 495s.

**Source:** Burlet et al. (2011).

**Comments:** The sample was characterized electron microprobe analyses. For the Raman spectrum of heterogenite see also Burlet et al. (2014).

**Heterosite**  $\text{Fe}^{3+}(\text{PO}_4)$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 532 nm laser radiation. The nominal laser radiation power was 3 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1123s, 1078s, 1064s, 962, 912, 660, 602, 587, 575w, 516w, 492, 400w, 339, 308, 246, 199w, 175s, 107.

**Source:** Burba and Frech (2004).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Heulandite**  $(\text{Ca},\text{Na},\text{K})_5(\text{Si}_{27}\text{Al}_9)\text{O}_{72}\cdot26\text{H}_2\text{O}(?)$ 

**Origin:** Paterson, Passaic Co., New Jersey, USA.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using Nd-YAG laser radiation. The laser radiation power at the sample was 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 1138w, 799w, 611w, 483s, 404s, 147.

**Source:** Mozgawa (2001).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Hexacelsian**  $\text{Ba}(\text{Al}_2\text{Si}_2\text{O}_8)$ 

**Origin:** Hatrurim complex, Negev Desert, Israel.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm solid-state laser radiation. The laser radiation power at the sample was 44 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1119, 1087w, 961, 924, 890, 809w, 678, 594, 480w, 461w, 406s, 296w, 107s.

**Source:** Galuskina et al. (2016b).

**Comments:** The sample was characterized by electron microprobe analyses. The empirical formula of the sample used is  $(\text{Ba}_{0.911}\text{K}_{0.059}\text{Ca}_{0.042}\text{Na}_{0.010})\text{Al}_{1.891}\text{Fe}^{3+}_{0.072}\text{Si}_{2.034}\text{O}_8$ . For the Raman spectra of hexacelsian see also Colomban et al. (2000), Kremenović et al. (2003), and Dondur et al. (2005).

**Hexaferrum** (Fe,Os,Ru,Ir)**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a high-purity polycrystalline Fe sample at pressures from 15 to 152 GPa. A 35° incidence angle for the exciting radiation was employed. No characteristics of the laser radiation are indicated.**Raman shifts (cm<sup>-1</sup>):** 245sh, 210 (at 22 GPa); 260 (at 82 GPa); 300 (at 152 GPa).**Source:** Merkel et al. (2000).**Comments:** No independent analytical data are provided for the sample used.**Hexahydrite** Mg(SO<sub>4</sub>)·6H<sub>2</sub>O**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powdered sample in the spectral region from 50 to 4300 cm<sup>-1</sup> using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 15 mW.**Raman shifts (cm<sup>-1</sup>):** 3540sh, 3428, 3258sh, 1655, 1146w, 1085w, 984s, 610w, 466w, 445w, 364, 245, 223.**Source:** Wang et al. (2006a).**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of hexahydrite see also Apopei et al. (2015).**Hexahydroborite** Ca[B(OH)<sub>4</sub>]<sub>2</sub>·2H<sub>2</sub>O**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 300 mW.**Raman shifts (cm<sup>-1</sup>):** 859s, 755s, 389w.**Source:** Jun et al. (1995).**Comments:** The sample was characterized by powder X-ray diffraction data.**Hiärneite** (Ca,Mn<sup>2+</sup>,Na)<sub>2</sub>(Zr,Mn<sup>3+</sup>)<sub>5</sub>(Sb,Ti,Fe)<sub>2</sub>O<sub>16</sub>**Origin:** Långban deposit, Bergslagen ore region, Filipstad district, Värmland, Sweden (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 200 mW.**Raman shifts (cm<sup>-1</sup>):** 672, 602, 515, 453, 426s, 398s, 388s, 378, 305, 268, 215sh, 195, 167, (159), 141.**Source:** Holtstam (1997).**Comments:** The sample was characterized by powder and single-crystal X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is Na<sub>0.17</sub>Ca<sub>1.57</sub>Mn<sup>2+</sup><sub>0.62</sub>Zr<sub>4.19</sub>Hf<sub>0.02</sub>Sb<sup>5+</sup><sub>1.37</sub>Ti<sub>0.59</sub>Mn<sup>3+</sup><sub>0.36</sub>Mg<sub>0.02</sub>Fe<sub>0.09</sub>O<sub>16</sub>. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

**Hibonite-(Fe)**  $(\text{Fe}, \text{Mg})\text{Al}_{12}\text{O}_{19}$ **Origin:** Allende meteorite.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1067s, 1014, 748, 728, 490, 432.**Source:** Ma (2010).**Comments:** The sample was characterized by electron microprobe data and electron microprobe analyses. The empirical formula of the sample used is  $(\text{Fe}^{2+}_{0.34}\text{Mg}_{0.27}\text{Na}_{0.12}\text{Al}_{0.11}\text{Ca}_{0.03})(\text{Al}_{11.77}\text{Si}_{0.23})\text{O}_{19}$ .**Hibonite**  $(\text{Ca}, \text{Ce})(\text{Al}, \text{Ti}, \text{Mg})_{12}\text{O}_{19}$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 532 nm Nd-YAG laser radiation. The laser radiation output power was 100 mW. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 910s, 873, 837, 796, 774, 741, 684, 640, 625, 565, 530, 489, 458, 450, 399, 332s, 274, 251, 209, 194sh.**Source:** Hofmeister et al. (2004).**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analysis. The crystal structure is solved.**Hidalgoite**  $\text{PbAl}_3(\text{SO}_4)(\text{AsO}_4)(\text{OH})_6$ **Origin:** Gold Hill mine, Tooele Co., Utah, USA.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3477, 3351sh, 3185sh, 1730, 1093, 1014s, 998sh, 879s, 853sh, 649, 631sh, 595, 528s, 513sh, 480, 433, 351sh, 334, 265, 234sh, 210s, 157, 142sh, 107.**Source:** Frost et al. (2011o).**Comments:** No independent analytical data are provided for the sample used.**Hieratite**  $\text{K}_2\text{SiF}_6$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power was between 80 and 200 mW.**Raman shifts (cm<sup>-1</sup>):** 655s, 478w, 408.**Source:** Rissom et al. (2008).**Comments:** The sample was characterized by powder X-ray diffraction data.

**Hilarionite**  $\text{Fe}^{3+}_2(\text{SO}_4)(\text{AsO}_4)(\text{OH})_6\text{H}_2\text{O}$ **Origin:** Hilarion Mine, Lavrion, Greece (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514 nm diode laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 1015s, 877sh, 843sh, 807, 585w, 495, 448sh, 390w, 365, 292, 191, 143sh, 123.**Source:** Liu et al. (2017).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.**Hingganite-(Y)**  $\text{BeY}(\text{SiO}_4)(\text{OH})$ **Origin:** Oppach, Lusatian Mts., Germany.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 45 mW.**Raman shifts (cm<sup>-1</sup>):** 3540, 922, 724, 332w.**Source:** Thomas and Davidson (2017).**Comments:** The sample was characterized by electron microprobe analyses. Fluorescence lines are excluded.**Hinsdalite**  $\text{PbAl}_3(\text{SO}_4)(\text{PO}_4)(\text{OH})_6$ **Origin:** Sylvester mine, Zeehan, Tasmania, Australia.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3603sh, 3472w, 3247w, 1021s, 1007s, 997sh, 982s, 930w, 614, 581sh, 506, 463, 374, 279sh, 250s, 187, 143, 108.**Source:** Frost et al. (2011k).**Comments:** No independent analytical data are provided for the sample used.**Hiortdahlite**  $(\text{Na,Ca})_2\text{Ca}_4\text{Zr}(\text{Mn,Ti,Fe})(\text{Si}_2\text{O}_7)_2(\text{F,O})_4$ **Origin:** Langezundfjord, Norway.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 1047, 947s, 796, 661s, 258.**Source:** Sharygin et al. (1996a, b).**Comments:** No independent analytical data are provided for the sample used.**Hisingerite**  $\text{Fe}_2\text{Si}_2\text{O}_5(\text{OH})_4 \cdot 2\text{H}_2\text{O}$ **Origin:** McMurdo Dry Valleys, Antarctica.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 1055, 1031, 983, 899w, 863w, 782, 736, 666s, 546s, 504, 450, 388, 288, 236, 189, 145w, 121w.

**Source:** Edwards et al. (2004).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

### Hochelagaite $\text{CaNb}_4\text{O}_{11}\cdot8\text{H}_2\text{O}$

**Origin:** Mont Saint-Hilaire, Québec, Canada (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 925, 878s, 663s, 587, 477, 387, 325w, 300w, 234, 196sh.

**Source:** Haring and McDonald (2017).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

### Hoelite $\text{C}_{14}\text{H}_8\text{O}_2$

**Origin:** Kladno, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 3076w, 1665s, 1597, 1583, 1439w, 1387w, 1317, 1306w, 1239w, 1214, 1176s, 1146, 1080w, 1030s, 976w, 818w, 790w, 767, 682, 520w, 495w, 475, 437, 362, 238s.

**Source:** Jehlička et al. (2007b).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of hoelite see also Jehlička et al. (2009a).

### Hoganite $\text{Cu}(\text{CH}_3\text{COO})_2\cdot\text{H}_2\text{O}$

**Origin:** Potosi Pit, Broken Hill, Yancowinna Co., New South Wales, Australia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3478, 3024s, 2989, 2941s, 2922s, 2862, 2788, 1449, 1440, 1418, 1360, 948s, 938, 703, 684, 322s, 297s, 266, 252, 230, 212, 184.

**Source:** Musumeci and Frost (2007).

**Comments:** The sample was characterized by powder X-ray diffraction data and chemical analysis. The empirical formula of the sample used is  $\text{C}_4\text{H}_{7.89}\text{O}_{5.07}\text{Cu}_{1.00}\text{Fe}_{0.01}$ .

### Hogarthite $(\text{Na},\text{K})_2\text{CaTi}_2\text{Si}_{10}\text{O}_{26}\cdot8\text{H}_2\text{O}$

**Origin:** Poudrette (Demix) quarry, Mont Saint-Hilaire, Rouville RCM (Rouville Co.), Montérégie, Québec, Canada (type locality).

**Experimental details:** Raman scattering measurements have been performed with a laser beam perpendicular to the {010} cleavage of a single using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3607, 3411sh, 3239sh, 1608w, 1190, 1052, 942s, 902sh, 794w, 714w, 679, 548s, 448s, 295s, 258w, 225, 173, 135, 105.

**Source:** McDonald et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Na}_{0.78}\text{K}_{0.62}\square_{0.51}\text{Ca}_{0.09})\text{Ca}(\text{Ti}_{1.85}\text{Zr}_{0.09}\text{Nb}_{0.06})\text{Si}_{10.09}\text{O}_{26}\cdot8\text{H}_2\text{O}$ .

**Hohmannite**  $\text{Fe}^{3+}\text{O}(\text{SO}_4)_2\cdot8\text{H}_2\text{O}$

**Origin:** Sierra Gorda District, Antofagasta Province, Antofagasta Region, Chile.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was less than 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 3495sh, 3438w, 3292sh, 3204w, 1204w, 1166w, 1125, 1098s, 1075w, 1058, 1031s, 1018, 659w, 628w, 605w, 580w, 496w, 470w, 400s, 334s, 258s, 245sh, 227sh, 198, 163, 144w, 129w, 73, 49.

**Source:** Ventruti et al. (2015).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data. The crystal structure is solved.

**Holdawayite**  $\text{Mn}^{2+}\text{}_6(\text{CO}_3)_2(\text{OH})_7(\text{Cl},\text{OH})$

**Origin:** Udachnaya-East kimberlite, Yakutia, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 1087s, ~700.

**Source:** Mernagh et al. (2011).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts have been determined for a polymineral aggregate. The Raman shifts of holdawayite from the RRUFF Project database (sample R090029) are: 1087s, 900, 701, 222, 164, 151.

**Holfertite**  $(\text{UO}_2)_{1.75}\text{Ca}_{0.25}\text{TiO}_4\cdot3\text{H}_2\text{O}$

**Origin:** Starvation Canyon, Thomas Range, Juab Co., Utah, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3500w, 3406sh, 2925w, 2866sh, 1628w, 1555sh, 1128w, 828s, 749s, 641sh, 474, 389s, 328, 257, 201sh, 144.

**Source:** Frost (2011a).

**Comments:** No independent analytical data are provided for the sample used.

**Hollandite**  $\text{Ba}(\text{Mn}^{4+}\text{}_6\text{Mn}^{3+}\text{}_2)\text{O}_{16}$

**Origin:** Jhabua district, Madhya Pradesh, India.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed in the spectral region from 10 to 1200 cm<sup>-1</sup> using 514.5 nm

$\text{Ar}^+$  laser radiation. The nominal laser radiation power was 10 mW. A nearly 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 705w, 628, 586, 558w, 507, 395w.

**Source:** Julien et al. (2004).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Hollingworthite RhAsS

**Origin:** No data.

**Experimental details:** Experimental details are not indicated. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1093w, 986w, 557w, 381sh, 360s, 347sh, 283, 272sh, 256s, 214, 146, 77sh.

**Source:** Bakker (2014).

**Comments:** The sample was characterized by electron microprobe data. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

### Holmquistite $\square\text{Li}_2(\text{Mg}_3\text{Al}_2)\text{Si}_8\text{O}_{22}(\text{OH})_2$

**Origin:** Martin Marietta quarry, Bessemer, North Carolina, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3661s, 3646s, 3631s, 3614, 1127, 1102sh, 1085s, 1045sh, 1022s, 791, 753, 694sh, 679s, 613, 582sh, 565sh, 551, 530sh, 502, 471, 456, 423, 408sh, 390s, 343, 309w, 297.

**Source:** Kloporgge et al. (2001a).

**Comments:** The sample was characterized by powder X-ray diffraction data and qualitative electron-microprobe analysis. The analytical data are insufficient for the mineral identification. For the Raman spectrum of holmquistite see also Kloporgge et al. (2001c).

### Honessite $(\text{Ni}_{1-x}\text{Fe}^{3+})_x(\text{SO}_4)_{x/2}(\text{OH})_2 \cdot n\text{H}_2\text{O}$ ( $x < 0.5$ , $n < 3x/2$ )

**Origin:** Linden, Upper Mississippi Valley district, Iowa Co., Wisconsin, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3614w, 2988sh, 2956, 2244, 1061w, 973, 852w, 527s, 460, 167w.

**Source:** Bindi et al. (2015a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $[(\text{Ni}^{2+})_{0.902}\text{Ca}^{2+}_{0.002})(\text{Co}^{3+}_{0.072}\text{Fe}^{3+}_{0.024})](\text{OH})_{1.884}\text{Cl}_{0.012}(\text{H}_2\text{O})_{0.004}(\text{SO}_4)_{0.100} \cdot 0.900\text{H}_2\text{O}$ .

### Hopeite $\text{Zn}_3(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$

**Origin:** Kabwe (Broken Hill)mine, Kabwe district, Central province, Zambia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power at the sample was 1 mW. The

Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3456w, 3247sh, 1150, 1059w, 1000sh, 995s, 940.

**Source:** Frost (2004a).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of hopeite see also O'Neill et al. (2006).

### **Hopeite Zn<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>·4H<sub>2</sub>O**

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1149, 1059, 998s, 942, 598, 368sh, 315.

**Source:** O'Neill et al. (2006).

**Comments:** The sample was characterized by powder X-ray diffraction data, but no independent analytical data are provided for the sample used. For the Raman spectrum of hopeite see also Frost (2004a).

### **Hörnesite Mg<sub>3</sub>(AsO<sub>4</sub>)<sub>2</sub>·8H<sub>2</sub>O**

**Origin:** Allchar (Alšar) deposit, Rožde, Kavadarci, Republic of Macedonia.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 875w, 808s, 468w, 430, 403, 365, 301w, 271, 262sh, 242, 205, 180w, 158, 138.

**Source:** Makreski et al. (2015b).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of hörnesite see also Frost et al. (2003g).

### **Hsianghualite Li<sub>2</sub>Ca<sub>3</sub>Be<sub>3</sub>(SiO<sub>4</sub>)<sub>3</sub>F<sub>2</sub>**

**Origin:** Xianghualing (Hsianghualing) mine, Linwu Co., Hunan province, China (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power was in the range from 300 to 380 mW.

**Raman shifts (cm<sup>-1</sup>):** 930, 894.

**Source:** Yuran and Li (1998).

**Comments:** No independent analytical data are provided for the sample used.

### **Huanghoite-(Ce) BaCe(CO<sub>3</sub>)<sub>2</sub>F**

**Origin:** Bayan Obo deposit, Baotou prefecture, Inner Mongolia Autonomous Region, China (type locality).

**Experimental details:** Raman scattering measurements have been performed using 488 nm laser radiation. The nominal laser radiation power was 300 mW. Raman spectrum was obtained in the spectral regions from 200 to 1200 cm<sup>-1</sup> and from 1300 to 3200 cm<sup>-1</sup>.

**Raman shifts (cm<sup>-1</sup>):** 2746, 2718sh, 2183, 1840w, 1596, 1525, 1374sh, 1089s, 720, 695, 649, 354, 273, 224, 106.

**Source:** Hong et al. (1999).

**Comments:** No independent analytical data are provided for the sample used. Raman bands in the range from 1300 to 2800 cm<sup>-1</sup> are mainly due to luminescence.

### Huanzalaite Mg(WO<sub>4</sub>)

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 2 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 917s, 809, 713, 684w, 552, 518, 420, 405w, 385w, 352, 314w, 294, 277, 267sh, 215w, 185, 156, 97s.

**Source:** Ruiz-Fuertes et al. (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Hubeite Ca<sub>2</sub>Mn<sup>2+</sup>Fe<sup>3+</sup>Si<sub>4</sub>O<sub>12</sub>(OH)·2H<sub>2</sub>O

**Origin:** Fengjiashan Mine, Daye Co., Huangshi prefecture, Hubei province, China (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The nominal laser radiation power was 0.23 mW.

**Raman shifts (cm<sup>-1</sup>):** 1083w, 1033, 966s, 912w, 899, 892, 864, 740, 664s, 575, 498, 489s, 468, 406sh, 400s, 366s, 292, 254, 195, 176, 145, 125, 117.

**Source:** Ferras et al. (2016).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

### Hübnerite Mn<sup>2+</sup>(WO<sub>4</sub>)

**Origin: Synthetic.**

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 685 nm Nd-YAG laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 885, 775, 697, 672, 543, 509, 445, 395, 353, 325, 290, 255, 202, 174, 161, 126.

**Source:** Frost et al. (2004b).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of hübnriter see also Kloprogge et al. (2004b) and Almeida et al. (2012).

### Hughesite Na<sub>3</sub>AlV<sub>10</sub>O<sub>28</sub>·22H<sub>2</sub>O

**Origin:** Sunday mine, Gypsum valley, San Miguel Co., Colorado, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal with the laser beam perpendicular to the (001) cleavage surface (orientation 1) and with the laser beam parallel to the cleavage surface (orientation 2) in the spectral region from 100 to

1500 cm<sup>-1</sup> using 632 nm He-Ne laser radiation. The nominal laser radiation power was 1 mW and 0.5 mW, respectively.

**Raman shifts (cm<sup>-1</sup>):** 1007s, 994sh, 972, 959sh, 945sh, 877w, 596, 471w, 363, 319, 270sh, 247, 235, 218w, 201sh, 192 (orientation 1); 999s, 972s, 854, 591, 469w, 362sh, 318, 260, 231w, 214w, 182 (orientation 2).

**Source:** Rakovan et al. (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is Na<sub>2.99</sub>Al<sub>1.05</sub>(V<sub>10</sub>O<sub>28</sub>)·22H<sub>2</sub>O.

### Humberstonite K<sub>3</sub>Na<sub>7</sub>Mg<sub>2</sub>(SO<sub>4</sub>)<sub>6</sub>(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O

**Origin:** Artificial (a component of gypsum-based plaster).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm diode laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1067, 1048, 1013, 723, 632, 183.

**Source:** Morillas et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Humboldtine Fe<sup>2+</sup>(C<sub>2</sub>O<sub>4</sub>)·2H<sub>2</sub>O

**Origin:** Bohemia, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3315, 1708w, 1555w, 1468s, 1450sh, 913, 856w, 582, 518, 293w, 246s, 203s.

**Source:** Frost (2004d).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of humboldtine see also Frost and Weier (2003), Echigo and Kimata (2008), and D'Antonio et al. (2009).

### Humite Mg<sub>7</sub>(SiO<sub>4</sub>)<sub>3</sub>(F,OH)<sub>2</sub>

**Origin:** Monte Somma, Somma-Vesuvius complex, Naples, Italy.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3576, 3572, 3560, 966, 930, 876, 859, 844, 831, 784, 757, 747, 606, 587, 570, 549, 547, 539, 442, 428, 391.

**Source:** Frost et al. (2007k).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The empirical formula of the sample used is Mg<sub>6.33</sub>Fe<sup>2+</sup><sub>0.50</sub>(SiO<sub>4</sub>)<sub>3</sub>(OH)<sub>1.66</sub>, which corresponds to the OH-analogue of humite.

**Humite**  $Mg_7(SiO_4)_3(F,OH)_2$ 

**Origin:** Monte Somma, Somma-Vesuvius complex, Naples, Italy.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3576, 3572, 3560, 966, 930, 876, 859, 844, 831, 784, 757, 747, 606, 587, 570, 549, 547, 539, 442, 428, 391.

**Source:** Frost et al. (2007k).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The empirical formula of the sample used is  $Mg_{6.33}Fe^{2+}_{0.50}(SiO_4)_3(OH)_{1.66}$ , which corresponds to the OH-analogue of humite.

**Hummerite**  $KMgV^{5+}_5O_{14}\cdot 8H_2O$ 

**Origin:** Hummer mine, Paradox valley, Montrose Co., Colorado, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3599, 3526, 3416, 3404, 3296, 3230, 3223, 2929, 2902, 1621, 1600, 999s, 962s, 833w, 817sh, 590, 532, 442w, 360sh, 326s, 314sh, 254sh, 241, 227sh, 208, 183s, 146.

**Source:** Frost et al. (2004e, 2005a).

**Comments:** No independent analytical data are provided for the sample used.

**Hungchaoite**  $MgB_4O_5(OH)_4\cdot 7H_2O$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample in the spectral region from 300 to 1800 cm<sup>-1</sup> using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 1628w, 1352, 1045, 949s, 897w, 855s, 816, 787s, 716w, 583s, 556w, 519, 491s, 450, 408s, 371, 345, 316s.

**Source:** Li et al. (1995) and Jia et al. (2001).

**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Huntite**  $CaMg_3(CO_3)_4$ 

**Origin:** No data.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed in the spectral region from 50 to 1200 cm<sup>-1</sup> using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 2905w, 1761w, 1459w, 1123s, 878, 742w, 723, 705w, 386w, 364w, 316, 272, 253, 231w, 155, 118.

**Source:** Edwards et al. (2005).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of huntite see also Scheetz and White (1977).

**Hureaulite**  $Mn^{2+} \cdot 5(PO_3OH)_2(PO_4)_2 \cdot 4H_2O$

**Origin:** Cigana mine, Conselheiro Pena, Rio Doce valley, Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm Nd-YAG laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3424, 3322, 3185, 2973sh, 2818, 1648, 1571, 1109sh, 1083, 1047, 1024, 1007sh, 989, 950, 941sh, 778w, 726, 598sh, 582, 564sh, 543sh, 531, 455, 414, 398sh, 381, 304w, 267w, 237sh, 221w, 194w, 155w, 137w, 120w, 104w.

**Source:** Frost et al. (2013aj).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. Powder X-ray diffraction data are not provided in the cited paper. The empirical formula of the sample used is  $(Mn_{3.23}Fe_{1.04}Ca_{0.19}Mg_{0.13})(PO_4,HPO_4)_{4.13}(OH,H_2O)_x$ , which indicates a significant deficit of (Mn,Fe,Ca,Mg)-cations.

**Hurlbutite**  $CaBe_2(PO_4)_2$

**Origin:** Nanping no. 31 granitic pegmatite dyke, Fujian province, southeastern China.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample. No other details are indicated.

**Raman shifts (cm<sup>-1</sup>):** 1021, 587, 575, 550, 404, 132.

**Source:** Rao et al. (2011).

**Comments:** The sample was characterized by electron microprobe analyses.

**Hydroboracite**  $CaMg[B_3O_4(OH)_3]_2 \cdot 3H_2O$

**Origin:** Kohnstein quarry, Thuringia, Germany.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3632s, 3563s, 3551sh, 3507s, 3384sh, 3371, 3255, 3138sh, 3076, 1685w, 1433w, 1394, 1379, 1318, 1268w, 1229, 1157, 1144sh, 1063sh, 1039s, 955w, 925, 910sh, 869w, 846, 825, 753, 730, 721sh, 696sh, 647, 612w, 582, 560s, 556sh, 526w, 491, 478sh, 459, 437, 421sh, 355sh, 342, 330sh, 304, 243, 229, 212, 168, 159sh, 135.

**Source:** Frost et al. (2014af).

**Comments:** No independent analytical data are provided for the sample used.

**Hydrocalumite**  $Ca_4Al_2(OH)_{12}(Cl,CO_3,OH)_2 \cdot 4H_2O$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power was 200 mW. The

Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1086, 1078sh, 712, 704sh, 531, 397, 359, 296sh, 281, 271sh.

**Source:** Frost et al. (2011j).

**Comments:** Questionable data: Raman spectra of samples with different Ca:Al ratios (from 2:1 to 4:1) are almost identical. According to powder X-ray diffraction data, the samples used may contain admixed calcite.

### Hydrocerussite Pb<sub>3</sub>(CO<sub>3</sub>)<sub>2</sub>(OH)<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed in the spectral region from 50 to 3600 cm<sup>-1</sup> using 1064 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1731w, 1467sh, 1365, 1050s, 862w, 837w, 707sh, 693sh, 679, 411, 321, 267w, 150sh, 113.

**Source:** Ciomartan et al. (1996).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of hydrocerussite see also Frost et al. (2003e) and Bouchard and Smith (2003).

### Hydrocerussite Pb<sub>3</sub>(CO<sub>3</sub>)<sub>2</sub>(OH)<sub>2</sub>

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3576, 3536w, 1736, 1705, 1679, 1479w, 1420w, 1378w, 1375w, 1365sh, 1053s, 1031sh, 887w, 866w, 837w, 737, 694w, 681, 671w, 417, 391, 376, 318, 221, 177w, 152.

**Source:** Frost et al. (2003e).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of hydrocerussite see also Ciomartan et al. (1996) and Bouchard and Smith (2003).

### Hydrodelhayelite-related compound KCa<sub>2</sub>Na(Si<sub>8</sub>O<sub>19</sub>)·5H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3500 (broad), 3300sh, 1636w, 1174, 1125sh, 1103, 848w, 783, 697, 610s, 496sh, 469, 437, 376, 351w, 317, 286, 240w, 190, 156, 127, 113, 98sh, 80sh.

**Source:** Cadoni and Ferraris (2009).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and semiquantitative electron microprobe analyses. The crystal structure is solved. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum

### Hydrohalite $\text{NaCl}\cdot 2\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample at  $-190^\circ\text{C}$ , in the spectral region from 2800 to  $4000\text{ cm}^{-1}$ , using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was between 1 and 1.5 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3536, 3432, 3418, 3402, 3321w, 3300w.

**Source:** Baumgartner and Bakker (2010).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of hydrohalite see also Bakker (2004), Sakurai et al. (2010), and Okotrub and Surovtsev (2013).

### Hydrohonessite $(\text{Ni}_{1-x}\text{Fe}^{3+}_x)(\text{SO}_4)_{x/2}(\text{OH})_2\cdot n\text{H}_2\text{O}$ ( $x < 0.5$ , $n > 3x/2$ )

**Origin:** Kambalda, Western Australia, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power at the sample was less than 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3493s, 3405, 1638w, 1135, 1115sh, 1008s, 671, 619, 579, 493, 414, 318w, 209w, 182, 164.

**Source:** Frost et al. (2003h).

**Comments:** No independent analytical data are provided for the sample used.

### Hydromagnesite $\text{Mg}_5(\text{CO}_3)_4(\text{OH})_2\cdot 4\text{H}_2\text{O}$

**Origin:** Salda Golulake, Turkey.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 2904w, 1871w, 1521w, 1487w, 1451w, 1119s, 757, 727, 706, 669w, 653sh, 329, 247, 232, 202, 184, 147.

**Source:** Edwards et al. (2005).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of hydromagnesite see also Frost (2011d) and Kristova et al. (2014).

### Hydroniumjarosite $(\text{H}_3\text{O})\text{Fe}^{3+}_3(\text{SO}_4)_2(\text{OH})_6$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power at the sample was in the range from 0.22 to 1 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3431, 3365, 2522, 2420, 1167, 1101s, 1019, 1013, 769, 633, 619, 565, 458, 420, 359, 281, 227.

**Source:** Murphy et al. (2009).

**Comments:** The sample was characterized by powder X-ray diffraction data and inductively coupled plasma-optical emission spectrometry. The empirical formula of the sample used is  $(\text{H}_3\text{O})\text{Fe}^{3+}_{2.93}(\text{SO}_4)_2(\text{OH})_{6.79}(\text{H}_2\text{O})_{0.2}$ . For the Raman spectra of hydroniumjarosite see also Frost et al. (2006r), Plášil et al. (2014b), and Apopei et al. (2014a).

**Hydroniumjarosite**  $(\text{H}_3\text{O})\text{Fe}^{3+}_3(\text{SO}_4)_2(\text{OH})_6$ 

**Origin:** Cerros Pintados, Pampa del Tamarugal, Iquique Province, Tarapacá Region, Chile.

**Experimental details:** Raman scattering measurements have been performed on an arbitrary oriented single crystal using 532 nm laser radiation. The nominal laser radiation power was 3 mW. Raman spectrum was obtained in the spectral region from 50 to 4000  $\text{cm}^{-1}$ .

**Raman shifts ( $\text{cm}^{-1}$ ):** 2989w, 2941w, 2878, 2328w, 2248, 2002w, 1742w, 1678w, 1622w, 1477w, 1449w, 1329w, 1164, 1103s, 1012s, 859w, 812w, 722w, 643sh, 620s, 569, 497w, 454sh, 424s, 367sh, 227s, 172w, 135, 62w.

**Source:** Plášil et al. (2014b).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{H}_3\text{O})^{+}_{0.77}\text{Na}_{0.20}\text{K}_{0.02}(\text{Fe}_{2.95}\text{Al}_{0.03})(\text{OH})_{6.12}[(\text{SO}_4)_{1.97}(\text{SiO}_4)_{0.03}]$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectra of hydroniumjarosite see also Frost et al. (2006r), Murphy et al. (2009), and Apopei et al. (2014a).

**Hydroromarchite**  $\text{Sn}^{2+}_3\text{O}_2(\text{OH})_2$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm laser radiation. The nominal laser radiation power was 400 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts ( $\text{cm}^{-1}$ ):** 264w, 226s, 184w, 53s.

**Source:** Chen and Grandbois (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Hydrotalcite-2H**  $\text{Mg}_6\text{Al}_2(\text{CO}_3)(\text{OH})_{16}\cdot 4\text{H}_2\text{O}$ 

**Origin:** Kovdor massif, Kola Peninsula, Russia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. Raman spectrum was obtained in the spectral region from 200 to 4000  $\text{cm}^{-1}$ . The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3573sh, 3487, 3371sh, 1237sh, 1223w, 1200w, 1101sh, 1064s, 1059sh, 1045sh, 973, 696w, 595sh, 558s, 484w, 408w, 151s, 111s.

**Source:** Frost et al. (2014y).

**Comments:** No independent analytical data are provided for the sample used. Based on the origin of the sample and its morphological features, one cannot exclude that it is quintinite.

**Hydrotalcite**  $\text{Mg}_6\text{Al}_2(\text{CO}_3)(\text{OH})_{16}\cdot 4\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample pressed as pellet using 1064 nm Nd-YAG laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1403, 1355, 1134(?), 1110, 1053, 1044s, 982, 936, 712, 694, 626, 611, 461, 453.

**Source:** Klopogge et al. (2002).

**Comments:** The sample was characterized by powder X-ray diffraction data. The empirical formula of the sample used is  $Mg_{5.8}Al_{2.2}(OH)_{16}(CO_3)_{0.92}(NO_3)_{0.26}\cdot nH_2O$ . For the Raman spectrum of hydrotalcite see also Palmer et al. (2011).

### Hydrotungstite $WO_2(OH)_2\cdot H_2O$

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on oriented and arbitrarily oriented samples in the spectral region from 150 to 1050 cm<sup>-1</sup> using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power was in the range from 0.06 to 0.15 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 956s, 677s, 661s, 580sh, 275w, 225w.

**Source:** Tarassov et al. (2002).

**Comments:** The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

### Hydroxyapophyllite-(K) $KCa_4Si_8O_{20}(OH,F)\cdot 8H_2O$

**Origin:** Pune (Poonah) district, Maharashtra State, India.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3626w, 3614sh, 3557s, 3365sh, 3085sh, 3007s, 2893sh, 2813sh, 1705w, 1683sh, 1626w, 1523w, 1114sh, 1086sh, 1059s, 1043sh, 1007w, 970w, 846w, 791, 765, 663s, 633sh, 583s, 538, 511, 485w, 462w, 431s, 409sh, 373, 337, 325sh, 297, 266w, 228, 209s, 185, 161, 132, 123, 106.

**Source:** Frost and Xi (2012o).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of hydroxyapophyllite-(K) see also Goryainov et al. (2012).

### Hydroxycalciobetafite (?) $(Ca,U)_2(Ti,Nb)_2O_6(OH)$

**Origin:** Antanifotsy, Betafo district, Madagascar.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 2184, 2075, 1956, 1584, 1456sh, 1327, 1161, 893, 810, 657, 601sh, 391, 325sh, 283, 218, 162, 149.

**Source:** Frost and Reddy (2010).

**Comments:** A metamict sample was used. For the Raman spectra of minerals and compounds related to the betafite group see also McMaster et al. (2013, 2014, 2015).

**Hydroxycalciomicrolite**  $\text{Ca}_{1.5}\text{Ta}_2\text{O}_6(\text{OH})$ 

**Origin:** Volta Grande pegmatite, Nazareno, Minas Gerais, Brazil (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm solid-state laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3614, 3586, 1028w, 892w, 803, 665, 638sh, 564sh, 519s, 440sh, 419, 398sh, 342, 311s, 285, 243, 230, 211, 195.

**Source:** Andrade et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Ca}_{1.48}\text{Na}_{0.06}\text{Mn}_{0.01})(\text{Ta}_{1.88}\text{Nb}_{0.11}\text{Sn}_{0.01})\text{O}_{6.00}[(\text{OH})_{0.76}\text{F}_{0.20}\text{O}_{0.04}]$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Hydroxycalciopyrochlore**  $(\text{Ca},\text{Na},\text{U},\square)_2(\text{Nb},\text{Ti})_2\text{O}_6(\text{OH})$ 

**Origin:** Bližná, Southwestern Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample in the spectral region from 70 to 6300 cm<sup>-1</sup> using 532.17 nm laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 3850, 3670sh, 2065s, 770, 635sh, 240, 95.

**Source:** Drábek et al. (2017).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe data. The empirical formula of the sample used is  $(\text{Ca}_{0.48}\text{Na}_{0.02}\text{Mg}_{0.06}\text{Mn}_{0.01}\text{Y}_{0.06}\text{REE}_{0.27}\text{Th}_{0.27}\text{U}_{0.01})(\text{Nb}_{1.06}\text{Ti}_{0.79}\text{Fe}_{0.14}\text{W}_{0.01})(\text{O}_{4.96}\text{OH}_{1.04})(\text{OH})_{0.81}\text{H}_2\text{O}$ . The Raman shifts were determined by us based on spectral curve analysis of the published spectrum. The band at 2065 cm<sup>-1</sup> may be due to fluorescence.

**Hydroxycalcioroméite**  $(\text{Ca},\text{Sb}^{3+})_2(\text{Sb}^{5+},\text{Ti})_2\text{O}_6(\text{OH})$ 

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3542sh, 3471w, 3328sh, 3200sh, 2920w, 2860w, 1965w, 1599w, 1447w, 1353w, 984, 806, 725, 611, 565, 517s, 507sh, 487sh, 400sh, 356, 300, 179sh, 150sh, 129s.

**Source:** Bahenne and Frost (2010b).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Hydroxyferroroméite**  $(\text{Fe}^{2+})_{1.5}\square_{0.5}\text{Sb}^{5+}_2\text{O}_6(\text{OH})$ 

**Origin:** Correc d'en Llinassos, Oms, Pyrénées-Orientales Department, France (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 532 nm laser radiation. The nominal laser radiation power was 80 mW.

**Raman shifts (cm<sup>-1</sup>):** 3634w, 3074w, 2936w, 1773w, 1706w, 1608, 709sh, 650s, 568sh, 466sh, 436, 358w, 271sh, 180.

**Source:** Mills et al. (2017b).

**Comments:** The sample was characterized by powder X-ray diffraction data, electron microprobe analyses, and X-ray photoelectron spectroscopy. The empirical formula of the sample used is  $(\text{Fe}^{2+})_{1.07}\text{Cu}^{2+}_{0.50}\text{Zn}_{0.03}\text{Sr}_{0.03}\text{Ca}_{0.01}\square_{0.36})(\text{Sb}^{5+}_{1.88}\text{Si}_{0.09}\text{Al}_{0.02}\text{As}_{0.01})\text{O}_6[(\text{OH})_{0.86}\text{O}_{0.14}]$ .

### Hydroxykenoelsmoreite ( $\square$ ,Pb)<sub>2</sub>(W,Fe<sup>3+</sup>,Al)<sub>2</sub>(O,OH)<sub>6</sub>(OH)

**Origin:** Masaka gold mine, Burundi (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 782 nm diode laser radiation. The nominal laser radiation power was 1.15 mW.

**Raman shifts (cm<sup>-1</sup>):** 3443, 2932w, 1610w, 929s, 853sh, 691, 476, 402, 298w, 225, 157.

**Source:** Mills et al. (2017a).

**Comments:** The sample was characterized by powder and single crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\square_{1.66}\text{Pb}_{0.315}\text{Ca}_{0.009}\text{Na}_{0.005}\text{K}_{0.003}\text{Ba}_{0.001})(\text{W}^{6+}_{1.487}\text{Fe}^{3+}_{0.357}\text{Al}_{0.156})[\text{O}_{4.119}(\text{OH})_{1.881}](\text{OH})$ .

### Hydroxylapatite Ca<sub>5</sub>(PO<sub>4</sub>)<sub>3</sub>OH

**Origin:** Tadano, Fukushima prefecture, Japan.

**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal thin section cut nearly perpendicular to the *c* axis using 532 nm laser radiation. The laser radiation output power was 11.8 mW.

**Raman shifts (cm<sup>-1</sup>):** 3561, 3537, 1080w, 1059, 1035, 968s, 612, 586, 449, 433.

**Source:** Banno et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is  $\text{Ca}_{5.022}(\text{P}_{2.943}\text{Si}_{0.024}\text{S}_{0.011})\text{O}_{11.960}(\text{OH}_{0.546}\text{F}_{0.406}\text{Cl}_{0.048})$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectra of hydroxylapatite see also Penel et al. (1998), Koutsopoulos (2002), O'Neill et al. (2006), and Pasteris et al. (2012).

### Hydroxylbastnäsite-(Ce) Ce(CO<sub>3</sub>)OH

**Origin:** Trimouns, Luzenac, France.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3637, 3567, 3492, 3257, 1475, 1431sh, 1415, 1100s, 1088s, 1082s, 1007, 872, 851, 786, 728w, 694, 665w, 582, 342, 257, 239sh, 195, 177, 156, 137, 118, 70w.

**Source:** Yang et al. (2008a).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Ce}_{0.50}\text{Nd}_{0.24}\text{La}_{0.23}\text{Y}_{0.03})(\text{CO}_3)[(\text{OH})_{0.65}\text{F}_{0.35}]$ . The Raman shifts were determined by us based on spectral curve analysis of the published spectrum. For the Raman spectra of hydroxylbastnäsite-(Ce) see also Frost and Dickfos (2007a) and Michiba et al. (2013).

### **Hydroxylchondrodite** $Mg_5(SiO_4)_2(OH)_2$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was about 60 mW.

**Raman shifts (cm<sup>-1</sup>):** 3571sh, 3554s, 3515s, 3226, 2930, 955, 921, 848sh, 835s, 754w, 723w, 597, 570, 535w, 473w, 420w, 368w, 327w, 282w, 222w.

**Source:** Lin et al. (1999).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of hydroxylchondrodite see also Mernagh et al. (1999).

### **Hydroxyclinohumite** $Mg_9(SiO_4)_4(OH)_2$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal in the spectral regions from 100 to 1600 cm<sup>-1</sup> and from 2700 to 4000 cm<sup>-1</sup> using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 3612w, 3580sh, 3564s, 3527s, 964, 856s, 847s, 838s, 826s, 765w, 737w, 716sh, 603, 583, 576w, 566w, 545w, 533sh, 499w, 468w, 456w, 430, 398w, 388sh, 378w, 364w, 342sh, 331w, 301w, 265w, 250w, 230w, 210w, 181w, 154w, 140w.

**Source:** Lin et al. (2000).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectrum of hydroxyclinohumite see also Hurai et al. (2014).

### **Hydroxyclinohumite** $Mg_9(SiO_4)_4F_2$

**Origin:** Namibwuste, Namibia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3579, 3570, 3560, 3412, 3390, 967, 877sh, 862s, 846, 831, 808w, 785, 760, 744, 607, 587.

**Source:** Frost et al. (2007k).

**Comments:** The sample described as “clinohumite” was characterized by powder X-ray diffraction data and electron microprobe analysis. Actually, the empirical formula  $Mg_{7.35}Fe^{2+}_{0.13}Ti_{0.08}Ca_{0.50}Al_{0.46}(SiO_4)_4Cl_{0.05}(OH)_{1.61}$  corresponds to cation-deficient hydroxyclinohumite.

### **Hydroxylegrewite** $Ca_9(SiO_4)_4(OH)_2$

**Origin:** Upper Chegem caldera, Northern Caucasus, Kabardino-Balkaria, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 514.5 nm laser radiation. The nominal laser radiation power was in the range from 30 to 50 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3550, 3475w, 923, 890w, 840w, 821sh, 814, 559, 527w, 419sh, 404, 394sh, 324w, 295, 256, 166, 160sh.

**Source:** Galuskin et al. (2012d).

**Comments:** The sample was characterized by powder and single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The sample used is a member of the solid-solution series  $\text{Ca}_9(\text{SiO}_4)_4(\text{F},\text{OH})_2$  with F:OH = 63:37.

### Hydroxylelestadite $\text{Ca}_5(\text{SiO}_4)_{1.5}(\text{SO}_4)_{1.5}\text{OH}$

**Origin:** Cioclovina Cave, řureanu Mts., Romania.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was 100 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3564, 3517sh, 1144, 1122, 1066w, 1002s, 954s, 853s, 642sh, 625, 579, 530, 462, 431sh, 397sh, 312w.

**Source:** Onac et al. (2006).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $\text{Ca}_{10.27}[(\text{SiO}_4)_{2.53}(\text{SO}_4)_{2.17}(\text{PO}_4)_{1.27}][(\text{OH})_{1.66}\text{F}_{0.21}\text{Cl}_{0.16}]$ . For the Raman spectrum of hydroxylelestadite see also Comodi et al. (1999).

### Hydroxylherderite $\text{CaBe}(\text{PO}_4)(\text{OH})$

**Origin:** Bennett pegmatite, Buckfield, Oxford Co., Maine, USA.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal with polarizers and without polarizers using 458 nm laser radiation. The laser radiation power at the sample was 18 mW. Polarized spectra were collected in scattering geometries with three different polarized angles, 0, 45 and 90° from an arbitrary reference plane.

**Raman shifts (cm<sup>-1</sup>):** 3620s, 3610sh, 3575sh, 3565s, 1142s, 1130sh, 1087w, 1005s, 985sh, 915, 910, 875sh, 770, 705sh, 680, 615sh, 598s, 590sh, 580, 532, 519, 448, 428w, 353w, 340w, 328w, 305w, 272w, 257w, 228w, 197w, 185w, 170w, 145w, 125w.

**Source:** Gatta et al. (2014).

**Comments:** The sample was characterized by single-crystal X-ray and neutron diffraction data, electron microprobe analyses and inductively coupled plasma-atomic emission spectroscopy. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Ca}_{1.01}\text{Na}_{0.01})(\text{Be}_{0.98}\text{Li}_{0.01})(\text{P}_{0.98}\text{Si}_{0.03})\text{O}_4[(\text{OH})_{0.67}\text{F}_{0.33}]$ . For the Raman spectrum of hydroxylherderite see also Frost et al. (2014a).

### Hydrozincite $\text{Zn}_5(\text{CO}_3)_2(\text{OH})_6$

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne or 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was 30 mW or less than 30 mW, respectively.

**Raman shifts (cm<sup>-1</sup>):** 1544, 1371, 1061s, 732, 704, 389, 340w, 230, 152s, 139, 121, 81.

**Source:** Bouchard and Smith (2003).

**Comments:** No independent analytical data are provided for the sample used.

**Hypersthene**  $(\text{Mg}, \text{Fe})\text{SiO}_3$ 

**Origin:** Pietra Nera, Agrigento, Sicilia, Italy.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm solid-state laser radiation. The laser radiation power is not indicated. A nearly 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1006s, 681s, 661, 339, 233, 129.

**Source:** Andò and Garzanti (2014).

**Comments:** No independent analytical data are provided for the sample used.

**Ianbruceite**  $\text{Zn}_2\text{O}[\text{AsO}_3(\text{OH})](\text{H}_2\text{O})_{3.53}$ 

**Origin:** Tsumeb mine, Otjikoto (Oshikoto) region, Namibia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was 12.5 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3600w, 3441sh, 3224w, 2740sh, 840s, 773sh, 534, 448, 420, 192.

**Source:** Cooper et al. (2012a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The crystal-chemical formula of the sample used is  $\text{K}_{0.02}(\text{Zn}_{1.93}\text{Fe}^{2+}_{0.03}\text{Al}_{0.02}\text{Mn}^{2+}_{0.01})(\text{OH})_{0.96}(\text{H}_2\text{O})(\text{As}^{5+}\text{O}_4)[\text{As}^{3+}(\text{OH})_2\text{O}]_{0.04}(\text{H}_2\text{O})_{1.96}$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Iangreyite**  $\text{Ca}_2\text{Al}_7(\text{PO}_4)_2(\text{PO}_3\text{OH})_2(\text{OH}, \text{F})_{15} \cdot 8\text{H}_2\text{O}$ 

**Origin:** Silver Coin mine, Nevada, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1345, 1200, 1095, 1078w, 1033, 1009s, 979, 923, 707, 622s, 510, 485w, 455, (377), 362, 338, 332, 271, 189s, 107, 114.

**Source:** Mills et al. (2011a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $\text{Ca}_{1.42}\text{K}_{0.22}\text{Na}_{0.09}\text{Ba}_{0.03}\text{Sr}_{0.01}\text{Al}_{6.51}\text{Mg}_{0.09}\text{Fe}_{0.02}\text{Cu}_{0.01}\text{Zn}_{0.01}\text{P}_{3.81}\text{F}_{5.24}\text{H}_{30.21}\text{O}_{33.76}$ . In the cited paper an erroneous figure of the Raman spectrum with displaced scale of Raman shifts is given. The Raman shifts listed above have been determined based on the analysis the correct spectral curve from the manuscript submitted to the Mineralogical Magazine, which was kindly provided by the authors.

**Ice**  $\text{H}_2\text{O}$ 

**Origin:** Artificial.

**Experimental details:** Raman scattering measurements have been performed at -190 °C on an arbitrarily oriented sample in the spectral region from 2800 to 4000 cm<sup>-1</sup> using 532.2 nm Nd-YAG laser radiation. The laser radiation power at the sample was in the range from 1 to 1.5 mW.

**Raman shifts (cm<sup>-1</sup>):** 3370sh, 3321w, 3218, 3090s.

**Source:** Baumgartner and Bakker (2010).

**Comments:** For the Raman spectra of ice see also Gigu  re and Harvey (1956) and Garcia et al. (2006).

The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

### Idaite $\text{Cu}_3\text{FeS}_4$

**Origin:** No data.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 466s, 403w, 356w, 265w, 209.

**Source:** Parker et al. (2008).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

### Idrialite $\text{C}_{22}\text{H}_{14}$

**Origin:** Idrija mercury ore field, External Dinarides, Slovenia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 1064 nm Nd-YAG and 785 nm diode laser radiations. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3049, 2905sh, 2891, 1617s, 1579s, 1445w, 1437sh, 1428sh, 1393s, 1375, 1367, 1352w, 1301, 1268, 1209, 1183, 1151, 1017s, 1009w, 911w, 960w, 825, 752s, 728sh, 710s, 679sh, 663, 642, 611, 599, 590sh, 579, 563sh, 552, 522, 498, 130 (?).

**Source:** Jehli  ka et al. (2006).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Ikaite $\text{Ca}(\text{CO}_3)\cdot 6\text{H}_2\text{O}$

**Origin:** Ika fjord, Ivigtut, southern Greenland (type locality).

**Experimental details:** Raman scattering measurements have been performed at -80 °C on an arbitrarily oriented sample in the spectral region from 400 to 4000 cm<sup>-1</sup> using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 8 mW.

**Raman shifts (cm<sup>-1</sup>):** 3421, 3240, 3182, 1483w, 1072s, 873w, 722.

**Source:** Coleyshaw et al. (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of ikaite see also Mikkelsen et al. (1999), Shahar et al. (2005), and S  nchez-Pastor et al. (2016).

### Ikaite $\text{Ca}(\text{CO}_3)\cdot 6\text{H}_2\text{O}$

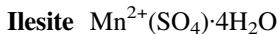
**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed at 4°C on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 10 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3432, 3336, 3257sh, 3165sh, 1066s, 715, 263, 214sh, 199s, 183, 156sh, 137, 116sh.

**Source:** S  nchez-Pastor et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction analysis. For the Raman spectra of ikaite see also Mikkelsen et al. (1999), Coleyshaw et al. (2003), and Shahar et al. (2005).



**Origin:** Artificial (degradation product from black slag).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample in the spectral region from 200 to 2000  $\text{cm}^{-1}$  using 514.5 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts ( $\text{cm}^{-1}$ ):** 1024s, 622, 488, 427, 263, 207.

**Source:** Gómez-Nubla et al. (2013).

**Comments:** No independent analytical data are provided for the sample used.



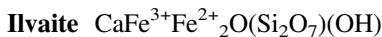
**Origin:** Lunar basalt from Taurus–Littrow floor, 15 m northeast of a 10 m diameter crater with blocky ejecta.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts ( $\text{cm}^{-1}$ ):** 679s, 449, 370, 330, 254, 227, 200w, 190w, 162w.

**Source:** Ling et al. (2011).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of ilmenite see also Andò and Garzanti (2014).



**Origin:** Sasa, Macedonia.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample in the spectral region from 100 to 1300  $\text{cm}^{-1}$  using 514.5 nm  $Ar^+$  laser radiation. The laser radiation power is not indicated.

**Raman shifts ( $\text{cm}^{-1}$ ):** 1084s, 614s, 563w, 530w, 492w, 440w, 370w, 223s, 153w, 140.

**Source:** Makreski et al. (2007).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectrum of ilvaite see also Jovanovski et al. (2009).



**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 1024 nm laser radiation. The nominal laser radiation power was 800 mW. A 180°-scattering geometry was employed.

**Raman shifts ( $\text{cm}^{-1}$ ):** 959, 925, 866, 698w, 550sh, 514s, 400sh, 367s, 251, 118s, 107.

**Source:** Creton et al. (2008).

**Comments:** The sample was characterized by inductive coupled plasma atomic emission spectroscopy analysis. The wavelength of 1024 nm indicated by the authors may be a misprint. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

**Inderite**  $MgB_3O_3(OH)_5 \cdot 5H_2O$ **Origin:** Boron, Kern Co., California, USA.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3616s, 3479sh, 3429, 3365shg, 3292w, 3254, 3127, 3067, 2988w, 2931, 2843w, 2750w, 1397w, 1349, 1282sh, 1249, 1195, 1167sh, 1138sh, 1058w, 1006, 948s, 879, 811w, 743, 664, 637, 580, 551, 492s, 440, 420, 379, 347w, 313, 248w, 193, 166.**Source:** Kloporgge and Frost (1999a).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of inderite see also Frost et al. (2013f).**Indite**  $FeIn_2S_4$ **Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 785 nm diode laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 370s, 334sh, 329sh, 313, 271sh, 253s, 231sh, 182, 167w, 96, 82.**Source:** Guc et al. (2012).**Comments:** The sample was characterized by electron microprobe analysis.**Inesite**  $Ca_2Mn^{2+}Si_{10}O_{28}(OH)_2 \cdot 5H_2O$ **Origin:** N'chwaning mine, Kalahari Manganese Fields, South Africa.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3661sh, 3642, 3612sh, 3496sh, 3420, 3362sh, 3300sh, 3246sh, 1856sh, 1825, 1775, 1730sh, 1671sh, 1653, 1608, 1546sh, 1383sh, 1365w, 1207sh, 1090sh, 1067sh, 1051sh, 1031s, 997sh, 958w, 933, 907sh, 764sh, 736sh, 716sh, 684sh, 653s, 631sh, 608sh, 467sh, 448sh, 428sh, 410, 374sh, 354, 301sh, 283, 248, 218, 156sh, 140s, 114s.**Source:** Frost et al. (2014r).**Comments:** No independent analytical data are provided for the sample used.**Innsbruckite**  $Mn_{33}(Si_2O_5)_{14}(OH)_{38}$ **Origin:** Staffelsee (Geier), Navis valley, Tyrol, Austria (type locality).**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample in the spectral regions from 100 to 1250 cm<sup>-1</sup> and from 3520 to 3700 cm<sup>-1</sup> using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 30 mW. Raman spectra were collected inscattering geometries with a 90° sample rotation between the data collections.

**Raman shifts (cm<sup>-1</sup>):** 1190w, 1032s, 1016w, 1010w, 998w, 792w, 777w, 717w, 693w, 671w, 649, 629, 609, 477w, 455w, 417, 405, 394, 360w, 352w, 336sh, 327w, 322w, 315, 312w, 305sh, 288, 277, 259, 252, 231, 221, 199sh, 193, 185, 178sh, 169, 160, 137, 131sh, 118w, 114w, 108w.

**Source:** Krüger et al. (2014).

**Comments:** The sample was characterized by single-crystal synchrotron radiation diffraction analysis and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is Mn<sub>31.58</sub>Fe<sub>0.19</sub>Mg<sub>1.29</sub>Si<sub>27.82</sub>Al<sub>0.20</sub>O<sub>108</sub>H<sub>37.97</sub>.

### Insizwaite PtBi<sub>2</sub>

**Origin:** No data.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532.1 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 126, 114s, 96.

**Source:** Bakker (2014).

**Comments:** No independent analytical data are provided for the sample used.

### Inyoite CaB<sub>3</sub>O<sub>3</sub>(OH)<sub>5</sub>·4H<sub>2</sub>O

**Origin:** Mount Blanco mine, Black Mountains, Death Valley, Inyo Co., California, USA.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3444w, 3389sh, 3153w, 2828w, 1689sh, 1656w, 1430w, 1376w, 1336sh, 1322w, 1254w, 1204w, 1177sh, 1062w, 1048sh, 1013w, 971sh, 957, 925sh, 910, 808w, 731, 615s, 596sh, 535, 521sh, 503, 474sh, 465, 408, 388, 352, 326w, 268sh, 258w, 206sh, 192sh, 182sh, 1721, 160sh.

**Source:** Frost et al. (2015i).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

### Iodargyrite AgI

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal with the *c* axis normal to the scattered plane using 457.9, 488.0, 546.1 nm Ar<sup>+</sup> and 568.2, 647.1 nm Kr<sup>+</sup> laser radiations. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 104w, 85w, 37w, 17s.

**Source:** Hanson et al. (1975).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts are given for the *z*(yy)–*z* scattering geometry.

**Iowaite**  $Mg_6Fe^{3+} \cdot 2(OH)_{16}Cl_2 \cdot 4H_2O$ **Origin:** Australia.**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3720w, 3707, 3700w, 3691sh, 3685, 3674sh.**Source:** Reddy et al. (2010).**Comments:** The sample was characterized by electron paramagnetic resonance. Raman shifts are given for region from 3600 to 3740 cm<sup>-1</sup>.**Iowaite**  $Mg_6Fe^{3+} \cdot 2(OH)_{16}Cl_2 \cdot 4H_2O$ **Origin:** Mount Keith, Western Australia.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 708sh, 690, 620, 527s, 495sh, 456, 430w, 386, 348w, 312, 298w, 282, 231, 188, 153, 146w, 140w, 132w.**Source:** Frost et al. (2010d).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of iowaite see also Reddy et al. (2010).**Iranite**  $CuPb_{10}(CrO_4)_6(SiO_4)_2(OH)_2$ **Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm Nd-YAG laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 916sh, 891sh, 865s, 846s, 818s, 790, 535sh, 404, 389, 380sh, 369s, 354sh, 343, 333, 307, 240, 222, 196, 163, 139.**Source:** Frost (2004c).**Comments:** No independent analytical data are provided for the sample used.**Irarsite** IrAsS**Origin:** Santa Elena Nappe, Costa Rica.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 399, 375s, 353s, 289, 263s, 219, 211sh, 177, 145.**Source:** Zaccarini et al. (2010).**Comments:** The sample was characterized by electron microprobe analyses. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Iriginitie**  $(\text{UO}_2)\text{Mo}^{6+}_2\text{O}_7 \cdot 3\text{H}_2\text{O}$ 

**Origin:** Hervey's Range deposit, 55 km W of Townsville, Queensland, Australia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm Nd-YAG laser radiation. The laser radiation power at the sample was 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 965sh, 950s, 888, 826sh, 818, 693sh, 668, 487s, 457, 413, 373, 337, 301, 246s, 198, 164s.

**Source:** Frost et al. (2004c).

**Comments:** No independent quantitative analytical data are provided for the sample used.

**Irinarassite**  $\text{Ca}_3\text{Sn}_2(\text{SiAl}_2)\text{O}_{12}$ 

**Origin:** Upper Chegem caldera, Northern Caucasus, Kabardino-Balkaria, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample in the spectral region from 100 to 4000 cm<sup>-1</sup> using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation output power was in the range from 30 to 50 mW. A 0°-scattering geometry was employed. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 915w, 818, 787, 739, 578, 503s, 420, 316, 269sh, 250, 197, 156, 112w.

**Source:** Galuskina et al. (2013a).

**Comments:** The sample was characterized by single-crystal electron backscatter diffraction and electron microprobe analyses. The empirical formula of the sample used is  $(\text{Ca}_{2.965}\text{Fe}^{2+}_{0.035})(\text{Sn}_{1.016}\text{Zr}_{0.410}\text{Ti}_{0.262}\text{Sb}^{5+}_{0.237}\text{Fe}^{2+}_{0.035}\text{U}^{6+}_{0.017}\text{Sc}_{0.014}\text{Hf}_{0.006}\text{Nb}_{0.004})(\text{Al}_{1.386}\text{Fe}^{3+}_{0.804}\text{Si}_{0.446}\text{Ti}^{4+}_{0.364})\text{O}_{12}$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Iron** Fe

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation output power was 4–5 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** (187), 139w.

**Source:** Campos et al. (2004b).

**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

**Iseite**  $\text{Mn}_2\text{Mo}_3\text{O}_8$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed at 400 K on a powdered sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 920s, 870, 815, 425w, 360, 325, 260w.

**Source:** Das et al. (2009).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Isocubanite** CuFe<sub>2</sub>S<sub>3</sub>**Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented thin section of a sample using 532 nm laser radiation. The laser radiation power at the sample was about 20 mW.**Raman shifts (cm<sup>-1</sup>):** 440w, 386s, 350.**Source:** White (2009).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of isocubanite see also Chandra et al. (2011a, b).**Isokite** CaMg(PO<sub>4</sub>)F**Origin:** Ehrenfriedersdorf, Erzgebirge (Ore Mts.), Germany.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 150 mW.**Raman shifts (cm<sup>-1</sup>):** 1021, 955s, 607, 457, 425, 273.**Source:** Thomas et al. (1998).**Isomertieite** Pd<sub>11</sub>Sb<sub>2</sub>As<sub>2</sub>**Origin:** No data.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.**Raman shifts (cm<sup>-1</sup>):** 136.**Source:** Bakker (2014).**Comments:** No independent analytical data are provided for the sample used.**Ivsite** Na<sub>3</sub>H(SO<sub>4</sub>)<sub>2</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample in the spectral region from 30 to 4000 cm<sup>-1</sup> using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1198, 1162, 1112, 1004s, 973sh, 636s, 613s, 605s, 525w, 493w, 437s, 115, 80s.**Source:** Damak et al. (1985).**Comments:** The sample was characterized by powder X-ray diffraction data.**Iwateite** Na<sub>2</sub>BaMn(PO<sub>4</sub>)<sub>2</sub>**Origin:** Tanohata mine, Iwate Prefecture, Japan (type locality).**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 100 mW.**Raman shifts (cm<sup>-1</sup>):** 1004w, 990w, 973s, 808w, 584w, 577w, 428w.

**Source:** Nishio-Hamane et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is  $\text{Na}_{2.026}(\text{Ba}_{0.993}\text{Sr}_{0.101})(\text{Mn}_{0.801}\text{Mg}_{0.164})\text{P}_{1.971}\text{O}_8$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

### Iyoite $\text{MnCuCl(OH)}_3$

**Origin:** Sadamisaki Peninsula, Ehime Prefecture, Japan (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 3558w, 3521s, 3513sh, 458, 438.

**Source:** Nishio-Hamane et al. (2016b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $\text{Mn}_{1.085}\text{Cu}_{0.915}\text{Cl}_{1.058}(\text{OH})_{2.942}$ .

### Jáchymovite $(\text{UO}_2)_8(\text{SO}_4)(\text{OH})_{14}\cdot 13\text{H}_2\text{O}$

**Origin:** Jáchymov, Krušné Hory (Czech Ore Mts.), Bohemia, Czech Republic (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3504w, 3180w, 2257w, 1688w, 1614w, 1348w, 1125sh, 1094, 1068sh, 1015, 1010sh, 1003sh, 839sh, 828s, 807sh, 800sh, 667, 562, 542, 474sh, 454, 434, 405, 357sh, 337, 322sh, 276sh, 261, 252sh, 242sh, 208sh, 195, 172, 147, 114.

**Source:** Čejka et al. (2009a).

**Comments:** The sample was characterized by powder X-ray diffraction data and wet chemical analyses. The empirical formula of the sample used is  $(\text{UO}_2)_{8.01}(\text{SO}_4)_{0.95}(\text{OH})_{14.12}\cdot 13.06\text{H}_2\text{O}$ .

### Jacobsite $\text{Mn}^{2+}\text{Fe}^{3+}_2\text{O}_4$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 646s, 563sh, 456w, 340.

**Source:** Rafique et al. (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectrum of jacobsitesee also Clark et al. (2007).

### Jadeite $\text{NaAlSi}_2\text{O}_6$

**Origin:** Uru River area (?), north-central Myanmar.

**Experimental details:** Raman scattering measurements have been performed on an oriented thin section of a sample with the *b* axis parallel to the laser beam using 532 nm laser radiation. The nominal laser radiation power was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 1309, 991, 700s, 575, 524, 434, 374, 292, 223, 203s, 144, 80.

**Source:** Leander et al. (2014).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectrum of jadeite see also Többens et al. (2005).

### Jakobssonite $\alpha\text{-CaAlF}_5$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a pressed-disk sample in the spectral region from 280 to 800 cm<sup>-1</sup> using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. A 90°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 588, 440.

**Source:** Kawamoto and Kono (1986) and Inoue et al. (1988).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Jalpaite $\text{Ag}_3\text{CuS}_2$

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was not higher than 0.3 mW.

**Raman shifts (cm<sup>-1</sup>):** 258.

**Source:** De Caro et al. (2016).

**Comments:** The sample was characterized by electron microprobe analysis.

### Jamborite $\text{Ni}^{2+}_{1-x}\text{Co}^{3+}_x(\text{OH})_{2x}(\text{SO}_4)_x \cdot n\text{H}_2\text{O}$ [ $x \leq 1/3$ , $n \leq (1-x)$ ]

**Origin:** Rio Vesale, Sestola, Val Panaro, Modena province, Italy.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3614w, 2988sh, 2956, 2244, 1061w, 973, 852w, 527s, 460, 167w.

**Source:** Bindi et al. (2015a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Ni}^{2+}_{0.902}\text{Co}^{3+}_{0.072}\text{Fe}^{3+}_{0.024}\text{Ca}_{0.002})(\text{OH})_{1.884}\text{Cl}_{0.012}(\text{SO}_4)_{0.100} \cdot 0.904\text{H}_2\text{O}$ .

### Jamesonite $\text{Pb}_4\text{FeSb}_6\text{S}_{14}$

**Origin:** Zlatá Baňa, Slanské Vrchy Mts., central Slovakia.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample in the spectral region from 10 to 600 cm<sup>-1</sup> using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 344sh, 326s, 298, 277, 269sh, 251, 236, 225, 215sh, 199, 173, 163sh, 147, 128, 110, 92, 75, 59sh.

**Source:** Kharbish and Jeleň (2016).

**Comments:** The sample was characterized by electron microprobe analyses. The empirical formula of the sample used is  $\text{Pb}_{4.01}\text{Fe}_{0.99}\text{Sb}_{6.01}\text{S}_{14.00}$ .

**Jarosite**  $\text{KFe}^{3+}_3(\text{SO}_4)_2(\text{OH})_6$

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented thin section of a sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power at the sample was about 1 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3415, 3395sh, 1156, 1102s, 1008s, 643sh, 626, 573, 551sh, 454sh, 434s, 354, 301, 223s, 140.

**Source:** Maubec et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The empirical formula of the sample used is  $(\text{K}_{0.8}\text{Na}_{0.1})(\text{Fe}_{2.7}\text{Al}_{0.3})(\text{SO}_4)_{2.0}(\text{OH})_{5.9}$ . For the Raman spectra of jarosite see also Sasaki et al. (1998), Makreski et al. (2005a), Frost et al. (2006a), Murphy et al. (2009), Chio et al. (2010), Ciobotă et al. (2012), and Spratt et al. (2013).

**Jeffbenite**  $\text{Mg}_3\text{Al}_2\text{Si}_3\text{O}_{12}$

**Origin:** An inclusion in an alluvial diamond, São Luizriver, Juina district, Mato Grosso, Brazil (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 532 nm laser radiation. The nominal laser radiation power was in the range from 3 to 5 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 1056sh, 995, 926s, 865s, 635, 610sh, 542w, 499, 393w, 318s, 284, 233, 204.

**Source:** Nestola et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Mg}_{0.82}\text{Fe}^{3+}_{0.12})(\text{Al}_{1.86}\text{Cr}_{0.16})(\text{Mg}_{1.80}\text{Fe}^{2+}_{0.15}\text{Mn}_{0.05}\text{Ca}_{0.01}\text{Na}_{0.01})(\text{Si}_{2.82}\text{Al}_{0.18})\text{O}_{12}$ .

**Jennite**  $\text{Ca}_9(\text{Si}_3\text{O}_9)_2(\text{OH})_6 \cdot 8\text{H}_2\text{O}$

**Origin:** Maroldsweisach, Bavaria, Germany.

**Experimental details:** Raman scattering measurements have been performed on an oriented sample with longest axis corresponding to the [010] direction parallel and perpendicular with respect to laser polarization using 532 nm laser radiation. The nominal laser radiation power was 9 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3631, 3590sh, 3580s, 3534, 3489, 3464, ~3149, ~1640w, 1048, 1015sh, 1000s, 986s, 969s, 950sh, 906, 677sh, 658s, 632sh, 507sh, 492s, 479sh, 361sh, 335s, 312, 287, 270, 251, 204sh, 185s, 165sh, 142, 127, 113.

**Source:** Müller et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is  $\text{Ca}_{8.57-9.43}\text{Si}_{5.56-7.28}\text{Al}_{0.02-0.07}\text{O}_{18}(\text{OH})_6 \cdot n\text{H}_2\text{O}$ . The Raman shifts are given for total spectrum including all scattering geometries. For the Raman spectrum of jennite see also Kirkpatrick et al. (1997).

**Ježekite**  $\text{Na}_8[(\text{UO}_2)(\text{CO}_3)_3](\text{SO}_4)_2 \cdot 3\text{H}_2\text{O}$ 

**Origin:** Jáchymov, Krušné Hory (Czech Ore Mts.), Bohemia, Czech Republic (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm solid-state laser radiation. The nominal laser radiation power was 2.5 mW.

**Raman shifts (cm<sup>-1</sup>):** 3680, 3380sh, 2740w, 1710w, 1656w, 1600w, 1550w, 1375w, 1355w, 1195w, 1130w, 1110sh, 1060s, 1050w, 996s, 896w, 825s, 731, 715, 688w, 629, 622, 458, 379sh, 277, 248, 188s, 161s, 85.

**Source:** Plášil et al. (2015a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $\text{Na}_{7.88}(\text{UO}_2)(\text{CO}_3)_3(\text{S}_{1.01}\text{O}_4)_2 \cdot 3\text{H}_2\text{O}$ .

**Jixianite**  $(\text{Pb},\square)_2(\text{W},\text{Fe}^{3+})_2(\text{O},\text{OH})_7$ 

**Origin:** Yanhe Mine, Ji Co., Tianjin Municipality, China (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 1064 nm Nd-YAG laser radiation. The laser radiation output power was in the range 300–380 mW.

**Raman shifts (cm<sup>-1</sup>):** 907, 709, 433w, 371sh, 288, 174.

**Source:** Yuran and Li (1998).

**Comments:** No independent analytical data are provided for the sample used.

**Joaquinite-(Ce)**  $\text{NaBa}_2\text{Fe}^{2+}\text{Ti}_2\text{Ce}_2(\text{Si}_4\text{O}_{12})_2\text{O}_2(\text{OH})\cdot\text{H}_2\text{O}$ 

**Origin:** Benitoite Gem Mine, Southern San Benito Co., California (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3584sh, 3572sh, 3559sh, 3548w, 3509w, 3494sh, 3384sh, 3340sh, 3316w, 3242w, 1111, 1038, 1022, 991, 925, 902s, 891sh, 864w, 732s, 720sh, 686sh, 664s, 636s, 601s, 542, 492, 469, 440, 432, 377s, 358, 313, 299, 276, 250, 200, 180sh, 150.

**Source:** Frost and Pinto (2007).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis, however barium content is not indicated.

**Joegoldsteinite**  $\text{MnCr}_2\text{S}_4$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample hot-pressed as a pellet using 488.0 nm and 514.5 nm Ar<sup>+</sup> and 647.1 nm and 676.4 nm Kr<sup>+</sup> laser radiations. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 378s, 282w, 251.

**Source:** Lutz et al. (1989).

**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts are given for the 647.1 nm radiation.

**Joëlbruggerite**  $\text{Pb}_3\text{Zn}_3\text{Sb}^{5+}\text{As}_2\text{O}_{13}(\text{OH})$

**Origin:** Black Pine mine, Montana, USA (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed in the spectral region from 150 to 3500  $\text{cm}^{-1}$  using 785 nm diode laser radiation. The laser radiation power is not indicated.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3030w, 3015w, 818, 680, 506, 475, 427, 383, 235, 200, 183, 168, 150.

**Source:** Mills et al. (2009).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $\text{Pb}_{3.112}(\text{Zn}_{2.689}\text{Fe}^{2+}_{0.185})(\text{Sb}^{5+}_{0.650}\text{Te}^{6+}_{0.451})(\text{As}_{1.551}\text{P}_{0.203}\text{Si}_{0.160})\text{O}_{13.335}(\text{OH})_{0.665}$ .

**Johachidolite**  $\text{CaAlB}_3\text{O}_7$

**Origin:** An unknown locality in Myanmar.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts ( $\text{cm}^{-1}$ ):** 1191, 1112, 684sh.

**Source:** Chadwick and Breeding (2008).

**Comments:** The sample was characterized by laser-ablation inductively coupled plasma mass spectroscopy analysis and by energy-dispersive X-ray fluorescence analysis.

**Johannite**  $\text{Cu}(\text{UO}_2)_2(\text{SO}_4)_2(\text{OH})_2 \cdot 8\text{H}_2\text{O}$

**Origin:** Saint Agnes, Cornwall, England.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3593, 3523w, 3387sh, 3234w, 1147, 1100, 1090, 1042, 975, 948sh, 812s, 788sh, 756sh, 539, 481, 384, 302s, 277s, 205s, 184sh.

**Source:** Frost et al. (2005e).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of johannite see also Driscoll et al. (2014).

**Johannite**  $\text{Cu}(\text{UO}_2)_2(\text{SO}_4)_2(\text{OH})_2 \cdot 8\text{H}_2\text{O}$

**Origin:** Geevor mine, Pendeen, Cornwall, UK.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 325 nm He-Cd, as well as 532 and 785 nm diode laser radiations. The laser radiation output power was 270, 380, and 370 mW, respectively.

**Raman shifts ( $\text{cm}^{-1}$ ):** 1095, 1045, 836s, 448w, 352w, 244w, 203w.

**Source:** Driscoll et al. (2014).

**Comments:** The Raman shifts are given for 785 nm laser excitation. The sample was characterized by electron microprobe analysis. The proposed empirical formula of the sample used is  $\text{Cu}_{1.4}(\text{UO}_2)_2(\text{SO}_4)_{1.8}\cdot n\text{H}_2\text{O}$ . For the Raman spectrum of johannite see also Frost et al. (2005e).

**Johnbaumite**  $\text{Ca}_5(\text{AsO}_4)_3(\text{OH})$

**Origin:** Franklin or Sterling Hill, New Jersey, USA.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 960w, 888w, 865s, 840, 830.

**Source:** Crimmins (2012).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is  $(\text{Ca}_{4.87}\text{Pb}_{0.07}\text{Mn}_{0.05}\text{Sr}_{0.01})[(\text{As}_{0.94}\text{P}_{0.06})\text{O}_4]_3[(\text{OH})_{0.94}\text{Cl}_{0.06}]$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Johninnesite**  $\text{Na}_2\text{Mn}^{2+}_9\text{Mg}_7(\text{AsO}_4)_2(\text{Si}_6\text{O}_{17})_2(\text{OH})_8$

**Origin:** Schmorrasgrat deposit, Schams nappes, Val Ferrera, Graubünden, Switzerland.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1662w, 1616w, 1424w, 1322w, 1084w, 1055w, 1029, 1015, 939, 886w, 836s, 799s, 785s, 705, 667, 401, 347.

**Source:** Brugger and Berlepsch (1997).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is  $\text{Na}_{2.01}\text{Mn}^{2+}_{9.00}(\text{Mg}_{3.74}\text{Mn}_{2.66}\text{Fe}_{0.01})(\text{As}_{1.74}\text{V}_{0.03})\text{Si}_{12.58}\text{O}_{42}(\text{OH})_8$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Jordisite**  $\text{MoS}_2$

**Origin:** Zunyi Formation, southern China.

**Experimental details:** Experimental details are not indicated. Raman scattering measurements have been performed on an arbitrarily oriented sample. Raman spectrum was obtained in the spectral region from 150 to 1800 cm<sup>-1</sup>.

**Raman shifts (cm<sup>-1</sup>):** 600w, 438sh, 403 (h-MoS<sub>2</sub>), 370 (h-MoS<sub>2</sub>), 339w, 303w, 258sh, 216, 184sh, 148sh.

**Source:** Orberger et al. (2007).

**Comments:** The sample was characterized by a combination of methods including electron microprobe analysis, inductively coupled plasma mass spectroscopy, inductively coupled plasma atomic emission spectroscopy analysis, and proton-induced X-ray emission analysis.

**Joteite**  $\text{Ca}_2\text{CuAl}(\text{AsO}_4)[\text{AsO}_3(\text{OH})]_2(\text{OH})_2 \cdot 5\text{H}_2\text{O}$ 

**Origin:** Jotemine, Tierra Amarilla, Copiapó Province, Atacama, Chile (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was about 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 3429w, 3260w, 3068sh, 2930sh, 900sh, 861s, 849s, 822sh, 725, 521sh, 506s, 461s, 451sh, 414, 384, 349, 334, 317, 300, 283, 270, 259, 201, 162, 140, 119, 112sh.

**Source:** Kampf et al. (2013c).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved. The empirical formula of the sample used is  $\text{Ca}_{1.98}\text{Cu}_{1.00}\text{Al}_{1.15}\text{As}_{2.87}\text{H}_{14.24}\text{O}_{19}$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Kaersutite**  $\text{NaCa}_2(\text{Mg}_3\text{AlTi}^{4+})(\text{Si}_6\text{Al}_2)\text{O}_{22}\text{O}_2$ 

**Origin:** An unknown locality in Czech Republic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1183w, 1063sh, 1013w, 975w, 893w, 788sh, 764s, 666, 590s, 544sh, 514sh, 423sh, 363, 347sh, 331sh, 306sh, 292w, 249, 189w, 157, 144sh, 125w.

**Source:** Apopei et al. (2011).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of kaersutite see also Andò and Garzanti (2014) and Leissner et al. (2015).

**Kainite**  $\text{KMg}(\text{SO}_4)\text{Cl} \cdot 3\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm or 785 nm laser radiation. The laser radiation power at the sample was no more than 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 1196w, 1040s, 1023s, 630w, 450w.

**Source:** Morillas et al. (2016).

**Comments:** The sample was characterized by electron microprobe analysis.

**Kalgoorlieite**  $\text{As}_2\text{Te}_3$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 632.8 nm He-Ne laser radiation. The laser radiation output power was below 0.3 mW.

**Raman shifts (cm<sup>-1</sup>):** 193, 171s, 142, 137sh, 128s, 123sh, 119sh, 99s, 91w, 67w, 49.

**Source:** Cuenca-Gotor et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Kaliborite**  $\text{KHMg}_2\text{B}_{12}\text{O}_{16}(\text{OH})_{10}\cdot 4\text{H}_2\text{O}$ 

**Origin:** Inder boron deposit, Atyrau region, Kazakhstan.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3603sh, 3597s, 3590sh, 3517sh, 3398sh, 3360sh, 3336, 3245sh, 3202, 3172sh, 3133, 3041sh, 2929, 1595w, 1448sh, 1444, 1309w, 1229w, 1144, 1084sh, 1065, 967sh, 944, 881, 847w, 793w, 775sh, 756, 670, 639, 630sh, 609, 567, 551, 526, 519sh, 485, 476sh, 454w, 426sh, 414sh, 402, 394sh, 387, 337, 327sh, 320, 310sh, 286w, 259, 252sh, 242, 218, 197, 184, 177sh, 1709sh, 151, 121.

**Source:** López et al. (2015a).

**Comments:** No independent analytical data are provided for the sample used.

**Kalicinite**  $\text{KH}(\text{CO}_3)_3$ 

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on a powder sample using Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was about 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 1037s, 678, 637.

**Source:** Kagi et al. (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data. The crystal structure is solved by the Rietveld method. For the Raman spectrum of kalicinite see also Frezzotti et al. (2012).

**Kalininite**  $\text{ZnCr}_2\text{S}_4$ 

**Origin:** Synthetic

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 647.1 nm Kr<sup>+</sup> laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 392s, 293, 260s.

**Source:** Lutz et al. (1989).

**Comments:** The sample was characterized by powder X-ray diffraction analysis. For the Raman spectrum of kalininite see also Kushwaha (2008).

**Kalinite**  $\text{KAl}(\text{SO}_4)_2\cdot 11\text{H}_2\text{O}$ 

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3528sh, 3379, 1678, 1630, 1132, 1104sh, 990s, 975, 618, 536sh, 501sh, 454, 440sh, 327w.

**Source:** Frost and Kloprogge (2001).

**Comments:** No independent analytical data are provided for the sample used.

**Kaliophilite**  $\text{KAlSiO}_4$ **Origin:** Artificial.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using  $514.5\text{ nm}$   $\text{Kr}^+ \text{-Ar}^+$  laser radiation. The laser radiation power at the sample was no more than  $2\text{ mW}$ . A  $180^\circ$ -scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 402, 357.**Source:** Jay and Cashion (2013).**Comments:** The sample was characterized by electron microprobe analysis.**Kalsilite**  $\text{KAlSiO}_4$ **Origin:** San Venanzo, Terni province, Umbria, Italy.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):**  $\sim 350\text{s}$ .**Source:** Uchida et al. (2006).**Comments:** The sample was characterized by single-crystal X-ray diffraction data. The crystal structure is solved. The empirical formula of the sample used is  $(\text{K}_{0.92}\text{Na}_{0.07})(\text{Al}_{0.93}\text{Fe}^{3+}_{0.04}\text{Si}_{1.03})\text{O}_4$ .**Kamacite** (Fe,Ni)**Origin:** Almahata Sitta meteorite.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using  $532\text{ nm}$  Nd-YAG laser radiation. The nominal laser radiation power was  $22.5\text{ mW}$ . A  $180^\circ$ -scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 275, 214, 175sh, 153sh.**Source:** Kaliwoda et al. (2013).**Comments:** The sample was characterized by electron microprobe analyses. It contains about 4 wt% Ni and 0.2 wt% Co. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.**Kamotoite-(Y)**  $\text{Y}_2\text{O}_4(\text{UO}_2)_4(\text{CO}_3)_3 \cdot 14\text{H}_2\text{O}$ **Origin:** Kamoto East open cut, Kolwezi, Shaba Cu belt, Democratic Republic of Congo (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a  $633\text{ nm}$  He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3516w, 3361w, 1634sh, 1551w, 1338w, 1131, 1125sh, 815s, 810sh, 745, 584, 547sh, 418, 336.**Source:** Frost et al. (2006k).**Comments:** No independent analytical data are provided for the sample used.**Kampelite**  $\text{Ba}_6\text{Mg}_3\text{Sc}_8(\text{PO}_4)_{12}(\text{OH})_6 \cdot 7\text{H}_2\text{O}$

**Origin:** Kovdor phoscorite-carbonatite complex, Kola Peninsula, Russia (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1604w, 1092, 975s, 932sh, 848, 715, 591, 456, (402), 297w, 172, 77s.

**Source:** Yakovenchuk et al. (2017).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### Kamphaugite-(Y) CaY(CO<sub>3</sub>)<sub>2</sub>(OH)·H<sub>2</sub>O

**Origin:** Goudini carbonatite, South Africa.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 3473sh, 3383s, 3298s, 3208s, 3140s, 2953w, 2668, 2500, 2357w, 2206w, 1087s, 1041sh, 953w, 761w, 523w, 433w, 250.

**Source:** Verwoerd (2008).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is (Ca<sub>1.84</sub>REE<sub>x</sub>)(Y<sub>1.46</sub>REE<sub>0.54-x</sub>)(CO<sub>3</sub>)<sub>4</sub>(OH)<sub>1.65</sub>·2H<sub>2</sub>O. For the Raman spectrum of kamphaugite-(Y) see also Frost et al. (2015a).

### Kangite (Sc,Ti,Al,Zr,Mg,Ca,□)<sub>2</sub>O<sub>3</sub>

**Origin:** Allende meteorite. (2015a)

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented polished section of a sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** No Raman shifts for kangite can be distinguished because of strong fluorescence features due to high concentrations of REEs in the sample.

**Source:** Ma et al. (2013).

**Comments:** The empirical formula of the sample used is (Sc<sub>0.54</sub>Al<sub>0.16</sub>Y<sub>0.07</sub>V<sub>0.03</sub>Gd<sub>0.01</sub>Dy<sub>0.01</sub>Er<sub>0.01</sub>)(Ti<sub>0.66</sub>Zr<sub>0.13</sub>)<sub>0.79</sub>(Mg<sub>0.11</sub>Ca<sub>0.06</sub>Fe<sub>0.02</sub>)<sub>0.19</sub>O<sub>3</sub>. In the cited paper a figure of the Raman spectrum of synthetic Sc<sub>2</sub>O<sub>3</sub> is given.

### Kaňkite Fe<sup>3+</sup>(AsO<sub>4</sub>)·3.5H<sub>2</sub>O

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power at the sample was less than 0.1 mW in the hydroxyl stretching region. The laser radiation power in the other spectral regions was not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3408w, 3221, 3112sh, 1629, 1469, 1065, 881s, 832sh, 808sh, 790, 733w, 564, 492s, 398w, 373w, 290w, 240, 228, 198, 179w.

**Source:** Frost and Kloprogge (2003).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of kaňkite see also Frost et al. (2015w) and Culka et al. (2016b).

**Kanoite** MnMgSi<sub>2</sub>O<sub>6</sub>**Origin:** Artificial.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm laser radiation. The laser radiation power at the sample was in the range 0.2–1 mW.**Raman shifts (cm<sup>-1</sup>):** 1010, 930w, 666, 563, 531, 393, 325, (231w).**Source:** Tomasini et al. (2015).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.**Kaolinite** Al<sub>2</sub>Si<sub>2</sub>O<sub>5</sub>(OH)<sub>4</sub>**Origin:** Washington County, Georgia, USA.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3683s, 3657w, 3644w, 3616s, 912, 789, 745, 462, 430, 334, 274.**Source:** Wang et al. (2015).**Comments:** The sample was characterized by powder X-ray diffraction data and by electron microprobe analyses. For the Raman spectra of kaolinite see also Frost et al. (1993) and Frost (1995).**Kapellasite** Cu<sub>3</sub>Zn(OH)<sub>6</sub>Cl<sub>2</sub>**Origin:** Sounion No. 19 mine, Kamariza, Lavrion, Greece (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 633 nm laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 3457, ~908w, 481, 409, 326, ~279sh, ~266sh, 247, ~232.**Source:** Krause et al. (2006).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is (Cu<sub>3.24</sub>Zn<sub>0.75</sub>)(OH)<sub>5.94</sub>Cl<sub>2.0</sub>.**Kapundaite** CaNaFe<sup>3+</sup><sub>4</sub>(PO<sub>4</sub>)<sub>4</sub>(OH)<sub>3</sub>·5H<sub>2</sub>O**Origin:** Tom's quarry, Kapunda, Mt. Lofty Ranges, South Australia, Australia (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using 633 nm He-Ne and 785 nm laser radiations. The laser radiation powers are not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3530w, 3449sh, 3311w, 3151sh, 2905w, 1687w, 1616w, 1549sh, 1443w, 1391w, 1203w, 1159sh, 1128sh, 1114s, 1089s, 1077sh, 1062sh, 1040sh, 1024, 1009sh, 988sh, 972, 963sh, 940, 912w, 675sh, 667sh, 658sh, 646, 633sh, 609, 588sh, 562sh, 547sh, 491sh, 475sh, 460sh, 448sh, 435, 412sh, 395s, 381sh, 361s, 295sh, 275s, 257s, 244sh, 221sh, 186sh, 162s, 137sh, 113sh.**Source:** Frost et al. (2014q).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

### Karelianite $\text{V}_2\text{O}_3$

**Origin:** Merelani Hills gem zoisite deposit, Tanzania.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power at the sample was 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 506, 354, 219.

**Source:** Giuliani et al. (2008).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectrum of karelianite see also Voloshin et al. (2014).

### Karelianite $\text{V}_2\text{O}_3$

**Origin:** Pyrrhotite gorge, Khibiny Mts., Kola Peninsula, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The nominal laser radiation power was 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 972w, 712w, 644w, 576w, 503s, 305s, 227.

**Source:** Voloshin et al. (2014).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectrum of karelianite see also Giuliani et al. (2008).

### Karrooite $\text{MgTi}_2\text{O}_5$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal with the *b* axis oriented parallel to the laser beam and the *c*-axis vertical using 785 nm Ti-sapphire laser radiation. The nominal laser radiation power was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 1446, 1366, 1253, 1165, 1112, 913w, 790s, 632w, 522w, 499w, 422, 370, 329, 270s, 207, 165, 140, 124, 105, 88.

**Source:** Liermann et al. (2006).

**Comments:** No independent analytical data are provided for the sample used.

### Karpenkoite $\text{Co}_3(\text{V}_2\text{O}_7)(\text{OH})_2 \cdot 2\text{H}_2\text{O}$

**Origin:** Little Eva mine, Grand Co., Utah, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 532 nm diode laser radiation. The laser radiation output power was 4 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** ~3500, 1670w, 823s, 474, 443, 312, 253.

**Source:** Kasatkin et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is  $(\text{Co}_{2.06}\text{Zn}_{0.72}\text{Ni}_{0.13}\text{Mn}_{0.09}\text{Ca}_{0.02}\text{Cu}_{0.02}\text{Mg}_{0.01})\text{V}_{1.98}\text{O}_7(\text{OH})_2 \cdot 2\text{H}_2\text{O}$ .

### Kashinite $\text{Ir}_2\text{As}_3$

**Origin:** No data.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was in the range from 1 to 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 389, 367, 311, 290s, 200, 169, 152.

**Source:** Bakker (2014).

**Comments:** The sample was characterized by electron microprobe analysis. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of kashinite see also Zaccarini et al. (2016).

### Kasolite Pb(UO<sub>2</sub>)(SiO<sub>4</sub>)·H<sub>2</sub>O

**Origin:** Sierra Albarrana, Córdoba, Spain.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 972w, 949w, 912w, ~800sh, 768s, 553, 424, 237, 217, 107.

**Source:** Bonales et al. (2015).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectra of kasolite see also Frost et al. (2006e) and Driscoll et al. (2014).

### Kassite CaTi<sub>2</sub>O<sub>4</sub>(OH)<sub>2</sub>

**Origin:** Prairie Lake carbonatite, Ontario, Canada.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm solid-state laser radiation. The nominal laser radiation power was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 3440sh, 3200–3194sh, 3161–3157, 3088sh, 2662w, 2596w, 2501w, 696–693s, 614sh, 472–463, 450–446, 398, 368, 336–332, 300–299s, 248sh, 193, 190sh, 165w, 147–146w, 124–123.

**Source:** Martins et al. (2014).

**Comments:** The sample was characterized by X-ray diffraction data and by electron microprobe analyses. The empirical formula of the sample used is (Ca<sub>0.90</sub>Ce<sub>0.03</sub>Nd<sub>0.02</sub>La<sub>0.01</sub>Mn<sub>0.01</sub>)(Ti<sub>1.94</sub>Fe<sub>0.04</sub>Si<sub>0.01</sub>Al<sub>0.01</sub>Nb<sub>0.01</sub>)O<sub>4</sub>(OH)<sub>2</sub>.

### Katayamalite KLi<sub>3</sub>Ca<sub>7</sub>Ti<sub>2</sub>(SiO<sub>3</sub>)<sub>12</sub>(OH)<sub>2</sub>

**Origin:** Iwagi Island, Inland Sea, Ehime prefecture, Japan (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm solid-state laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~3678, 1141, 1115w, 1019w, 982s, 960s, 915w, 904w, 700w, 668w, 570s, 514w, 495sh, 488, 454, 412, 376s, 297, 278, 257, 230w, 218, 195w.

**Source:** Andrade et al. (2013b).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is (K<sub>0.89</sub>Na<sub>0.12</sub>)Li<sub>3.21</sub>(Ca<sub>6.87</sub>Mn<sub>0.04</sub>Ba<sub>0.02</sub>)(Ti<sub>1.79</sub>Zr<sub>0.14</sub>Fe<sub>0.04</sub>Sn<sub>0.02</sub>)(SiO<sub>3</sub>)<sub>12</sub>(OH<sub>1.55</sub>F<sub>0.45</sub>). The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

### Katoite Ca<sub>3</sub>Al<sub>2</sub>(OH)<sub>12</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal from the (110) face of the crystal with parallel ( $A_{1g}$  and  $E_g$ ) and cross ( $F_{2g}$ ) polarizations of the incident and scattered light using 488 and 514.5 nm  $Ar^+$  laser radiations. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3648s, 534, 327 ( $A_{1g} + E_g$ ); 3653, 780w, 688sh, 535w, 388w, 331w, 231w, 163 ( $F_{2g}$ ).

**Source:** Kolesov and Geiger (2005).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Kawazulite $Bi_2Te_2Se$

**Origin:** Ozernyi district, Salla-Kuolayarvi, Kola Peninsula, Russia.

**Experimental details:** Methods of samples preparation are not described. Raman scattering measurements have been performed using 514.5 nm  $Ar^+$  and 785 nm diode laser radiations. The nominal laser radiation power was 50 and 500 mW, respectively.

**Raman shifts (cm<sup>-1</sup>):** 141–140, 103s, 61s.

**Source:** Voloshin et al. (2015a).

**Comments:** The samples were characterized by electron microprobe analyses. The empirical formulae of the samples used are  $Bi_{2.052}Te_{1.797}Se_{1.151}$  and  $(Bi_{1.986}Ni_{0.068})Te_{2.011}Se_{0.936}$ . For the Raman spectra of kawazulite see also Akrap et al. (2012) and Gehring et al. (2013).

### Kazanskyite $BaNa_3Ti_2Nb(Si_2O_7)_2O_2(OH)_2(H_2O)_4$

**Origin:** Kukisvumchorr Mt., Khibiny alkaline massif, Kola Peninsula, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was in the range from 5 to 12.5 mW.

**Raman shifts (cm<sup>-1</sup>):** 3628w, 3545, 3462sh, 1071w, 1001w, 935, 885s, 822, 722w, 680, 580, 521w, 455, 411, 317, 214w, 151.

**Source:** Cámara et al. (2012b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(Na_{2.55}Mn_{0.31}Ca_{0.11}Fe^{2+}_{0.03})(Ba_{0.70}Sr_{0.28}K_{0.21}Ca_{0.03})(Ti_{2.09}Nb_{0.63}Mn_{0.26}Al_{0.02})Si_{4.05}O_{21.42}H_{9.45}F_{0.59}$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

### Keilite FeS

**Origin:** Zakłodzie meteorite.

**Experimental details:** Raman scattering measurements have been performed in the spectral region from 100 to 4000 cm<sup>-1</sup> on an arbitrarily oriented sample using 514.5 nm laser radiation. The laser radiation power at the sample was 1.2 mW.

**Raman shifts (cm<sup>-1</sup>):** ~335w, ~280.

**Source:** Ma et al. (2012a).

**Comments:** The sample was characterized by electron backscatter diffraction and electron microprobe analysis. The empirical formula of the sample used is  $(\text{Fe}_{0.43}\text{Mn}_{0.35}\text{Mg}_{0.16}\text{Cr}_{0.02}\text{Ca}_{0.02})\text{S}$ . The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

### Keiviite-(Yb) $\text{Yb}_2\text{Si}_2\text{O}_7$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal and on a powdered sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was 4 W.

**Raman shifts (cm<sup>-1</sup>):** 952s, 923s, 663, 521, 484w, 424, 413, 370, 362, 277, 203w, 145s, 88w.

**Source:** Bretheau-Raynal et al. (1979).

**Comments:** The sample was characterized by electron microprobe analysis. The Raman shifts are given for a powdered sample.

### Kemmlitzite $\text{SrAl}_3(\text{AsO}_4)(\text{SO}_4)(\text{OH})_6$

**Origin:** Oschatz, Saxony, Germany (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3566sh, 3441s, 3374sh, 3269sh, 3047w, 1591w, 1524sh, 1356sh, 984s, 957sh, 825, 772sh, 690, 631sh, 564w, 482sh, 427, 388sh, 342s, 218, 208, 199, 149, 108w.

**Source:** Frost et al. (2012a).

**Comments:** No independent analytical data are provided for the sample used.

### Kempite $\text{Mn}^{2+}_2\text{Cl}(\text{OH})_3$

**Origin:** Artificial.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using 785 nm laser. The laser radiation power at the sample was less than 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 506, 478, 413w, 293s.

**Source:** Vallette Campos and Alvarado Aguayo (2015).

**Comments:** No independent analytical data are provided for the sample used.

### Kentrolite $\text{Pb}_2\text{Mn}^{3+}_2\text{O}_2(\text{Si}_2\text{O}_7)$

**Origin:** Artificial.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 950, 893, 593s, 540, 344, 305.

**Source:** Vieira Ferreira et al. (2014).

**Comments:** No independent analytical data are provided for the sample used.

**Kenyaite**  $\text{Na}_2\text{Si}_{22}\text{O}_{41}(\text{OH})_8 \cdot 6\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 1064 nm Nd-YAG laser radiation. The laser radiation power at the sample was 90 mW.**Raman shifts (cm<sup>-1</sup>):** 3200w, 1179, 1061, 1049, 819, 801w, 780w, 622, 493sh, 465s, 431sh, 398w, 376, 349, 316, 258, 242w, 204, 166, 162, 155w, 148w, 139w, 129w, 123w, 115w, 106.**Source:** Huang et al. (1999a).**Comments:** The sample was characterized by powder X-ray diffraction data.**Kerimasite**  $\text{Ca}_3\text{Zr}_2(\text{SiFe}^{3+})_2\text{O}_{12}$ **Origin:** Kerimasi volcano, northern Tanzania (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3537w, 3420sh, 3400w, 3380sh, 3240w, 875w, 830sh, 785sh, 732, 573w, 500s, 414w, 298s, 243, 152.**Source:** Zaitsev et al. (2010).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Ca}_{3.00}\text{Mn}_{0.01}\text{Ce}_{0.01}\text{Nd}_{0.01})(\text{Zr}_{1.72}\text{Nb}_{0.14}\text{Ti}_{0.08}\text{Mg}_{0.02}\text{Y}_{0.02})(\text{Fe}^{3+}_{1.23}\text{Si}_{0.86}\text{Al}_{0.82}\text{Ti}_{0.09})\text{O}_{12}$ . For the Raman spectra of kerimasite see also Galuskina et al. (2013a) and Uher et al. (2015).**Kermesite**  $\text{Sb}_2\text{OS}_2$ **Origin:** Pernek, Slovak Republic.**Experimental details:** Raman scattering measurements have been performed on an oriented crystal with the laser polarization parallel and perpendicular to the cleavage and elongation of kermesite. 632.8 nm He-Ne and 785 nm solid-state laser radiations were used. The nominal laser radiation power was 1.7 and 8.5 mW, respectively. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 334, 317s, 303w, 289w, 276w, 245, 237w, 231, 206w, 175w, 162w, 148, 130, 111w, 105, 97w, 84w, 72w, 64, 59, 48s.**Source:** Kharbish et al. (2009).**Comments:** The sample was characterized by electron microprobe analysis. The empirical formula of the sample used is  $\text{Sb}_{1.9}\text{S}_{2.1}\text{O}$ . The Raman shifts are given as the sum of the spectra of all scattering geometries with He-Ne laser excitation.**Keyite**  $\text{Cu}^{2+}_3\text{Zn}_4\text{Cd}_2(\text{AsO}_4)_6 \cdot 2\text{H}_2\text{O}$ **Origin:** Tsumeb, Namibia (?).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 856, 803, 735, 590, 505, 411, 355, 307sh, 288, 239, 195, 134, 65.**Source:** Schlüter et al. (2013).**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

**Khademite** Al(SO<sub>4</sub>)F·5H<sub>2</sub>O

**Origin:** Kladno mine, Central Bohemia, Czech Republic (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. Raman spectrum was obtained in the spectral region from 200 to 4000 cm<sup>-1</sup>. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3380, 3146sh, 2991sh, 1763sh, 1609w, 1449sh, 1132, 1104sh, 991s, 975sh, 618, 534sh, 505sh, 455, 324sh, 253sh, 226sh, 192, 150, 113sh.

**Source:** Frost et al. (2013m).

**Comments:** No independent analytical data are provided for the sample used.

**Khatyrkite** CuAl<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 260, 103.

**Source:** Bahrami et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Khesinite** Ca<sub>4</sub>(Mg<sub>3</sub>Fe<sup>3+</sup><sub>9</sub>)O<sub>4</sub>(Fe<sup>3+</sup><sub>9</sub>Si<sub>3</sub>)O<sub>36</sub>

**Origin:** Gurim anticline, near Arad city, Hatrurim Complex, Negev Desert, Israel (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm solid-state laser radiation. The laser radiation power at the sample was in the range from 10 to 20 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1638, 1495sh, 1403, 1132w, 947, 814sh, 749sh, 696, 610, 522, 481sh, 336sh, 310s, 256sh, 208sh, 159, 121.

**Source:** Galuskina et al. (2017).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is Ca<sub>4</sub>(Fe<sup>3+</sup><sub>8.528</sub>Mg<sub>1.635</sub>Ca<sub>0.898</sub>Ti<sup>4+</sup><sub>0.336</sub>Ni<sup>2+</sup><sub>0.217</sub>Mn<sup>2+</sup><sub>0.155</sub>Cr<sup>3+</sup><sub>0.132</sub>Fe<sup>2+</sup><sub>0.098</sub>)[(Fe<sup>3+</sup><sub>6.827</sub>Al<sub>2.506</sub>Si<sub>2.667</sub>O<sub>40</sub>].

**Khvorovite** Pb<sub>4</sub>Ca<sub>2</sub>[Si<sub>8</sub>B<sub>2</sub>(Si,B)<sub>2</sub>O<sub>28</sub>]F

**Origin:** Dara-I Pioz glacier, Dara-I Pioz alkaline massif, Tien Shan Mts., Tajikistan (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1100w, 1017s, 937, 783, 713, 642, 531s, 485, 425s, 296, 256s, 221w, 203w, 170, 162.

**Source:** Pautov et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is (Pb<sup>2+</sup><sub>2.76</sub>Ba<sub>0.62</sub>K<sub>0.56</sub>Na<sub>0.16</sub>)(Ca<sub>1.86</sub>Sr<sub>0.06</sub>Y<sub>0.04</sub>Na<sub>0.04</sub>)[Si<sub>8</sub>B<sub>2</sub>(Si<sub>1.46</sub>B<sub>0.65</sub>)O<sub>28</sub>](F<sub>0.71</sub>O<sub>0.29</sub>).

**Kiddcreekite** Cu<sub>6</sub>SnWS<sub>8</sub>

**Origin:** Zijin Cu-Au mine, China.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 860, 654, 430, 345, 291, 256.

**Source:** Liu et al. (2012).

**Comments:** No independent analytical data are provided for the sample used.

**Kidwellite** NaFe<sup>3+</sup><sub>9+x</sub>(PO<sub>4</sub>)<sub>6</sub>(OH)<sub>11</sub>·3H<sub>2</sub>O ( $x \gg 0.33$ )

**Origin:** Savannah River, Girard Barke Co., Georgia, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. Raman spectrum was obtained in the spectral region from 200 to 4000 cm<sup>-1</sup>. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3580, 3466, 3356, 3231, 3122, 1188, 1144w, 1129, 1082, 1063, 1050w, 1034, 1014s, 978s, 931w, 919, 875w, 653w, 644w, 631w, 588, 570, 557, 539, 500, 490, 467, 453, 444, 418w, 405, 333, 322, 285, 271, 253w, 223, 189, 181, 169, 144, 139, 118, 111.

**Source:** Frost et al. (2014k).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

**Kieftite** CoSb<sub>3</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polished plate cut perpendicular to the [101] direction of a single crystal using 476.5, 488, and 514.5 nm Ar<sup>+</sup> laser radiations. The laser radiation power is not indicated. A 135°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 188, 180, 171w, 154s.

**Source:** Nolas et al. (1996).

**Comments:** The sample was characterized by X-ray diffraction data. The Raman shifts are given for 514.5 nm laser radiation.

**Kieserite** Mg(SO<sub>4</sub>)·H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 15 mW.

**Raman shifts (cm<sup>-1</sup>):** 3297, 1509, 1215w, 1117, 1046s, 629, 481, 436, 272, 218.

**Source:** Wang et al. (2006a).

**Comments:** The sample was characterized by powder X-ray diffraction analysis. For the Raman spectrum of kieserite see also Wang et al. (2008).

**Kilchoanite** Ca<sub>6</sub>(SiO<sub>4</sub>)(Si<sub>3</sub>O<sub>10</sub>)

**Origin:** Birkhin massif, Baikal Lake area, Siberia, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was in the range from 30 to 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 1012, 988, 967, 927, 911w, 871sh, 864s, 828s, 782w, 671s, 596w, 571w, 552w, 485w, 401, 358w, 333w, 306w, 259w, 246w, 208w, 195w, 188w, 163, 133, 121w, 112sh.

**Source:** Galuskin et al. (2012b).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Killalaite** Ca<sub>6.4</sub>[H<sub>0.6</sub>Si<sub>2</sub>O<sub>7</sub>]<sub>2</sub>(OH)<sub>2</sub>

**Origin:** Upper Chegem caldera, Northern Caucasus, Kabardino-Balkaria, Russia.

**Experimental details:** Raman scattering measurements have been performed on an approximately oriented crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation output power was in the range from 30 to 50 mW. A 180°-scattering geometry was employed. Spectra were collected on a cross-section approximately perpendicular to z-axis (I scattering geometry) and on a cross-section approximately parallel to z-axis (II scattering geometry).

**Raman shifts (cm<sup>-1</sup>):** 3562, 3523, 994, 943, 912, 677, 551, 433, 371, 302, 284, 266, 185, 129 (I scattering geometry); 3567, 3530, 1077, 999, 945, 912, 883, 678, 552, 435, 367, 284, 266, 185, 148, 107 (II scattering geometry).

**Source:** Armbruster et al. (2012).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

**Kimzeyite** Ca<sub>3</sub>Zr<sub>2</sub>(SiAl<sub>2</sub>)O<sub>12</sub>

**Origin:** Wiluy River basin, Sakha-Yakutia, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 937w, 879w, 785, 728, 499s, 303s, 248sh, 153.

**Source:** Galuskina et al. (2005).

**Comments:** The sample was characterized by electron microprobe analyses.

**Kinoite** Ca<sub>2</sub>Cu<sub>2</sub>Si<sub>3</sub>O<sub>10</sub>·2H<sub>2</sub>O

**Origin:** Christmas mine, Gila Co., Arizona, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3572sh, 3519, 3441sh, 3237w, 3022w, 1585w, 1186, 1052, 1000, 994sh, 975sh, 951s, 859sh, 847s, 765, 742, 642, 543sh, 531s, 486s, 456s, 422s, 400s, 352sh, 339, 324sh, 309, 301, 286, 266sh, 251, 233sh, 225, 194, 183, 163sh, 153s, 138s, 118sh, 110.

**Source:** Frost and Xi (2012c).

**Comments:** No independent analytical data are provided for the sample used.

**Kinoshitalite** BaMg<sub>3</sub>(Si<sub>2</sub>Al<sub>2</sub>O<sub>10</sub>)(OH)<sub>2</sub>

**Origin:** Hokkejino, Kyoto prefecture, Kinki region, Honshu Island, Japan.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 780 nm laser radiation. The nominal laser radiation power was 600 mW.

**Raman shifts (cm<sup>-1</sup>):** 653s, 210, 150, 140.

**Source:** Manuella et al. (2012).

**Comments:** The sample was characterized by X-ray diffraction data.

**Kintoreite** PbFe<sup>3+</sup><sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>(PO<sub>3</sub>OH)(OH)<sub>6</sub>

**Origin:** Broken Hill, New South Wales, Australia (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3435sh, 3391sh, 3225, 2968sh, 1413, 1229, 1140, 1110, 1075, 1021, 1003, 975, 851, 814, 625, 573sh, 562, 551, 477sh, 459sh, 440s, 422sh, 420sh, 372, 336, 307, 253, 219, 204.

**Source:** Frost et al. (2006p).

**Comments:** No independent analytical data are provided for the sample used.

**Kipushite** Cu<sub>6</sub>(PO<sub>4</sub>)<sub>2</sub>(OH)<sub>6</sub>·H<sub>2</sub>O

**Origin:** Miedzianka (former Kupferberg), Sudety Mts., SW Poland.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 40 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3549, 3482, 3444sh, 3251sh, 1078sh, 1045w, 1021w, 975s, 942w, 875sh, 869s, 843sh, 814, 796sh, 639w, 617w, 552sh, 521w, 493sh, 464, 438w, 396, 369sh, 317w, 297w, 256w, 221w.

**Source:** Ciesielczuk et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The Raman shifts are given for As-bearing kipushite with 1.21 *apfu* P and 0.67 *apfu* As.

**Kirschsteinite** CaFe<sup>2+</sup>(SiO<sub>4</sub>)

**Origin:** Artificial.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented polished sample cross-section using 785 nm laser radiation. The laser radiation power at the sample was 6.6 mW.

**Raman shifts (cm<sup>-1</sup>):** 932, 901w, 849sh, 815s, 635w, 566w, 522w, 391, 291, 249.

**Source:** Kramar et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

**Kladnoite**  $\text{C}_6\text{H}_4(\text{CO})_2\text{NH}$ 

**Origin:** Kladno (Schöller) mine, Libušín, Kladno, Bohemia, Czech Republic (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 3085, 3071w, 3068sh, 3046, 1755s, 1726, 1606, 1468w, 1386, 1373, 1305, 1165, 1142, 1091w, 1047w, 1012s, 901w, 809w, 805w, 795w, 743s, 666w, 641, 550, 531w, 350, 260, 200, 163s, 72.

**Source:** Jehlička et al. (2007b).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of kladnoite see also Moroz et al. (2004) and Jehlička et al. (2009a).

**Klaprothite**  $\text{Na}_6(\text{UO}_2)(\text{SO}_4)_4 \cdot 4\text{H}_2\text{O}$ 

**Origin:** Blue Lizard mine, San Juan Co., Utah, USA (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3620, 3440, 1640, 1248, 1216w, 1175, 1161, 1070, 1036, 997s, 974, 944, 830s, 658, 624, 540w, 495w, 456, 430, 335w, 287w, 230sh, 215, 146w, 130w, 98w, 78w.

**Source:** Kampf et al. (2016g).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $\text{Na}_{6.01}(\text{U}_{1.03}\text{O}_2)(\text{S}_{0.993}\text{O}_4)_4(\text{H}_2\text{O})_4$ . The Raman shifts were determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of klaprothite see also Plášil et al. (2015d).

**Klebensbergite**  $\text{Sb}^{3+} \text{O}_4(\text{SO}_4)(\text{OH})_2$ 

**Origin:** Pereta mine, Grosseto province, Tuscany, Italy.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3457sh, 3435w, 3357w, 1142, 1139sh, 1089sh, 1074, 1029, 971s, 936sh, 723, 662, 627sh, 611sh, 604s, 581s, 489s, 481sh, 446, 435, 410, 326, 303, 266w, 238s, 225s, 205s, 194sh, 170s, 160sh, 142, 130, 116.

**Source:** Frost and Bahfenne (2011c).

**Comments:** No independent analytical data are provided for the sample used.

**Klockmannite**  $\text{Cu}_{5.2}\text{Se}_6$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 263s, 206w, 192w, 45sh, 43s, 17.

**Source:** Ishii et al. (1993).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Knorrtingite**  $Mg_3Cr_2(SiO_4)_3$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a polished surface of an arbitrarily oriented single crystal using 632 nm He-Ne laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 936, 908, 866, 718, 551s, 368.**Source:** Bykova et al. (2014).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $Mg_{3.21}Cr_{1.58}Si_{3.21}O_{12}$ .**Kobokoboite**  $Al_6(PO_4)_4(OH) \cdot 11H_2O$ **Origin:** No data.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 1630, 1463, 1170sh, 1095, 1046, 980sh, 916, 764, 600, 514, 490sh.**Source:** Sanchez-Moral et al. (2011).**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.**Koechlinite**  $Bi_2MoO_6$ **Origin:** Pittong, Victoria, Australia.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm Nd-YAG laser radiation. The laser radiation power at the sample was 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 843, 797, 773sh, 715, 401, 349, 321, 293sh, 281, 268sh, 228, 195, 154sh, 141.**Source:** Frost et al. (2004c).**Comments:** No independent analytical data are provided for the sample used.**Kojonenite**  $Pd_{7-x}SnTe_2$  ( $0.3 \leq x \leq 0.8$ )**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a polished surface of an arbitrarily oriented crystal using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was in the range from 1 to 2 mW.**Raman shifts (cm<sup>-1</sup>):** 197w.**Source:** Vymazalová et al. (2014).**Comments:** The sample was characterized by electron microprobe analysis.**Kokchetavite**  $K(AlSi_3O_8)$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 60 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 835, 390s, 109s.

**Source:** Kanzaki et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of kokchetavite see also Hwang et al. (2004) and Ferrero et al. (2016).

### Koktaite $(\text{NH}_4)_2\text{Ca}(\text{SO}_4)_2 \cdot \text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 3353sh, 3149, 2852w, 1723w, 1677w, 1453, 1419, 1153, 1132, 1104w, 1087, 996s, 980s, 656, 642, 625, 616, 603, 487, 474, 437, 423.

**Source:** Jentzsch et al. (2012a).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Kolskyite $\text{CaNa}_2\text{Ti}_4(\text{Si}_2\text{O}_7)_2\text{O}_4(\text{H}_2\text{O})_7$

**Origin:** Kirovskii mine, Kukisvumchorr Mt., Khibiny alkaline massif, Kola Peninsula, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1072w, 997w, 925s, 800w, 685s, 586, 505w, 435, 420, 397, 297, 214w, 151.

**Source:** Cámara et al. (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Na}_{1.93}\text{Mn}_{0.04}\text{Ca}_{0.03})(\text{Ca}_{0.67}\text{Sr}_{0.45}\text{Ba}_{0.19}\text{K}_{0.15})(\text{Ti}_{2.93}\text{Nb}_{0.46}\text{Mn}_{0.33}\text{Mg}_{0.17}\text{Fe}^{2+}_{0.10}\text{Zr}_{0.01})\text{Si}_{4.00}\text{O}_{24.67}\text{H}_{13.60}\text{F}_{0.33}$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

### Kolwezite $(\text{Cu},\text{Co})_2(\text{CO}_3)(\text{OH})_2$

**Origin:** Mupine, Shaba province, Zaire.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3439sh, 3389, 3310sh, 3284sh, 1515sh, 1495, 1456sh, 1363, 1093s, 1059s, 757w, 718w, 530, 431, 346, 264, 176, 159.

**Source:** Frost (2006).

**Comments:** No independent analytical data are provided for the sample used.

### Konyaite $\text{Na}_2\text{Mg}(\text{SO}_4)_2 \cdot 5\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 3295, 3185sh, 1179w, 1144w, 1091, 1003s, 981s, 648w, 619sh, 610, 602sh, 471sh, 455sh, 448.

**Source:** Jentzsch et al. (2011).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of konyaite see also Jentzsch et al. (2013). The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum.

### Koritnigite Zn(AsO<sub>3</sub>OH)·H<sub>2</sub>O

**Origin:** Jáchymov ore district, Krušné Hory Mts., Bohemia, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3474w, 3297sh, 3182w, 3005w, 2770w, 2434sh, 2285w, 1755sh, 1597w, 1303w, 877s, 842s, 813s, 766, 330, 261, 284, 237, 219, 187, 172s, 154, 140, 120, 110.

**Source:** Frost et al. (2011q).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The empirical formula of the sample used is  $(\text{Zn}_{0.79}\text{Co}_{0.14}\text{Ni}_{0.02})[\text{AsO}_3(\text{OH})_{0.99}\text{F}_{0.01}]_{1.00}\text{H}_2\text{O}$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of koritnigite see also Frost et al. (2014a).

### Kornelite Fe<sup>3+</sup><sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>·7H<sub>2</sub>O(?)

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3587w, 3352sh, 3123, 1696sh, 1658w, 1613sh, 1182, 1151sh, 1124w, 1078w, 1033s, 1021sh, 993w, 838w, 672w, 636, 597, 476, 452, 439, 269, 248, 209, 187.

**Source:** Ling and Wang (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of kornelite see also Ling et al. (2009) and Kong et al. (2011a).

### Kornerupine (Mg,Fe<sup>2+</sup>,Al,□))<sub>10</sub>(Si,Al,B)<sub>5</sub>O<sub>21</sub>(OH,F)<sub>2</sub>(?)

**Origin:** Mautia Hill, Tanzania.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3619sh, 3612s, 3599sh, 3556sh, 3547s, 3538sh, 3521w, 3275w, 1084w, 1051, 1035sh, 995, 947sh, 923, 668, 648sh, 620, 586sh, 554w, 507sh, 487, 477sh, 459sh, 403, 394sh, 364w, 355w, 336, 324, 316sh, 298w, 261, 254sh, 236w, 224, 219sh, 191sh, 180, 150, 138sh, 123.

**Source:** Frost et al. (2015t).

**Comments:** The sample was characterized by qualitative electron microprobe analysis. For the Raman spectrum of kornerupine see also Wopenka et al. (1999).

**Kosmochlor**  $\text{NaCr}^{3+}\text{Si}_2\text{O}_6$

**Origin:** Morasko iron meteorite.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 1055, 1033s, 991, 952w, 863, 680, 565sh, 552s, 520, 413, 380w, 339s, 320w, 294, 252, 202, 142w.

**Source:** Karwowski et al. (2013).

**Comments:** The sample was characterized by electron microprobe analyses. The empirical formula of the sample used is  $\text{Na}_{0.91}\text{Ca}_{0.07}\text{Mg}_{0.09}\text{Fe}_{0.02}\text{Cr}_{0.82}\text{Al}_{0.01}\text{V}_{0.01}\text{Ti}_{0.07}\text{Si}_{2.00}\text{O}_{6.00}$ . The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of kosmochlor see also Leander et al. (2014).

**Kosnarite**  $\text{KZr}_2(\text{PO}_4)_3$

**Origin:** Jenipapo district, Itinga, Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1149w, 1116w, 1088, 1079sh, 1063, 1060, 1031sh, 1026s, 1022sh, 1017sh, 979sh, 638, 595, 561w, 437s, 421, 405, 387w, 318, 290s, 263, 188sh, 175, 156, 141sh, 122.

**Source:** Frost et al. (2012i).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

**Kotoite**  $\text{Mg}_3(\text{BO}_3)_2$

**Origin:** Snezhnoye deposit, East Verkhoyan'ye, Sakha Yakutia, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented polished sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was less than 20 mW. A 0°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1255w, 1088w, 920s, 866w, 847, 708, 796, 691, 553, 357s, 327, 310.

**Source:** Galuskina et al. (2008).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectra of kotoite see also Frost and Xi (2013c) and Kipcak et al. (2013).

**Köttigite**  $\text{Zn}_3(\text{AsO}_4)_2 \cdot 8\text{H}_2\text{O}$

**Origin:** Ojuela Mine, Mapini, Durango, Mexico.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3458sh, 3215w, 868sh, 835s, 810sh, 790s, 547, 479sh, 451s, 432s, 371w, 332w, 286sh, 249s, 220s, 194sh, 142w.

**Source:** Frost et al. (2003g).

**Comments:** No independent analytical data are provided for the sample used.

### Kotulskite Pd(Te,Bi)<sub>2-x</sub> ( $x \approx 0.4$ )

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was in the range from 1 to 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 97.

**Source:** Vymazalová et al. (2014).

**Comments:** The sample was characterized by electron microprobe analysis.

### Kovdorskite Mg<sub>2</sub>(PO<sub>4</sub>)(OH)·3H<sub>2</sub>O

**Origin:** Kovdor massif, Kola Peninsula, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm solid-state laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3681, 3395, 3219, 2967, 1550, 1089w, 1056, 964s, 870w, 566sh, 536, 453, 410w, 375, 345, 320w, 303, 255w, 228, 201, 158s, 135.

**Source:** Morrison et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is Mg<sub>2.00</sub>PO<sub>4.00</sub>(OH)·2.67H<sub>2</sub>O. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman spectrum of kovdorskite see also Frost et al. (2013a).

### Kozyrevskite Cu<sub>4</sub>O(AsO<sub>4</sub>)<sub>2</sub>

**Origin:** Arsenatnaya fumarole, Tolbachik volcano, Kamchatka, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm diode laser radiation. The laser radiation power at the sample was about 3 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 875s, 840sh, 826s, 757sh, 497w, 445, 394, 340, 216, 170sh, 137sh, 112.

**Source:** Pekov et al. (2014c).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is (Cu<sub>3.95</sub>Zn<sub>0.07</sub>Fe<sub>0.01</sub>)(As<sub>1.83</sub>P<sub>0.09</sub>S<sub>0.03</sub>V<sub>0.02</sub>Si<sub>0.01</sub>)O<sub>9</sub>.

### Kremersite (NH<sub>4</sub>)<sub>2</sub>Fe<sup>3+</sup>Cl<sub>5</sub>·H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using He-Ne laser radiation. The nominal laser radiation power was 50 mW. A 135°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 359w, 296s, 211, 194, 130sh, 115w.

**Source:** Sharma and Pandya (1974).

**Comments:** No independent analytical data are provided for the sample used.

### Krieselite Al<sub>2</sub>(GeO<sub>4</sub>)F<sub>2</sub>

**Origin:** Tsumeb mine, Namibia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632 nm He-Ne laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 862, ~802sh, 718w, 294s, 224.

**Source:** Schläter et al. (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The empirical formula of the sample used is (Al<sub>1.860</sub>Ga<sub>0.102</sub>As<sup>3+</sup><sub>0.036</sub>Zn<sub>0.020</sub>Mg<sub>0.016</sub>Fe<sup>3+</sup><sub>0.012</sub>Na<sub>0.009</sub>Sb<sup>3+</sup><sub>0.005</sub>Ti<sub>0.003</sub>Cu<sub>0.001</sub>)(Ge<sub>0.844</sub>Al<sub>0.143</sub>Si<sub>0.013</sub>O<sub>4</sub>(F<sub>1.103</sub>OH<sub>0.897</sub>).

### Kröhnikite Na<sub>2</sub>Cu(SO<sub>4</sub>)<sub>2</sub>·2H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 488 and 514.5 nm Ar<sup>+</sup> laser radiations. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3280w, 3200w, 3140w, 3100w, 1660w, 1610w, 1590w, 1182w, 1175w, 1162, 1150, 1128w, 1090w, 1045s, 989s, 840w, 740, 715w, 655, 645, 615, 585w, 560, 464s, 444s, 430sh, 300s, 280w, 260, 210w, 175w, 145w, 100s, 80, 70, 55.

**Source:** Pillai et al. (1997).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of kröhnikite see also Frost et al. (2013v) and Majzlan et al. (2015).

### Krotite CaAl<sub>2</sub>O<sub>4</sub>

**Origin:** Northwest Africa 1934 meteorite (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 789, 686w, 647w, 543s, 520s, 456w, 404w, 312w, 174, 150, 141.

**Source:** Ma et al. (2011b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is Ca<sub>1.02</sub>Al<sub>1.99</sub>O<sub>4</sub>. For the Raman spectrum of krotite see also Janáková et al. (2007).

### Krut'aite CuSe<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> and 632.8 nm He-Ne lasers radiations. The nominal laser radiation power was 70 and 50 mW, respectively. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 270sh, 260, 115w.

**Source:** Anastassakis (1973).

**Comments:** No independent analytical data are provided for the sample used.

**Kryzhanovskite**  $(\text{Fe}^{3+}, \text{Mn}^{2+})_3(\text{PO}_4)_2(\text{OH}, \text{H}_2\text{O})_3$ 

**Origin:** Hagendorf South pegmatite, Waidhaus, Upper Palatinate, Bavaria, Germany.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3562, 3531, 3432w, 1596w, 1530sh, 1379w, 1114sh, 1081sh, 1046s, 1020sh, 1001sh, 970s, 907sh, 829w, 622sh, 601s, 581sh, 547, 512sh, 477, 414, 363sh, 329, 283s, 251sh, 199s, 179sh, 147sh, 113.

**Source:** Frost et al. (2016d).

**Comment** The sample was characterized by qualitative electron microprobe analysis.

**Ktenasite**  $(\text{Cu}, \text{Zn})_5(\text{SO}_4)_2(\text{OH})_6 \cdot 6\text{H}_2\text{O}$ 

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 994, 981, 973, 604, 475, 449.

**Source:** Frost et al. (2013a).

**Comments:** No independent analytical data are provided for the sample used.

**Kuksite**  $\text{Pb}_3\text{Zn}_3\text{TeO}_6(\text{PO}_4)_2$ 

**Origin:** Blue Bell claims, California, USA, and Black Pine mine, Montana, USA.

**Experimental details:** Methods of samples preparation are not described. Raman scattering measurements have been performed using 785 nm diode laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3036w, 1006, 734, 529, 493, 416 (for a sample from Blue Bell claims); 1017, 731, 497, 476, 424 (for a sample from Black Pine mine).

**Source:** Mills et al. (2010).

**Comments:** The samples were characterized by powder X-ray data and electron microprobe analyses. The crystal structure is solved. The empirical formulae of the samples used are  $(\text{Pb}_{2.89}\text{Bi}_{0.10})(\text{Zn}_{2.84}\text{Cu}_{0.20}\text{Fe}_{0.02})\text{Te}_{1.05}(\text{P}_{1.52}\text{Si}_{0.44}\text{As}_{0.02})\text{O}_{14}$  and  $\text{Pb}_{2.93}(\text{Zn}_{2.74}\text{Cu}_{0.06}\text{Fe}_{0.01})(\text{Te}_{0.58}\text{Sb}_{0.33})(\text{P}_{1.44}\text{As}_{0.74}\text{Si}_{0.11})\text{O}_{14}$ , respectively.

**Kulanite**  $\text{BaFe}^{2+} \text{Al}_2(\text{PO}_4)_3(\text{OH})_3$ 

**Origin:** Rapid Creek, Dawson Mining District, Yukon, Canada (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3533, 3513w, 3339sh, 3211, 3095w, 2960sh, 2754sh, 1303w, 1235w, 1182sh, 1146, 1110, 1076sh, 1039sh, 1022s, 1012sh, 1006sh, 967, 928w, 665w, 624sh, 616, 585, 569, 553, 525, 492, 456, 438, 418, 358w, 343, 317w, 279, 213, 196sh, 186sh, 161sh, 137, 122.

**Source:** Frost et al. (2013k).

**Comments:** No independent analytical data are provided for the sample used.

### Kullerudite NiSe<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline thin film using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power density on the surface was of the order of 100 kW cm<sup>-2</sup>. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 243, 214s, 170, 152.

**Source:** De las Heras and Agulló-Rueda (2000).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of kullerudite see also Zhuo et al. (2015).

### Kumdykolite Na(AlSi<sub>3</sub>O<sub>8</sub>)

**Origin:** Village of Staré, České Středohoří Mts., Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 492s, 464, 407w, 284sh, 265, 222, 155s.

**Source:** Kotková et al. (2014).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectra of kumdykolite see also Hwang et al. (2009) and Ferrero et al. (2016).

### Kumtyubeite Ca<sub>5</sub>(SiO<sub>4</sub>)<sub>2</sub>F<sub>2</sub>

**Origin:** Upper Chegem volcanic structure, Kabardino-Balkaria, Northern Caucasus, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was in the range from 20 to 40 mW. A 0°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3561, 3553s, 3544, 925w, 901, 849, 822s, 547, 525w, 420, 397, 323, 299w, 281.

**Source:** Galuskina et al. (2009).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is Ca<sub>5</sub>(Si<sub>1.99</sub>Ti<sub>0.01</sub>)O<sub>8</sub>(F<sub>1.39</sub>OH<sub>0.61</sub>).

### Kuramite Cu<sub>3</sub>SnS<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 346s, 333s, 316s, 289.

**Source:** Gusain et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Kuranakhite**  $\text{PbMn}^{4+}\text{Te}^{6+}\text{O}_6$

**Origin:** Moctezuma, Sonora, Mexico.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm  $\text{Ar}^+$  laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 677, 619s, 508, 380, 320, 310.

**Source:** Grundler et al. (2008).

**Comments:** The sample was characterized by electron microprobe analyses. Raman spectrum of presumed kuranakhite published by Frost and Keeffe (2009e) without accompanying analytical data is questionable.

**Kuratite**  $\text{Ca}_2(\text{Fe}^{2+}, \text{Ti})\text{O}_2[\text{Si}_4\text{Al}_2\text{O}_{18}]$

**Origin:** D'Orbigny angrite meteorite (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 996, 856, 699s, 563, 500sh, 351.

**Source:** Hwang et al. (2016).

**Comments:** The sample was characterized by selected area electron diffraction and electron microprobe analysis. The empirical formula of the sample used is  $(\text{Ca}_{3.88}\text{Na}_{0.02}\text{REE}^{3+}_{0.03}\text{Mn}_{0.03}\text{Mg}_{0.01}\text{Ni}_{0.02}\text{Zn}_{0.01}\text{Sr}_{0.01})(\text{Fe}^{2+}_{9.98}\text{Ti}_{2.00})(\text{Si}_{7.80}\text{Al}_{3.52}\text{Fe}^{3+}_{0.64}\text{P}_{0.05}\text{S}_{0.02})\text{O}_{39.98}\text{F}_{0.01}\text{Cl}_{0.01}$ .

**Kurnakovite**  $\text{MgB}_3\text{O}_3(\text{OH})_5 \cdot 5\text{H}_2\text{O}$

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 944, 850s, 627, 466w, 422, 391.

**Source:** Jun et al. (1995).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Kusachiite**  $\text{Cu}^{2+}\text{Bi}^{3+}_2\text{O}_4$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powder sample using 1064 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 914, 879, 625, 599, 560, 497, 482s, 451s, 415.

**Source:** Anandan et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Kushiroite** CaAlAlSiO<sub>6</sub>**Origin:** ALH 85085 CH chondrite.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 and 514.5 nm Ar<sup>+</sup> laser radiations. The nominal laser radiation power was in the range from 12 to 20 mW.**Raman shifts (cm<sup>-1</sup>):** 959, 675, 520w, 410sh, 369, 334.**Source:** Kimura et al. (2009).**Comments:** The sample was characterized by electron backscatter diffraction and electron microprobe analyses. The empirical formula of the sample used is Ca<sub>1.008</sub>(Mg<sub>0.094</sub>Fe<sub>0.034</sub>Al<sub>0.878</sub>)(Al<sub>0.921</sub>Si<sub>1.079</sub>)O<sub>6</sub>. For the Raman spectrum of kushiroite see also Ma et al. (2009).**Kutnohorite** CaMn<sup>2+</sup>(CO<sub>3</sub>)<sub>2</sub>**Origin:** No data.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation output power was in the range from 200 to 300 mW. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 1740w, 1420w, 1086s, 716, 284.**Source:** Herman et al. (1987).**Comments:** The sample was characterized by powder X-ray diffraction data and by quantitative chemical analysis.**Kuzminite** HgBr**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal using 514.5 nm Ar<sup>+</sup> and 632.8 nm He-Ne laser radiations. The nominal laser radiation power was in the range from tens to hundreds mW. Spectra were collected in the (zz), (xz), and (yz) scattering geometries.**Raman shifts (cm<sup>-1</sup>):** 208, 128, 85, 35.**Source:** Markov and Roginskii (2011).**Comments:** No independent analytical data are provided for the sample used. The Raman shifts are given as the sum of the Raman shifts for different scattering geometries. For the Raman spectrum of kuzminite see also Ōsaka (1971).**Kyanite** Al<sub>2</sub>OSiO<sub>4</sub>**Origin:** Harts Range, Northern Territory, Australia.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 60 mW.**Raman shifts (cm<sup>-1</sup>):** 998w, 952s, 900w, 669sh, 654, 632, 606, 562, 486s, 437, 419, 405, 386, 360, 325, 302.**Source:** Mernagh and Liu (1991).**Comments:** The sample was characterized by electron microprobe analysis. The Raman shifts were partly determined by us based on spectral curve analysis of the published spectrum. For the Raman

spectra of kyanite see also Makreski et al. (2005b), Yang et al. (2007b), Andò and Garzanti (2014), and Culka et al. (2016a).

### Kyawthuite $\text{Bi}^{3+}\text{Sb}^{5+}\text{O}_4$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was less than 10 mW. A 180°-scattering geometry was employed. The Raman shifts for asymmetric peaks have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts ( $\text{cm}^{-1}$ ):** 783w, 730w, 636w, 603w, 452, 420w, 394, 387sh, 319w, 252, 158s, 137s, 133sh, 56s.

**Source:** Errandonea et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectrum of kyawthuite see also Loubbidi et al. (2014).

### Laachite $(\text{Ca},\text{Mn})_2\text{Zr}_2\text{Nb}_2\text{TiFeO}_{14}$

**Origin:** Dellen (Ziegłowski) pumice quarry, 1.5 km NE of Mendig, Laacher See volcano, Eifel region, Rhineland-Palatinate, Germany (typical locality).

**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal using 532 nm diode laser radiation. The laser radiation power about 6 mW. Raman spectra were collected with the polarization of the laser beam parallel to the  $a$  axis of the crystal (A) and with the polarization of the laser beam lying in the plane (010), perpendicular to the  $a$  axis of the crystal (B) scattering geometries. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts ( $\text{cm}^{-1}$ ):** 1568w, 1190w, 821sh, 752, 584s, 468sh, 300s, 183w (A); 1175w, 832sh, 757, 588s, 485, 371sh, 330, 213sh, 192 (B).

**Source:** Chukanov et al. (2014a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Ca}_{0.66}\text{Mn}_{0.37}\text{Th}_{0.25}\text{Y}_{0.20}\text{La}_{0.11}\text{Ce}_{0.34}\text{Nd}_{0.11})(\text{Zr}_{1.36}\text{Mn}_{0.64})(\text{Nb}_{1.81}\text{Ti}_{1.19})(\text{Fe}_{0.69}\text{Al}_{0.17}\text{Mn}_{0.14})\text{O}_{14.00}$ .

### Lacroixite $\text{NaAl}(\text{PO}_4)\text{F}$

**Origin:** Ehrenfriedersdorf, Germany.

**Experimental details:** No data.

**Raman shifts ( $\text{cm}^{-1}$ ):** 1001s, 623, 609.

**Source:** Frezzotti et al. (2012).

**Comments:** No independent analytical data are provided for the sample used.

### Lafossaitite $\text{TlCl}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented polished crystals using 457.9 nm, 476.5 nm, and 514.5 nm  $\text{Ar}^+$  laser radiations. The sample was

immersed in pumped liquid helium or in liquid nitrogen. The laser radiation power at the sample was below 200 mW.

**Raman shifts (cm<sup>-1</sup>):** 340s, 237, 190, 172s, 147, 111, 98, 85sh, 70sh, 36, 26sh.

**Source:** Nanba et al. (1987).

**Comments:** No independent analytical data are provided for the sample used. In lafossaaite, the first order Raman scattering process is forbidden by the inversion symmetry (the alternative prohibition rule). However, the second order Raman scattering spectrum is allowed. Raman shifts are given for a sample at 77 K.

### Laihunite (Fe<sup>3+</sup>,Fe<sup>2+</sup>,□)<sub>2</sub>(SiO<sub>4</sub>)

**Origin:** Lau-Hi, China.

**Experimental details:** Experimental details are not indicated. Raman scattering measurements have been performed on an arbitrarily oriented polished sample.

**Raman shifts (cm<sup>-1</sup>):** 896s, 785w, 592sh, 568s, 506w, 428w, 355sh, 312s.

**Source:** Kuebler et al. (2011).

**Comments:** The sample was characterized by electron microprobe analyses.

### Lakargiite CaZrO<sub>3</sub>

**Origin:** Upper Chegem caldera, Kabardino-Balkaria, Northern Caucasus, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented polished sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was in the range from 40 to 60 mW. A 0°-scattering geometry was employed. Raman spectrum was obtained in the spectral region from 50 to 4000 cm<sup>-1</sup>.

**Raman shifts (cm<sup>-1</sup>):** ~800w, ~715w, ~525w, ~470, ~442s, ~355s, ~285s, ~262s, ~240w, ~215w, ~182w, ~152w.

**Source:** Galuskin et al. (2011b).

**Comments:** The sample was characterized by powder X-ray diffraction analysis and by electron microprobe analyses. Raman shifts are given for lakargiite with the following chemical composition: lakargiite CaZrO<sub>3</sub> 67%, megawite CaSnO<sub>3</sub> 27%, perovskite CaTiO<sub>3</sub> 2%, and others 4%.

### Lamprophyllite Na<sub>3</sub>(SrNa)Ti<sub>3</sub>(Si<sub>2</sub>O<sub>7</sub>)<sub>2</sub>O<sub>2</sub>(OH)<sub>2</sub>

**Origin:** Rasvumchorr Mt., Khibiny massif, Kola Peninsula, Russia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1113w, 1072w, 1049w, 1028w, 1001w, 972w, 940s, 918s, 888sh, 861w, 852sh, 801w, 782sh, 707, 671, 595sh, 576, 538w, 516w, 459w, 445sh, 411w, 349, 319w, 294sh, 282sh, 270, 257sh, 227w, 208sh, 201, 177sh, 168sh, 151, 137sh, 114w.

**Source:** Frost et al. (2015ab).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

**Lanarkite**  $\text{Pb}_2\text{O}(\text{SO}_4)$ **Origin:** Leadhills, Scotland, UK.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented polished cross-section of the sample using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was in the range from 0.02 to 2 mW.**Raman shifts (cm<sup>-1</sup>):** 1070, 1055, 976s, 619w, 601w, 439w, 426w, 334, 284, 147s.**Source:** Correia et al. (2007).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.**Långbanite**  $\text{Mn}^{2+}{}_4\text{Mn}^{3+}{}_9\text{Sb}^{5+}\text{O}_{16}(\text{SiO}_4)_2$ **Origin:** Långban mine, Bergslagen ore district, Filipstad, Värmland, Sweden (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals. Other experimental details are not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3699sh, 3680w, 3476sh, 3076sh, 2636w, 2488w, 2240w, 1947w, 1718w, 1432w, 1200sh, 1130, 1094sh, 1034sh, 1012sh, 986s, 964s, 897sh, 872, 671, 646sh, 558sh, 542, 463w, 415sh, 386, 351, 330sh, 258w, 202.**Source:** Bahfenne and Frost (2010a).**Comments:** No independent analytical data are provided for the sample used.**Langbeinite**  $\text{K}_2\text{Mg}_2(\text{SO}_4)_3$ **Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 514 nm and 785 nm lasers radiations. The laser radiation power at the sample was less than 1 mW.**Raman shifts (cm<sup>-1</sup>):** 1245w, 1134w, 1123w, 1053s, 626w, 466w, 457w.**Source:** Morillas et al. (2016).**Comments:** The sample was characterized by electron microprobe analysis.**Langite**  $\text{Cu}_4(\text{SO}_4)_6 \cdot 2\text{H}_2\text{O}$ **Origin:** Cornwall, UK.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 780 nm Nd-YAG laser radiation. The nominal laser radiation power was less than 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3587, 3564, 3405, 3372, 3260w, 1911, 1906, 1266, 1172, 1149, 1128, 1102, 1076, 982sh, 974s, 911w, 773w, 732, 621, 609, 596s, 507, 481, 449, 420, 391, 317, 273sh, 258sh, 241, 226sh, 1912, 183sh, 175, 167, 155, 147, 139, 130sh, 118sh.**Source:** Martens et al. (2003a).**Comments:** No independent analytical data are provided for the sample used.

**Lanmchangite**  $\text{TiAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** The stimulated Raman scattering measurements have been performed on an oriented sample using 532 nm and 1064 nm Nd-YAG laser radiations. The laser radiation power is not indicated. Raman spectra were collected in the scattering geometries with pumping and registration along [110] direction and polarization both emissions perpendicular to the [110] direction.**Raman shifts (cm<sup>-1</sup>):** 991s.**Source:** Kaminskii et al. (2004).**Comments:** No independent analytical data are provided for the sample used.**Lansfordite**  $\text{Mg}(\text{CO}_3) \cdot 5\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed below 0°C on an arbitrarily oriented microcrystalline sample using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was about 8 mW.**Raman shifts (cm<sup>-1</sup>):** 3264s, 1705w, 1514w, 1424w, 1098s, 774w, 698w, 225s.**Source:** Coleyshaw et al. (2003).**Comments:** No independent analytical data are provided for the sample used.**Lanthanite-(Nd)**  $\text{Nd}_2(\text{CO}_3)_3 \cdot 8\text{H}_2\text{O}$ **Origin:** Whitianga quarry, Coromandel Peninsula, New Zealand.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystal blades using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 25 mW. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 3471s, 3280s, 3072s, 2865s, 1702w, 1636w, 1615w, 1612w, 1581, 1576w, 1559w, 1557w, 1513w, 1505w, 1487w, 1459w, 1454w, 1418w, 1394w, 1365, 1294w, 1292w, 1286w, 1173w, 1093s, 968w, 762w, 732w, 686w, 372w, 356w, 277w, 233.**Source:** Graham et al. (2007).**Comments:** The sample was characterized by powder X-ray diffraction data, electron microprobe analysis and laser-ablation inductively coupled plasma mass spectrometry. The empirical formula of the sample used is  $(\text{Nd}_{0.63}\text{La}_{0.59}\text{Ce}_{0.35}\text{Pr}_{0.15}\text{Sm}_{0.10}\text{Gd}_{0.069}\text{Y}_{0.06}\text{Eu}_{0.03}\text{Dy}_{0.02}\text{Ga}_{0.01})(\text{CO}_3)_3 \cdot 8\text{H}_2\text{O}$ .**Lapeyreite**  $\text{Cu}_3\text{O}[\text{AsO}_3(\text{OH})_2] \cdot \text{H}_2\text{O}$ **Origin:** Alpes-Maritimes Region, Nice, France (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented fragment of the holotype sample using 532 nm He-Ne laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1047, 627, 405, 214s, 198sh, 188sh, 141, 100.**Source:** Hatipoglu and Babalik (2012).

**Larnite**  $\text{Ca}_2(\text{SiO}_4)$ **Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 17 mW. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 1577w, 1112w, 1085w, 976, 949, 914, 897w, 871sh, 858s, 845sh, 669w, 564w, 554w, 536, 524sh, 516sh, 443, 368w, 300, 274sh, 252w, 241, 222w, 201w, 165, 146, 101w, 76w.**Source:** Sokol et al. (2015).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectrum of larnite see also Piriou and McMillan (1983).**Laueite**  $\text{Mn}^{2+}\text{Fe}^{3+}_2(\text{PO}_4)_2(\text{OH})_2\cdot 8\text{H}_2\text{O}$ **Origin:** Cigana mine, Conselheiro Pena, Minas Gerais, Brazil.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power at the sample was 0.1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3515sh, 3478sh, 3430, 3379, 3297sh, 3080sh, 1692sh, 1613w, 1504sh, 1096sh, 1069, 1045s, 1021, 997sh, 980s, 864w, 731, 551, 542, 525, 472, 456, 404, 357, 335, 279, 265, 253s, 240, 226sh, 186, 172, 161s, 138, 115, 110.**Source:** Frost et al. (2016b).**Comments:** The empirical formula based on the semiquantitative chemical analyses of the sample used is  $(\text{Mn}^{2+}_{0.85}\text{Fe}^{2+}_{0.10}\text{Mg}_{0.05})(\text{Fe}^{3+}_{1.90}\text{Al}_{0.10})(\text{PO}_4)_2(\text{OH})_2\cdot 8\text{H}_2\text{O}$ .**Laumontite**  $\text{CaAl}_2\text{Si}_4\text{O}_{12}\cdot 4\text{H}_2\text{O}$ **Origin:** Grodziszcz, Poland.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using Nd-YAG laser radiation. The laser radiation power at the sample was 300 mW.**Raman shifts (cm<sup>-1</sup>):** 1023, 948, 817, 674, 593, 517s, 493s, 385, 327s, 201, 164.**Source:** Mozgawa (2001).**Comments:** The sample was characterized by powder X-ray diffraction data.**Laurentianite**  $[\text{NbO}(\text{H}_2\text{O})]_3(\text{Si}_2\text{O}_7)_2[\text{Na}(\text{H}_2\text{O})_2]_3$ **Origin:** Poudrette quarry, Mont Saint-Hilaire, Quebec, Canada (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 532 laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 3421, 33267, 3024, 1103w, 1054w, 920s, 841s, 771w, 700, 628w, 597, 560w, 486w, 467w, 405, 344w, 309, 292, 241, 218sh, 193sh, 176, 138sh, 122, 90.**Source:** Haring et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $[(Nb_{0.99}Ti_{0.01})O(H_2O)]_3(Si_{2.00}O_7)_2[(Na_{0.86}□_{0.10}K_{0.02}Ca_{0.01})(H_2O)_2]_3$ .

### Laurionite PbCl(OH)

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline and on an oriented single crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. 90° and 180°-scattering geometries were employed in single-crystal experiments. Raman spectra were obtained in the spectral region from 50 to 4000 cm<sup>-1</sup>. Polarized spectra were collected in the *c*(*xx*)–*c*, *c*(*yy*)–*c*, *a*(*zz*)–*a*, *a*(*yx*)*c*, *a*(*zx*)*c*, and *a*(*zy*)*c* scattering geometries.

**Raman shifts (cm<sup>-1</sup>):** 3517s, 665sh, 595, 505w, 446w, 327, 272, 175w, 123sh, 111s, 105s, 87sh, 51s.

**Source:** Lutz et al. (1995).

**Comments:** The sample was characterized by powder X-ray diffraction analysis. The Raman shifts are given for a polycrystalline sample.

### Laurite RuS<sub>2</sub>

**Origin:** Santa Elena Nappe, Costa Rica.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532.6 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~395w, 330s.

**Source:** Zaccarini et al. (2010).

**Comments:** The sample was characterized by electron microprobe analyses.

### Laurite RuS<sub>2</sub>

**Origin:** No data.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532.1 nm Nd-YAG laser radiation. The laser radiation power at the sample was in the range from 1 to 2 mW.

**Raman shifts (cm<sup>-1</sup>):** ~395sh, 364–351s.

**Source:** Bakker (2014).

**Comments:** No independent analytical data are provided for the sample used.

### Lausenite Fe<sup>3+</sup><sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>·5H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3425sh, 3323sh, 3195, 3057sh, 1653w, 1605w, 1189, 1119w, 1087w, 1052sh, 1036s, 1017, 799w, 652w, 631w, 614w, 599w, 494, 468, 457, 441sh, 416sh, 281, 253.

**Source:** Ling and Wang (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Lautarite**  $\text{Ca}(\text{IO}_3)_2$ **Origin:** Synthetic.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 830s, 808w, 794s, 775, 759s, 737s, 427, 394, 362sh, 351, ~333sh, 326, ~315sh, 266w, 235.**Source:** Alici et al. (1992).**Comments:** The sample was characterized by powder X-ray diffraction data.**Lavendulan**  $\text{NaCaCu}_5(\text{AsO}_4)_4\text{Cl}\cdot 5\text{H}_2\text{O}$ **Origin:** Alice Mary Mine, Kundip, Western Australia, Australia.**Experimental details:** Experimental details are not indicated. Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 1053w, 981w, 893sh, 878sh, 856s, 783, 614w, 543s, 406, 342w, 278w, 226, 176.**Source:** Frost et al. (2007m).**Comments:** No independent analytical data are provided for the sample used.**Lavinskyite**  $\text{K}(\text{LiCu})\text{Cu}_6(\text{Si}_4\text{O}_{11})_2(\text{OH})_4$ **Origin:** Wessels mine, Kalahari Manganese Fields, South Africa (type locality).**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm solid-state laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3694, 3662s, 3630sh, 3390, 1090, 1043, 991, 919, 891, 685s, 580w, 562, 503, 445+424s, 401.**Source:** Yang et al. (2014).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{K}_{0.99}\text{Ba}_{0.01})(\text{Li}_{1.04}\text{Cu}_{0.93}\text{Na}_{0.10})(\text{Cu}_{5.57}\text{Mg}_{0.43}\text{Mn}_{0.01})(\text{Si}_{4.00}\text{O}_{11})_2(\text{OH})_4$ .**Lawrencite**  $\text{FeCl}_2$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed at 277 K using 647.1 nm Kr<sup>+</sup> laser radiation. The laser light was directed along the *c* face of the crystal with polarization in the plane of incidence. In this configuration the scattered light is largely depolarised and there were no polarization effects. The nominal laser radiation power was about 100 mW. A 90°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 246, 144s.**Source:** Johnstone et al. (1978).**Comments:** No independent analytical data are provided for the sample used.

**Lawsonite**  $\text{CaAl}_2(\text{Si}_2\text{O}_7)(\text{OH})_2 \cdot \text{H}_2\text{O}$ 

**Origin:** Tiburon Peninsula, California, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed at different pressures, on an arbitrarily oriented single-crystal slice oriented parallel to (001), using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3541, 961sh, 940s, 918sh, 800, 696, 565s, 462w, 434w, 364w, 330, 282, 280.

**Source:** Daniel et al. (2000).

**Comments:** The sample was characterized by powder X-ray diffraction data. Raman shifts are given for sample at ambient conditions (pressure 0.1 MPa).

**Lazaridisite**  $\text{Cd}_3(\text{SO}_4)_3 \cdot 8\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented microcrystal using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1117, 1004s, 625w, 460, 330w.

**Source:** Falgayrac et al. (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Lazulite**  $\text{MgAl}_2(\text{PO}_4)_2(\text{OH})_2$ 

**Origin:** Gentil mine, Mendes Pimentel, east of Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3478w, 3402s, 3385sh, 3373sh, 3146w, 1684w, 1528sh, 1509w, 1271w, 1214w, 1139sh, 1137s, 1102, 1089sh, 1060s, 1019, 1004sh, 865w, 790w, 742, 714w, 669sh, 648, 633sh, 623, 613sh, 605sh, 580w, 568w, 527w, 479, 460w, 425, 414, 394sh, 378, 365sh, 347, 333sh, 322, 282, 254, 225, 197sh, 195sh, 190s, 173, 137.

**Source:** Frost et al. (2013p).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectrum of lazulite see also Frezzotti et al. (2012).

**Lazurite**  $\text{Na}_3\text{Ca}(\text{Si}_3\text{Al}_3)\text{O}_{12}\text{S}$ 

**Origin:** Badakhshan, Afghanistan.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 1090, 970w, 801w, 636w, 582sh, 545s, 413w, 258.

**Source:** Caggiani et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction analysis and by energy-dispersive X-ray scan analysis. For the Raman spectra of lazurite see also Ostroumov et al. (2002).

**Lead Pb**

**Origin:** Karrantza Valley, the westerner area of the Basque Co., Spain.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 153s.

**Source:** Goienaga et al. (2011).

**Comments:** No independent analytical data are provided for the sample used.

**Leadhillite Pb<sub>4</sub>(SO<sub>4</sub>)<sub>2</sub>(CO<sub>3</sub>)<sub>2</sub>(OH)<sub>2</sub>**

**Origin:** Hard Luck Claim, near Baker, San Bernardino Co., California, USA.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3481, 3386sh, 1719, 1704, 1674, 1375, 1097sh, 1054s, 1016sh, 964s, 856, 703w, 677w, 626w, 599w, 458sh, 428s, 360w, 307w, 262w, 220sh, 195sh, 173s.

**Source:** Frost et al. (2003e).

**Comments:** No independent analytical data are provided for the sample used.

**Lechatelierite SiO<sub>2</sub>**

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 3 mW.

**Raman shifts (cm<sup>-1</sup>):** 1110w, 802, 603, 493, 441, ~300sh.

**Source:** Kowitz et al. (2013).

**Comments:** The sample was characterized by energy-dispersive X-ray scan analysis. Raman shifts are given for a sample subjected to a shock more than 36 GPa.

**Leguernite Bi<sub>12.67</sub>O<sub>14</sub>(SO<sub>4</sub>)<sub>5</sub>**

**Origin:** La Fossa crater, Vulcano, Aeolian Islands, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 532 nm laser radiation. The nominal laser radiation power was 1.4 mW.

**Raman shifts (cm<sup>-1</sup>):** 2430, 1145sh, 1019, 970s, 603sh, 473, 429, 279s, 243, 183, 150.

**Source:** Garavelli et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The crystal structure is solved. The empirical formula of the sample used is (Bi<sub>12.40</sub>Pb<sub>0.15</sub>)S<sub>5.08</sub>O<sub>34</sub>.

**Leightonite K<sub>2</sub>Ca<sub>2</sub>Cu(SO<sub>4</sub>)<sub>4</sub>·2H<sub>2</sub>O**

**Origin:** Chuquicamata mine, Antofagasta region, Chile (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The

Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3457sh, 3435, 3386sh, 3364sh, 3350s, 3329s, 3310sh, 3206w, 3088w, 2911w, 2856w, 1803w, 1748w, 1700sh, 1670w, 1446w, 1177w, 1163w, 1137w, 1120w, 1047, 990sh, 975sh, 912, 864w, 846sh, 823, 753w, 654, 640sh, 612, 601, 589sh, 513, 463, 446, 425sh, 413, 394, 361, 298, 266, 238w, 217, 155sh, 149, 137, 126sh, 120, 106.

**Source:** Frost et al. (2013j).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

### Leiteite ZnAs<sup>3+</sup><sub>2</sub>O<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample and oriented crystal using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. Polarized spectra were collected in the *c(bb)c*, *c(ba)c*, *c(aa)c*, *b(ac)b*, *b(aa)b*, *a(bb)a*, *a(bc)a*, and *a(cc)a* scattering geometries. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 804, 763, 647w, 600, 566sh, 548, 457s, 3768w, 366w, 304w, 265sh, 254s, 217, 199w.

**Source:** Bahfenne et al. (2011b).

**Comments:** The sample was characterized by powder X-ray diffraction analysis and electron microprobe analysis. For the Raman spectra of leiteite see also Origlieri et al. (2009) and Frost and Bahfenne (2010d).

### Lemanskiite NaCaCu<sub>5</sub>(AsO<sub>4</sub>)<sub>4</sub>Cl·5H<sub>2</sub>O

**Origin:** El Guanqco mine, Antofagsta, Chile (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1369, 1264, 1165w, 910w, 878s, 853s, 800w, 775w, 545, 479w, 440w, 400w, 345, 280sh, 262w, 243w, 220, 172.

**Source:** Frost et al. (2007m).

**Comments:** No independent analytical data are provided for the sample used.

### Lemoynite Na<sub>2</sub>CaZr<sub>2</sub>Si<sub>10</sub>O<sub>26</sub>·5-6H<sub>2</sub>O

**Origin:** Poudrette quarry, Mont Saint-Hilaire, Montérégie, Quebec, Canada (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 952–961, ~600–605s, 533–540s, 426–429s, (~360w), (~325w), (~280), (~250w).

**Source:** McDonald et al. (2015).

**Comments:** No independent analytical data are provided for the sample used.

**Leogangite** Cu<sub>10</sub>(AsO<sub>4</sub>)<sub>4</sub>(SO<sub>4</sub>)(OH)<sub>6</sub>·8H<sub>2</sub>O

**Origin:** Monte Avanza Mine, Formi Avoltri, Udine Province, Fruili Venezia Giulia, Italy.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3619sh, 3496, 3316, 3181sh, 2929, 2884sh, 2854w, 1627w, 1576w, 1461sh, 1441w, 1070w, 996w, 904sh, 868s, 827sh, 628w, 606sh, 519, 498sh, 431, 416sh, 336sh, 324, 312sh, 263, 228sh, 205, 153, 139sh, 106.

**Source:** Frost et al. (2011t).

**Comments:** No independent analytical data are provided for the sample used.

**Leószilárdite** Na<sub>6</sub>Mg(UO<sub>2</sub>)<sub>2</sub>(CO<sub>3</sub>)<sub>6</sub>·6H<sub>2</sub>O

**Origin:** Markey Mine, San Juan County, Utah, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm diode laser radiation. The nominal laser radiation power was 200 mW.

**Raman shifts (cm<sup>-1</sup>):** 1535w, 1396w, 1328w, 1078, 1062, 1052, 824s, 742, 728, 705w, 695w, 345, 290, 254, 193sh, 172sh, 161s, 144s, 125s.

**Source:** Olds et al. (2016b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is Na<sub>5.60</sub>Mg<sub>0.90</sub>U<sub>2</sub>O<sub>28</sub>C<sub>6</sub>H<sub>12.60</sub>.

**Lepidocrocite** Fe<sup>3+</sup>O(OH)

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm diode laser radiation. The output laser radiation power was more than 300 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 647w, 524s, 374s, 345s, ~315w, 284s, 249sh, 214, 140.

**Source:** Das and Hendry (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of lepidocrocite see also De Faria et al. (1997) and Bouchard and Smith (2003).

**Letovicite** (NH<sub>4</sub>)<sub>3</sub>H(SO<sub>4</sub>)<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed at different temperatures on an oriented crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 4 W. A 90°-scattering geometry was employed. Spectra were collected in (yy) scattering geometry.

**Raman shifts (cm<sup>-1</sup>):** ~670sh, ~655, ~480s, ~275w, ~200w, ~90.

**Source:** Schwalowsky et al. (1996).

**Comments:** The sample was characterized by powder X-ray diffraction data and synchrotron diffraction analysis. The Raman shifts are given for a sample at 298 K.

**Leucite**  $K(AlSi_2O_6)$ 

**Origin:** Swan City, Colorado, USA.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 488 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 600 mW. A 90°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1066, 984sh, 786w, 678w, 618w, 528sh, 498s, 432w, 394w, 338, 304, 272w, 266w, 216, 180, 152, 112, 76.

**Source:** Matson et al. (1986).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of leucite see also Castriota et al. (2008).

**Leucophosphite**  $KFe^{3+}_2(PO_4)_2(OH)\cdot 2H_2O$ 

**Origin:** Sapucaia mine, Conselheiro Pena pegmatite district, Brazil.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3535sh, 3456, 3355sh, 3225, 3171sh, 2892sh, 1632w, 1255w, 1177, 1135, 1104, 1087sh, 1058s, 1028sh, 1014sh, 994s, 973sh, 850w, 789w, 630s, 611s, 589sh, 550w, 497sh, 481, 436, 420, 407sh, 380sh, 336sh, 310sh, 303s, 282sh, 262sh, 226sh, 215, 204sh, 190sh, 164, 152, 142, 129sh, 117.

**Source:** Frost et al. (2013ac).

**Comments:** The sample was characterized by powder X-ray diffraction data and qualitative electron microprobe analysis.

**Lévyne-Ca**  $Ca_3(Si_{12}Al_6)O_{36}\cdot 18H_2O$ 

**Origin:** Stolpen, Germany.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using Nd-YAG laser radiation. The laser radiation power at the sample was 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 917w, 709s, 430s, 290, 264w, 202s.

**Source:** Mozgawa (2001).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Leydetite**  $Fe(UO_2)(SO_4)_2\cdot 11H_2O$ 

**Origin:** Mas d'Alary, Lodève, France (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was 2.5 mW.

**Raman shifts (cm<sup>-1</sup>):** 3492, 3404, 3237, 3130, 1679, 1649, 1203, 1180, 1150, 1139, 1135, 1113, 1099, 1038s, 1030, 1023, 1015, 937, 930, 858, 851, 846, 843, 836, 828, 686s, 675, 666, 608, 538, 522, 504, 485, 464, 443, 420, 394, 373, 290, 260, 236, 223, 196, 182, 165, 138, 123, 116, 102, 89, 77, 65.

**Source:** Plášil et al. (2013a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $(\text{Fe}_{0.93}\text{Mg}_{0.07}\text{Al}_{0.04}\text{Cu}_{0.01})(\text{U}_{1.01}\text{O}_2)(\text{S}_{1.96}\text{Si}_{0.02})\text{O}_8(\text{H}_2\text{O})_{11}$ .

### Libethenite $\text{Cu}_2(\text{PO}_4)(\text{OH})$

**Origin:** Banská Bystrica, central Slovakia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 17 mW. A  $180^\circ$ -scattering geometry was employed. Polarized spectra were collected in parallel and perpendicular to the *c*-axis scattering geometries. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3485–3475, 1130w, 1102w, 1075sh, 1052, 1022s, 1008sh, 979s, 944sh, 864w, 818w, 650w, 625, 590, 561, 461, 430sh, 392, 371sh, 319sh, 301s, 270w, 250w, 227s, 195s, 160s, 140sh, 113w, 92sh, 74s.

**Source:** Kharbish et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. Raman shifts are given as sum of spectra at parallel and perpendicular to the *c*-axis scattering geometries. For the Raman spectra of libethenite see also Frost et al. (2002g), Bouchard and Smith (2003), Belik et al. (2007, 2011), and Majzlan et al. (2015).

### Liebenbergite $\text{Ni}_2(\text{SiO}_4)$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed at different pressures on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was about 60 mW. A  $180^\circ$ -scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 952, 889, 868sh, 831s, 819s, 593sh, 560, 521, 414, 344w, 298, 272w, 252w, 221w, 191w, 181w.

**Source:** Lin (2001).

**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts are given for a sample at ambient conditions.

### Liebigite $\text{Ca}_2(\text{UO}_2)(\text{CO}_3)_3 \cdot 11\text{H}_2\text{O}$

**Origin:** Kroderen, Snarum, Norway.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3468s, 3258s, 1566, 1409, 1381, 1087s, 1073sh, 1007w, 838sh, 822s, 816sh, 758w, 747sh, 248.

**Source:** Frost et al. (2005g).

**Comments:** No independent quantitative analytical data are provided for the sample used.

**Likasite** Cu<sub>3</sub>(NO<sub>3</sub>)(OH)<sub>5</sub>·2H<sub>2</sub>O**Origin:** Great Australian Mine, Queensland, Australia.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3567sh, 3522s, 3452sh, 3338sh, 3281, 3040w, 1628w, 1394w, 1319w, 1050, 1049, 980w, 831, 763, 715w, 706w, 529, 514, 493, 459w, 377w, 341w, 233w, 210w, 190w, 175w, 165w, 140w.**Source:** Frost et al. (2005h).**Comments:** No independent analytical data are provided for the sample used.**Lime** CaO**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 10 mW.**Raman shifts (cm<sup>-1</sup>):** ~680w.**Source:** Schmid and Dariz (2015).**Comments:** No independent analytical data are provided for the sample used. The CaO phase has halite structure with cubic unit cell (Fm3m) and does not have the first-order Raman scattering. The given Raman shift belongs to the second-order Raman scattering.**Linarite** CuPb(SO<sub>4</sub>)(OH)<sub>2</sub>**Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632 nm He-Ne laser radiation with output radiation power 30 mW, and 514.5 nm Ar<sup>+</sup> laser radiation with a low radiation power.**Raman shifts (cm<sup>-1</sup>):** 3471sh, 3448, 3220w, 1141, 1019, 968s, 818w, 632, 610, 594w, 513, 461, 436, 365, 345sh, 326w, 230w, 163.**Source:** Bouchard and Smith (2003).**Comments:** The sample was characterized by powder X-ray diffraction analysis. For the Raman spectra of linarite see also Buzgar et al. (2009) and Hrazdil et al. (2016).**Lindbergite** Mn(C<sub>2</sub>O<sub>4</sub>)·2H<sub>2</sub>O**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 100 mW.**Raman shifts (cm<sup>-1</sup>):** 3326s, 1469s, 908, 579, 517, 240, 199.**Source:** Echigo and Kimata (2008).**Comments:** The sample was characterized by powder X-ray diffraction data.

**Lindbergite** Mn(C<sub>2</sub>O<sub>4</sub>)·2H<sub>2</sub>O**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 1064 nm Nd-YAG laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1625w, 1465s, 1410w, 909, 855w, 579, 517.**Source:** Mancilla et al. (2009a).**Comments:** No independent analytical data are provided for the sample used.**Lindgrenite** Cu<sub>3</sub>(Mo<sup>6+</sup>O<sub>4</sub>)<sub>2</sub>(OH)<sub>2</sub>**Origin:** Broken Hill, NSW, Australia.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm Nd-YAG laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 932s, 887w, 839w, 798w, 775w, 496w, 399, 349, 325, 313, 302s, 287w, 251, 217sh, 190w, 171, 158, 123w.**Source:** Frost et al. (2004c).**Comments:** The sample was characterized by qualitative electron microprobe analysis.**Lindsleyite** (Ba,Sr)(Zr,Ca)(Fe,Mg)<sub>2</sub>(Ti,Cr,Fe)<sub>18</sub>O<sub>38</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632 nm He-Ne laser radiation. The nominal laser radiation power was in the range from 2 to 4 mW.**Raman shifts (cm<sup>-1</sup>):** 1702s, 661s, 560, 433, 327.**Source:** Konzett et al. (2005).**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analysis. The formula of the sample used is Ba(Ti<sub>12</sub>Cr<sub>4</sub>Fe<sub>2</sub>ZrMg<sub>2</sub>)O<sub>38</sub>.**Lingunite** NaAlSi<sub>3</sub>O<sub>8</sub>**Origin:** Shocked Sixiangkou L6 chondrite.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was about 16 mW. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 975, 844, 798sh, 767s, 717w, 625, 595w, 531w, 494, 430sh, 277, 213.**Source:** Liu and El Gorsey (2007).**Comments:** No independent analytical data are provided for the sample used.**Lingunite K-analogue** KAlSi<sub>3</sub>O<sub>8</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystals using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was about 10 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1726w, 1601w, 1580w, 1452w, 1043, 952w, 866sh, 838w, 761s, 721sh, 655w, 621, 539, 521sh, 405w, 380sh, 283, 214s.

**Source:** Liu et al. (2009).

**Comments:** The sample was characterized by X-ray diffraction data.

### Linnæite Co<sup>2+</sup>Co<sup>3+</sup><sub>2</sub>S<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a bulk sample and on an ultrathin sheet. Other experimental details are not described.

**Raman shifts (cm<sup>-1</sup>):** ~400, ~340, ~235w.

**Source:** Liu et al. (2015d).

**Comments:** The samples were characterized by X-ray diffraction and SAED data.

### Linzhiite FeSi<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on the oriented single crystals in the forms as thin crystalline needles and plaques in different scattering geometries, using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 100 mW. A 90°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** ~340w, ~298w, ~270–275w, ~245s, and a series of peaks below 200 cm<sup>-1</sup>.

**Source:** Guizzetti et al. (1997).

### Liroconite Cu<sub>2</sub>Al(AsO<sub>4</sub>)(OH)<sub>4</sub>·4H<sub>2</sub>O

**Origin:** Cornwall deposit, UK.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 0.97 mW.

**Raman shifts (cm<sup>-1</sup>):** 3580w, 3550w, 865s, 846sh, 567w, 418w, 376w, 316sh, 299, 182, 165, 109.

**Source:** Makreski et al. (2015a).

**Comments:** The sample was characterized by powder X-ray diffraction data and thermal analysis.

### Liskeardite (Al,Fe)<sub>32</sub>(AsO<sub>4</sub>)<sub>18</sub>(OH)<sub>42</sub>(H<sub>2</sub>O)<sub>22</sub>·52H<sub>2</sub>O

**Origin:** Penberthy Croft Mine, St. Hilary, Cornwall, England UK.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3618sh, 3577, 3504, 3446sh, 3289sh, 3077sh, 2930, 2762sh, 1687sh, 1611w, 1554w, 1532w, 1453w, 1138w, 1124w, 1111sh, 1007w, 987w, 931sh, 914sh, 893s, 867s, 843s, 813sh, 769sh, 750w, 723w, 651w, 624w, 579, 554sh, 528sh, 514s, 499sh, 485sh, 477s, 454, 431w, 406w, 386sh, 373, 343w, 336sh, 305, 285, 263sh, 245sh, 230sh, 217sh, 196sh, 182sh, 162s, 143, 126sh, 110w.

**Source:** Frost et al. (2015w).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

**Litharge** PbO**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 1064 nm Nd-YAG laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 381w, 339, 288w, 146s, 82w.**Source:** Ciomartan et al. (1996).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of litharge see also Bouchard and Smith (2003).**Lithiophilite** LiMn<sup>2+</sup>(PO<sub>4</sub>)**Origin:** Cigana pegmatite, Conselheiro Pena, Minas Gerais, Brazil.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 1081w, 1068, 1018w, 1000, 955sh, 950s, 944sh, 627w, 591w, 575w, 443w, 424sh, 403sh, 317w, 288w, 247w, 235w, 199w, 154sh, 146w, 135sh, 105w.**Source:** Frost et al. (2013ak).**Comments:** The sample was characterized by electron microprobe analysis. The empirical formula of the sample used is Li<sub>1.01</sub>(Mn<sub>0.60</sub>Fe<sub>0.41</sub>Mg<sub>0.01</sub>Ca<sub>0.01</sub>)(PO<sub>4</sub>)<sub>0.99</sub>.**Lithiophorite** (Al,Li)(Mn<sup>4+</sup>,Mn<sup>3+</sup>)<sub>2</sub>O<sub>2</sub>(OH)<sub>2</sub>**Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation output power was 0.2 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3458–3465w, 1600w, (1183), (1058), (938), 621–629s, 575–579s, 541sh, 482–487, 460sh, 378–383w.**Source:** Burlet et al. (2014), Burlet and Vanbrabant (2015).**Comments:** The sample was characterized by powder X-ray diffraction data, energy-dispersive X-ray scan analysis, and flame emission analysis.**Lithiophosphate** Li<sub>3</sub>(PO<sub>4</sub>)**Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed at different temperatures using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation output power was 120 mW.**Raman shifts (cm<sup>-1</sup>):** 1061w, 1022, 942s, ~630s, 586s, 474, 442, 376, 352.**Source:** Popović et al. (2003).**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts are given for a sample at room temperature.

**Lithiotantite**  $\text{LiTa}_3\text{O}_8$ 

**Origin:** Eastern Brazilian Pegmatite Province, Minas Gerais, Brazil.

**Experimental details:** Experimental details are not indicated. Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 902, 826, 682s, 630w, 565s, 463w, 426sh, 416w, 370w, 342, 283, 259w, 229, 180.

**Source:** Menezes Filho et al. (2016).

**Comments:** The sample was characterized by electron microprobe analysis.

The empirical formula of the sample used is  $(\text{Li}_{0.96}\text{Mn}_{0.02}\text{Fe}_{0.01}\text{Na}_{0.01})(\text{Ta}_{2.18}\text{Nb}_{0.79}\text{Sn}_{0.03})\text{O}_{8.00}$ .

**Liversidgeite**  $\text{Zn}_6(\text{PO}_4)_4 \cdot 7\text{H}_2\text{O}$ 

**Origin:** Broken Hill, New South Wales, Australia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 17 mW.

**Raman shifts (cm<sup>-1</sup>):** 3220, 2895, 1645w, 1142w, 1050w, 1004, 986, 958s, 610, 584, 476, 464, 430, 244, 210.

**Source:** Elliott et al. (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is  $\text{Pb}_{0.01}(\text{Zn}_{5.86}\text{Mn}_{0.06})(\text{P}_{4.01}\text{As}_{0.05}\text{S}_{0.04})\text{O}_{16.20} \cdot 6.8\text{H}_2\text{O}$ .

**Livingstonite**  $\text{HgSb}_4\text{S}_6(\text{S})_2$ 

**Origin:** Huitzoco, Mexico.

**Experimental details:** Methods of sample preparation are not described. The Raman signal was excited by a 532 nm solid-state laser. The nominal laser radiation power was 0.5 mW.

**Raman shifts (cm<sup>-1</sup>):** 308s, 284s, 238, 191, 157w, 125w, 106w, 75w.

**Source:** Števko et al. (2015).

**Comments:** The empirical formula of the sample used is  $\text{Hg}_{1.01}(\text{Sb}_{3.89}\text{As}_{0.08})\text{S}_{8.01}$ .

**Lizardite**  $\text{Mg}_3\text{Si}_2\text{O}_5(\text{OH})_4$ 

**Origin:** Monte Fico, Elba Island, Italy

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power was 120 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1096w, 690s, 630w, 510w, 388s, 350w, 233s.

**Source:** Rinaudo et al. (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectra of lizardite see also Auzende et al. (2004) and Frezzotti et al. (2012).

**Löllingite** FeAs<sub>2</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal, using 676.4 nm Kr<sup>+</sup> laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed. Polarized spectra were collected in the z(xxy)z-, y(xx)y-, x(xy)x-, y(xz)y-, and z(xy)z- scattering geometries.**Source:** Lutz and Müller (1991).**Raman shifts (cm<sup>-1</sup>):** 271s, 269sh, 241sh, 236s.**Comments:** The Raman shifts are given for the scattering geometry z(xxy)z-. The notation z(xxy)z- means that the incident laser light is polarized parallel to x, scattered light is of all polarizations (x, y). No independent analytical data are provided for the sample used.**Lomonosovite** Na<sub>5</sub>Ti<sub>2</sub>(Si<sub>2</sub>O<sub>7</sub>)(PO<sub>4</sub>)O<sub>2</sub>**Origin:** Kirovskii apatite mine, Kukisvumchorr Mt., Khibiny Massif, Kola Peninsula, Russia.**Experimental details:** Raman scattering measurements have been performed in the spectral regions from 100 to 550 and from 750 to ~3800 cm<sup>-1</sup> on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 1084w, 1080w, 1070w, 999, 975, 939sh, 925sh, 909s, 882sh, 853, 838sh, 803, 789sh, ..., 534, 509sh, 499w, 457, 440sh, 427sh, 408s, 393sh, 368sh, 351, 319w, 302w, 284sh, 272, 223sh, 204, 173sh, 150sh, 145s, 112.**Source:** Frost et al. (2015m).**Comments:** The sample was characterized by qualitative electron microprobe analysis.**Lonecreekite** (NH<sub>4</sub>)Fe<sup>3+</sup>(SO<sub>4</sub>)<sub>2</sub>·12H<sub>2</sub>O**Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 1131, 1108w, 1099w, 991s, 701, 636, 615, 525, 463, 435, 307.**Source:** Frost and Kloprogge (2001).**Comments:** The sample was analyzed for chemical composition, and some substitution with Al<sup>3+</sup> for Fe<sup>3+</sup> was detected. Raman shifts are given for sample at 77 K because of the fluorescence at 298 K. For the Raman spectrum of lonecreekite see also Jentzsch et al. (2013).**Lonsdaleite** C**Origin:** Popigai crater, Siberia, Russia.**Experimental details:** Raman scattering measurements have been performed on the arbitrarily oriented carbon platelets with the lonsdaleite fraction in the range from 0.29 to 0.565 using 325 nm He-Cd laser radiation. The laser radiation power at the sample was 0.5 mW. A 180°-scattering geometry was employed. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1303–1292, 1244–1219w.

**Source:** Goryainov et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data. The lonsdaleite/diamond molar ratio was estimated using the Rietveld method.

### Lópezite K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 6 mW.

**Raman shifts (cm<sup>-1</sup>):** 950w, 938w, 935, 913w, 910w, 893, 744, 564, 553sh, 527, 385, 370sh, 357sh, 230, 220sh, 130w.

**Source:** Mathur et al. (1968).

**Comments:** No independent analytical data are provided for the sample used.

### Lorándite TlAsS<sub>2</sub>

**Origin:** Allchar, Republic of Macedonia.

**Experimental details:** Raman scattering measurements have been performed on an oriented sample using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 17 mW. A 180°-scattering geometry was employed. Polarized spectra were collected with the laser polarization parallel to the *b*- and *c*-axes scattering geometries.

**Raman shifts (cm<sup>-1</sup>):** 398, 380s, 366sh, 325, 317sh, 311sh, 275, 263sh, 211, 203sh, 193, 172, 157sh, 135w.

**Source:** Kharbish (2011).

**Comments:** The sample was characterized by single-crystal X-ray diffraction and electron microprobe analyses. The Raman shifts are given for the scattering geometry with the laser polarization parallel to the *b*-axes. For the Raman spectra of lorándite see also Minceva-Sukarova et al. (2003) and Makreski et al. (2014).

### Lorenzenite Na<sub>2</sub>Ti<sub>2</sub>O<sub>3</sub>(Si<sub>2</sub>O<sub>6</sub>)

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a pellet of pressed powdered sample using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was about 300 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1049w, 984, 963, 899w, 856w, 834w, 704, 637s, 579w, 538, 486, 451, 349, 305s, 274, 258sh, 233w, 215.

**Source:** Su et al. (2000).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Löweite Na<sub>12</sub>Mg<sub>7</sub>(SO<sub>4</sub>)<sub>13</sub>·15H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 1210, 1142w, 1117w, 1079, 1039s, 1001s, 980, 971sh, 641sh, 622, 606sh, 471sh, 462, 453sh.

**Source:** Jentzsch et al. (2011).

**Comments:** No independent analytical data are provided for the sample used.

**Luddenite**  $\text{Cu}_2\text{Pb}_2\text{Si}_5\text{O}_{14}\cdot14\text{H}_2\text{O}$

**Origin:** Artillery Peak, Mohave Co., Arizona, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3329sh, 3317, 3284sh, 1658sh, 1603, 1557sh, 1482, 1455sh, 1368sh, 1346, 1301, 1276sh, 1160, 1148sh, 1122sh, 986sh, 978, 970sh, 831sh, 808, 801sh, 696sh, 676, 648sh, 501sh, 473sh, 464s, 449sh, 413w, 403, 394sh, 356, 344sh, 263, 213sh, 201, 174sh, 167.

**Source:** Frost et al. (2015u).

**Comments:** No independent analytical data are provided for the sample used.

**Ludjibaite**  $\text{Cu}_3(\text{PO}_4)(\text{OH})_3$

**Origin:** Banská Bystrica, central Slovakia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 17 mW. A 180°-scattering geometry was employed. Polarized spectra were collected in parallel and perpendicular to the *c*-axis scattering geometries.

**Raman shifts (cm<sup>-1</sup>):** 3470, 1115, 1072sh, 1046sh, 1019, 981s, 925sh, 855w, 815w, 784w, 736sh, 633, 586, 557sh, 449, 402sh, 387, 368sh, 301s, 263sh, 226, 190sh, 160s.

**Source:** Kharbish et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction analysis and by electron microprobe analyses. For the Raman spectrum of ludjibaite see also Frost et al. (2002g).

**Ludlamite**  $\text{Fe}^{2+}_3(\text{PO}_4)_2\cdot4\text{H}_2\text{O}$

**Origin:** Boa Vista mine, Galiléia, Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3190sh, 3137, 3013sh, 2896, 2730, 2605, 1160w, 1080, 1044, 992sh, 973sh, 950s, 916sh, 774w, 665sh, 634, 599, 564sh, 548, 494, 465, 371sh, 369, 345w, 302, 286, 266, 249, 244sh, 207sh, 199, 182sh, 172, 164sh, 145, 140sh, 103.

**Source:** Frost et al. (2013w).

**Comments:** The empirical formula of the sample used is  $(\text{Fe}_{2.35}\text{Mn}_{0.25}\text{Mg}_{0.22})(\text{PO}_4)_{2.08}\cdot4.0\text{H}_2\text{O}$ .

**Ludlockite**  $\text{PbFe}^{3+}_4\text{As}^{3+}_{10}\text{O}_{22}$

**Origin:** Tsumeb mine, Tsumeb, Namibia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts

have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 798s, 756s, 743sh, 674sh, 666, 639, 611w, 579sh, 549s, 536sh, 524sh, 501sh, 486s, 470sh, 436w, 420, 408sh, 381sh, 368, 348, 332, 287, 266sh, 246s, 221, 204, 193sh.

**Source:** Bahfenne and Frost (2009).

**Comments:** No independent analytical data are provided for the sample used.

### Ludwigite Mg<sub>2</sub>Fe<sup>3+</sup>O<sub>2</sub>(BO<sub>3</sub>)

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 20 mW. A nearly 180°-scattering geometry was employed. Polarized spectra were collected in the (zz) scattering geometry.

**Raman shifts (cm<sup>-1</sup>):** 640s, 568, 480sh, 456w, 399s, 367sh, 298, 269, 233, 191, 160, 132w, 109.

**Source:** Leite et al. (2002).

**Comments:** No independent analytical data are provided for the sample used.

### Lueshite NaNbO<sub>3</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 868w, 599s, 428w, 238s.

**Source:** Wu et al. (2010b).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of lueshite see also Fresno et al. (2016).

### Lulzacite Sr<sub>2</sub>Fe<sup>2+</sup><sub>3</sub>Al<sub>4</sub>(PO<sub>4</sub>)<sub>4</sub>(OH)<sub>10</sub>

**Origin:** Saint-Aubin-des-Châteauax, Loire-Atlantique, France.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 989s, 918, 842, 568, 505, 420, 290, 142.

**Source:** Moëlo et al. (2000).

**Comments:** The sample was characterized by powder X-ray diffraction analysis and by electron microprobe analyses. The empirical formula of the sample used is (Sr<sub>0.96</sub>Ba<sub>0.04</sub>)<sub>2</sub>Fe<sup>2+</sup>(Fe<sup>2+</sup><sub>0.63</sub>Mg<sub>0.37</sub>)<sub>2</sub>Al<sub>4</sub>[(P<sub>0.98</sub>V<sub>0.02</sub>)O<sub>4</sub>]<sub>4</sub>(OH)<sub>10</sub>.

### Lüneburgite Mg<sub>3</sub>[B<sub>2</sub>(OH)<sub>6</sub>(PO<sub>4</sub>)<sub>2</sub>]·6H<sub>2</sub>O

**Origin:** Mejillones Peninsula, Antofagasta Province, Chile.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 325 nm laser radiation. The laser radiation power at the sample was about 8 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3504sh, 3438sh, 3392s, 3272, 3207, 1087, 1032, 999sh, 877, 734, 590, 465.

**Source:** Korybska-Sadło et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

### **Luogufengite Fe<sub>2</sub>O<sub>3</sub>**

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 532 nm Nd-YAG laser radiation. The output laser radiation power was in the range from 0.2 to 30 mW.

**Raman shifts (cm<sup>-1</sup>):** 1641, 1474, 1435, 1378, 1329, 1276, 1188, 829, 731, 704, 669, 643, 597, 579, 559, 488, 461, 439, 419, 397, 378, 362, 346, 330, 299, 267, 214, 195, 165, 146, 116.

**Source:** López-Sánchez et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### **Lusernaite-(Y) Y<sub>4</sub>Al(CO<sub>3</sub>)<sub>2</sub>(OH,F)<sub>11</sub>·6H<sub>2</sub>O**

**Origin:** Luserna valley, Piedmont, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 473.1 nm Nd-YAG and 632.8 nm He-Ne lasers radiations. The laser radiations powers are not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1096.

**Source:** Biagioni et al. (2013a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The empirical formula of the sample used is (Y<sub>3.41</sub>Dy<sub>0.16</sub>Er<sub>0.15</sub>Yb<sub>0.09</sub>Gd<sub>0.07</sub>Ca<sub>0.05</sub>Pb<sub>0.02</sub>Sm<sub>0.01</sub>)Al<sub>1.06</sub>(CO<sub>3</sub>)<sub>2.00</sub>(OH<sub>10.35</sub>F<sub>0.65</sub>)·6H<sub>2</sub>O. Due to the strong luminescence only one Raman band was registered in the spectrum, confirming the presence of CO<sub>3</sub><sup>3-</sup> groups in the structure.

### **Macedonite PbTiO<sub>3</sub>**

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on PbTiO<sub>3</sub> single crystals with the tetragonal *c* axis normal to the scattered plane, using a 633 nm He-Ne laser. Polarized spectra were collected in *x(zz)y*, *x(zx)y*, and *x(yx)y* scattering geometry.

**Raman shifts (cm<sup>-1</sup>):** 508s, 440, 290s, 220, 130, 89.

**Source:** Fontana et al. (1991).

**Comments:** The sample was identified by electron microprobe analysis; boron was determined by LA-ICP-MS. The Raman shifts are given for the scattering geometry *x(zx)y*.

### **Mackayite Fe<sup>3+</sup>Te<sup>4+</sup><sub>2</sub>O<sub>5</sub>(OH)**

**Origin:** An unknown locality in Nevada, USA (?).

**Experimental details:** Raman spectra of unoriented samples were obtained using a He-Ne laser with the wavelengths of laser excitation line of 633 nm. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 907w, 872w, 782w, 732, (644), 635s, (602w), 579, 513, (502w), 436, 424s, 379s, 349, 306, 177s, 150, 124.

**Source:** Frost and Dickfoss (2009).

**Comments:** The IR spectra of presumed mackayite given in the cited paper are wrong: the strongest IR bands correspond to a sulfate. Possibly, the correct locality is Bambolla mine, Moctezuma, Sonora, Mexico.

### Mackinawite (Fe,Ni)<sub>1+x</sub>S ( $x = 0\text{--}0.07$ )

**Origin:** Synthetic (corrosion film formed after exposure of iron to saline H<sub>2</sub>S saturated acetic solution).

**Experimental details:** Raman spectrum of an unoriented sample was obtained at the wavelength of laser excitation line of 532.1 nm.

**Raman shifts (cm<sup>-1</sup>):** (587), 474w, 385, 274s, 208.

**Source:** Genchev and Erbe (2016).

### Macquartite Cu<sub>2</sub>Pb<sub>7</sub>(CrO<sub>4</sub>)<sub>4</sub>(SiO<sub>4</sub>)<sub>2</sub>(OH)<sub>2</sub>

**Origin:** No data.

**Experimental details:** Raman spectra of crystals oriented to provide maximum intensity were obtained using a He-Ne laser with the wavelengths of laser excitation line of 785 nm. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 968w, 936w, 857, 840, 814s, 463, 439, 374, 349s, 340, 194, 152.

**Source:** Frost (2004c).

**Comments:** The sample was identified by electron microprobe analysis; boron was determined by LA-ICP-MS. The Raman shifts are given for the scattering geometry  $y(z)z)y$ , in which the Raman intensities are most strong.

### Magadiite Na<sub>2</sub>Si<sub>14</sub>O<sub>29</sub>·11H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an unoriented sample using a 1064.1 nm Nd<sup>3+</sup>:YAG laser. The laser radiation power at the sample was about 90 mW.

**Raman shifts (cm<sup>-1</sup>):** 3266w, 1151w, 1131w, 1101w, 1085w, 1064, 1049w, 992s, 823w, 792w, 705w, 645w, 632w, 620, 587w, 488sh, 464s, 442sh, 398w, 373w, 338w.

**Source:** Huang et al. (1999b).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Magbasite KBaFe<sup>3+</sup>Mg<sub>7</sub>Si<sub>8</sub>O<sub>22</sub>(OH)<sub>2</sub>F<sub>6</sub>

**Origin:** Eldor carbonatite complex, Quebec, Canada.

**Experimental details:** Polarized single-crystal Raman spectra were collected in the range from 3200 to 3800 cm<sup>-1</sup> with the polarizer parallel and perpendicular to the length of the crystal using 460 and 532 nm laser radiations with a nominal output power of 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 3735w, 3719w, 3636s.

**Source:** Welch et al. (2014)

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The Raman shifts are given for the radiation polarization parallel to the length of the crystal.

### Maghemite $\text{Fe}_2\text{O}_3$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdery sample using a 636.4 nm tuneable dye laser. The laser radiation power at the sample was 0.34 mW.

**Raman shifts (cm<sup>-1</sup>):** 648s, 527, 377, 350, 309, 250w, 220w.

**Source:** Nieuwoudt et al. (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Magnesio-arfvedsonite $\text{NaNa}_2(\text{Mg}_4\text{Fe}^{3+})\text{Si}_8\text{O}_{22}(\text{OH})_2$

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed in the region of O–H-stretching vibrations, in backscattering geometry using a 514.5 nm Ar<sup>+</sup> laser.

**Raman shifts (cm<sup>-1</sup>):** 3666.

**Source:** Leissner et al. (2015).

**Comments:** The sample was characterized by EMPA and ICP-MS. The empirical formula of the sample used is  $(\text{Na}_{0.25}\text{K}_{0.13})(\text{Na}_{0.89}\text{Ca}_{0.11})_2(\text{Mg}_{0.70}\text{Fe}^{3+}_{0.26}\text{Al}_{0.01}\text{Mn}_{0.01})_5(\text{Si}_{0.99}\text{Al}_{0.01})_8\text{O}_{22}(\text{OH})_{1.7}\text{F}_{0.3}$ .

### Magnesiocarpholite $\text{MgAl}_2\text{Si}_2\text{O}_6(\text{OH})_4$

**Origin:** Monte Leoni, Monticiano-Roccastrada Unit, Northern Apennine, southern Tuscany, Italy.

**Experimental details:** Raman scattering measurements have been performed on single crystals in four different orientations, using a 514.5 nm Ar<sup>+</sup> laser. The laser emission power was 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 3633w, 3594s, 3571sh, 1098w, 1037w, 936, 879, 783s, 747, 688, 560, 445, 351, 278w, 263, 207w, 161w, 117w.

**Source:** Fuchs et al. (2001).

**Comments:** The sample was characterized electron microprobe analyses and Mössbauer spectroscopy. The Raman shifts are given for the scattering geometry with *c* axis vertical and most developed crystal face normal to the polarization direction.

### Magnesiochloritoid $\text{MgAl}_2(\text{SiO}_4)\text{O}(\text{OH})_2$

**Origin:** Synthetic

**Experimental details:** Raman scattering measurements have been performed on single crystals with different orientations using a 514.5 nm Ar<sup>+</sup> laser.

**Raman shifts (cm<sup>-1</sup>):** 3455, 3076, 1096, 985, 909, 881, 847, 805, 738, 594, 551, 531, 513, 411–412.

**Source:** Koch-Müller et al. (2002).

**Comments:** Band intensities are not indicated in the cited paper.

**Magnesiochromite** MgCr<sub>2</sub>O<sub>4</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an unoriented sample using a 514.5 nm Ar<sup>+</sup> laser.**Raman shifts (cm<sup>-1</sup>):** 684s, 613, 543s, 447.**Source:** Yong et al. (2012).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of magnesiochromite see also Hosterman (2011), Lenaz and Lughí (2013), Andò and Garzanti (2014), and D'Ippolito et al. (2015).**Magnesiocopiapite** MgFe<sup>3+</sup><sub>4</sub>(SO<sub>4</sub>)<sub>6</sub>(OH)<sub>2</sub>·20H<sub>2</sub>O**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an unoriented sample using a 532 nm Nd-YAG laser.**Raman shifts (cm<sup>-1</sup>):** 3499, 3331, 3314, 3167, 1645, 1225, 1218, 1129, 1102, 1019, 1004, 995, 639, 613, 597, 557, 305, 270, 252, 227.**Source:** Kong et al. (2011b).**Comments:** The sample was characterized by powder X-ray diffraction data. Band intensities are not indicated in the cited paper. For the Raman spectra of magnesiocopiapite see also Frost (2011c) and Rull et al. (2014).**Magnesioferrite** MgFe<sup>3+</sup><sub>2</sub>O<sub>4</sub>**Origin:** Synthetic.**Experimental details:** The spectrum of an unoriented sample was recorded using 632.8 nm line of a He-Ne laser.**Raman shifts (cm<sup>-1</sup>):** 707\*s, 661sh, 596\*w, 550w, 479\*, 377w, 332\*, 214\*.**Source:** D'Ippolito et al. (2015).**Comments:** The modes marked with an asterisk are provoked by the inversion. For the Raman spectra of magnesioferrite see also Lenaz and Lughí (2013) and Aramendia et al. (2014).**Magnesio-foitite** (Mg<sub>2</sub>Al)Al<sub>6</sub>(Si<sub>6</sub>O<sub>18</sub>)(BO<sub>3</sub>)<sub>3</sub>(OH)<sub>3</sub>(OH)**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on single crystals with the electrical field vector of the linearly polarized laser light parallel to the crystallographic *c* axis using a 488 or 473 nm laser. The laser radiation power at the sample was 30 or 12 mW. The Raman shifts in the region of O–H-stretching vibrations have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3657w, 3619w, 3551, 3511, 3459, 688, ~370s, 311, 267, 228.**Source:** Berryman et al. (2016).**Comments:** The sample was characterized by powder and single-crystal X-ray diffraction data and electron microprobe analysis. For the Raman spectrum of magnesio-foitite see also Fantini et al. (2014).

**Magnesiohögbonite-2N4S**  $(\text{Mg},\text{Fe}^{2+})_{10}\text{Al}_{22}\text{Ti}^{4+}_2\text{O}_{46}(\text{OH})_2$ 

**Origin:** Central Sør Rondane Mts., Queen Maud Land, East Antarctica (type locality).

**Experimental details:** Raman scattering measurements have been performed on an unoriented single crystal using a 532.1 nm Ar<sup>+</sup> laser.

**Raman shifts (cm<sup>-1</sup>):** ~3400, 872s, 780, 709, 659, 536, 498, 479, 419, 342w, 302, 263w, 217, 142, 104w.

**Source:** Shimura et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Magnesio-hornblende**  $\text{Ca}_2(\text{Mg}_4\text{Al})(\text{Si}_7\text{Al})\text{O}_{22}(\text{OH})_2$ 

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed in backscattering geometry using a 514.5 nm Ar<sup>+</sup> laser.

**Raman shifts (cm<sup>-1</sup>):** 3672–3673. Only a figure of the Raman spectrum of magnesio-hornblende is given in the spectral range from 10 to 1200 cm<sup>-1</sup>.

**Source:** Leissner et al. (2015).

**Comments:** The sample was characterized by electron microprobe analyses and ICP-MS. The empirical formula of the sample used is  $(\text{Na}_{0.45}\text{K}_{0.04})(\text{Ca}_{0.87}\text{Fe}_{0.10}\text{Mn}_{0.02}\text{Na}_{0.01})_2(\text{Mg}_{0.52}\text{Fe}_{0.36}\text{Al}_{0.12})_5(\text{Si}_{0.86}\text{Al}_{0.14})_8\text{O}_{22}(\text{OH})_{2.00}$ .

**Magnesiotaaffeite-2N'2S**  $\text{Mg}_3\text{BeAl}_8\text{O}_{16}$ 

**Origin:** Ratnapura district, Sri Lanka (type locality).

**Experimental details:** No data

**Raman shifts (cm<sup>-1</sup>):** 809w, 758, 703, 662w, 489, 447, 435, 415s, 305s.

**Source:** Kiefert and Schmetzer (1998).

**Comments:** The sample was characterized by chemical and X-ray diffraction data.

**Magnesiotaaffeite-6N'3S**  $\text{Mg}_2\text{BeAl}_6\text{O}_{12}$ 

**Origin:** Casey Bay, Antarctica.

**Experimental details:** No data

**Raman shifts (cm<sup>-1</sup>):** 803, 713s, 660, 564w, 489, 443, 412s, 326s.

**Source:** Kiefert and Schmetzer (1998).

**Comments:** The sample was characterized by chemical and X-ray diffraction data.

**Magnesite**  $\text{Mg}(\text{CO}_3)$ 

**Origin:** Brumado, Bahia, Brazil.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented polished sample using 514.5 and 532 nm Ar<sup>+</sup> lasers.

**Raman shifts (cm<sup>-1</sup>):** 1763w, 1446w, 1095s, 738w, 331s, 214.

**Source:** Perrin et al. (2016).

**Comments:** The sample was characterized by electron microprobe analysis. For the Raman spectra of magnesite see also Rutt and Nicola (1974), Edwards et al. (2005), Frezzotti et al. (2012), and Bernardino et al. (2016).

### Magnetite $\text{Fe}^{2+}\text{Fe}^{3+}_2\text{O}_4$

**Origin:** Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed using a 632.8 nm He-Ne laser. Laser beam was focused on the sample to give a spot size of *ca.* 1  $\mu\text{m}$ . The laser radiation power at the sample was 0.7 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 663s, 534, 513, 302.

**Source:** De Faria et al. (1997).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of magnetite see also Castriota et al. (2008), Nieuwoudt et al. (2011), Hosterman (2011), Saheb et al. (2011), Das and Hendry (2011), Andò and Garzanti (2014), and D'Ippolito et al. (2015).

### Magnetoplumbite $\text{PbFe}^{3+}_{12}\text{O}_{19}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented nanoparticles using a 514.5 nm Ar<sup>+</sup> laser. The laser radiation power at the sample was 20 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 1320 (broad), 680s, 608, 519, 403, (328w), 325s, (290), 206w, 176.

**Source:** Yang et al. (2007c).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of magnetoplumbite see also Kreisel et al. (1999), Konzett et al. (2005), and Zhukova et al. (2016).

### Majorite $\text{Mg}_3(\text{MgSi})(\text{SiO}_4)_3$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline aggregate using a micro-Raman system with an argon ion laser. The laser radiation power at the sample was in the range from 5 to 50 mW.

**Raman shifts ( $\text{cm}^{-1}$ ):** 1065, 989, 931s, 889, 802, 602s, 458, 367, 311, 226s, 159.

**Source:** De La Pierre and Belmonte (2016).

### Makatite $\text{Na}_2\text{Si}_4\text{O}_8(\text{OH})_2 \cdot 4\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an aggregate of arbitrarily oriented particles using a 1064.1 nm Nd-YAG laser.

**Raman shifts ( $\text{cm}^{-1}$ ):** 3368sh, 3122w (broad), 1244w, 1060w, 1025s, 986w, 945w, 919w, 793w, 567s, 482, 460, 414, 381w, 339w, 324, 292s, 266w, 226w, 219w, 194w, 167w, 151w, 122, 100.

**Source:** Huang et al. (1999a).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Malachite** Cu<sub>2</sub>(CO<sub>3</sub>)(OH)<sub>2</sub>**Origin:** Eisenzeche, Germany.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented aggregate using a 532 nm Nd-YAG laser. The nominal laser radiation power was 100 mW.**Raman shifts (cm<sup>-1</sup>):** 3383, 3311w, 1639w, 1495s, 1462, 1369, 1098, 1059, 821w, 755, 722, 597w, 537, 435s, 355, 270s, 215s.**Source:** Buzgar and Apopei (2009).**Comments:** For the Raman spectra of malachite see also Frost et al. (2002g), Bouchard and Smith (2003), Frezzotti et al. (2012), Capitani et al. (2014), and Coccato et al. (2016).**Malayaite** CaSnO(SiO<sub>4</sub>)**Origin:** Skarn approximately 4 km north of Ash Mountain, near Mc-Dame, northern British Columbia, Canada.**Experimental details:** Raman scattering measurements have been performed on a sample with continuously variable polarization directions using a 488 nm Ar<sup>+</sup> laser.**Raman shifts (cm<sup>-1</sup>):** 895w, 837s, 802w, 595s, 520s, 510w, 450w, 412w, 340s, 328w, 305s, 295w, 280s, 250s, 227w, 197w, 176s, 142s, 109s, 75w.**Source:** Groat et al. (1996).**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. For the Raman spectrum of malayaite see also Heyns and Harden (1999).**Malladrite** Na<sub>2</sub>SiF<sub>6</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 4358 Å laser.**Source:** Begun and Rutenberg (1967).**Raman shifts (cm<sup>-1</sup>):** 592, 559s, 477, 300, 252.**Mallardite** Mn(SO<sub>4</sub>)·7H<sub>2</sub>O**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using a 4358 Å laser.**Raman shifts (cm<sup>-1</sup>):** 3467, 3399, 1148, 1085, 1084, 993–994, 693, 603, 457, 330.**Source:** Rao (1941).**Comments:** Krishnamurti (1958) notes that actually this study does not reveal the existence of lines at 330 and 693 cm<sup>-1</sup> and, based on the crystallization conditions, it is probable that the results refer to MnSO<sub>4</sub>·5H<sub>2</sub>O.**Mallestigite** Pb<sub>3</sub>Sb(SO<sub>4</sub>)(AsO<sub>4</sub>)(OH)<sub>6</sub>·3H<sub>2</sub>O**Origin:** A waste dump from a Cu-Pb-Zn mine, 1 km NW of Mallestiger, Carinthia, Austria.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1261w, 1234w, 1158, 1151, 1062w, 978s, 865w, 827, 803, 641, 631w, 619w, 606, 460, 449s, 437s, 416w, 374, 340w.

**Source:** Frost et al. (2011p).

**Comments:** The IR spectrum of presumed mallestigite published in the cited paper corresponds to quartz.

### Mandarinoite Fe<sup>3+</sup><sub>2</sub>(Se<sup>4+</sup>O<sub>3</sub>)<sub>3</sub>·6H<sub>2</sub>O

**Origin:** El Dragon Mine, Potosí, Bolivia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3507, 3189s, (3046), 2926, (2796w), 1666w, 1563, 814s, 744, 723, 695w, 553, 474, 398w, 355w, 262, 212, 186, 129.

**Source:** Frost and Keeffe (2009a).

**Comments:** No independent analytical data are provided for the sample used.

### Manganite Mn<sup>3+</sup>O(OH)

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 632.8 nm He-Ne laser. In spite of the strong opacity of the mineral, it was possible to record a Raman spectrum by using a very weak laser beam intensity of 1 mW and a long duration of 500 s.

**Raman shifts (cm<sup>-1</sup>):** 622, 558s, 530, 490w, 387, 357.

**Source:** Bouchard and Smith (2003).

**Comments:** For the Raman spectrum of manganite see also Bernard et al. (1993a).

### Manganlotharmeyerite CaMn<sup>3+</sup><sub>2</sub>(AsO<sub>4</sub>)<sub>2</sub>(OH)<sub>2</sub>

**Origin:** Starlera Fe-Mn deposit, Middle Penninic domain, Eastern Swiss Alps.

**Experimental details:** Unpolarized Raman spectrum was obtained on an arbitrarily oriented single crystal using a 488 nm Ar<sup>+</sup> laser.

**Raman shifts (cm<sup>-1</sup>):** 3000 (broad), 880, 830 (broad), 765, 475, 426, 365, 344.

**Source:** Brugger et al. (2002).

**Comments:** The sample was characterized by optical and structural data and electron microprobe analysis. The band at 475 cm<sup>-1</sup> is absent in the figure of manganlotharmeyerite given in the cited paper. The strongest band in this figure has a maximum at ~520 cm<sup>-1</sup>.

### Manganochromite Mn<sup>2+</sup>Cr<sub>2</sub>O<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdery sample consisting of octahedral nanocrystals using a Raman microscope.

**Raman shifts (cm<sup>-1</sup>):** 652, 555s.

**Source:** Tong et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of manganochromite see also Chen et al. (2007c).

**Manganolangbeinite**  $K_2Mn^{2+}_2(SO_4)_3$ **Origin:** Synthetic.**Experimental details:** Unpolarized and polarized (with different scattering geometries) Raman scattering measurements have been performed on single crystals using a 488 nm Ar<sup>+</sup> laser at the power of 5 mW.**Raman shifts (cm<sup>-1</sup>):** 1224w, 1153w, 1138w, 1113w, 1107w, 1031, 1022sh, 651w, 645w, 628, 620, 604, 597sh, 590w, 473sh, 447, 436w, 426w.**Source:** Kreske and Devarajan (1982).**Comments:** The Raman shifts are given for the scattering geometry z(yz)x.**Manganosite** MnO**Origin:** Synthetic (Alfa Aesar).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 514.5 nm Ar<sup>+</sup> laser.**Raman shifts (cm<sup>-1</sup>):** 654, (591), 531s, 250w.**Source:** Julien et al. (2004).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of manganosite see also Mironova-Ulmane et al. (2009).**Manjirite**  $Na(Mn^{4+}_7Mn^{3+})O_{16}$ **Origin:** Bahariya depression, Western Desert, Egypt.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily sample using a 532 nm Nd-YAG laser. The laser radiation power at the sample was between 20 and 200 μW.**Raman shifts (cm<sup>-1</sup>):** ~1300, 643, ~395, ~292.**Source:** Ciobotă et al. (2012).**Comments:** No independent analytical data are given for the sample used.**Marcasite** FeS<sub>2</sub>**Origin:** A seafloor hydrothermal vent field.**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using a 532 nm laser. The maximum laser radiation power was 20 mW.**Raman shifts (cm<sup>-1</sup>):** 386, 323s.**Source:** White (2009).**Comments:** For the Raman spectra of marcasite see also Lutz and Müller (1991), Mernagh and Trudu (1993), and Frezzotti et al. (2012).**Margarite** CaAl<sub>2</sub>Si<sub>2</sub>Al<sub>2</sub>O<sub>10</sub>(OH)<sub>2</sub>**Origin:** Rekwika, Troms, Norway.**Experimental details:** Micro-Raman scattering measurements have been performed on a single crystal using a 514.5 nm Ar<sup>+</sup> laser. Sample orientation is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3635s, 917s, 711s, 676, 648, (553), 489, 393s, (348), 315, 271s, 248s, (225), 115s, 84.

**Source:** Tlili et al. (1989).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectra of margarite see also Graeser et al. (2003) and Wang et al. (2015).

### Margarosanite $\text{Ca}_2\text{PbSi}_3\text{O}_9$

**Origin:** Franklin, New Jersey, USA.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 437 nm laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 1014s, 966, 907, 659s, 581, 498, 443, 389, 262, 128.

**Source:** Gaft et al. (2013).

**Comments:** Weak peaks are not indicated.

### Marićite $\text{NaFe}^{2+}(\text{PO}_4)$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented powder using 532 nm Ar<sup>+</sup> laser radiation. The power at the laser beam was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 1125w, 1080w, 1052w, 972s, 943sh.

**Source:** Burba and Frech (2006).

**Comments:** For the Raman spectrum of marićite see also Burba (2006).

### Markascherite $\text{Cu}_3(\text{MoO}_4)(\text{OH})_4$

**Origin:** Copper Creek, Pinal Co., Arizona, USA (type locality).

**Experimental details:** Micro-Raman scattering measurements have been performed on a randomly oriented crystal using 532 nm laser radiation. The laser radiation power at the sample was 200 mW.

**Raman shifts (cm<sup>-1</sup>):** 3560sh, 3541sh, 3527s, 3510, 911s, 886sh, 864sh, 489w, 449w, 425, 402w, 329s.

**Source:** Yang et al. (2012).

**Comments:** The sample was characterized by powder and single-crystal X-ray diffraction data and electron microprobe analyses.

### Marokite $\text{CaMn}^{3+}_2\text{O}_4$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm laser radiation. The laser radiation power at the sample was 3 mW.

**Raman shifts (cm<sup>-1</sup>):** 720, 679, 633s, 614s, 577, 536, 517w, 475, 397s, 376s, 350, 299s, 284sh, 272, 241, 221w, 206, 192w, 177s, 123.

**Source:** Wang et al. (2003).

**Comments:** For the Raman spectrum of marokite see also Ivanov et al. (2014).

### Marthozite $\text{Cu}^{2+}(\text{UO}_2)_3(\text{Se}^{4+}\text{O}_3)_2\text{O}_2 \cdot 8\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystal using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3180, 3271s, 3381, 3524, 1672, 1616, 1414w, 1358w, 1283w, 869, 812s, 797s, 739, 571w, 449, 424s, 360, 257, 199, 139.

**Source:** Frost et al. (2008e).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The IR spectrum of presumed marthozite given in the cited paper is wrong and corresponds to malachite.

### Martyite Zn<sub>3</sub>(V<sub>2</sub>O<sub>7</sub>)(OH)<sub>2</sub>·2H<sub>2</sub>O

**Origin:** Little Eva mine, Grand Co., Utah, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented polycrystalline aggregate using 532 nm laser radiation. The output power of the laser beam was about 4 mW.

**Raman shifts (cm<sup>-1</sup>):** 3475, 1600w, 943sh, 864sh, 844s, 800sh, 483, 440, 319, 258, 111.

**Source:** Kasatkin et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

### Maruyamaite K(MgAl<sub>2</sub>)(Al<sub>5</sub>Mg)(BO<sub>3</sub>)<sub>3</sub>(Si<sub>6</sub>O<sub>18</sub>)(OH)<sub>3</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation with laser beam perpendicular and parallel to the *c*-axis.

**Raman shifts (cm<sup>-1</sup>):** 3572, 1106sh, 1091, 977, 789s, 703s, 669, 538w, 500w, 367s, 242, 212s, 155w.

**Source:** Lussier et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The Raman shifts are given for the spectrum obtained with laser beam perpendicular to the *c*-axis.

### Mascagnite (NH<sub>4</sub>)<sub>2</sub>(SO<sub>4</sub>)

**Origin:** Synthetic (commercial reactant).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the objective lens was about 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 975s, ~615w, ~610w, ~450w.

**Source:** Sakurai et al. (2010).

**Comments:** For the Raman spectrum of maskagnite see also Morillas et al. (2016).

### Maskelynite A feldspar glass

**Origin:** Sixiangkou meteorite (L6 chondrite).

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 1090 (broad), 575sh, 487s (broad).

**Source:** Gillet et al. (2000).

**Comments:** The Raman spectrum contains numerous narrow peaks of admixed lingunite, the high-pressure hollandite-type phase  $\text{KAlSi}_3\text{O}_8$ .

#### Massicot PbO

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single sample using 1064 nm Nd-YAG laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 423w, 384, 341w, 289s, 248sh, 217w, 174sh, 143s, 88w, 73w.

**Source:** Ciomartan et al. (1996).

**Comments:** For the Raman spectra of massicot see also Madsen and Weaver (1998), Bouchard-Abouchakra (2001), Bouchard and Smith (2003), and Lepot et al. (2006).

#### Mathesiusite $\text{K}_5(\text{UO}_2)_4(\text{SO}_4)_4(\text{VO}_5)(\text{H}_2\text{O})_4$

**Origin:** Jáchymov, Krušné Hory Mts. (Ore Mts.), Bohemia, Czech Republic (type locality).

**Experimental details:** Raman scattering measurements have been performed on the {110} face of a single crystal using depolarized 780 nm radiation of a frequency-stabilized single mode diode laser. The laser radiation power at the sample was between 4 and 8 mW.

**Raman shifts (cm<sup>-1</sup>):** 1329w, 1210w, 1114w, 1007s, 982, 896, 888sh, 844sh, 830s, 742, 644, 619, 598, 557w, 480, 460s, 447sh, 370w, 276, 248.

**Source:** Plášil et al. (2014c).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

#### Mathiasite $(\text{K},\text{Ba},\text{Sr})(\text{Zr},\text{Fe})(\text{Mg},\text{Fe})_2(\text{Ti},\text{Cr},\text{Fe})_{18}\text{O}_{38}$

**Origin:** Synthetic.

**Experimental details:** Unpolarized micro-Raman spectrum was obtained on an arbitrarily oriented sample using 632 nm He-Ne laser radiation. The laser radiation power at the sample was between 4 and 8 mW.

**Raman shifts (cm<sup>-1</sup>):** 649s, 550, 450, 337, 243w.

**Source:** Konzett et al. (2005).

**Comments:** The sample was characterized by electron microprobe analysis.

#### Matildite $\text{AgBiS}_2$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample consisting of nanocrystals using 514 nm laser radiation.

**Raman shifts (cm<sup>-1</sup>):** ~140, ~120.

**Source:** Guin et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Matioliite**  $\text{NaMgAl}_5(\text{PO}_4)_4(\text{OH})_6 \cdot 2\text{H}_2\text{O}$ 

**Origin:** Gentil mine, Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystal using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3643w, 3630s, 3399w, 3281s, (3253), 3232s, (3231), 3072, 2920w, 1751w, 1714w, 1610w, 1562w, 1230w, 1211, 1181, 1155w, 1104, 1068s, 1048s, 1025s, (1007), (994), 985, 965, 892w, 811,

**Source:** Scholz et al. (2013b).

**Comments:** The sample was characterized by electron microprobe analysis.

**Matlockite**  $\text{PbClF}$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 632.8 nm He-Ne laser. In spite of the strong opacity of the mineral, it was possible to record a Raman spectrum by using a very weak intensity laser (1 mW) and a long duration of 500 s.

**Raman shifts (cm<sup>-1</sup>):** 238, 227, 163s, 155, 132, 105, 84.

**Source:** Bouchard and Smith (2003).

**Comments:** For the Raman spectrum of matlockite see also Bouchard-Abouchakra (2001).

**Mattagamite**  $\text{CoTe}_2$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 121s.

**Source:** McKendry et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Matteuccite**  $\text{NaH}(\text{SO}_4) \cdot \text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** No data

**Raman shifts (cm<sup>-1</sup>):** 2940w, 1656, 1549w, 1308, 1268w, 1241w, 1191, 1060s, 874s, 655, 612, 577, 435, 411, 278w, 224w, 188w, 140w, 87.

**Source:** Baran et al. (1999a).

**Maxwelllite**  $\text{NaFe}^{3+}(\text{AsO}_4)\text{F}$ 

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 954w, 814sh, 894sh, 871s, (849), 812, 753, 542, (523), (487), 455w, (373), 360sh, (346), 327, 309sh, (291), (274w), 259w, (164w), 151, (140w), 111w.

**Source:** Frost et al. (2014aa).

**Comments:** The sample was characterized by qualitative electron microprobe analysis. For the Raman spectrum of maxwellite see also Downs et al. (2012).

### Mbobomkulite (Ni,Cu)Al<sub>4</sub>(NO<sub>3</sub>,SO<sub>4</sub>)<sub>2</sub>(OH)<sub>12</sub>·3H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements of SO<sub>4</sub>-free analogue of mbobomkulite have been performed on arbitrarily oriented sample using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3647, 3576, 3544w, 3468s, 3447w, 3422w, 3250s, 2900, 1645w, 1413, 1342w, 1058, 1050, 1045, 713w, 676, 614, 570, 545w, 541, 494, 447w, 350, 340, 337w, 324w, 297w, 217w, 184w, 181w, 160w, 142w.

**Source:** Frost et al. (2005f).

**Comments:** No independent analytical data are provided for the sample used.

### Mcallisterite Mg<sub>2</sub>[B<sub>6</sub>O<sub>7</sub>(OH)<sub>6</sub>]<sub>2</sub>·9H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 951, 637s, 526w, 488w, 410s, 321.

**Source:** Kipcak et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and may contain admixture of admontite. For the Raman spectrum of mcallisterite see also Derun and Tugce (2014).

### Mcalpineite Cu<sub>3</sub>Te<sup>6+</sup>O<sub>6</sub>

**Origin:** Gambatesa mine, eastern Liguria, Italy.

**Experimental details:** Micro-Raman scattering measurements have been performed on earthy mcalpineite aggregate using 633 nm laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 740s, 690s.

**Source:** Carbone et al. (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

### Mcconnellite Cu<sup>1+</sup>CrO<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Micro-Raman scattering measurements have been performed on a single crystal using 632 nm He-Ne laser radiation. The laser radiation power at the sample was 0.3 mW. Incident beam power with a 3 μm spot size (4000 W/cm<sup>2</sup>) was used. Polarized spectra were collected in the z(yz)z and z(yx)z scattering geometries.

**Raman shifts (cm<sup>-1</sup>):** 692s, 351w.

**Source:** Aktas et al. (2011).

**Comments:** The Raman shifts are given for the scattering geometry  $z(yy)z$ . For the Raman spectra of mconnellite see also Shu et al. (2009) and Elkhouni et al. (2013).

**Mcguinnessite** CuMg(CO<sub>3</sub>)(OH)<sub>2</sub>

**Origin:** Red Mountain, Mendocino Co., California, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystal using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3594, 3522s, 3381, 3309, 1567w, 1540, 1494s, 1359, 1090s, 1060, 914w, 741w, 707w, 516, 433, 269, 166, 147.

**Source:** Frost (2006).

**Megawite** CaSnO<sub>3</sub>

**Origin:** Upper Chegem caldera, Kabardino-Balkaria, Northern Caucasus, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power was in the range from 40 to 60 mW.

**Raman shifts (cm<sup>-1</sup>):** 705w, 557 (broad), 474w, 443, 355s, 283, 262, 183, 159.

**Source:** Galuskin et al. (2011b).

**Comments:** The sample was characterized by electron data and electron microprobe analyses. The empirical formula of the sample used is CaSn<sub>0.6</sub>Zr<sub>0.3</sub>O<sub>3</sub>. For the Raman spectrum of megawite see also Zheng et al. (2012).

**Meisserite** Na<sub>5</sub>(UO<sub>2</sub>)(SO<sub>4</sub>)<sub>3</sub>(SO<sub>3</sub>OH)(H<sub>2</sub>O)

**Origin:** Blue Lizard mine, San Juan Co., Utah, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm frequency-stabilized single mode diode laser radiation. The laser radiation power at the sample was 3 mW.

**Raman shifts (cm<sup>-1</sup>):** 3497w, 3366w, 1239, 1213, 1186, 1153, 1139, 1102, 1068, 1045, 1031s, 1019s, 990, 975, 847s, 633, 606, 589, 464, 448, 414, 241, 199, 171, 123, 96, 61.

**Source:** Plášil et al. (2013c).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Meixnerite** Mg<sub>6</sub>Al<sub>2</sub>(OH)<sub>16</sub>(OH)<sub>2</sub>·4H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm Ar<sup>+</sup> laser radiation. The output power of the laser was set to 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 3492w (broad), 2392w, 1808, 1512, 1368w, 1165w, 936s, 827s, 748s, 686s, 629, 572, 555, 491, 416, 394w, 342, 313w, 238s, 207w, 180, 157, 128, 101, 76w, 60w.

**Source:** Kagunya et al. (1998).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Melanarsite**  $K_3Cu_7Fe^{3+}O_4(AsO_4)_4$ 

**Origin:** Arsenatnaya fumarole, Tolbachik volcano, Kamchatka Peninsula, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 532 nm laser radiation. The laser output power was 4 mW.

**Raman shifts (cm<sup>-1</sup>):** 854s, 789, 632w, 550w, 464, 403, 352s, 331, 241, 187, 164, 142.

**Source:** Pekov et al. (2016d).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Melanophlogite**  $C_2H_{17}O_5 \cdot Si_{46}O_{92}$ 

**Origin:** Mt. Hamilton, California, USA.

**Experimental details:** Polarized (XX and XY) Raman spectra have been obtained on a single crystal using 514.5 or 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 3050w, 2909, 2900, 2321, 1380, 1277w, 803, 590, 364w, 268s, 165.

**Source:** Kolesov and Geiger (2003).

**Comments:** The Raman shifts are given with the XX polarization. For the Raman spectrum of melanophlogite see also Tribaudino et al. (2008).

**Melanterite**  $Fe(SO_4) \cdot 7H_2O$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 3385, 1147, 1074, 992s, 612, 480, 457, 284, 241w, 214w.

**Source:** Buzgar et al. (2009).

**Comments:** For the Raman spectra of melanterite see also Chio et al. (2007), Sobron and Alpers (2013), Jentzsch et al. (2013), Wang and Zhou (2014), Apopei et al. (2015), Buzatu et al. (2016), and Kompanchenko et al. (2016).

**Meliphanite**  $Ca_4(Na,Ca)_4Be_4AlSi_7O_{24}(F,O)_4$ 

**Origin:** Østskogen larvikittbrudd, Tvedalen, Larvik kommune, Vestfold fylke, Norway.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3805w, 3693w, 3595w, 3503, 3412, 3330, 3304w, 3207w, 3155w, 1095w, 1050w, 1016s, 991, 968, 932, 893w, 870w, 774, 745w, 721, 666s, 636w, 625s, 611w, 555w, 534w, 510w, 472, 421w, 382, 285w, 258, 207, 180, 147s, 113.

**Source:** Frost et al. (2015o).

**Mellite**  $Al_2C_6(COO)_6 \cdot 16H_2O$ 

**Origin:** Bílina, near Most, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power was 350 mW.

**Raman shifts (cm<sup>-1</sup>):** 3250w (broad), 1552, 1467s, 1386w, 1343, 1224, 805 (broad), 772, 538w, 376sh, 353w, 325, 242, 202sh, 178s, 162w, 151w, 134, 117w.

**Source:** Jehlička and Edwards (2008).

### Mellizinkalite K<sub>3</sub>Zn<sub>2</sub>Cl<sub>7</sub>

**Origin:** Glavnaya Tenoritovaya fumarole, Tolbachik volcano, Kamchatka, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented polycrystalline sample using 532 nm laser radiation. The laser radiation power at the sample was about 3–3.5 mW.

**Raman shifts (cm<sup>-1</sup>):** 310, 274s, 264s, 188, 128s.

**Source:** Pekov et al. (2015f).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### Mendipite Pb<sub>3</sub>O<sub>2</sub>Cl<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 632.8 nm He-Ne laser.

**Raman shifts (cm<sup>-1</sup>):** 3504, 732, 601w, 474w, 435, 330s, 273s, 134s.

**Source:** Bouchard and Smith (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of mendipite see also Frost and Williams (2004).

### Mercallite KH(SO<sub>4</sub>)

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 1174, 1126w, 1027s, 1001s, 872sh, 855, 581, 572, 448, 412.

**Source:** Ayta et al. (2010).

**Comments:** A Mn-doped crystal characterized by ESR was used.

### Merelaniite Mo<sub>4</sub>Pb<sub>4</sub>VSbS<sub>15</sub>

**Origin:** Merelani Tanzanite deposit, Lelatema Mts., Manyara Region, Tanzania (type locality).

**Experimental details:** Raman scattering measurements have been performed on a curved surface of a cylindrical whisker using 633 nm laser radiation. The laser radiation power at the sample was less than 3 mW.

**Raman shifts (cm<sup>-1</sup>):** 780w, 570w, 450, 401s, 390, 379, 324, 245, 133.

**Source:** Jaszczak et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Merenskyite** PdTe<sub>2</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. Neutral filter was used to decrease the laser radiation power to prevent sample damage.**Raman shifts (cm<sup>-1</sup>):** 132s, (105).**Source:** Bakker (2014).**Comments:** For the Raman spectrum of merenskyite see also Vymazalová et al. (2014).**Meridianiite** Mg(SO<sub>4</sub>)·11H<sub>2</sub>O**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 513 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 20 mW.**Raman shifts (cm<sup>-1</sup>):** 3520sh, 3395s, 1116, 1071, 990s, 620, 155sh, 444, 233w, 190.**Source:** Genceli et al. (2007).**Comments:** The sample was characterized by single-crystal X-ray diffraction data. The crystal structure is solved. For the Raman spectra of meridianiite see also Genceli et al. (2009) and Sakurai et al. (2010).**Merrillite Na-free analogue** Ca<sub>9.5</sub>Mg(PO<sub>4</sub>)<sub>7</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 20 mW.**Raman shifts (cm<sup>-1</sup>):** 1071, 1010, 966s, 951s, 761, 656w, 618, 601, 548, 437, 406.**Source:** Jolliff et al. (2006).**Comments:** The empirical formula of the sample used is Ca<sub>18.70</sub>REE<sub>0.05</sub>(Mg,Fe)<sub>2.00</sub>Na<sub>0.17</sub>P<sub>13.90</sub>Si<sub>0.16</sub>O<sub>56</sub>.**Merrillite** Ca<sub>9</sub>NaMg(PO<sub>4</sub>)<sub>7</sub>**Origin:** Suizhou meteorite, Dayanpo, Hubei, China.**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 514 nm Ar<sup>+</sup> laser radiation.**Raman shifts (cm<sup>-1</sup>):** 1080, 1026w, 972s, 956s, 604, 550w, 445, 408, 178.**Source:** Xie et al. (2002).**Comments:** The empirical formula of the sample used is Ca<sub>8.82</sub>Na<sub>0.88</sub>Mg<sub>0.91</sub>Fe<sub>0.07</sub>P<sub>7.14</sub>O<sub>28</sub>. For the Raman spectra of merrillite see also Cooney et al. (1999) and Xie et al. (2015).**Merwinite** Ca<sub>3</sub>Mg(SiO<sub>4</sub>)<sub>2</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented polycrystalline sample using 5145 or 4880 Å laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 1011, 991w, 980w, 939, 921, 911, 887s, 872s, 860, 845, 667w, 640w, 579, 540, 529, 424, 394, 374w, 330, 270, 227w, 203w, 194w, 156s, 143s, 126, 119, 78, 42.

**Source:** Piriou and McMillan (1983).

**Comments:** The sample was characterized by electron microprobe analysis. For the Raman spectrum of merwinite see also Zedgenizov et al. (2014).

#### Mesolite Na<sub>2</sub>Ca<sub>2</sub>(Si<sub>9</sub>Al<sub>6</sub>)O<sub>30</sub>·8H<sub>2</sub>O

**Origin:** Talisker, Isle of Skye, Scotland.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 3583s, 3510s, 3412s, 3329, 3242s, 1666, 1652, 1099s, 1073, 1049s, 1023, 1007, 990s, 955, 951, 762, 757s, 753, 735, 727, 717, 710, 708s, 673s, 668, 538s, 496, 441s, 409s, 381s, 374, 368, 346, 330s, 283s, 273, 255s, 225s, 204, 183s, 158s, 143.

**Source:** Wopenka et al. (1998).

**Comments:** Bands whose intensities are definitely dependent upon polarization are indicated in the cited paper. For the Raman spectra of mesolite see also Pechar (1983) and Mozgawa (2001).

#### Meta-ankoleite K(UO<sub>2</sub>)(PO<sub>4</sub>)·3H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 1–4 mW.

**Raman shifts (cm<sup>-1</sup>):** 3805, 3498, 3375, 3237, 3110, 2786, 1004s, 994s, 831s, 826s, 400, 291, 195, 173, 113, 108.

**Source:** Clavier et al. (2016).

**Comments:** For the Raman spectrum of meta-ankoleite see also Pham-Thi et al. (1985).

#### Meta-autunite Ca(UO<sub>2</sub>)<sub>2</sub>(PO<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O

**Origin:** Autun, France (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using a 633 nm He-Ne laser. Power at the sample was measured as 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3508, 3456, 3244, 1093, 1033, 1018, 1007s, 989, 915, 890, 850, 833s, 818, 643, 507, 453, 387s, 263, 222, 190.

**Source:** Frost and Weier (2004d).

**Comments:** For the Raman spectra of meta-autunite see also Frost (2004b) and Stefaniak et al. (2009).

#### Metacinnabar β-HgS

**Origin:** No data.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 339, 280w, 253s.

**Source:** Radepont (2013).

**Metahewettite**  $\text{CaV}^{5+}\text{O}_{16}\cdot 3\text{H}_2\text{O}$ 

**Origin:** The Fish, Eureka Co., Nevada, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystal using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1013, 994s, 954s, 878, 692, 530, 470, 425, 404, 290, 280s, 240, 188, 154, 140s.

**Source:** Frost et al. (2005d).

**Metakirchheimerite**  $\text{Co}(\text{UO}_2)_2(\text{AsO}_4)_2\cdot 8\text{H}_2\text{O}$ 

**Origin:** Jáchymov, Krušné Hory Mts. (Ore Mts.), Bohemia, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 730 nm laser radiation. The laser radiation power at the sample was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 908, 896sh, 883sh, 816s, 801sh, 449, 320w, 206sh, 191.

**Source:** Plášil et al. (2009).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Metalodèvite**  $\text{Zn}(\text{UO}_2)_2(\text{AsO}_4)_2\cdot 10\text{H}_2\text{O}$ 

**Origin:** Jánská vein, Březové Hory deposit, Příbram ore district, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532.2 nm laser radiation. The laser radiation power was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 3418, 994, 977, 892, 866, 819s, 522s, 469, 447, 399, 319, 303, 280w, 191.

**Source:** Plášil et al. (2010d).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Metamunirite**  $\text{NaV}^{5+}\text{O}_3$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed using 4880 Å Ar<sup>+</sup> laser radiation on the (110) cleavage plate, with incident light perpendicular to the plane, and polarized perpendicular to the scattering plane. The laser radiation power at the sample was 100 mW. No analyser was in the path of the scattered radiation but a polarization scrambler was used.

**Raman shifts (cm<sup>-1</sup>):** 948s, 911, 887s, 737, 557, 431, 288, 257, 203, 168, 135, 124, 81w, 53w.

**Source:** Seetharaman et al. (1983).

**Metarauchite**  $\text{Ni}(\text{UO}_2)_2(\text{AsO}_4)_2\cdot 8\text{H}_2\text{O}$ 

**Origin:** Jáchymov, Krušné Hory Mts. (Ore Mts.), Bohemia, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power was 10 mW. The Raman shifts have been partly determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3265w (broad), 3079, 1124w, 911sh, 898s, 893w, 883w, 878w, 817s, 804sh, 785sh, 771sh, 682w, 534w, 445, 395, 361w, 330, 319, 248, 211, 204w.

**Source:** Plášil et al. (2010c).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

### Metarossite CaV<sup>5+</sup><sub>2</sub>O<sub>6</sub>·2H<sub>2</sub>O

**Origin:** Blue Cap mine, San Juan Co., Utah, USA.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 532 nm laser radiation. The laser radiation power was 150 mW.

**Raman shifts (cm<sup>-1</sup>):** 3398, 3240, 3189, 2954, 2904.

**Source:** Kobsch et al. (2016).

**Comments:** The sample was characterized by the crystal structure refinement based on single-crystal X-ray diffraction data. For the Raman spectrum of metarossite see also Frost et al. (2005d).

### Metastibnite Sb<sub>2</sub>S<sub>3</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 25 mW.

**Raman shifts (cm<sup>-1</sup>):** 290s, 170.

**Source:** Watanabe et al. (1983).

**Comments:** The sample used was prepared as amorphous film by thermal evaporation of bulk Sb-S alloy with corresponding composition.

### Metastudtite UO<sub>4</sub>·2H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 6 mW.

**Raman shifts (cm<sup>-1</sup>):** 3446s, 3245w, 1716sh, 1621, 1111w, 927s, 909s, 791w, 558w, 474.

**Source:** Bastians et al. (2004).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Metathénardite Na<sub>2</sub>(SO<sub>4</sub>)

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed at 523 K on a single crystal, in different scattering geometries, using 457.9 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 150 mW.

**Source:** Choi and Lockwood (1989).

**Raman shifts (cm<sup>-1</sup>):** 1175, 1100, 993.5s, 628–626s, 467sh, 464s.

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of metathénardite see also Murugan et al. (2000).

**Metatorbernite**  $\text{Cu}(\text{UO}_2)_2(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was 10 mW.**Raman shifts (cm<sup>-1</sup>):** 1630w, 1514w, 1414w, 1014w, 997s, 986w, 905w, 831w, 827s, 806w, 627w, 602w, 560w, 541w, 464w, 443w, 429w, 412w, 406, 399w, 291w, 253w, 221w, 196, 145w, 125w, 113w, 99, 81w.**Source:** Sánchez-Pastor et al. (2013).**Comments:** The sample was characterized electron microprobe analysis. For the Raman spectra of metatorbernite see also Čejka Jr (1984), Frost (2004b), Frost and Weier (2004a), and Faulques et al. (2015a, b).**Metatyuyamunite**  $\text{Ca}(\text{UO}_2)_2(\text{VO}_4)_2 \cdot 3\text{H}_2\text{O}$ **Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation.**Raman shifts (cm<sup>-1</sup>):** 962, 829, 747s, 646w, 582, 570, 532, 467, 411w, 369s, 310.**Source:** Botto et al. (1989).**Comments:** The sample was characterized by powder X-ray diffraction data and analysis of H<sub>2</sub>O.**Metauranocircite-I**  $\text{Ba}(\text{UO}_2)_2(\text{PO}_4)_2 \cdot 6\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was 10 mW.**Raman shifts (cm<sup>-1</sup>):** 1635, 1543, 1420, 1039, 1023, 1003, 989s, 960, 821, 815s, 809, 627, 566, 502, 425, 409, 398, 376, 222.**Source:** Sánchez-Pastor et al. (2013).**Comments:** The sample was characterized electron microprobe analysis.**Metauranospinite**  $\text{Ca}(\text{UO}_2)_2(\text{AsO}_4)_2 \cdot 8\text{H}_2\text{O}$ **Origin:** Příbram, Central Bohemia region, Czech Republic.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3549w, 3428, 3238w, 2106w, 1891w, 1787w, 1617w, 1518w, 1366w, 907w, 896, 815s, 806, 458, 397, 321, 275, 196, 187s, 150, 111.**Source:** Čejka et al. (2009b).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Metavariscite**  $\text{Al}(\text{PO}_4) \cdot 2\text{H}_2\text{O}$ **Origin:** Mt Lucia, Utah, USA.**Experimental details:** Raman scattering measurements have been performed at 77 K on an arbitrarily oriented sample using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 1889, 1628, 1362, 1249, 1150, 1081s, 1063, 1033, 1018s, 643, 585, 574, 553, 499, 460, 446, 427s, 400, 387, 380, 374, 367, 360, 353s, 347, 340, 329s, 302, 297, 290, 280, 273, 258, 253, 244, 239, 230s, 211, 201, 187s, 171, 152, 147, 133, 124.**Source:** Frost et al. (2004l).**Metavivianite**  $\text{Fe}^{2+}\text{Fe}^{3+}(\text{PO}_4)_2(\text{OH})_2 \cdot 6\text{H}_2\text{O}$ **Origin:** Boa Vista pegmatite, near Galiléia, Minas Gerais, Brazil.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 10 mW.**Raman shifts (cm<sup>-1</sup>):** 3431, 3378w, 3299w, 3257sh, 3194sh, 1089w, 1022, 972s, 579, 506s, 461, 374w, 322sh, 289, 256, 236, 197, 166, 143.**Source:** Chukanov et al. (2012b).**Comments:** The sample was characterized by powder X-ray diffraction data, Mössbauer spectroscopy, electron microprobe analysis and gas-chromatographic determination of H<sub>2</sub>O. The empirical formula of the sample used is  $(\text{Fe}^{3+}_{1.64}\text{Fe}^{2+}_{1.23}\text{Mg}_{0.085}\text{Mn}_{0.06})_{\Sigma 3.015}(\text{PO}_4)_{1.98}(\text{OH})_{1.72} \cdot 6.36\text{H}_2\text{O}$ . The crystal structure is solved. For the Raman spectrum of metavivianite see also Frost et al. (2004m).**Metazeunerite**  $\text{Cu}(\text{UO}_2)_2(\text{AsO}_4)_2 \cdot 8\text{H}_2\text{O}$ **Origin:** Gilgai, New England, New South Wales, Australia, or Wheal Edward Bottalock, Cornwell, England (not specified in the cited paper).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3371, 3238, 3136, 910, 888, 819s, 809, 793, 449, 398, 320, 276, 240, 218.**Source:** Frost (2004b).**Comments:** For the Raman spectra of metazeunerite see also Frost and Weier (2004c) and Frost et al. (2004k).**Meurigite-Na**  $[\text{Na}(\text{H}_2\text{O})_{2.5}][\text{Fe}^{3+}_8(\text{PO}_4)_6(\text{OH})_7(\text{H}_2\text{O})_4]$ **Origin:** Silver Coin mine, Valmy, Iron Point district, Nevada, USA (type locality).**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 3270, 1125, ~1005s, ~960s, ~925, 876, 568, 490, 441s, 401, 281, 222, 170.**Source:** Kampf et al. (2009a).**Comments:** Maybe, an erroneous spectrum: wavenumbers of the strongest bands of phosphate groups in the range from 900 to 1100 cm<sup>-1</sup> are anomalously high. The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### Meyerhofferite $\text{CaB}_3\text{O}_3(\text{OH})_5 \cdot \text{H}_2\text{O}$

**Origin:** Bigadic deposits, Turkey.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3608s, (3505w), 3483s, (3421w), 3400s, 3344w, 3287, 3232, (3092), 3031s, (2908w), 1621w, (1592w), 1551w, 1367w, 1201, 1135, 1110, 1046, 1002, 958, 944, 935, 880, 728, 698w, (627w), 609s, 592, 493, 474, 435, 398w, 381w, 366w, 336, 235w, 227, 204, 189, 164, 124, 118.

**Source:** Frost et al. (2013h).

**Comments:** The sample was characterized by powder X-ray diffraction data and qualitative electron microprobe analysis.

### Meymacite monoclinic analogue $\text{WO}_3 \cdot 2\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdery sample using Ar<sup>+</sup> laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 3530, 3370sh, 3160s, ~1600, 960s, 685s, 662s, 380, 268, 235, 210, 110.

**Source:** Daniel et al. (1987).

### Miargyrite $\text{AgSbS}_2$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 447, 370w, 322w, 250s, 185s, 134w, 115.

**Source:** Minceva-Sukarova et al. (2003).

**Comments:** For the Raman spectrum of miargyrite see also Makreski et al. (2013b).

### Microcline $\text{K}(\text{AlSi}_3\text{O}_8)$

**Origin:** Čanište, Macedonia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 1139sh, 1124, 1099, 1051w, 994, 814w, 750, 651, 585w, 513s, 475s, 454, 402, 372, 331w, 285, 266, 258, 199, 179, 155, 127, 108.

**Source:** Makreski et al. (2009).

**Comments:** The sample was characterized by electron microprobe analysis. For the Raman spectra of microcline see also Ciobotă et al. (2012) and Frezzotti et al. (2012).

### Miersite $\text{AgI}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed at 573 K on a single crystal using 6328 Å He-Ne laser radiation. The laser radiation power at the sample was 10 mW. Polarized spectra were collected in the  $y[z(x/y)]z$  and  $y(zx)z$  scattering geometries.

**Raman shifts (cm<sup>-1</sup>):** ~100 (broad), ~30s (broad).

**Source:** Delaney and Ushioda (1976).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. The Raman shifts are given for the scattering geometry  $y[z(x/y)]z$ . In the scattering geometry  $y(zx)z$  only a peak at ~30 cm<sup>-1</sup> is observed.

**Mikasaite** Fe<sup>3+</sup><sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>

**Origin:** Synthetic.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 1123s, 1098s, 1078s, 1069, 1040, 677, 657, 628, 613, 600, 468, 461, 448, 295, 234, 178.

**Source:** Ling and Wang (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of mikasaite see also Apopei et al. (2015).

**Milarite** KCa<sub>2</sub>(Be<sub>2</sub>AlSi<sub>12</sub>)O<sub>30</sub>·H<sub>2</sub>O

**Origin:** Giuv Tavetsch, CH.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 785 nm laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 1126, 834, 538, 479s, 436w, 382w, 288w, 161w.

**Source:** Jehlička and Vandenabeele (2015).

**Comments:** For the Raman spectra of milarite see also Lengauer et al. (2009) and Jehlička et al. (2012).

**Millerite** β-NiS

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm laser radiation. The laser radiation power was 15 mW.

**Raman shifts (cm<sup>-1</sup>):** 372, 350, 301, 283, 246s, 222, 181, 174s, 142.

**Source:** Bishop et al. (2000).

**Comments:** The sample was characterized by powder X-ray diffraction.

**Millosevichite** Al<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1053, 1009, 990s, 979, 726, 630, 614, 572, 496, 459, 446.

**Source:** Kloprogge and Frost (1999c).

**Mimetite**  $\text{Pb}_5(\text{AsO}_4)_3\text{Cl}$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using Nd-YAG laser radiation. The laser radiation power at the sample was 300 mW.**Raman shifts (cm<sup>-1</sup>):** 1043, 1000w, 982w, 949, 920s, 812s, 791sh, 744sh, 553w, 546sh, 426sh, 411sh, 409, 391, 372, 338s, 314s.**Source:** Bajda et al. (2011).**Comments:** The empirical formula of the sample used is  $\text{Pb}_5[(\text{AsO}_4)_{2.4}(\text{PO}_4)_{0.6}]\text{Cl}$ . The bands in the ranges 900–1050 and 540–560 cm<sup>-1</sup> correspond to phosphate groups. For the Raman spectra of mimetite see also Levitt and Condrate, Sr (1970), Adams and Gardner (1974), Bartholomäi and Klee (1978), Frost et al. (2007c), and Bajda (2010).**Minguzzite**  $\text{K}_3\text{Fe}^{3+}(\text{C}_2\text{O}_4)_3 \cdot 3\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using 514.5 nm laser radiation.**Raman shifts (cm<sup>-1</sup>):** 1720, 1451s, 1252, 898, 782, 558s, 370, 257s, 136s.**Source:** Narsimhulu et al. (2015).**Minium**  $\text{Pb}^{2+}{}_2\text{Pb}^{4+}\text{O}_4$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 632.8 nm He-Ne laser. In spite of the strong opacity of the mineral, it was possible to record a Raman spectrum by using a very weak intensity laser (1 mW) and a long duration of 500 s.**Raman shifts (cm<sup>-1</sup>):** 549s, 480, 391, 313, 223, 150, 120s, 84, 70, 60, 51.**Source:** Bouchard and Smith (2003).**Comments:** For the Raman spectra of minium see also Bouchard-Abouchakra (2001), Burgio and Clark (2001), and Lepot et al. (2006).**Minnesotaite**  $\text{Fe}^{2+}{}_3\text{Si}_4\text{O}_{10}(\text{OH})_2$ **Origin:** No data in the cited paper.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power at the sample was about 13 mW.**Raman shifts (cm<sup>-1</sup>):** 3654s, 3639s, 3625s, 660s, 545, 440, 407, 350, 251, 188.**Source:** Wang et al. (2015).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.**Minyulite**  $\text{KAl}_2(\text{PO}_4)_2\text{F} \cdot 4\text{H}_2\text{O}$ **Origin:** Minyulo Well, Australia (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3692w, 3669, 3661w, 3324 (broad), 3225 (broad), 1584w, (1190w), 1176w, 1155w, (1136w), (1105w), 1091, 1077, (1047), 1012s, (991w), 657, (628w), (606w), 592s, 575, (551w), (535w), (522w), (506), 494s, (481), 448, (420w), 407.

**Source:** Frost et al. (2014l).

**Comments:** The empirical formula of the sample used is  $(K_{0.82}Ca_{0.05}Na_{0.03})Al_{2.04}Fe_{0.08}(PO_4)_2[F_{0.55}(OH)_{0.45}] \cdot 4H_2O$ .

### Mirabilite $Na_2(SO_4) \cdot 10H_2O$

**Origin:** No data in the cited paper.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 3506s, 3340, 1129w, 989s, 627, 458.

**Source:** Frezzotti et al. (2012).

**Comments:** For the Raman spectrum of mirabilite see also Sakurai et al. (2010).

### Misakiite $Cu_3Mn(OH)_6Cl_2$

**Origin:** Sadamisaki Peninsula, Ehime prefecture, Japan (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 3552w, 3505, 3460s, 470, 397s, 321, 265.

**Source:** Nishio-Hamane et al. (2016b).

**Comments:** The sample was characterized by powder and single-crystal X-ray diffraction data, and electron microprobe analyses.

### Mitscherlichite $K_2CuCl_4 \cdot 2H_2O$

**Origin:** Synthetic.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 3340, 3275, 3250, 3235, 3170, 1630–1628, 685, 633, 550, 404, 395.

**Source:** Thomas et al. (1974).

### Mixite $Cu_6Bi(AsO_4)_3(OH)_6 \cdot 3H_2O$

**Origin:** Smrkovec ore occurrence, the Slavkovský Les Mts., western Bohemia, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3470, 3392, 1588w, 1513w, 995w, (855), 850s, 805, 553, 529, (494), 472s, (460), 421, 390, 311, 284, 252, 232, 192, 169, 138, (112), 105s.

**Source:** Frost et al. (2009f).

**Comments:** The sample was characterized by X-ray diffraction data and electron microprobe analyses. For the Raman spectrum of mixite see also Frost et al. (2006m).

**Moctezumite**  $\text{Pb}(\text{UO}_2)(\text{Te}^{4+}\text{O}_3)_2$ 

**Origin:** Moctezuma (Bambolla) mine, Sonora, Mexico.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 826, 758, 723s, 656s, 623, 511w, 455, 356, 308w, 252, 212, 142.

**Source:** Frost et al. (2009b).

**Comments:** IR spectrum of presumed moctezumite given in the cited paper corresponds to quartz.

**Mogánite**  $\text{SiO}_2 \cdot n\text{H}_2\text{O}$ 

**Origin:** Mogán, Gran Canaria (Grand Canary), Las Palmas Province, Canary Islands, Spain (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 1177w, 1171w, 1084w, 1058w, (978w), (950w), 833w, 792w, 693w, 501s, 463, 449, 432w, 398w, 377w, 370w, 317w, 265w, 220s, 141, 129s.

**Source:** Kingma and Hemley (1994).

**Comments:** No independent analytical data are provided for the sample used.

**Mohite**  $\text{Cu}_2\text{SnS}_3$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 or 785 nm laser radiation. The laser radiation power at the sample was below 0.4 mW.

**Raman shifts (cm<sup>-1</sup>):** 374w, 352s, 314, 290s, 263sh, 248sh, 224w.

**Source:** Fontané et al. (2013).

**Comments:** No independent analytical data are provided for the sample used.

**Mohrite**  $(\text{NH}_4)_2\text{Fe}^{2+}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** Micro-Raman scattering measurements have been performed on arbitrarily oriented individual particles using 532 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 3355, 3290, 3101sh, (2913w), (2852w), 1705w, 1678w, 1430w, 1148sh, 1129, 1091, 1067, 980s, 622, 610, 457sh, 450.

**Source:** Jentzsch et al. (2013).

**Comments:** No independent analytical data are provided for the sample used.

**Moissanite** SiC

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 or 488 nm laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 963, 783s, 762, 150.

**Source:** Andò and Garzanti (2014).

**Comments:** For the Raman spectra of moissanite see also Xu et al. (2008, 2015b) and Kompanchenko et al. (2016).

**Mojaveite** Cu<sub>6</sub>[Te<sup>6+</sup>O<sub>4</sub>(OH)<sub>2</sub>](OH)<sub>7</sub>Cl

**Origin:** Blue Bell claims, near Baker, San Bernardino Co., California, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on a single crystal (probably on the (001) face) using 514.3 nm laser radiation. The laser radiation power at the sample was 2 mW.

**Raman shifts (cm<sup>-1</sup>):** ~3500w, 1112w, 967w, 694s, 654, 624, 555, 510, 475sh, 414w, 286, 254, 233w, 203, 172.

**Source:** Mills et al. (2014b).

**Comments:** The sample was characterized by powder and single-crystal X-ray diffraction data and electron microprobe analyses.

**Molybdenite** MoS<sub>2</sub>

**Origin:** Wolfram Camp, Qld., Australia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was between 1 and 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 451, 408s, 382s, 285.

**Source:** Mernagh and Trudu (1993).

**Comments:** For the Raman spectra of molybdenite see also Windom et al. (2011) and Štengl and Henych (2013).

**Molybdite** MoO<sub>3</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdery sample using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 15 mW.

**Raman shifts (cm<sup>-1</sup>):** 995s, 820s, 666, 285s, 158.

**Source:** Windom et al. (2011).

**Comments:** For the Raman spectra of molybdite see also Seguin et al. (1995), Nitta et al. (2006), and Camacho-López et al. (2011).

**Molybdoformacite** CuPb<sub>2</sub>(MoO<sub>4</sub>)(AsO<sub>4</sub>)(OH)

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm Nd-YAG laser radiation. The laser radiation power at the sample was 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 1089, 1048, 1014, 855, 713, 666, 558, 387, 355, 320, 278, 226, 196, 159, 152.

**Source:** Frost (2004c).

**Comments:** The data are questionable: no information on the sample origin and no independent analytical data on the sample used are given. Band intensities are not indicated.

**Molybdophyllite**  $\text{Pb}_8\text{Mg}_9[\text{Si}_{10}\text{O}_{28}(\text{OH})_8\text{O}_2(\text{CO}_3)_3]\cdot\text{H}_2\text{O}$ 

**Origin:** Långban deposit, Bergslagen ore region, Filipstad district, Värmland, Sweden (type locality).

**Experimental details:** Raman scattering measurements have been performed on a single crystal using unpolarized 633 nm laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 3696s, ~3600, ~1050, ~998.

**Source:** Kolitsch et al. (2012).

**Comments:** The sample was characterized by single crystal X-ray diffraction data.

**Molysite**  $\text{FeCl}_3$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 632.8 nm He-Ne laser. Laser radiation power of 30 mW at the source was reduced considerably by various filters.

**Raman shifts (cm<sup>-1</sup>):** 667, 598, 373, 293s, 259.

**Source:** Bouchard and Smith (2003).

**Comments:** For the Raman spectrum of molysite see also Bouchard-Abouchakra (2001).

**Monazite-(Ce)**  $\text{Ce}(\text{PO}_4)$ 

**Origin:** Synthetic.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 He-Ne laser radiation. The laser radiation power behind the microscope objective was 8 mW.

**Raman shifts (cm<sup>-1</sup>):** 1073, 1056, 992, 970s, 620, 572w, 467, 397, 220, 102, 88.

**Source:** Ruschel et al. (2012).

**Comments:** The sample was characterized by electron microprobe analysis. For the Raman spectra of monazite-(Ce) see also Begun et al. (1981), O'Neill et al. (2006), Silva et al. (2006), Andò and Garzanti (2014), and Heuser et al. (2014).

**Monazite-(La)**  $\text{La}(\text{PO}_4)$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 1073, 1065w, 1055s, 1025w, 991, 967s, 619, 589w, 572, 537w, 465, 414, 394, 271, 255w, 227, 220, 183w, 170, 151, 131w, 120w, 100, 90.

**Source:** Begun et al. (1981).

**Comments:** For the Raman spectra of monazite-(La) see also Silva et al. (2006), Frezzotti et al. (2012), and Heuser et al. (2014).

**Monazite-(Nd)**  $\text{Nd}(\text{PO}_4)$ 

**Origin:** Synthetic.

**Experimental details:** Polarized Raman scattering measurements have been performed on a single crystal using 488 nm laser radiation. Scattering geometry is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1079, 1061, 1033, 998, 977s, 625s, 601, 575, 539, 471s, 419, 398, 291, 264, 236, 228, 183, 175, 160, 154, 106, 89.

**Source:** Silva et al. (2006).

**Comments:** For the Raman spectra of monazite-(Nd) see also Begun et al. (1981) and Heuser et al. (2014).

### Monazite-(Sm) Sm(PO<sub>4</sub>)

**Origin:** Synthetic.

**Experimental details:** Polarized Raman scattering measurements have been performed on a single crystal using 514.5 nm Ar<sup>+</sup>laser radiation. Scattering geometry is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1084, 1065, 1035, 999, 983s, 629s, 603, 577, 542, 474s, 424, 404, 293, 265, 243, 231, 185, 177, 159, 155, 107, 88.

**Source:** Silva et al. (2006).

**Comments:** For the Raman spectra of monazite-(Sm) see also Begun et al. (1981) and Heuser et al. (2014).

### Moncheite Pt(Te,Bi)<sub>2</sub>

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532.068 nm laser radiation. The laser radiation power at the sample was in the range from 1 to 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 155, 115s.

**Source:** Bakker (2014).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of moncheite see also Mernagh and Hoatson (1995).

### Monetite Ca(PO<sub>3</sub>OH)

**Origin:** Synthetic (commercial reactant).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 1064.1 nm Nd-YAG laser radiation. The laser radiation power at the sample was below 320 mW.

**Raman shifts (cm<sup>-1</sup>):** 2814w, 2421w, 1617w, 1133, 1095, 988s, 901s, 779, 693, 591, 574, 562, 474w, 420, 395, 274w, 182w, 143w.

**Source:** Xu et al. (1999).

**Comments:** For the Raman spectrum of monetite see also Frost et al. (2013r).

### Monipite MoNiP

**Origin:** Allende meteorite.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented grain in a polished section using 514.5 nm laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 430, 350s, 280.

**Source:** Ma et al. (2014a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Monohydrocalcite**  $\text{Ca}(\text{CO}_3)\cdot\text{H}_2\text{O}$ 

**Origin:** Sainte Guillaume vein, St.-Marie-aux-Mines, Haut Rhin, France.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser adiation. The laser emitted power was about 8 mW.

**Raman shifts (cm<sup>-1</sup>):** 3425w, 3326, 3224, 1069s, 876w, 723w, 699w, 208.

**Source:** Coleyshaw et al. (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Montebrasite**  $\text{LiAl}(\text{PO}_4)\text{OH}$ 

**Origin:** Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 200 mW.

**Raman shifts (cm<sup>-1</sup>):** 3329s, 1189w, 1108, 1057s, 1046s, 1012s, 799, 645, 627, 601w, 483w, 429, 298s, 278, and a series of weak bands below 270 cm<sup>-1</sup>.

**Source:** Rondeau et al. (2006).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectrum of montebrasite see also Dias et al. (2011).

**Monteponite** CdO

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power was 2.48 mW.

**Raman shifts (cm<sup>-1</sup>):** 938w, 390s, 330sh, 259.

**Source:** Thema et al. (2015).

**Comments:** For the Raman spectrum of monteponite see also Falgayrac et al. (2013).

**Montgomeryite**  $\text{Ca}_4\text{MgAl}_4(\text{PO}_4)_6(\text{OH})_4\cdot12\text{H}_2\text{O}$ 

**Origin:** Katies Bower, Chifley Cave, Jenolan Caves, New South Wales, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1709, 1669w, 1606, (1582w), 1339, (1286), 1260, 1214, 1143, 1088, 1011s, 979s, 655w, (609), 591, 511s, 475, 457s, 391, 318, 292s, 268, (251), 202, 176, 161s, 146.

**Source:** Frost et al. (2012e).

**Comments:** Powder X-ray diffraction data indicate that the sample used contains minor admixture of variscite.

**Monticellite**  $\text{CaMg}(\text{SiO}_4)$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 or 488.0 nm laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 950, 900, 852s, 818s.

**Source:** Piriou and McMillan (1983).

**Comments:** For the Raman spectrum of monticellite see also Mouri and Enami (2008).

**Montmorillonite**  $(\text{Na,Ca})_{0.3}(\text{Al,Mg})_2\text{Si}_4\text{O}_{10}(\text{OH})_2 \cdot n\text{H}_2\text{O}$

**Origin:** Bidahochi formation, Cheto district, Apache Co., Arizona, USA.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 1064 nm laser radiation. The nominal laser radiation power was 0.2 mW.

**Raman shifts (cm<sup>-1</sup>):** 1112, 1029, 917, 885, 840, 792, 709s, 705sh, 571w, 505sh, 433s, 330, 290, 262, 200s, 176, 81.

**Source:** Bishop and Murad (2004).

**Comments:** The sample was characterized by chemical analyses. For the Raman spectrum of montmorillonite see also Frost and Rintoul (1996).

**Montroseite**  $(\text{V}^{3+},\text{Fe}^{2+},\text{V}^{4+})\text{O(OH)}$

**Origin:** Akouta mine, Niger.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 514.5 nm Ar<sup>+</sup> laser radiation.

**Source:** Forbes and Dubessy (1988).

**Raman shifts (cm<sup>-1</sup>):** 990s, 960, 925, 905w, 845, 780, 750w, 690, 560w, 515, 470, 400, 340w, 295sh, 280s, 144.

**Comments:** The sample was characterized by powder X-ray diffraction data and chemical analysis.

**Montroydite** HgO

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 568, 327s, 120w.

**Source:** Zhou et al. (1998).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Moolooite** Cu(C<sub>2</sub>O<sub>4</sub>)·nH<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 1620, 1513s, 1486s, 922, 845, 608, 584s, 558s, 300, 209s.

**Source:** D'Antonio et al. (2007).

**Comments:** The sample was characterized by powder X-ray diffraction data and TG analysis. For the Raman spectra of moolooite see also Frost and Weier (2003), Frost (2004d), Castro et al. (2008), and Romann et al. (2009).

**Mopungite**  $\text{NaSb}^{5+}(\text{OH})_6$ **Origin:** Pereta mine, Tuscany, Italy.**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 20 mW. The Raman shifts have been partly determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3423s, 3353, 3331, 3239, 3178s, 3134, (671), (648), 626s, (605), 362, 350, 204, 189.**Source:** Bittarello et al. (2015).**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analysis. For the Raman spectra of mopungite see also Bahfenne (2011) and Rintoul et al. (2011).**Moraskoite**  $\text{Na}_2\text{Mg}(\text{PO}_4)\text{F}$ **Origin:** Morasko IAB-MG iron meteorite, Poland (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was between 30 and 50 mW.**Raman shifts (cm<sup>-1</sup>):** 1114s, 1027s, 962s, 589, 438w, 336w, 308w, 279w, 262w, 244w, 193w, 184w, 147w, 131w.**Source:** Karwowski et al. (2015).**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses.**Mordenite**  $(\text{Na}_2,\text{Ca},\text{K}_2)_4(\text{Al}_8\text{Si}_{40})\text{O}_{96}\cdot28\text{H}_2\text{O}$ **Origin:** Faröes Islands.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using Nd-YAG laser radiation. The nominal laser radiation power was 300 mW.**Raman shifts (cm<sup>-1</sup>):** 1087w, 1046, 977w, 713w, 534s, 448, 427, 297w, 229w, 160.**Source:** Mozgawa (2001).**Comments:** The sample was characterized by powder X-ray diffraction data.**Morenosite**  $\text{Ni}(\text{SO}_4)\cdot7\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Micro-Raman spectrum was recorded with a medium Hilger quartz spectrophotograph using the  $\lambda = 2536.5 \text{ \AA}$  resonance radiation of mercury.**Raman shifts (cm<sup>-1</sup>):** 3532w, 3437s, 3266, 1158w, 1139, 1095, 1057s, 985s, 642, 622w, 612s, 463s, 442s, 419w, 402, 251s, 233w, 207s, 152s, 131w, 111s, 88, 75s, 60.**Source:** Krishnamurti (1958).

**Moschelite** HgI**Origin:** Synthetic.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 194, 113, 65, 31.**Source:** Ōsaka (1971).**Comments:** For the Raman spectrum of moschelite see also Cooney et al. (1968).**Mosesite** (Hg<sub>2</sub>N)Cl**Origin:** No data.**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily sample using 785 nm laser radiation.**Raman shifts (cm<sup>-1</sup>):** ~547, ~538.**Source:** Cooper et al. (2013a).**Mottramite** PbCu(VO<sub>4</sub>)(OH)**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3162w, (2927)w, (891w), (849), (841), 829s, (821), 802, (796), (747w), 716w, 612w, 500w, 451w, 411, 366, (354), 333, (307), (301), 293, 247w, 227, 202w, 172w, 151, (136), (129), 118.**Source:** Frost et al. (2014ai).**Comments:** The sample was characterized by qualitative electron microprobe analysis. For the Raman spectrum of mottramite see also Frost et al. (2001).**Mountkeithite** (Mg<sub>1-x</sub>Fe<sup>3+</sup><sub>x</sub>)(SO<sub>4</sub>)<sub>x/2</sub>(OH)<sub>2</sub>·nH<sub>2</sub>O ( $x < 0.5$ ,  $n > 3x/2$ )**Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3698, 3688, 3654, 2240w, 1937, 1679s, 1613s, 1525s, 1439, 1273s, 1122, 1109, 920, 691, 621w, 528, 468w, 390, 348w, 233, 202w.**Source:** Frost et al. (2003h).**Comments:** No independent analytical data are provided for the sample used.**Moydite-(Y)** YB(OH)<sub>4</sub>(CO<sub>3</sub>)**Origin:** Evans-Lougranitic pegmatite, near Wakefield, Quebec, Canada (type locality).**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was between 20 and 50 mW.**Raman shifts (cm<sup>-1</sup>):** 1610s, 1410, 1124s, 1106, 765, 700w.

**Source:** Grice et al. (1986).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. There are discrepancies between Raman shifts and figure of the Raman spectrum given in the cited paper.

**Mukhinite**  $\text{Ca}_2(\text{Al}_2\text{V}^{3+})[\text{Si}_2\text{O}_7][\text{SiO}_4]\text{O}(\text{OH})$

**Origin:** Pyrrhotite gorge, Khibiny Mts., Kola Peninsula, Russia.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented polished surface using 633 nm He-Ne laser radiation. The laser radiation power at the sample was between 2 and 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 1235w, 1213w, 1087w, 1052w, 965, 910, 849, 805, 741, 693, 623, 596s, 547, 518s, 485, 322, 284, 235, 155, 125, 85s.

**Source:** Voloshin et al. (2014).

**Comments:** The sample was characterized by electron microprobe analyses.

**Mukhinite V-rich analogue**  $\text{Ca}_2(\text{AlV}^{3+})_2[\text{Si}_2\text{O}_7][\text{SiO}_4]\text{O}(\text{OH})$

**Origin:** Pyrrhotite gorge, Khibiny Mts., Kola Peninsula, Russia.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented polished surface using 633 nm He-Ne laser radiation. The laser radiation power at the sample was between 2 and 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 1089s, 1012s, 929, 891, 816, 700, 668, 607, 552, 499, 389s, 357, 328, 229w, 136w.

**Source:** Voloshin et al. (2014).

**Comments:** The sample was characterized by electron microprobe analyses.

**Mullite**  $\text{Al}_{4+2x}\text{Si}_{2-2x}\text{O}_{10-x}$  ( $x \approx 0.4$ )

**Origin:** NW of Ormsaig, Ross of Mull, Scotland, UK (type locality).

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 457 nm Ar<sup>+</sup> laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 1130, 1035, 960s, 870s, 720, 600s, 415, 340, 305.

**Source:** Bost et al. (2016).

**Comments:** For the Raman spectrum of mullite see also Shoval et al. (2001).

**Muscovite**  $\text{KAl}_2(\text{Si}_3\text{Al})\text{O}_{10}(\text{OH})_2$

**Origin:** Rebra Valley, Rodnei (Rodna) Mts., Romania.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single sample using 532 nm laser radiation. The laser radiation power at the sample was 35 mW.

**Raman shifts (cm<sup>-1</sup>):** 119, 957, 914, 755, 704s, 641, 412s, 266s, 219.

**Source:** Buzgar (2008).

**Comments:** According to the Raman Spectra Database, Siena ([http://www.dst.unisi.it/geofluids/raman/spectrum\\_frame.htm](http://www.dst.unisi.it/geofluids/raman/spectrum_frame.htm)), Raman spectrum of muscovite contains also a band of O-H-stretching vibrations at 3627 cm<sup>-1</sup>. For the Raman spectra of muscovite see also Haley et al. (1982), Tlili et al. (1989), Wada and Kamitakahara (1991), Graeser et al. (2003), and Frezzotti et al. (2012).

**Nabiasite** BaMn<sub>9</sub>(VO<sub>4</sub>)<sub>6</sub>(OH)<sub>2</sub>

**Origin:** Nabias hamlet, Central Pyrenees, France (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 880sh, 867, 807s, 768.

**Source:** Brugger et al. (1999).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analysis. The crystal structure is solved.

**Nabimusaite** KCa<sub>12</sub>(SiO<sub>4</sub>)<sub>4</sub>(SO<sub>4</sub>)<sub>2</sub>O<sub>2</sub>F

**Origin:** Jabel Harmun, Palestinian Autonomy, Israel (type locality).

**Experimental details:** Methods of sample preparation are not described. Micro-Raman scattering measurements have been performed using 488 nm solid-state laser radiation. The laser radiation power at the sample was 44 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1121, 993s, 948, 930sh, 885, 849sh, 831, 637, 563, 524, 463, 403, 129.

**Source:** Galuskin et al. (2015d).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Nacrite** Al<sub>2</sub>Si<sub>2</sub>O<sub>5</sub>(OH)<sub>4</sub>

**Origin:** Commonwealth Scientific and Industrial Research Organization, Division of Soils, Glen Osmond, South Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 1064 nm Nd-YAG laser. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1175, 1160, 1085, 1020, 920s, 810, 720, 710, 660, 550, 520, 480s, 400, 340s, 275s, 250s.

**Source:** Frost et al. (1993).

**Comments:** No independent analytical data are provided for the sample used.

**Nadorite** PbSb<sup>3+</sup>O<sub>2</sub>Cl

**Origin:** Harstigen mine, Pajsberg, near Filipstad, Värmland, Sweden.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was in the range from 20 to 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 214, 165–117.

**Source:** Jonsson (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Nafertisite**  $\text{Na}_3\text{Fe}^{2+}_{10}\text{Ti}_2(\text{Si}_6\text{O}_{17})_2\text{O}_2(\text{OH})_6\text{F}(\text{H}_2\text{O})_2$ 

**Origin:** Kukisvumchorr, Khibiny alkaline massif, Kola peninsula, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 633 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1030, 922, 688s, 658s, 569, 530, 490, 420w, 345, 297, 240, 212w, 184, 145.

**Source:** Cámara et al. (2014b).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data, electron microprobe analyses, and Mössbauer spectroscopy. The crystal structure is solved.

**Nagelschmidtite**  $\text{Ca}_7(\text{SiO}_4)_2(\text{PO}_4)_2$ 

**Origin:** Artificial (component of slags produced from a solid radioactive waste).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1176, 1075, 1008s, 916, 843w, 702, 535w, 352, 217.

**Source:** Malinina and Stefanovsky (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Nahcolite**  $\text{NaH}(\text{CO}_3)$ 

**Origin:** Ryoke metamorphic rocks, Kasado Island, Yamaguchi prefecture, Japan.

**Experimental details:** Raman scattering measurements have been performed on a microscopic inclusion using 532 nm laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1268, 1046s, 687.

**Source:** Hoshino et al. (2006).

**Comments:** No independent analytical data are provided for the sample used.

**Nahcolite**  $\text{NaH}(\text{CO}_3)$ 

**Origin:** No data in the cited paper.

**Experimental details:** No data in the cited paper.

**Raman shifts (cm<sup>-1</sup>):** 1432w, 1271, 1048s, 688.

**Source:** Frezzotti et al. (2012).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of nahcolite see also Edwards et al. (2007), Kaminsky et al. (2009), and Frezzotti et al. (2012).

**Nahpoite**  $\text{Na}_2(\text{PO}_3\text{OH})$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed at 84°C on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 30 mW.

**Raman shifts (cm<sup>-1</sup>):** 1139, 1072, 1001w, 939s, 855, 583w, 571w, 556, 501w, 461, 397.

**Source:** Ghule et al. (2003).

**Comments:** The sample was characterized by TG data.

**Namibite** Cu(BiO)<sub>2</sub>(VO<sub>4</sub>)(OH)**Origin:** Lodi No. 4 mine, Plumas Co., California, USA.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 899w, 846s, (842), (769w), 736, 677w, 563s, 410w, 370s, 328s, 288, 247, 212.**Source:** Frost et al. (2006i)**Comments:** No independent analytical data are provided for the sample used.**Nantokite** CuCl**Origin:** Synthetic.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** ~197, ~155, ~117s, ~58, ~40sh.**Source:** Vardeny and Brafman (1979).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of nantokite see also Bouchard-Abouchakra (2001) and Frost et al. (2003i).**Naquite** FeSi**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an oriented crystal at 340 K. The laser wavelength and the laser radiation power are not indicated.**Raman shifts (cm<sup>-1</sup>):** 436, (333w), 315s, (260), 219, (193), 180s.**Source:** Nyhus et al. (1995).**Comments:** No independent analytical data are provided for the sample used.**Narsarsukite** Na<sub>2</sub>(Ti,Fe<sup>3+</sup>)Si<sub>4</sub>(O,F)<sub>11</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on pellets of pressed powder using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was about 300 mW. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 1009, 907, 764s, 518w, 480w, 422w, 362.**Source:** Su et al. (2000).**Comments:** The sample was characterized by powder X-ray diffraction data.**Natalytite** NaV<sup>3+</sup>Si<sub>2</sub>O<sub>6</sub>**Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Micro-Raman scattering measurements have been performed in the backscattering configuration, using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1042, 1025w, 972s, 954s, ~910w, ~865, ~830, ~680, ~640w, ~550s, ~505, ~390, ~360, ~345sh, ~340s, and a series of bands below 340 cm<sup>-1</sup>.**Source:** Konstantinović et al. (2002).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of natalite see also Popović et al. (2006) and Ullrich et al. (2009).

### Natisite $\text{Na}_2\text{TiO}(\text{SiO}_4)$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on pellets of pressed powder using 488 nm  $\text{Ar}^+$  laser radiation. The laser radiation power at the sample was about 300 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 926w, 898, 869, 851s, 830s, 677w, 533w, 497w, 379sh, 360.

**Source:** Su et al. (2000).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Natrite $\text{Na}_2(\text{CO}_3)$

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-Yag laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1429w, 1080s, 702, 290.

**Source:** Buzgar and Apopei (2009).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of natrite see also Edwards et al. (2007), Frezzotti et al. (2012), and Shatskiy et al. (2013).

### Natroalunite $\text{NaAl}_3(\text{SO}_4)_2(\text{OH})_6$

**Origin:** No data.

**Experimental details:** Micro-Raman scattering measurements have been performed on a thin section using 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power at the sample was 20 or 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 1183, 1163w, 1024s, 652s, 572, 519, 482, 395, 345, 234s, 163.

**Source:** Maubec et al. (2012).

**Comments:** The sample was characterized by electron microprobe analysis. Its empirical formula is  $\text{Na}_{0.6}\text{K}_{0.4}\text{Al}_{2.9}(\text{SO}_4)_{2.1}(\text{OH})_{5.5}$ .

### Natrochalcite $\text{NaCu}_2(\text{SO}_4)_2(\text{OH}) \cdot \text{H}_2\text{O}$

**Origin:** Chuquicamata, Chile.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3196, 3156, 1046, 1023, 997s, 930, 709, 636s, 607, 466, 445, 429, 402, 212.

**Source:** Frost and Weier (2004e).

**Comments:** No independent analytical data are provided for the sample used.

**Natrodufrénite**  $\text{NaFe}^{2+}\text{Fe}^{3+}_5(\text{PO}_4)_4(\text{OH})_6 \cdot 2\text{H}_2\text{O}$ 

**Origin:** Divino das Laranjeiras, eastern Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3573, 3187, (3119), 1634, 1335w, 1188, 1059, 1003, 961, 914, 814, 668, 619w, 582, 560, 507, 477s, (444), 425, 376, 356, 298, 217, 194, 163, 142, 120.

**Source:** López et al. (2013b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Natrojarosite**  $\text{NaFe}^{3+}_3(\text{SO}_4)_2(\text{OH})_6$ 

**Origin:** The sample was obtained from the Dogan Paktunc of Mineral Resources Laboratories, CANMET, Ottawa, ON, Canada. The locality is not indicated.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 785 nm solid-state laser radiation. The laser radiation output power was above 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 1105, 1008s, 618, 555, 356, 288, 221, 134.

**Source:** Das and Hendry (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of natrojarosite see also Sasaki et al. (1998), Frost et al. (2006r), Murphy et al. (2009), and Chio et al. (2010).

**Natrolemoynite**  $\text{Na}_4\text{Zr}_2\text{Si}_{10}\text{O}_{26} \cdot 9\text{H}_2\text{O}$ 

**Origin:** Poudrette (Demix) quarry, Mont Saint-Hilaire, Rouville RCM (Rouville Co.), Montérégie, Québec, Canada (type locality) (?).

**Experimental details:** Raman scattering measurements have been performed with laser radiation perpendicular to the {010} cleavage of a single crystal using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 968s, ~610, 538, 428, ~290w.

**Source:** McDonald et al. (2015).

**Comments:** No independent analytical data are provided for the sample used.

**Natrolite**  $\text{Na}_2(\text{Si}_3\text{Al}_2)\text{O}_{10} \cdot 2\text{H}_2\text{O}$ 

**Origin:** Chimney Rock Quarry, Bound Brook, New Jersey, USA (?).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 3543s, 3476, 3329s, 3231, 1637, 1093, 1085, 1071, 1064, 1042s, 1019, 1009, 987, 977, 966, 727s, 718, 707s, 534s, 443s, 417, 393, 360s, 333s, 308s, 290, 276, 259, 241, 218s, 207, 186, 163s, 145s.

**Source:** Wopenka et al. (1998).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectra of natrolite see also Belitsky et al. (1992), Goryainov and Smirnov (2001), Mozgawa (2001), Jehlička et al. (2012), and Jehlička and Vandenabeele (2015).

### Natron $\text{Na}_2(\text{CO}_3) \cdot 10\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 or 514.5 nm laser radiation. The nominal laser radiation power was in the range from 5 to 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1061–1070s, 335w, 224w, 185w.

**Source:** Edwards et al. (2007).

**Comments:** No independent analytical data are provided for the sample used.

### Natroniobite $\text{NaNbO}_3$

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed at 560 K in backscattering geometry using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~570s, ~240, ~205, ~160, ~120, ~50.

**Source:** Yuzyuk et al. (2005).

**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts are given for a sample at 560 K.

### Natropalermoite $\text{Na}_2\text{SrAl}_4(\text{PO}_4)_4(\text{OH})_4$

**Origin:** Palermo No. 1 mine, Groton, New Hampshire, USA (type locality).

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm solid-state laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~3215, ~1145s, ~1079, ~1008s, ~935, ~640, ~622, ~595, ~524, ~431s, ~413, ~318, and a series of bands below 300 cm<sup>-1</sup>.

**Source:** Schumer et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### Natrophilite $\text{NaMn}^{2+}(\text{PO}_4)$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an aggregate of microtubes using 1064 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1054, 1010, 948, 614, 579, 454, 410.

**Source:** Shi et al. (2005).

**Comments:** The sample was characterized by powder X-ray diffraction data and energy dispersive X-ray spectral analysis.

**Natrosilite**  $\text{Na}_2\text{Si}_2\text{O}_5$ **Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 510.5 nm, 10 kHz pulsed copper vapor laser radiation with the laser radiation power at the sample of about 30 kW within a pulse.**Raman shifts (cm<sup>-1</sup>):** 1072s, ~1010w, ~955w, ~760w, 517s, ~470w, 384, 337, 270, 223, 149.**Source:** You et al. (2001).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of natrosilite see also Fleet and Henderson (1997).**Natrouranospinite**  $\text{Na}_2(\text{UO}_2)_2(\text{AsO}_4)_2 \cdot 5\text{H}_2\text{O}$ **Origin:** Měděnec deposit, the Krušné Hory (Ore Mts.), northern Bohemia, Czech Republic.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3493, (3450), 3404, 3260sh, 1136, 1008s, (904w), 893, 816s, (810), 671, 621, 579w, 494, 461, 415s, 400sh, 322, 267, (245), 209sh, (199), 188s, 156sh, 148, (140), 110.**Source:** Čejka et al. (2009c).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.**Natroxalate**  $\text{Na}_2(\text{C}_2\text{O}_4)$ **Origin:** Alluaiv Mt., Lovozero massif, Kola Peninsula, Russia.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 1750, 1643, 1614, 1456s, 1358s, 884, 875, 567, 481, 221, 156, 117.**Source:** Frost (2004d).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of natroxalate see also Frost and Weier (2003) and Frost et al. (2003k).**Natrozippeite**  $\text{Na}_5(\text{UO}_2)_8(\text{SO}_4)_4\text{O}_5(\text{OH})_3 \cdot 12\text{H}_2\text{O}$ **Origin:** Mecsek Mountains, Hungary.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1239, 1137, 1099w, 1009, 825s, 665w, 461, 409, 273.**Source:** Stefaniak et al. (2009).**Comments:** The sample was characterized by electron microprobe analysis. For the Raman spectra of natrozippeite see also Frost et al. (2007f) and Driscoll et al. (2014).

**Naumannite** Ag<sub>2</sub>Se**Origin:** Synthetic.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 141.**Source:** Ge and Li (2003).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.**Nealite** Pb<sub>4</sub>Fe(AsO<sub>3</sub>)<sub>2</sub>Cl<sub>4</sub>·2H<sub>2</sub>O**Origin:** Lavrion, Greece.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3451, 3431, 3387w, 3357sh, 3215m 2892w, 2849w, 1015w, 831w, 732, 808s, 632, 604sh, 548, 471, 418sh, 393, 371sh, 342sh, 320, 299sh, 245, 212, 194sh, 183sh, 160sh, 149s, 137, 129sh, 119.**Source:** Frost and Bahfenne (2011a).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of nealite see also Bahfenne (2011).**Negevite** NiP<sub>2</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on nanoparticles using 532 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 454, 586s.**Source:** Zhuo et al. (2015).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.**Neighborite** NaMgF<sub>3</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed in the geometry y(zz)-y. Characteristics of laser radiation are not indicated.**Raman shifts (cm<sup>-1</sup>):** ~230s, ~212w, ~187s, ~140, ~130sh, ~105.**Source:** Oçafrain et al. (1996).**Comments:** The sample was characterized by optical methods.**Nekoite** Ca<sub>3</sub>Si<sub>6</sub>O<sub>15</sub>·7H<sub>2</sub>O**Origin:** Iron Cap Mine, near Klondyke, Cochise Co., Arizona, USA.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts

have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** (3567), 3502, 3380sh, 3071sh, 2810sh, (1647), 1623, 1567sh, 1132sh, 1092s, 1061s, 1023, 994sh, 974, 774, 661s, (560), 588s, 525, 437, 416sh, 398, 362sh, 345, 303, 287, (259), 240, 198, 180, 156, 136, 106w.

**Source:** Frost and Xi (2012n).

**Comments:** No independent analytical data are provided for the sample used.

### Nenadkevichite (Na, $\square$ )<sub>8</sub>Nb<sub>4</sub>(Si<sub>4</sub>O<sub>12</sub>)<sub>2</sub>(O,OH)<sub>4</sub>·8H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The output laser radiation power was 25 mW.

**Raman shifts (cm<sup>-1</sup>):** 940w, 878w, 668s, ~500w, ~480w, 226s.

**Source:** Rocha et al. (1996).

**Comments:** A sample with the Ti:Nb molar ratio of 0.8 was used. The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of nenaskevichite see also Rocha et al. (1996).

### Nepheline NaAlSiO<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 488 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 600 mW. A 90°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1081, 984, 973, 690w, 616w, 497, 469, 427s, 399s, 331, 264, 214, 151, 138w, 123.

**Source:** Matson et al. (1986).

**Comments:** No independent analytical data are provided for the sample used.

### Nesquehonite Mg(CO<sub>3</sub>)·3H<sub>2</sub>O

**Origin:** A natural sample. The locality is not indicated.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 2905w, 1890w, 1708w, 1515w, 1428w, 1100s, 772w, 703w, 344w, 311w, 273w, 228, 199, 187, 119.

**Source:** Edwards et al. (2005).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of nesquehonite see also Coleyshaw et al. (2003), Kloprogge et al. (2003), and Kristova et al. (2014).

### Nestolaite CaSeO<sub>3</sub>·H<sub>2</sub>O

**Origin:** Little Eva mine, Grand County, Utah, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm diode laser radiation. The laser radiation power at the sample was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 1680w, 825s, 750s, 470w, 405w, 360w.

**Source:** Kasatkin et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### Newberryite $\text{Mg}(\text{PO}_3\text{OH}) \cdot 3\text{H}_2\text{O}$

**Origin:** Lava Cave, Skipton, Victoria, Australia (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3514, 3479, 3456, 3381, 3265, 3181, 2880, 1648, 1620, 1272, 1195, 1154, 984s, 967, 893, 555, 498, 400, 369, 327, 283, 266, 244, 219, 199, 180, 158, 139.

**Source:** Frost et al. (2005j).

**Comments:** No independent analytical data are provided for the sample used.

### Nežilovite $\text{PbZn}_2\text{Mn}^{4+}_2\text{Fe}^{3+}_8\text{O}_{19}$

**Origin:** “Mixed series” metamorphic complex, near the Nežilovo village, 40 km SW of Veles, Pelagonian massif, Macedonia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** Raman shifts of presumed nežilovite given in the cited paper (*i. e.* 1099s, 725w, 483w, 340w, 300, 176) correspond to associated dolomite.

**Source:** Stamatovska et al. (2011).

### Nickelaustinite $\text{CaNi}(\text{AsO}_4)(\text{OH})$

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3344, 3320, 917, 828s, 811, 799, 777, 495, 475s, 430s, 398, 369, 348s, 332, 216, 164, 147.

**Source:** Martens et al. (2003c).

**Comments:** No independent analytical data are provided for the sample used.

### Nickelbischofite $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed at 80 K on oriented single crystal using Kr<sup>+</sup> laser radiation. The laser radiation power is not indicated. Polarized spectra were collected in different scattering geometries.

**Raman shifts (cm<sup>-1</sup>):** 3503, 3424, 3411, 3371, 3160, 1671, 1623, 869, 699, 685, 571, 543, 372, 362.

**Source:** Agulló-Rueda et al. (1987).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of nickelbischofite see also Cariati et al. (1989).

#### Nickelboussingaultite $(\text{NH}_4)_2\text{Ni}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$

**Origin:** Cameron, Coconino Co., Arizona, USA.

**Experimental details:** Micro-Raman scattering measurements have been performed on a fine-grained sample using 785 nm diode laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3280w, 2940w, 1660w, 1460w, 1149w, 1093w, 1063w, 1027, 990s, 652w, 624w, 602w, 482w, 457, 440w, 341w, 312w, <240.

**Source:** Culka et al. (2009).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts have been partly determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

#### Nickelhexahydrite $\text{Ni}(\text{SO}_4) \cdot 6\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 253.65 nm radiation of mercury. The radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3441s, 3403s, 3302, 3250, 1131, 1088, 1050w, 987s, 971w, 639, 620, 596.

**Source:** Krishnamurti (1958).

**Comments:** The sample was characterized by optical methods.

#### Nickeline NiAs

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation at a power below 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 218, 154

**Source:** Watté et al. (1994).

**Comments:** The sample was characterized by powder X-ray diffraction data.

#### Nickelpicromerite $\text{K}_2\text{Ni}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 253.65 nm radiation of mercury. The incident light was normal to the (110) face and the scattered light was taken parallel to the (110) face and roughly perpendicular to the (001) face. The radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3310s, 3234, 3148, 3050–3540, 1230w, 1155, 1127, 1113, 1085s, 990s, 910w, 845w, 800w, 634, 611, 462, 448, (374), 320sh, 305w, 269w, 225, (184), 132sh, 115, (93w), 74sh, 62, 46.

**Source:** Ananthanarayanan (1961).

**Comments:** The sample was characterized by morphological features.

**Nierite hexagonal polyborph**  $\beta\text{-Si}_3\text{N}_4$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented polycrystalline sample using 488 nm laser radiation. The laser radiation power at the sample was 50 mW.**Raman shifts (cm<sup>-1</sup>):** 1045, 937, 927, 863, 730w, 618w, 525s, 449w, 227, 206, 183.**Source:** Muraki et al. (1997).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of  $\beta\text{-Si}_3\text{N}_4$  see also Honda et al. (1999).**Nifontovite**  $\text{Ca}_3[\text{BO}(\text{OH})_2]_6 \cdot 2\text{H}_2\text{O}$ **Origin:** Fuka Mine, Okayama Prefecture, Japan.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was about 20 mW.**Raman shifts (cm<sup>-1</sup>):** 3650w, 3611s, 3575s, 3434s, 3393, 3311, 3217sh, 3177s, 1607w, 1235w, 1208w, 1186w, 1154w, 1122w, 1030w, 991w, 932w, 918w, 896w, 831w, 806w, 749sh, 720, 653s, 633sh, 574w, 558w, 543w, 441w, 420, 391w, 371w, 348w, 322w, 306, 275w, 262sh, 225w, 213w, 190w, 171w, 140w, 123.**Source:** Bermanec et al. (2010).**Comments:** The sample was characterized by powder X-ray diffraction and thermal data.**Nimite**  $(\text{Ni},\text{Mg},\text{Al})_6(\text{Si},\text{Al})_4\text{O}_{10}(\text{OH})_8$ **Origin:** Bon Accord, Barberton, South Africa.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 3645, 678, 547, 279, 196.**Source:** Villanova-de-Benavent et al. (2014).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.**Niningerite** MgS**Origin:** Meteorite Sahara 97158.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 2 mW.**Raman shifts (cm<sup>-1</sup>):** ~280s, ~220.**Source:** Avril et al. (2013).**Comments:** Fe,Mn-bearing sample with the formula  $(\text{Mg}_{0.73}\text{Fe}_{0.16}\text{Mn}_{0.11})\text{S}$  was used.**Nioboholtite**  $(\text{Nb}_{0.6}\square_{0.4})\text{Al}_6\text{BSi}_3\text{O}_{18}$ **Origin:** Szklary pegmatite, Lower Silesia, Poland (type locality).**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was about 5.5 mW.

**Raman shifts (cm<sup>-1</sup>):** ~1110, ~1045, ~965sh, ~945s, ~895sh, ~710w, ~612, ~555s, ~507s, ~460, ~420, ~380, ~270w, ~205w.

**Source:** Pieczka et al. (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

### Niter K(NO<sub>3</sub>)

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power was between 80 and 200 mW.

**Raman shifts (cm<sup>-1</sup>):** 1359, 1345, 1050s.

**Source:** Rissom et al. (2008).

**Comments:** No independent analytical data are provided for the sample used.

### Nitratine Na(NO<sub>3</sub>)

**Origin:** Dolomite Cave of Pozalagua, Karrantza, Basque Co., northern Spain.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm diode laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** See comment below.

**Source:** Martínez-Arkarazo et al. (2007).

**Comments:** In the cited paper Raman spectra of nitratine-bearing polymimetal samples are given. Raman shifts of pure nitratine are: 1066s, 725, 185s (see RRUFF ID R050394, for an unoriented sample).

### Nitrobarite Ba(NO<sub>3</sub>)<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 785 nm diode laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1631w, 1402w, 1045s, 1025w, 729.

**Source:** Maguregui et al. (2008).

**Comments:** No independent analytical data are provided for the sample used.

### Nitrocalcite Ca(NO<sub>3</sub>)<sub>2</sub>·4H<sub>2</sub>O

**Origin:** Dolomite Cave of Pozalagua, Karrantza, Basque Co., northern Spain.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm diode laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** See comment below.

**Source:** Martínez-Arkarazo et al. (2007).

**Comments:** In the cited paper Raman spectra of nitrocalcite-bearing polymimetal samples are given. Raman shifts of pure nitratine are: 1067s, 740, 282w, ~195 (RRUFF ID R120047, for an unoriented sample, with 780 nm radiation).

**Nitromagnesite**  $Mg(NO_3)_2 \cdot 6H_2O$ **Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 785 or 514 nm laser radiation. The nominal laser radiation power was 350 or 50 mW.**Raman shifts (cm<sup>-1</sup>):** 1059s.**Source:** Morillas et al. (2016).**Comments:** No independent analytical data are provided for the sample used.**Nobleite**  $CaB_6O_9(OH)_2 \cdot 3H_2O$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a sample held in a pyrex tube using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 300 mW.**Raman shifts (cm<sup>-1</sup>):** 996w, 956w, 855s, 745, 636, 572w, 460, 383.**Source:** Jun et al. (1995).**Comments:** The sample was characterized by chemical analyses.**Noelbensonite**  $BaMn^{3+} _2Si_2O_7(OH)_2 \cdot H_2O$ **Origin:** Postmasburg manganese field, Northern Cape Province, South Africa.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 925s, 904, 650, 572, 523s, 436, 386, 331w, 304w, 245, 185, 160.**Source:** Costin et al. (2015).**Comments:** The sample was characterized by electron backscatter diffraction and electron microprobe analyses.**Nolanite**  $(V^{3+}, Fe^{3+}, Fe^{2+})_{10}O_{14}(OH)_2$ **Origin:** Vihanti, Northern Ostrobothnia region, Finland.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 633 nm He-Ne laser radiation. The nominal laser radiation power was 2 or 20 mW.**Raman shifts (cm<sup>-1</sup>):** 587, 504, 478, 323w, 293w, 221s, 85s.**Source:** Voloshin et al. (2014).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.**Nontronite**  $Na_{0.3}Fe^{3+} _2(Si, Al)_4O_{10}(OH)_2 \cdot nH_2O$ **Origin:** No data.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632.8 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~3575s, ~3410, ~890, ~810w, ~760w, ~680, ~570w, ~520, ~420, ~360, ~290s, ~240s.

**Source:** Wang et al. (1998a).

**Comments:** No independent analytical data are provided for the sample used.

### Norbergite Mg<sub>3</sub>(SiO<sub>4</sub>)F<sub>2</sub>

**Origin:** Franklin Limestone quarry, Franklin, Sussex Co., New Jersey, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3583, 3488, 979, 955, 900, (884w), 855s, 614, 572, 555s, 435s, 382.

**Source:** Frost et al. (2007k).

**Comments:** The sample was characterized by electron microprobe analysis. The empirical formula shows deficit of Mg+Fe.

### Nordenskiöldine CaSn(BO<sub>3</sub>)<sub>2</sub>

**Origin:** Gejiu tin deposit, Yunnan, China.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 458 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 120 mW.

**Raman shifts (cm<sup>-1</sup>):** 1453w, 1205s, 944w, 847w, 764, 743, 449s, 389, 277, 214w.

**Source:** Li et al. (1994).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

### Nordstrandite Al(OH)<sub>3</sub>

**Origin:** Gunong Kapor, Bau mining district, West Sarawak, Borneo.

**Experimental details:** Raman scattering measurements have been performed on grains placed on glass slide using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 25 mW.

**Raman shifts (cm<sup>-1</sup>):** 3623, 3567s, 3523w, 3490, 3349, 1093, 985, 959w, 898, 657, (633w), 596, 542s, 507, 492, 464w, 437w, 412, 390, 378, (355w), (344w), 305s, 286, (267w), 252, 228w, 177, 119s.

**Source:** Rodgers (1993).

**Comments:** The sample was identified by Raman spectrum only. No independent analytical data are provided for the sample used.

### Normandite Na<sub>2</sub>Ca<sub>2</sub>(Mn,Fe)<sub>2</sub>(Ti,Nb,Zr)<sub>2</sub>(Si<sub>2</sub>O<sub>7</sub>)<sub>2</sub>O<sub>2</sub>F<sub>2</sub>

**Origin:** Partomchorr Mt., Khibiny Massif, Kola Peninsula, Russia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 813s, 803, 782, 748s, 724, 667sh, 656, (649), 641sh, 520sh, 513s, (505), 477, 454, 412w, 404sh, 382w, 371w, 361w, (352w), 285, 267s, (259), 198, 179, 151s, 141, 125, 109.

**Source:** Frost et al. (2015p).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

### Norsethite BaMg(CO<sub>3</sub>)<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 488 or 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 200 mW.

**Raman shifts (cm<sup>-1</sup>):** 1115s, 695, 260, 130.

**Source:** Scheetz and White (1977).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of norsethite see also Schmidt et al. (2013) and Effenberger et al. (2014).

### Northupite Na<sub>3</sub>Mg(CO<sub>3</sub>)<sub>2</sub>Cl

**Origin:** Searles Lake, California, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1554, 1115s, 1107sh, 714w, 250, 213, 180, 148.

**Source:** Frost and Dickfos (2007a).

**Comments:** No independent analytical data are provided for the sample used.

### Nosean Na<sub>8</sub>(Si<sub>6</sub>Al<sub>6</sub>)O<sub>24</sub>(SO<sub>4</sub>)·H<sub>2</sub>O

**Origin:** Laacher See (Laach Lake) volcano, Eifel, Germany.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~1060, ~980s, ~630, ~605w, ~530, ~435.

**Source:** Hettmann et al. (2012).

**Comments:** No independent analytical data are provided for the sample used.

### Nováčekite-II Mg(UO<sub>2</sub>)<sub>2</sub>(AsO<sub>4</sub>)<sub>2</sub>·10H<sub>2</sub>O

**Origin:** Wheal Edward, St. Just, Cornwall, UK.

**Experimental details:** Methods of sample preparation are not indicated. Raman scattering measurements have been performed using 785 nm laser radiation. The nominal laser radiation power at the source was ~370 mW.

**Raman shifts (cm<sup>-1</sup>):** The strongest band is observed at 817 cm<sup>-1</sup>. Other Raman shifts are not indicated.

**Source:** Driscoll et al. (2014).

**Comments:** The sample was characterized by electron microprobe analysis.

**Novgorodovaite**  $\text{Ca}_2(\text{C}_2\text{O}_4)\text{Cl}_2 \cdot 2\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm solid-state laser radiation. The nominal laser radiation power was 10 mW.**Raman shifts (cm<sup>-1</sup>):** 3350sh, 3330s, 1717w, 1630w, 1477s, 1402w, 904s, 859s, 730w, 673w, 600w, 503s, 472s.**Source:** Piro et al. (2017).**Comments:** The sample was characterized by powder X-ray diffraction data.**Nsutite**  $\text{Mn}^{2+}_x\text{Mn}^{4+}_{1-x}\text{O}_{2-2x}(\text{OH})_{2x}$ **Origin:** No data.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 10 mW.**Raman shifts (cm<sup>-1</sup>):** 732, 634, 572, 515, 458, 382, 280.**Source:** Julien et al. (2004).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of nsutite see also Julien et al. (2003).**Nullagine**  $\text{Ni}_2(\text{CO}_3)(\text{OH})_2$ **Origin:** Otway Prospect, Nullagine district, Western Australia, Australia (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3506w, 1734w, (1441w), 1426, (1092), 1089s, 742, 528, 342s, 232**Source:** Frost (2006).**Comments:** Raman spectrum of presumed nullagine was published also by Frost et al. (2008I). However IR spectra of presumed nullagine published in this paper are wrong: the strongest bands correspond to a serpentine-type silicate.**Nyerereite**  $\text{Na}_2\text{Ca}(\text{CO}_3)_2$ **Origin:** Oldoinyo Lengai volcano, Tanzania (type locality).**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 20 mW.**Raman shifts (cm<sup>-1</sup>):** 1086s, 1078sh, 1001w, 723–725sh, 709, 682–684sh.**Source:** Golovin et al. (2015).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectra of nyerereite see also Kaminsky et al. (2009), Zaitsev et al. (2009), Golovin et al. (2014), and Shatskiy et al. (2015).

**Offretite**  $\text{KCaMg}(\text{Si}_{13}\text{Al}_5)\text{O}_{36} \cdot 15\text{H}_2\text{O}$ **Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 20 mW.**Raman shifts (cm<sup>-1</sup>):** 788w, 480s, 330.**Source:** Croce et al. (2013).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of offretite see also Mozgawa (2001).**Okenite**  $\text{Ca}_{10}\text{Si}_{18}\text{O}_{46} \cdot 18\text{H}_2\text{O}$ **Origin:** Pune (Poonah) district, Maharashtra, India.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** (3607), 3531, 3417, (3284), 3029w, 1631w, 1180, 1125sh, 1090s, (1075), 1048w, 1024, (1014), 973, 943, 801, 668, 651, 617, (603), (581), 569, 515, 496sh, 445, 423, 403, 385, 352, 302, 254, 228, 211sh, 190, 155sh, 133.**Source:** Frost and Xi (2012n).**Comments:** No independent analytical data are provided for the sample used.**Oldhamite** CaS**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 20 mW.**Raman shifts (cm<sup>-1</sup>):** ~485, ~350s, ~285s, ~215, 185, 160.**Source:** Avril et al. (2013).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.**Olgite**  $(\text{Ba},\text{Sr})(\text{Na},\text{Sr},\text{REE})_2\text{Na}(\text{PO}_4)_2$ **Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power was 50 mW.**Raman shifts (cm<sup>-1</sup>):** 1100w, 1001w, 952s, 608, 570, 423, 86.**Source:** Huang et al. (2007).**Comments:** The Raman spectrum was obtained for a Ce<sup>3+</sup>-doped sample. The sample was characterized by powder X-ray diffraction data.

**Olivenite** Cu<sub>2</sub>(AsO<sub>4</sub>)(OH)**Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 20 mW. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 854s, 818, 514, 498, 424w, 345w, 311, 284, 220, 184w, 157, 116, 95, 82, 67.**Source:** Majzlan et al. (2015).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of olivenite see also Yang et al. (2001), Frost et al. (2002e, 2009i), and Martens et al. (2003b).**Olivine P-rich variety** (Fe,Mg)<sub>2-x</sub>(SiO<sub>4</sub>,PO<sub>4</sub>)**Origin:** Prehistoric slag from Goldbichl, Igls, Tyrol, Austria.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm He-Ne laser radiation. The nominal laser radiation power was 170 mW.**Raman shifts (cm<sup>-1</sup>):** 1096, 1049, 975, 936s, 832+822s (unresolved doublet?), 725, 680, 631, 582, 561, 510, 457, 405, 368, 331, 291, 228, 163, 113.**Source:** Schneider et al. (2013).**Comments:** The sample was characterized by electron microprobe analyses. The contents of P and Fe are from 0.36 to 0.54 and from 0.77 to 1.08 atoms per formula unit, respectively.**Olmiite** CaMn[SiO<sub>3</sub>(OH)](OH)**Origin:** N'Chwaning II mine, Kalaharimanganese fields, South Africa (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** (3550), 3543, 3511, 3467sh, 2807, (064w), 953, 914w, 853s, 811, 799sh, 782sh, 726w, 513, 484, 436, 420, 400, 378w, 335.**Source:** Frost et al. (2013o).**Comments:** The sample was characterized by electron microprobe analysis.**Olshanskyite** Ca<sub>2</sub>[B<sub>3</sub>O<sub>3</sub>(OH)<sub>6</sub>]OH·3H<sub>2</sub>O**Origin:** Fuka mine, Okayama prefecture, Japan.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3621, 3536, 3482s, (3440), 3373, 3240, 3100sh, 2919, 1365w, 1206w, 1141w, 1069, 1025sh, (1014), 1003, 989, (976), 961, (919), 850sh, (696), 679s, (658), 579w, 516w, 463, 448w, 388w, 345, (335), 330, 322, 315, (303).**Source:** Frost et al. (2014ak).**Comments:** No independent analytical data are provided for the sample used.

**Omongwaite**  $\text{Na}_2\text{Ca}_5(\text{SO}_4)_6 \cdot 3\text{H}_2\text{O}$ 

**Origin:** A recent salt lake deposit at Omongwa pan, Namibia (type locality).

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 3527w, 1143, 1013s, 665w, 637, 608w, 476, 436w,

**Source:** Mees et al. (2008).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectra of omongwaite see also Tong et al. (2011).

**Omphacite**  $(\text{Ca},\text{Na})(\text{Mg},\text{Fe},\text{Al})\text{Si}_2\text{O}_6$ 

**Origin:** Uru River area (?), north-central Myanmar.

**Experimental details:** Raman scattering measurements have been performed on an oriented grain in a polished sample using 532 nm laser radiation, with laser beam parallel to the *b* axis. The nominal laser radiation power was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 1016, 684s, 567, 382, 144, 76.

**Source:** Leander et al. (2014).

**Comments:** The sample was characterized by electron microprobe analysis. For the Raman spectra of omphacite see also Buzatu and Buzgar (2010), and Andò and Garzanti (2014).

**Onoratoite**  $\text{Sb}_8\text{O}_{11}\text{Cl}_2$ 

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** ~477s, ~456s, ~430, ~372, ~325, ~225sh, ~205, ~195, and a series of weak bands below 190 cm<sup>-1</sup>.

**Source:** Orman et al. (2008), Orman (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Opal-A**  $\text{SiO}_2 \cdot n\text{H}_2\text{O}$ 

**Origin:** No data.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 1064 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~3460, 410s.

**Source:** Kiefert and Karampelas (2011).

**Comments:** No independent analytical data are provided for the sample used.

**Opal-CT**  $\text{SiO}_2 \cdot n\text{H}_2\text{O}$ 

**Origin:** No data.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 1064 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~3450, 335s.

**Source:** Kiefert and Karampelas (2011).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of opal-CT see also Ilieva et al. (2007) and Wilson (2014).

**Ophirite** Ca<sub>2</sub>Mg<sub>4</sub>[Zn<sub>2</sub>Mn<sup>3+</sup><sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>(Fe<sup>3+</sup>W<sub>9</sub>O<sub>34</sub>)<sub>2</sub>]:46H<sub>2</sub>O

**Origin:** Ophir Hill Consolidated mine, Ophir district, Oquirrh Mts., Tooele Co., Utah, USA (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power at the sample was between 0.5 and 5 mW.

**Raman shifts (cm<sup>-1</sup>):** ~955s, ~920sh, ~850, ~335w, ~220w.

**Source:** Kampf et al. (2014b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Oppenheimerite** Na<sub>4</sub>(UO<sub>2</sub>)(SO<sub>4</sub>)<sub>3</sub>·3H<sub>2</sub>O

**Origin:** Blue Lizard mine, San Juan Co., Utah, USA (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3526, 3400, 3218, ~1600w, 1215w, 1156w, 1060w, 1013, 1002, 986, 970s, 841s, 825sh, 651w, 603w, 459, 378sh, 345sh, 207, 188, 163, 153, 132, 110, 55.

**Source:** Kampf et al. (2015c).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Ordoñezite** ZnSb<sup>5+</sup><sub>2</sub>O<sub>6</sub>

**Origin:** Synthetic.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 830w, 798w, 748s, 730, 670s, 615, 570sh, 538s, 480w, 364w, 331sh, 323, 300sh, 292, 248sh, 261, 220w.

**Source:** Husson et al. (1979).

**Comments:** No independent analytical data are provided for the sample used.

**Orpiment** As<sub>2</sub>S<sub>3</sub>

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 379w, 364sh, 352s, 308s, 291, 200w, 178w, 153, 143w, 135w.

**Source:** Minceva-Sukarova et al. (2003).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of orpiment see also Forneris (1969), Trentelman et al. (1996), Burgio and Clark (2001), Frost et al. (2010c), and Kampf et al. (2011a).

### Orschallite $\text{Ca}_3(\text{S}^{4+}\text{O}_3)_2(\text{SO}_4)\cdot 12\text{H}_2\text{O}$

**Origin:** Hannebacher Ley volcano, Eifel, Germany (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3383, 1215w, 1096, (1011), 1005s, 984, 971sh, (657), 651, 532sh, 521, 492, 441, 244, 194, 173, 145, 119.

**Source:** Frost and Keeffe (2009d).

**Comments:** No independent analytical data are provided for the sample used.

### Orthoclase $\text{K}(\text{AlSi}_3\text{O}_8)$

**Origin:** Bahariya depression, Western Desert, Egypt.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was between 20 and 200 mW.

**Raman shifts (cm<sup>-1</sup>):** ~1125, ~750w, ~650, ~640, ~590, 515s, 475s, 453, ~403, 282.

**Source:** Ciobotă et al. (2012).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of orthoclase see also Frezzotti et al. (2012) and Culka et al. (2016a).

### Orthojoaquinite-(Ce) $\text{NaBa}_2\text{Fe}^{2+}\text{Ce}_2\text{Ti}_2(\text{SiO}_3)_8\text{O}_2(\text{O},\text{OH})\cdot\text{H}_2\text{O}$

**Origin:** Benitoite Gem Mine, San Benito Co., California, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3574sh, 3558, (3515), 3506, 3444sh, 3397, 3344+3317 (unresolved doublet?), 3230w, 3192w, 1112, 1033, 982, 956, 933, 896s, 732, 687sh, 668, 636, 600, 526, 494, 511, 375, 358, 304, 267, (202), 191, (165), 145, 112.

**Source:** Frost and Pinto (2007).

**Comments:** No independent analytical data are provided for the sample used.

### Osakaite $\text{Zn}_4(\text{SO}_4)(\text{OH})_6\cdot 5\text{H}_2\text{O}$

**Origin:** Block 14 Opencut, Broken Hill, New South Wales, Australia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 632.8 He-Ne laser radiation. The nominal laser radiation power was 17 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3633, 3550, 3510, 3455, 3330, 3257sh, 3243, 3175, ~1670w, ~1620w, 1160, 1112, 1051, 1024, 1011, 964s, 636, 604, 508, 456, 430, 398.

**Source:** Elliott (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### Osbornite TiN

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a coating deposited on silicon (111) substrate using He-Ne laser radiation. The nominal laser radiation power was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 563, 242.

**Source:** Barshilia and Rajam (2004).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of osbornite see also Spengler et al. (1978).

### Oskarssonite AlF<sub>3</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powder sample using 1064 nm Nd-YAG or 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was up to 400 mW or 10–25 mW, respectively.

**Raman shifts (cm<sup>-1</sup>):** 478w, 382w, 157s, 96.

**Source:** Groß et al. (2007).

**Comments:** For the Raman spectrum of oskarssonite see also Daniel et al. (1990).

### Osumilite KFe<sub>2</sub>(Al<sub>5</sub>Si<sub>10</sub>)O<sub>30</sub>

**Origin:** Rundvågshetta, Lützow-Holm Complex, East Antarctica.

**Experimental details:** Raman scattering measurements have been performed on a grain included within a garnet porphyroblast using 532 nm laser radiation. The nominal laser radiation power was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 1103, 920, 549, 477s, 383w, 350w, 281.

**Source:** Kawasaki et al. (2011).

**Comments:** The sample was characterized by electron microprobe analyses.

### Otavite Cd(CO<sub>3</sub>)

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 488 and 514.5 nm Ar<sup>+</sup> laser radiations. The nominal laser radiation power was in the range from 100 to 500 mW.

**Raman shifts (cm<sup>-1</sup>):** 1718, 1388, 1084s, 712, 271, 158.

**Source:** Rutt and Nicola (1974).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of otavite see also Minch et al. (2010) and Falgayrac et al. (2013).

**Ottemannite**  $\text{Sn}_2\text{S}_3$ **Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power at the sample was below 0.4 mW.**Raman shifts (cm<sup>-1</sup>):** 310s, 303sh, 247w, 231w, 67w, 56, 48.**Source:** Fontané et al. (2013)**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of ottemannite see also Price et al. (1999).**Ottensite**  $\text{Na}_3(\text{Sb}_2\text{O}_3)_3(\text{SbS}_3)\cdot 3\text{H}_2\text{O}$ **Origin:** Pereta mine, Tuscany, Italy.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 20 mW.**Raman shifts (cm<sup>-1</sup>):** 766w, 615w, 538, 479w, 355s, 344sh, 299, 254w, 225w, 153.**Source:** Bittarello et al. (2015).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.**Ottohahnite**  $\text{Na}_6(\text{UO}_2)_2(\text{SO}_4)_5(\text{H}_2\text{O})_7 \cdot 1.5\text{H}_2\text{O}$ **Origin:** Blue Lizard mine, San Juan Co., Utah, USA (type locality).**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** ~3595, ~3490w, ~1630w, ~1220, ~1200, ~1155, ~1050, ~1010, ~980, ~930, ~840s, ~655, ~203s, and a series of weak bands in the range from 300 to 640 cm<sup>-1</sup>.**Source:** Kampf et al. (2016g).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.**Otwayite**  $\text{Ni}_2(\text{CO}_3)(\text{OH})_2 \cdot \text{H}_2\text{O}$ **Origin:** Mt. Grey, Tasmania, Australia.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3612, (3610), 3579, 3538, 3470sh, (3288), (2989), 2935, 2879sh, 1690, 1600, 1353w, 1073s, (1068), 981s, 937, (835), 708, 703, 617, (545), 529, (469), 445, 395, 308sh, 232, 216, 194sh, 177sh.**Source:** Frost et al. (2006o).**Comments:** No independent analytical data are provided for the sample used.

**Oxammite**  $(\text{NH}_4)_2(\text{C}_2\text{O}_4)\cdot\text{H}_2\text{O}$ **Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3235, 3030, 2995, 2900, 2879, 2161, 1902, 1737, 1695s, 1605, 1473, 1451, 1447, 1430, 1417, 1312, 892s, 866, 815, 642, 489s, 438, 278, 224, 210, 198, 181, 160.**Source:** Frost and Weier (2003).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of oxammite see also Frost et al. (2003k), Frost (2004d), and Frost and Weier (2004a).**Oxycalcioroméite**  $\text{Ca}_2\text{Sb}^{5+}_2\text{O}_7$ **Origin:** Bucadella Vena mine, Apuan Alps, Tuscany, Italy (type locality).**Experimental details:** Methods of sample preparation are not described. Micro-Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 913w, 777, 666, 540sh, 509s, 426, 295, 199w.**Source:** Biagioni et al. (2013c).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.**Oxy-dravite**  $\text{Na}(\text{Al}_2\text{Mg})(\text{Al}_5\text{Mg})(\text{Si}_6\text{O}_{18})(\text{BO}_3)_3(\text{OH})_3\text{O}$ **Origin:** No data available.**Experimental details:** Raman scattering measurements have been performed on an oriented crystal with the crystallographic *c* axis parallel to the Cartesian coordinate *z* axis using 514.5 and 488.0 nm Ar<sup>+</sup> laser radiations. The laser radiation power at the sample was 14 mW. Raman spectrum was obtained in the spectral region from 15 to 4000 cm<sup>-1</sup>. Polarized spectrum was collected in the -y(zz) *y* scattering geometry.**Raman shifts (cm<sup>-1</sup>):** 3776w, 3738w, 3674w, 3642w, 3567+3529 (unresolved doublet?), (3480w), ~700, 368s, 312, 242, 217, and a series of relatively weak bands in the range from 400 to 700 cm<sup>-1</sup>.**Source:** Watenphul et al. (2016a, b).**Comments:** The sample was characterized by electron microprobe and LA-ICP-MS analyses.**Oxykinoshitalite**  $\text{BaMg}_2\text{Ti}^{4+}\text{O}_2(\text{Si}_2\text{Al}_2)\text{O}_{10}$ **Origin:** S. Demetrio High, Hyblean plateau, Sicily, Italy.**Experimental details:** Micro-Raman scattering measurements have been performed on a grain in thin section using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 6 mW.**Raman shifts (cm<sup>-1</sup>):** 996, 880, 725s, 135, 122.**Source:** Manuella et al. (2012).**Comments:** The sample was characterized by electron microprobe analyses.

### Oxynatromicrolite $(\text{Na,Ca,U})_2(\text{Ta,Nb})_2\text{O}_6(\text{O,F})$

**Origin:** Guanpo, Henan province, China (type locality).

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** ~3450sh, ~770, ~650s.

**Source:** Guang et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses, and differential thermal analysis.

### Oxyplumboroméite $\text{Pb}_2\text{Sb}^{5+}_2\text{O}_7$

**Origin:** Synthetic.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 532.0 nm Nd-YAG laser radiation. The laser radiation power at the sample was between 0.8 and 4 mW.

**Raman shifts (cm<sup>-1</sup>):** 807w, 513s, 423, 355, 298, 230s, 190, 107s.

**Source:** Rosi et al. (2009).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of oxyplumboroméite see also Kendix et al. (2008).

### Oyelite $\text{Ca}_{10}\text{B}_2\text{Si}_8\text{O}_{29}\cdot12\text{H}_2\text{O}$

**Origin:** N'Chwaning II mine, Manganese Fields, Kalahari desert, Republic of South Africa.

**Experimental details:** Methods of sample preparation are not described. Non-polarized micro-Raman spectrum has been obtained in a nearly backscattered geometry using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~1025, ~1005, ~990, ~910, ~860, ~715s, ~685s, ~460, ~350, ~320.

**Source:** Biagioni et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Ozokerite

**Origin:** Boryslav, Poland.

**Experimental details:** Kind of sample preparation is not indicated. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation with the nominal radiation power of 10 mW (micro-Raman measurements) and/or 1064 nm Nd-YAG laser radiation with the power of 350 mW.

**Raman shifts (cm<sup>-1</sup>):** 2977, 2961w, 2930w, 2923s, 2917s, 2901w, 2880s, 2855, 2848w, 2836, 2733w, 2724, 1498w, 1486w, 1466, 1442, 1420w, 1416w, 1387w, 1369w, 1349w, 1321w, 1297w, 1169w, 1154w, 1133s.

**Source:** Jehlička et al. (2007a).

**Comments:** No independent analytical data are provided for the sample used.

### Pabstite $\text{BaSnSi}_3\text{O}_9$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdery sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 994w, ~876w, ~817w, 574s.

**Source:** Takahashi et al. (2008).

**Comments:** The sample was characterized by powder X-ray diffraction data.

#### Padmaite PdBiSe

**Origin:** Southern Sopchinskoe deposit, Monchegorsk district, Kola Peninsula, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 235s, 177w, 154, 115, 91, 82, 61s, 52sh.

**Source:** Voloshin et al. (2015a).

**Comments:** The sample was characterized electron microprobe analyses.

#### Pakhomovskyite Co<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>·8H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1043, 1023, 956s, 894, 560, 462, 370w, 260, 249, 202, 171.

**Source:** Shao et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data.

#### Palermoite Li<sub>2</sub>SrAl<sub>4</sub>(PO<sub>4</sub>)<sub>4</sub>(OH)<sub>4</sub>

**Origin:** Palermo No. 1 mine, Groton, New Hampshire, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm solid-state laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1077, 1026s, 1005s, 982sh, 657, 637, 603s, 534, 512, 345, 417, 367w, 328, 282, 253, 238.

**Source:** Schumer et al. (2016).

**Comments:** No independent analytical data are provided for the sample used.

#### Palladinite PdO

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 18794.59 cm<sup>-1</sup> laser radiation. The laser radiation power at the sample was between 1 and 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 723w, 650s, 445.

**Source:** Bakker (2014).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of palladinite see also McBride et al. (1991).

**Palladosilicide** Pd<sub>2</sub>Si**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a thin film using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was  $\leq 10$  mW.**Raman shifts (cm<sup>-1</sup>):** 115s, 90.**Source:** Nemanich (1986).**Palygorskite** (Mg,Al)<sub>2</sub>Si<sub>4</sub>O<sub>10</sub>(OH)·4H<sub>2</sub>O**Origin:** Glasgow, Virginia, USA.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on randomly oriented crystals in back-scattering geometry, using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power was 900 mW.**Raman shifts (cm<sup>-1</sup>):** 1109, 988, 971, 809, 774, 680, 638, 556, 512, 488, 473, 437, 406, 354, 327, 268, 205, 183, 167, 130 (A<sub>g</sub> modes); 1211, 1160, 1077, 986, 904, 800, 704, 658, 597, 540, 512, 456, 435, 410, 397, 353, 327, 243, 216, 205, 157, 139 (B<sub>g</sub> modes). The strongest peaks are observed in the ranges 250–300 and 650–720 cm<sup>-1</sup>.**Source:** McKeown et al. (2002).**Comments:** The empirical formula of the sample used is (Mg<sub>2.00</sub>Al<sub>1.96</sub>Fe<sub>0.06</sub>)Si<sub>7.94</sub>O<sub>21</sub>·nH<sub>2</sub>O.**Panguite** (Ti,Al,Sc,Mg,Zr,Ca)<sub>1.8</sub>O<sub>3</sub>**Origin:** Allende meteorite (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented grain in a polished section using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was  $\sim 5$  mW.**Raman shifts (cm<sup>-1</sup>):** 405, 380s.**Source:** Ma et al. (2012c).**Comments:** The sample was characterized by electron backscatter diffraction data and electron microprobe analyses.**Panichiite** (NH<sub>4</sub>)<sub>2</sub>SnCl<sub>6</sub>**Origin:** Synthetic.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):**  $\sim 430$ s,  $\sim 330$ s,  $\sim 290$ ,  $\sim 265$ ,  $\sim 210$ ,  $\sim 193$ ,  $\sim 148$ ,  $\sim 122$ .**Source:** Podsiadlo et al. (2015).**Comments:** The sample was characterized by X-ray diffraction data. The crystal structure is solved.**Papagoite** CaCuAlSi<sub>2</sub>O<sub>6</sub>(OH)<sub>3</sub>**Origin:** Cornelia mine, Ajo, Pima Co., Arizona, USA (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3614sh, 3573s, (3567), 3545s, (3533), (3490), 3453, (3368), (1079), 1053, 986, 942w, 867, 830sh, 812, 755, (644w), 630, 573, 536, 472sh, 460s, 438sh, 419s, 382, 298, 279, 264, 251, 243sh, 236sh, 205, (199), 185sh, 178, 170sh, 163, 156w, 150w, 147sh, 136, 131sh, 119, 113sh, 107.

**Source:** Frost and Xi (2013d).

**Comments:** No independent analytical data are provided for the sample used.

**Parabutlerite**  $\text{Fe}^{3+}(\text{SO}_4)(\text{OH}) \cdot 2\text{H}_2\text{O}$

**Origin:** Alcaparrosa mine, Cerritos Bayos, Calama, El Loa province, Antofagasta, Chile (type locality).

**Experimental details:** Methods of sample preparation are not described. Polarized Raman spectra have been obtained using 633 nm He-Ne laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3504sh, 3316, 3200sh, (3133), 1202, 1164, 1109s, (1095), 1044, 1026s, 1014, 990sh, 655sh, 614, 550, 468s, 406, 368, 263sh, 237, 214, 186, 155sh.

**Source:** Čejka et al. (2011b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Paracoquimbite**  $\text{Fe}^{3+}(\text{SO}_4)_3 \cdot 9\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3577, 3412, 3245, 3046, 1682, 1620, 1200, 1170, 1112, 1093, 1037, 1025s, 1012, 877, 675, 628, 602, 514, 502, 478, 286, 211.

**Source:** Ling and Wang (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Paragonite**  $\text{NaAl}_2(\text{Si}_3\text{Al})\text{O}_{10}(\text{OH})_2$

**Origin:** Rebra II Formation, Rodnei Mts., Eastern Carpathians, Romania.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power at the sample was 35 mW.

**Raman shifts (cm<sup>-1</sup>):** 911, 704, 612, 442s, 266, 217w.

**Source:** Buzgar (2008).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of paragonite see also Tlili et al. (1989), Graeser et al. (2003), and Frezzotti et al. (2012).

**Paraguanajuatite**  $\text{Bi}_2\text{Se}_3$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a crystal with the trigonal *c* axis parallel to the laser beam direction using 514.5 nm Ar<sup>+</sup> laser and 647.1 nm Kr<sup>+</sup> laser

radiations. The laser radiation power is not indicated. A 180°-scattering geometry was employed. Polarized spectra were collected in  $z(xx)$ -z and  $z(xy)$ -z scattering geometries.

**Raman shifts (cm<sup>-1</sup>):**  $z(xx)$ -z ( $A_{1g}$ ): 175, 72;  $z(xy)$ -z ( $E_g$ ): 132.

**Source:** Richter et al. (1977).

### Parahopeite $Zn_3(PO_4)_2 \cdot 4H_2O$

**Origin:** Reaphook Hill, Martins Well, Flinders Ranges, South Australia, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals in the spectral range from 700 to 4000 cm<sup>-1</sup> using a 633 nm He-Ne laser. The laser radiation power at the sample was 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3439sh, 3293, 3163, 3027, 1053, 1033, 1003s, 959.

**Source:** Frost (2004a).

**Comments:** No independent analytical data are provided for the sample used.

### Paramontroseite $VO_2$

**Origin:** Product of heating of karelianite from Pyrrhotite gorge, Khibiny massif by the laser beam.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 633 nm He-Ne laser radiation. The nominal laser radiation power was 2 or 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 991, 897w, 688, 405, 281, 222, 190, 139s, 98.

**Source:** Voloshin et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

### Paranatrolite $Na_2(Si_3Al_2)O_{10} \cdot 3H_2O$

**Origin:** Poudrette (Demix) quarry, Mont Saint-Hilaire, Rouville RCM (Rouville Co.), Montérégie, Québec, Canada.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** ~3465w, ~1095w, ~527s, ~430, ~330, ~135s.

**Source:** Belitsky et al. (1992).

**Comments:** No independent analytical data are provided for the sample used.

### Paraotwayite $Ni(OH)_{2-x}(SO_4,CO_3)_{0.5x}$

**Origin:** Otway deposit, Western Australia, Australia (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3606sh, 3590, 3568, (3566), 3532, 2909w, 2852w, 1115, 987s, (977), 642w, 606, 487, 473, 451, 416, 297w, (260), (238), (218), (196), (176).

**Source:** Frost et al. (2006o).

**Comments:** No independent analytical data are provided for the sample used.

**Parapierrotite**  $TlSb_5S_8$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a single crystal with the laser polarization parallel to the *b*- and *c*-axes using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 1.7 mW.**Raman shifts (cm<sup>-1</sup>):** 334, 321, 310 (very strong for  $E \parallel b$ ), 293, 275w, 260w, 242, 227 (very weak for  $E \parallel b$ ), 204w, 178w, 162w, 145w, 127, 115w, 106w, 94w, 94, 81, 62, 51 (strong for  $E \parallel c$ ), 41.**Source:** Kharbish (2011).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of parapierrotite see also Makreski et al. (2013b, 2014).**Pararealgar**  $As_4S_4$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 647.1 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 383w, 370w, 364, 346, 334, 340sh, 322w, 316w, 275, 236s, 230s, 204, 198, 191w, 175, 172, 167sh, 158, 152, 142, 135w, 118, 52sh, 45, 32.**Source:** Muniz-Miranda et al. (1996).**Comments:** For the Raman spectra of pararealgar see also Trentelman et al. (1996) and Burgio and Clark (2001).**Pararobertsite**  $Ca_2Mn^{3+}_3(PO_4)_3O_2 \cdot 3H_2O$ **Origin:** Tip Top mine, Custer, South Dakota, USA (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 780 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** ~1197w, ~1112w, ~1042, ~1035, ~983, ~965, ~953sh, ~896w, ~623s, ~547w, ~498w, ~461, ~403, ~365w, ~309, ~277, ~258.**Source:** Andrade et al. (2012).**Comments:** The sample was characterized by powder X-ray diffraction data.**Parascholzite**  $CaZn_2(PO_4)_2 \cdot 2H_2O$ **Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power at the sample was 1 mW.**Raman shifts (cm<sup>-1</sup>):** 1170, 1115, 1086, 999, 925s, 553s, 409, 302, 286, 271, 236.**Source:** Scholz et al. (2013a).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of parascholzite see also Frost (2004a).**Parascorodite**  $Fe^{3+}(AsO_4) \cdot 2H_2O$ **Origin:** Kaňk (near Kutná Hora) or Lehnschafter gallery in Mikulov (near Teplice), both Czech Republic.

**Experimental details:** Methods of sample preparation are not described. Micro-Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was between 1 and 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 892, 859, 815s, 800sh, 782s, 492, 458sh, 437s, 413sh, 382w, 349sh, 337, 292sh, 280, 269sh, 245, 231w, 181s, 164sh.

**Source:** Culka et al. (2016b).

**Comments:** The sample was characterized by powder X-ray diffraction data. Additionally, in the cited paper Raman spectra of parascorodite obtained with 785 and 532 nm lasers are given.

### Parasibirskite Ca<sub>2</sub>B<sub>2</sub>O<sub>5</sub>·H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powder sample was first pressed into a tablet using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 40 mW. Backscattered spectra were collected from focal spot of diameter of 2 μm.

**Raman shifts (cm<sup>-1</sup>):** 3354, 3309, 1278, 1250, 1153, 1086, 908, 712, 489, 295, 281, 263, 252, 216, 175, 147, 135.

**Source:** Goryainov et al. (2017).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Parasymplesite Fe<sup>2+</sup><sub>3</sub>(AsO<sub>4</sub>)<sub>2</sub>·8H<sub>2</sub>O

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3460, 3215, 860, 835, 810, 780, 545, 480, 450, 432, 371, 332, 286, 249, 220, 194, 142.

**Source:** Frost et al. (2003g).

**Comments:** In the cited paper the mineral is named “parasymplesite/symplesite.” Band intensities are not indicated. No independent analytical data are provided for the sample used.

### Paratacamite Cu<sup>2+</sup><sub>3</sub>(Cu,Zn)(OH)<sub>6</sub>Cl<sub>2</sub>

**Origin:** Widgiemooltha, Western Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3508, 3446, 3395, 3364, 3341, 3232, 942, 890, 732, 513, 501, 474, 404, 367, 277, 243, 148, 124.

**Source:** Frost et al. (2002b).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of paratacamite see also Chu et al. (2011).

**Paratellurite**  $\alpha\text{-TeO}_2$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed in a back-scattering geometry on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 150 mW.**Raman shifts (cm<sup>-1</sup>):** 786, 769, 649s, 642, 592, 575, 415, 392, 379, 330, 315, 297, 281, 259, 235, 218, 210, 179, 174, 157, 152s, 121s, 82, 62.**Source:** Mirgorodsky et al. (2000).**Comments:** For the Raman spectra of paratellurite see also Bürger et al. (1992), Berthereau (1995), and Noguera et al. (2003).**Paratooite-(La)**  $(\text{La,Ca,Na,Sr})_6\text{Cu}(\text{CO}_3)_8$ **Origin:** Paratoo Cu mine, Olary district, South Australia (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** ~1440w, 1095s, 1075s, ~220s, and a series of weak bands in the range from 300 to 900 cm<sup>-1</sup>.**Source:** Pring et al. (2006).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.**Paravauxite**  $\text{Fe}^{2+}\text{Al}_2(\text{PO}_4)_2(\text{OH})_2 \cdot 8\text{H}_2\text{O}$ **Origin:** Siglo XX mine, Bustillo province, Potosí department, Bolivia.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3648w, 3505s, 3421, 3315, (3215), 3086, 1639w, 1582sh, 1490sh, 1148, 1115sh, 1058sh, 1020s, 643, 609, 570, 537sh, 420sh, 393s, 253, 319, 299, 227sh, 214, 196w, 164, 148, 110.**Source:** Frost et al. (2013n).**Comments:** The sample was characterized by electron microprobe analysis.**Pargasite**  $\text{NaCa}_2(\text{Mg}_4\text{Al})(\text{Si}_6\text{Al}_2)\text{O}_{22}(\text{OH})_2$ **Origin:** Edenville, New York, USA.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.**Raman shifts (cm<sup>-1</sup>):** 1095w, 1045, 1009, 971w, 956w, 924, 910, 885, 758s, 663s, 581sh, 547, 526, 514, 475w, 415w, 322, 292s, 226s.**Source:** Apopei and Buzgar (2010).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of pargasite see also Apopei et al. (2011), Frezzotti et al. (2012), Andò and Garzanti (2014), and Leissner et al. (2015).

### Parisite-(Ce) $\text{CaCe}_2(\text{CO}_3)_3\text{F}_2$

**Origin:** Snowbird mine, Fish Creek, Alberton, Mineral Co., Montana, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3661sh, 3517sh, 3316, 3180, 1420w, 1088s, 742, 682w, 601, 263, 152.

**Source:** Frost and Dickfos (2007a).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of parisite-(Ce) see also Hong et al. (1999).

### Parisite-(La) $\text{CaLa}_2(\text{CO}_3)_3\text{F}_2$

**Origin:** Mula mine, Tapera village, Novo Horizonte Co., Bahia, Brazil (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm solid-state laser radiation. The nominal laser radiation power was 150 mW.

**Raman shifts (cm<sup>-1</sup>):** 1428, 1331w, 1098s, 1091s, 1081s, 970, 871, 737, 600, 453, 394, 350, 331, 262s, 162.

**Source:** Menezes Filho et al. (2017).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. All peaks above 1500 cm<sup>-1</sup> are due to fluorescence.

### Parnauite $\text{Cu}_9(\text{AsO}_4)_2(\text{SO}_4)(\text{OH})_{10}\cdot 7\text{H}_2\text{O}$

**Origin:** Cap Garonne, Var, France.

**Experimental details:** Raman scattering measurements have been performed on a surfaces nearly perpendicular to the {010} cleavage of a single crystal using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3544sh, 3457, 3365sh, 2926, 2880, 2848, 1608w, 1442, 1320w, 1118sh, 1039, 975, 849s, 814sh, 688sh, 604sh, 493s, 447sh, 378, 295, 268, 218sh, 168sh, 110s.

**Source:** Mills et al. (2013).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. For the Raman spectra of parnauite see also Frost et al. (2009j) and Frost and Keeffe (2011).

### Parsonsite $\text{Pb}_2(\text{UO}_2)(\text{PO}_4)_2$

**Origin:** Ranger U Mine, Northern Territory, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3404w, 3329, 1590, 1078, (1074), 1024, (998), (987), 967, (943), (872), (831), 807s, 796sh, 609, 595, (591), 582, 560, 540, 465, 439, 406, 394, 281, 255, 227sh, 206, 188sh, 171, 155, 136sh, 111sh.

**Source:** Frost et al. (2006f).

**Comments:** The sample was characterized by chemical analyses.

### Parthéite Ca<sub>2</sub>(Si<sub>4</sub>Al<sub>4</sub>)O<sub>15</sub>(OH)<sub>2</sub>·4H<sub>2</sub>O

**Origin:** Denezhkin Kamen' Mt., Middle Urals, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 532 and 633 nm laser radiations. The nominal laser radiation power was 100 and 17 mW, respectively.

**Raman shifts (cm<sup>-1</sup>):** 3574w, 3476sh, 3417, 3384, 3308w, 3256, ~1100w, ~1048, ~978, ~955, ~930, ~770, ~740, ~714, ~640, ~550, ~500s, ~450, ~420, ~400, ~360, ~310s, ~260w, ~250w, ~235w, ~220, ~200, ~180, ~160s, ~150, ~140, ~113.

**Source:** Lazic et al. (2012).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data. The crystal structure is solved.

### Partzite Cu<sub>2</sub>Sb<sup>5+</sup><sub>2</sub>O<sub>7</sub>

**Origin:** Blind Spring Hill district, near Benton, Mono Co., California, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3622w, 3586, 3563, 3485w, 3407, 3376, 3266, 2947sh, (1455w), (1396w), 1126, 1096, 1074, 982sh, 971s, (938), 907w, 837w, 777w, 730w, 675w, 620, 607, 594, 520s, 479, 449, 418, 387, 362, 316, 258sh, 241, 195.

**Source:** Bahfenne and Frost (2010c).

**Comments:** Questionable data. In particular, the strongest band at 971 cm<sup>-1</sup> may correspond to an impurity. No independent analytical data are provided for the sample used.

### Pašavaite Pd<sub>3</sub>Pb<sub>2</sub>Te<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 159s, 119.

**Source:** Bakker (2014).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of pašavaite see also Vymazalová et al. (2014).

**Pascoite**  $\text{Ca}_3\text{V}^{5+}_{10}\text{O}_{28}\cdot 17\text{H}_2\text{O}$ **Origin:** Vanadium Queen mine, San Juan Co., Utah, USA.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3570w, 3466, 3405, 3254, 3125, (1668), 1644, 1514w, 993s, 961s, 841, 621s, 588s, 540, 459, 360sh, 337, 320sh, 292, 238, 193, 159.**Source:** Frost and Palmer (2011c).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of pascoite see also Frost et al. (2004e, 2005d).**Patrónite** VS<sub>4</sub>**Origin:** Synthetic.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** ~990, ~690, ~400, ~280, ~190, ~140s, ~100.**Source:** Kozlova et al. (2015).**Comments:** The sample was characterized by powder X-ray diffraction data and qualitative electron microprobe analysis.**Pattersonite** PbFe<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>(OH)<sub>5</sub>·H<sub>2</sub>O**Origin:** Grube Vereinigung, near Eisenbach, Taunus, Hesse, Germany (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 3547, 3526s, 3291 (broad), ~1610 (broad), 1084s, 1046s, 996, 973s, 927, 636, 571s, 523, 504, 460s, 407, ~377, 360, 325s, ~296, ~273, 259.**Source:** Kolitsch et al. (2008).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.**Pauflerite** VO(SO<sub>4</sub>)**Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 488 and 514.5 nm Ar<sup>+</sup> laser radiations. The laser radiation power is not indicated. A 90°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 1125, 1112, 1095, 1075, 1002, 925s, 654, 596w, 488w, 425w, 395, 361w, 335w, 311w, 285, 269, 253w, 231, 184w, 167w, 136w, 96.**Source:** Boghosian et al. (1995).**Comments:** The sample was characterized by single-crystal X-ray diffraction data. The crystal structure is solved.

**Paulingite-K**  $K_{x_1}Ca_{x_2}Na_{x_3}Ba_{x_4}\square_{x_5}(Si,Al)_{42}O_{84}\cdot 34H_2O$ 

**Origin:** Vinařická Hora Hill, near Kladno, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3554s (broad), 3433sh, 3265sh, 2945w, 2330w, 1640w, 1110, 993, 937, 774, 557sh, 496s, 474, 422w.

**Source:** Gatta et al. (2015b).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Paulmooreite**  $Pb_2As^{3+}_2O_5$ 

**Origin:** Långban, Filipstad district, Värmland province, Sweden (type locality).

**Experimental details:** Raman scattering measurements have been performed from the *a* and *c* faces an oriented single crystal the using 633 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 751, 732, 658w, 562w, 501, 433, 410, 367, 344w, 312, 270, 210, 186s, 138s, 106w (for the spectrum collected from the *a*face of the crystal).

**Source:** Bahfenne et al. (2012).

**Comments:** For the Raman spectrum of paulmooreite see also Bahfenne (2011).

**Pauloabibite**  $NaNbO_3$ 

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 647.1 nm Kr<sup>+</sup> laser radiation. The nominal laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 790, 630sh, 590s, 505sh, 387, 295 (broad), 255w, 733s, 673w, 487, 476sh, 287, 257, 212, 202, 165.

**Source:** Baran et al. (1986).

**Comments:** No independent analytical data are provided for the sample used.

**Paulscherrerite**  $(UO_2)(OH)_2$ 

**Origin:** No. 2 Workings, Radium Ridge, Northern Flinders Ranges, South Australia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3340, ~3290, 864sh, (850), 843s, 831s, 557w, 505w, 460w, 360w.

**Source:** Brugger et al. (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectra of paulscherrerite see also Hoekstra and Siegel (1973), and Walenta and Theye (2012).

**Pavlovskyite**  $\text{Ca}_8(\text{SiO}_4)_2(\text{Si}_3\text{O}_{10})$ 

**Origin:** Lakargi Mt., Upper Chegem caldera, North Caucasus (cotype locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power at the sample was from 30 to 50 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1088w, 993s, 974, 925w, 908, 892, 858s, 847s, 821s, 669s, 569w, 546, 484w, 428w, 400, 358, 329, 305, 262w, 215w, 176w, 118s.

**Source:** Galuskin et al. (2012b).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Peatite-(Y)**  $\text{Li}_4\text{Na}_{12}(\text{Y},\text{Na},\text{Ca},\text{REE})_{12}(\text{PO}_4)_{12}(\text{CO}_3)_4(\text{F},\text{OH})_8$ 

**Origin:** Poudrette (Demix) quarry, Mont Saint-Hilaire, Rouville RCM (Rouville Co.), Montérégie, Québec, Canada (type locality).

**Experimental details:** Raman scattering measurements have been performed from a face of single crystal using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3659w, 1117sh, 1088s, 1042sh, 1000s, 623, 568, 494, 405sh, 370s, 260, 183, 139w.

**Source:** McDonald et al. (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Pecoraite**  $\text{Ni}_3\text{Si}_2\text{O}_5(\text{OH})_4$ 

**Origin:** Nullagine region, Western Australia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** (3638), (3613), 3586, 3535, 3460sh, 3271sh, 2934w, 2896w, 2854w, 1593, 1384, 1075s, 979s, 930w, 821, 761, 616, 451, 397, 235, 194, 151.

**Source:** Frost et al. (2008j).

**Comments:** No independent analytical data are provided for the sample used.

**Pectolite**  $\text{NaCa}_2\text{Si}_3\text{O}_8(\text{OH})$ 

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** (2896), 2879w, 2851w, 2809sh, 1615, 1444w, 1413sh, 1388, (1047), 1026s, 998, 974s, (953), 936sh, 911, 706w, 687, 667sh, 653s, (642), (532w), 518sh, 508+500w (unresolved doublet?), 463w, (432), 415, 378, (370), 358, 325sh, 317, 276, 259sh, 225, (217), 203, 186, 152, 143, 134sh, 111.

**Source:** Frost et al. (2015n).

**Comments:** The sample was characterized by qualitative electron microprobe analysis. For the Raman spectra of pectolite see also Mitchell et al. (2015) and Origlieri et al. (2017).

**Peisleyite**  $\text{Na}_3\text{Al}_{16}(\text{PO}_4)_{10}(\text{SO}_4)_2(\text{OH})_{17}\cdot 20\text{H}_2\text{O}$

**Origin:** Tom's phosphate quarry, near the town of Kapunda, South Australia (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3505s, 3429, 3272, 2888, 1358w, 1289w, 1247w, 1144, 1023s, 989w, 634, 547, 412s, 314w, 276, 207, 188w, 159w.

**Source:** Frost et al. (2004j).

**Comments:** The sample was characterized TG/DTG data.

**Péligotite**  $\text{Na}_6(\text{UO}_2)(\text{SO}_4)_4\cdot 4\text{H}_2\text{O}$

**Origin:** Blue Lizard mine, San Juan Co., Utah, USA (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~3460, ~1210, ~1165, ~1080, ~1045, ~1000s, ~980, ~960, ~945, ~830s, ~655, ~620.

**Source:** Kampf et al. (2016g).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Penkvilksite-2O**  $\text{Na}_2\text{TiSi}_4\text{O}_{11}\cdot 2\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 562 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3527w, 3471sh, 3410, 3354sh. In the spectral range below 3200 cm<sup>-1</sup>, only a figure of the Raman spectrum of Penkvilksite-2O is given by Cadoni and Ferraris (2008).

**Source:** Cadoni and Ferraris (2008).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data. The crystal structure is solved. For the Raman spectrum of penkvilksite see also Frost and Xi (2013b).

**Penroseite**  $(\text{Ni},\text{Co},\text{Cu})\text{Se}_2$

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed by means of back scattering technique. Characteristics of the laser radiation are not indicated.

**Raman shifts (cm<sup>-1</sup>):** 216.5.

**Source:** Yang et al. (2001).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Pentagonite $\text{CaV}^{4+}\text{OSi}_4\text{O}_{10}\cdot4\text{H}_2\text{O}$

**Origin:** Pune (Poonah) district, Maharashtra, India.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3640sh, (3580), 3532, (3499), 1634w, 1612w, 1191w, 1153w, 1089, 1047w, 971s, 765w, 651, 559, 524, 494w, 479w, 398, 344sh, 324, 305, 288, 261w, 230, 206, 158sh, 140, 123sh.

**Source:** Frost and Xi (2012h).

**Comments:** No independent analytical data are provided for the sample used.

### Pentahydrite $\text{Mg}(\text{SO}_4)\cdot5\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on randomly oriented fine grains using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 15 mW.

**Raman shifts (cm<sup>-1</sup>):** 3553sh, 3494, 3391, 3343, 3289, 1650w, 1159, 1106w, 1005s, 602, 447w, 371, 241, 206, 165, 119.

**Source:** Wang et al. (2006a).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of pentahydrite see also Ling et al. (2009) and Frezzotti et al. (2012).

### Pentahydroborite $\text{CaB}_2\text{O}(\text{OH})_6\cdot2\text{H}_2\text{O}$

**Origin:** Fuka mine, Okayama prefecture, Japan.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 3595w, 3499, 3445s, 3399, 3371sh, 3324s, 3196s, 3041s (broad), 2938w, 1610w, 1446w (broad), 1305, 1249, 1223, 1157, 1032, 981, 957, 918, 842, 781w, 725s, 678w, 611s, 584, 562, 508, 492, 472, 416sh, 401, 355, 330, 313sh, 272, 251, 243sh, 214.

**Source:** Bermanec et al. (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data and thermal analysis.

### Pentlandite $(\text{Ni},\text{Fe})_9\text{S}_8$

**Origin:** Kambalda, Western Australia, Australia.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was between 1 and 10 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 370.

**Source:** Mernagh and Trudu (1993).

**Comments:** No independent analytical data are provided for the sample used.

**Peretaite**  $\text{CaSb}^{3+}_4\text{O}_4(\text{SO}_4)_2(\text{OH})_2 \cdot 2\text{H}_2\text{O}$ 

**Origin:** Pereta mine, Scansano, Grosseto province, Tuscany, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3334, 1152, 1142, 1115w, 1092w, 1060, 980s, 710wm, 650w, 610sh, 595s, 589sh, 482w, 434, 417, 373w, 337, 229s, (219), 215sh, 196, 175w, 156, 137sh.

**Source:** Frost et al. (2010f).

**Comments:** No independent analytical data are provided for the sample used.

**Perhamite**  $\text{Ca}_3\text{Al}_{77}\text{Si}_3\text{P}_4\text{O}_{23.5}(\text{OH})_{14.1} \cdot 8\text{H}_2\text{O}$ 

**Origin:** Dunton Gem Quarry, Newry, Oxford Co., Maine, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1884, 1354, 1245, 1153, 1131, 1096, 1059w, 1032, 1005s, 996s, 929w, 708, 636, 615, 586w, 554, 520s, 506s, 468, 442w, 385, 375, 363w, 334, 276, 267, 207, 191, 170w, 148w, 129w.

**Source:** Frost et al. (2007l).

**Comments:** No independent analytical data are provided for the sample used.

**Perite**  $\text{PbBiO}_2\text{Cl}$ 

**Origin:** Homeward Bound mine, Mannahill, South Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 506, 484, 389, 367, 295, 253, 180, 157.

**Source:** Frost and Williams (2004).

**Comments:** The sample was characterized by X-ray diffraction and chemical analysis using ICP-AES techniques, but no analytical data are provided in the cited paper.

**Permingeatite**  $\text{Cu}_3\text{SbSe}_4$ 

**Origin:** Příbram, Central Bohemia region, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on grains mounted in a polished section in backscattering geometry using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was ~1 mW.

**Raman shifts (cm<sup>-1</sup>):** 374w, 366w, 357w, 318w, 276w, 251w, 137, 229s, 214, 205, 193, 184s, 176, 167, 159w, 140w, 127, 78, 75, 63, 59, 51w, 45, 40, 26s, 21s, 17, 14.

**Source:** Škácha et al. (2014a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Perovskite**  $\text{CaTiO}_3$

**Origin:** Rocca Castellaccio, Ciappanico, Malenco Valley, Sondrio province, Lombardy, Italy.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne or 488 nm  $\text{Ar}^+$  laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 638 (broad), 471, 248s, 227s, 182s.

**Source:** Andò and Garzanti (2014).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of perovskite see also Ma et al. (2013), Zajzon et al. (2013), and Martins et al. (2014).

**Pertsevite-(OH)**  $\text{Mg}_2(\text{BO}_3)(\text{OH})$

**Origin:** Snezhnoe boron deposit, Dogdo River basin, Saha Republic (Yakutia), Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on a polished section using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power at the sample was 20 mW. A 0°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3560 (broad), 919s, 862s, 738, 681, 602, 545.

**Source:** Galuskina et al. (2008).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Petalite**  $\text{LiAlSi}_4\text{O}_{10}$

**Origin:** Laghman province, Nuristan, Afghanistan.

**Experimental details:** Unpolarized Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1138, 1060w, 790w, 490s, 467w, 383s, 357s, 280, 143, 113, 85, 60w.

**Source:** Kaminskii et al. (2015).

**Comments:** The sample was characterized by X-ray diffraction data.

**Petersite-(Ce)**  $\text{Cu}_6\text{Ce}(\text{PO}_4)_3(\text{OH})_6 \cdot 3\text{H}_2\text{O}$

**Origin:** Yavapai County, Arizona, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm solid-state laser radiation. The nominal laser radiation power was 60 mW.

**Raman shifts (cm<sup>-1</sup>):** 3499, 3411, 3292, 3072, 2934, 2873, 2862, 1095, 1084, 1043s, 945, 580s, 528, 472s, 393.

**Source:** Morrison et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Petitjeanite**  $\text{Bi}_3\text{O}(\text{PO}_4)_2(\text{OH})$ 

**Origin:** Cetoraz, near Pacov, Czech Republic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 633 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1038, 952, 584w, 548w, 405, 298, 260, 222s, 177s, 102s.

**Source:** Losertová et al. (2014).

**Comments:** The sample was characterized by electron microprobe analyses.

**Petrukite**  $(\text{Cu},\text{Fe},\text{Zn},\text{Ag})_3(\text{Sn},\text{In})\text{S}_4$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdery sample using 644 nm laser radiation. The laser radiation power at the sample was 0.02 mW.

**Raman shifts (cm<sup>-1</sup>):** 990w, 940w, 637, 597sh, 346, 337, 317s, 292, 280, 261sh, 150, 130w, 99, 93.

**Source:** Dzhagan et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of petrukite see also Fernandes et al. (2010).

**Petterdite**  $\text{PbCr}_2(\text{CO}_3)_2(\text{OH})_4 \cdot \text{H}_2\text{O}$ 

**Origin:** Red Lead mine, Zeehan–Dundas mining field, Tasmania, Australia (type locality).

**Experimental details:** Raman scattering measurements have been performed on a powder sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation output power was 0.3 mW.

**Raman shifts (cm<sup>-1</sup>):** 3540, 3470, 3282w, 2948w, 2924, 2854w, 2072w, 1641w, 1516s, 1493sh, 1394sh, 1343s, 1122w, 1089w, 956w, 881sh, 852w, 830w, 812w, 744w, 650sh, 626w, 592w, 541, 504s, 433.

**Source:** Birch et al. (2000).

**Comments:** The sample was characterized by powder X-ray diffraction data, as well as by electron microprobe and HCN analyses.

**Petzite**  $\text{Ag}_3\text{AuTe}_2$ 

**Origin:** Coranda-Hondol open pit, Certej Au-Ag deposit, Romania.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632.8 He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~320, 174, 163s.

**Source:** Apopei et al. (2014b).

**Comments:** The sample was characterized by electron microprobe analyses.

**Pezzottaite**  $\text{CsLiBe}_2\text{Al}_2\text{Si}_6\text{O}_{18}$ 

**Origin:** Piława Górska, Lower Silesia, SW Poland.

**Experimental details:** Raman scattering measurements have been performed on a powder sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1106s, 1067s, 1024, 1007, 689s, 542, 461, 406s, 329, 250, 118s.

**Source:** Pieczka et al. (2016b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. Pezzottaite differs from beryl by intensive Raman bands at 118 and 1106 cm<sup>-1</sup>. For the Raman spectrum of pezzottaite see also Lambruschi et al. (2014).

### Pharmacolite Ca(AsO<sub>3</sub>OH)·2H<sub>2</sub>O

**Origin:** Jáchymov, Krušné Hory (Ore Mts.), Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3525, 3435, 3266sh, (3239), 3186, 1652w, 1179w, 885w, 865s, (858), 844, 706s, 676sh, 545w, 448, 397, 371, 357, 337sh, (309), 305, 286s, 195, (187), 176sh, 155, 133sh, 124.

**Source:** Frost et al. (2010b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

### Pharmacosiderite KFe<sup>3+</sup><sub>4</sub>(AsO<sub>4</sub>)<sub>3</sub>(OH)<sub>4</sub>·6-7H<sub>2</sub>O

**Origin:** Mokrsko-west Au deposit, Příbram district, Central Bohemia region, Czech Republic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532.2 nm diode laser radiation. The laser radiation power at the sample was 0.5 mW.

**Raman shifts (cm<sup>-1</sup>):** 886, 830sh, 803s, 475s, 383, 336, 290w, 279, 244w, 179, 137w.

**Source:** Filippi et al. (2007).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectra of pharmacosiderite see also Frost and Klopogge (2003) and Bossy et al. (2010).

### Pharmazincite KZn(AsO<sub>4</sub>)

**Origin:** Arsenatnaya fumarole, Tolbachik volcano, Kamchatka, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm laser radiation. The laser radiation output power was 30 mW.

**Raman shifts (cm<sup>-1</sup>):** 853s, 513sh, 453w, 430w, 406w, 343, 323, 291.

**Source:** Pekov et al. (2016a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### Phenakite Be<sub>2</sub>(SiO<sub>4</sub>)

**Origin:** San Miguel de Piracicaba, Minas Gerais, Brazil.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 785 nm diode laser radiation. The maximum output power of 300 mW was filtered to diminish the power at the sample.

**Raman shifts (cm<sup>-1</sup>):** 1021w, 952, 938, 918, 879s, 786, 775w, 761w, 728w, 702w, 686w, 666w, 616w, 601w, 527, 463w, 446, 384, 347w, 283w, 233w, 223.

**Source:** Jehlička et al. (2012).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of phenakite see also Hofmeister et al. (1987), Annen and Davis (1993), Pilati et al. (1998), and Jehlička and Vandenberghe (2015).

#### Philipsbornite PbAl<sub>3</sub>(AsO<sub>4</sub>)(AsO<sub>3</sub>OH)(OH)<sub>6</sub>

**Origin:** Red Lead Mine, Dundas mineral field, Zeehan district, West Coast municipality, Tasmania, Australia (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** (865), (857), 846+831s (unresolved doublet?), (820), 399, 376, 357s, 347, 336, 325, 189w, 180w, 134, 115w.

**Source:** Frost et al. (2013s).

**Comments:** No independent analytical data are provided for the sample used.

#### Philipsburgite (Cu,Zn)<sub>6</sub>(AsO<sub>4</sub>,PO<sub>4</sub>)<sub>2</sub>(OH)<sub>6</sub>·H<sub>2</sub>O

**Origin:** Miedzianka (former Kupferberg), Sudety Mts., SW Poland.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 40 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3550w, 3489, 3429w, 3215sh, 1060w, (994w), 970, (946w), 865s, 847sh, 809s, 791sh, 667w, 564sh, (491w), 474, 396, 368sh, 347sh, 317, 307sh, 249w, 218w.

**Source:** Ciesielczuk et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

#### Phillipsite-K K<sub>6</sub>(Si<sub>10</sub>Al<sub>6</sub>)O<sub>32</sub>·12H<sub>2</sub>O

**Origin:** Capo di Bove, Rome province, Latium, Italy (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using Nd-YAG laser radiation. The laser radiation power at the sample was 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 815, 743, 472s, 424sh, 187w.

**Source:** Mozgawa (2001).

**Comments:** The sample was characterized by powder X-ray diffraction data.

#### Philolithite Pb<sub>12</sub>O<sub>6</sub>Mn<sub>7</sub>(SO<sub>4</sub>)(CO<sub>3</sub>)<sub>4</sub>Cl<sub>4</sub>(OH)<sub>12</sub>

**Origin:** Långban, Värmland, Sweden (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** A group of bands around 3400 cm<sup>-1</sup>, 1122, 1111, 1073, 1011, 420.

**Source:** Kampf et al. (1998).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### Phlogopite KMg<sub>3</sub>(AlSi<sub>3</sub>O<sub>10</sub>)(OH)<sub>2</sub>

**Origin:** Arendal Fe Mines, Aust-Agder, Norway.

**Experimental details:** Micro-Raman scattering measurements have been performed on a single crystal using a 514.5 nm Ar<sup>+</sup> laser. Sample orientation is not indicated.

**Raman shifts (cm<sup>-1</sup>):** (1024), (1000), 675s, 650, 273, 190s, 97.

**Source:** Tlili et al. (1989).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectra of phlogopite see also McKeown et al. (1999), Tlili and Smith (2007), and Frezzotti et al. (2012).

### Phoenicochroite Pb<sub>2</sub>(CrO<sub>4</sub>)O

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 647.1 nm Kr<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 849, 838, 826s, 382, 356w, 343, 333w, 324.

**Source:** Roncaglia et al. (1985).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of phoenicochroite see also Frost (2004c).

### Phosgenite Pb<sub>2</sub>(CO<sub>3</sub>)Cl<sub>2</sub>

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne or 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was  $\leq 30$  mW.

**Raman shifts (cm<sup>-1</sup>):** 1063s, 668, 281, 252, 181w, 154, 129, 87s, 81, 53, 47s.

**Source:** Bouchard and Smith (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of phosgenite see also Frost et al. (2003j) and Frost and Williams (2004).

### Phosphammite (NH<sub>4</sub>)<sub>2</sub>(PO<sub>3</sub>OH)

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed at 260 K on crystals in a sealed glass cell using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was between 0.1 and 0.2 mW.

**Raman shifts (cm<sup>-1</sup>):** 3200sh, 3048s, 2805s, 2203, 1948, 1743, 1720, 1696, 1441w, 1404, 1094w, 1062w, 1052w, 997w, 949s, 900, 856w, 565, 557, 522, 510w, 400, 380.

**Source:** Hadrich et al. (2000).

**Comments:** No independent analytical data are provided for the sample used.

**Phosphohedyphane**  $\text{Ca}_2\text{Pb}_3(\text{PO}_4)_3\text{Cl}$ 

**Origin:** Root (Bonanza Hill) mine, Goodsprings district, Spring Mts., Clark Co., Nevada, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** (3421), 3395, 3344, 1226w, 1188w, (1084), 1073, (1030), (980), 975s, (966), 933s, 835, 812w, 595, 577sh, 557, 437s, (421), 400, 208, 148, 113sh, 106.

**Source:** Frost et al. (2014w).

**Comments:** No independent analytical data are provided for the sample used.

**Phosphophyllite**  $\text{Zn}_2\text{Fe}^{2+}(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ 

**Origin:** Hagendorf South pegmatite, Bavaria, Germany.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3567s, (3561), 3362sh, 3258, 3146, (3034), 1603, (1571), 1135, 1073, 995s, 939, 744w, 633, 592, 571sh, 505, 415, 322, (297), 269, 199, 181sh, 142, 130sh, 119.

**Source:** Scholz et al. (2013a).

**Comments:** The sample was characterized by qualitative electron microprobe analyses. No independent quantitative analytical data are provided.

**Phosphosiderite**  $\text{Fe}^{3+}(\text{PO}_4) \cdot 2\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1032sh, 1000sh, 988s, 570w, 485sh, 447, 330sh, 302, 258, 200, 126w, 70.

**Source:** Zaghbil and Julien (2005).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of phosphosiderite see also Frost et al. (2004l).

**Phosphuranylite**  $\text{KCa}(\text{H}_3\text{O})_3(\text{UO}_2)_7(\text{PO}_4)_4\text{O}_4 \cdot 8\text{H}_2\text{O}$ 

**Origin:** Bedford, Westchester Co., New York, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using 647.1 nm Kr<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1034, 981, 827s, 398, 264, 237.

**Source:** Faulques et al. (2015a, b).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of phosphuranylite see also Frost et al. (2008a) and Driscoll et al. (2014).

**Phurcalite**  $\text{Ca}_2(\text{UO}_2)_3\text{O}_2(\text{PO}_4)_2 \cdot 7\text{H}_2\text{O}$ 

**Origin:** Posey mine, Red Canyon, White Canyon district, San Juan Co., Utah, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3613w, 3538w, 3421, (3238), 1769w, 1615w, 1155w, 1118sh, 1108, 1059, (1009), 1004s, 995sh, 969, 960, 950sh, 864w, (819), 810, (800), 546, (434), 431, 408, 391sh.

**Source:** Čejka et al. (2014b).

**Comments:** The sample was characterized by powder X-ray diffraction data and qualitative electron microprobe analysis.

**Pickeringite**  $\text{MgAl}_2(\text{SO}_4)_4 \cdot 22\text{H}_2\text{O}$ 

**Origin:** San Bernardino Co., California, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power at the sample was 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3449, 3279, 3082sh, 1145w, 1114w, 1071w, (990), 986s, 975, 621, 530, 468, 424, 344w, 315, 221.

**Source:** Locke et al. (2007).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Picromerite**  $\text{K}_2\text{Mg}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 253.65 nm radiation of mercury. The incident light was normal to the (110) face and the scattered light was taken parallel to the (110) face and roughly perpendicular to the (001) face. The radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3344, 3308s, 3250, 3150, 1234w, 1156, 1129s, 1111, 1082s, 990s, 835w, 792w, 767w, 632, 614, 462s, 448s, 372, 320w, 305w, 269w, 225, 177, 136, 115, 93w, 74, 62, 46.

**Source:** Ananthanarayanan (1961).

**Comments:** The sample was characterized by morphological features. For the Raman spectrum of picromerite see also Bouchard and Smith (2003).

**Picropharmacolite**  $\text{Ca}_4\text{Mg}(\text{AsO}_3\text{OH})_2(\text{AsO}_4)_2 \cdot 11\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power was below 0.1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3448, 3212, (2922), 980, 866s, 750, 530, 460, 397, 325, 230.

**Source:** Frost and Kloprogge (2003).

**Comments:** No independent analytical data are provided for the sample used.

**Pieczkaite**  $Mn_5(PO_4)_3Cl$

**Origin:** Cross Lake pegmatite field, Manitoba, Canada (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The nominal laser radiation power was between 5 and 12.5 mW.

**Raman shifts (cm<sup>-1</sup>):** 1095s, 1000sh, 960sh, 795w, 560s, 480sh.

**Source:** Tait et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Piemontite**  $Ca_2(Al_2Mn^{3+})[Si_2O_7][SiO_4]O(OH)$

**Origin:** Prabornaz (Praborna) mine, Saint-Marcel, Aosta Valley, Italy.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne or 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 916s, 886s, 601, 565, 453s, 350s, 244, 172.

**Source:** Andò and Garzanti (2014).

**Comments:** No independent analytical data are provided for the sample used.

**Pigeonite**  $(Mg,Fe,Ca)_2Si_2O_6$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal in a polished thin section using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was  $\leq 1$  mW.

**Raman shifts (cm<sup>-1</sup>):** ~1035, ~1010, 685s, ~665, ~415, ~400, ~385w, 341s, ~300w, ~240.

**Source:** Tribaudino et al. (2011).

**Comments:** The Raman shifts are given for a Fe-free sample with the diopside to enstatite ratio of 15:85. In the cited paper Raman spectra of natural pigeonite samples with different Fe:Mg ratios are given.

**Pilsenite**  $Bi_4Te_3$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a thin film grown on Si (111) substrate using 532 nm Nd-YAG laser radiation. The material grew along its *c*-axis. The nominal laser radiation power was 2 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 204, 183w, 115, 101sh, 88s, 57, 37.

**Source:** Xu et al. (2015a).

**Comments:** The sample was characterized by X-ray diffraction data.

**Pilsenite**  $\text{Bi}_4\text{Te}_3$ 

**Origin:** Panarechensk volcanic-tectonic formation, Kola Peninsula, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 204w, 171–174, 131sh–133, 97–106s, 81.

**Source:** Voloshin et al. (2015a).

**Comments:** The samples used were characterized by electron microprobe analyses.

**“Pimelite”**  $\text{Ni}_3\text{Si}_4\text{O}_{10}(\text{OH})_2 \cdot 4\text{H}_2\text{O}$ 

**Origin:** Falcondo mine, Bonao, La Vega province, Dominican Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 1064 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 822, 735w, 675s, 640, 386, 362, 188s.

**Source:** Villanova-de-Benavent et al. (2012).

**Comments:** No independent analytical data are provided for the sample used.

**Pinakiolite**  $(\text{Mg},\text{Mn})_2(\text{Mn}^{3+},\text{Sb}^{5+})\text{O}_2(\text{BO}_3)$ 

**Origin:** Långban deposit, Bergslagen ore region, Filipstad district, Värmland, Sweden (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** See comment below.

**Source:** Frost (2011b).

**Comments:** All Raman spectra of presumed orthoborates (azoproite, fredrikssonite, pinakiolite and takéuchiite) given in the cited paper are almost identical and correspond to calcite. In particular, for “pinakiolite” the following Raman shifts have been determined: 1748w, 1435w, 1086s, 712, 283, 154. The correct Raman shifts of pinakiolite are (RRUFF (2007), sample R050636; cm<sup>-1</sup>): 686s, 644s, 550sh, 445, 391w, 352w, 322, 280, 200w, 153.

**Pinnosite**  $\text{MgB}_2\text{O}(\text{OH})_6$ 

**Origin:** Ider boron deposit, Atyrau region, Kazakhstan.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3579s, (3569), 3554s, (3415w), 3399s, 3290, 3179, (3085w), 1320, 1299, 1260, 1186, 1157, 1140sh, 1049, 1020, 945, 900s, 875, (799w), 745, 630, 605, (594w), 578, 538sh, 524, 508, 491w, 480, 468sh, 403sh, 388, 375, 357, (338), 288, 273, 260w, 230, 209sh, 193, 180, 172w, 143, 126.

**Source:** Frost and Xi (2014).

**Comments:** No independent analytical data are provided for the sample used.

**Pirssonite**  $\text{Na}_2\text{Ca}(\text{CO}_3)_2 \cdot 2\text{H}_2\text{O}$ 

**Origin:** Green River formation, Sweetwater Co., Wyoming, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3502, 3065, 1070s, 717, 659, 298, 253, (199), 126.

**Source:** Frost and Dickfoss (2007b).

**Comments:** No independent analytical data are provided for the sample used.

**Pitticite**  $[\text{Fe},\text{AsO}_4,\text{SO}_4,\text{H}_2\text{O}]$  (?)

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3490, 3327, 3186, (3060), (2723), (1182w), 1096, 916sh, 845+837s (unresolved doublet?), 617w, (504), 457, 428, 401sh, 372w, 349sh, 335, 322, 309, 297sh, 278, 260, 236, 221sh, 207w, 194w, 181w, 166w, 131sh, 118+111 (unresolved doublet?).

**Source:** Frost et al. (2012l).

**Comments:** No independent analytical data are provided for the sample used.

**Plancheite**  $\text{Cu}_8(\text{Si}_4\text{O}_{11})_2(\text{OH})_4 \cdot \text{H}_2\text{O}$ 

**Origin:** Tsumeb mine, Tsumeb, Namibia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** See comment below.

**Source:** Frost and Xi (2012d).

**Comments:** No independent analytical data are provided for the sample used. The Raman and IR spectra of presumed plancheite given in the cited paper are wrong and correspond to a carbonate. The correct Raman shifts of plancheite are (RRUFF (2007), sample R070233; cm<sup>-1</sup>): 780, 674s, 553, 499, 441s, 400, 336, 328sh, 316, 262, (248), (239).

**Plášilite**  $\text{Na}(\text{UO}_2)(\text{SO}_4)(\text{OH}) \cdot 2\text{H}_2\text{O}$ 

**Origin:** Blue Lizard mine, San Juan Co., Utah, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm diode-pumped solid-state laser radiation. The nominal laser radiation power was 3 mW.

**Raman shifts (cm<sup>-1</sup>):** 3600, 3520, 3385w, 1180, 1069w, 1035, 997, 986.5, 905w, 838s, 824, 645w, 603, 480, 445, 349, 243, 210, 186, 170.

**Source:** Kampf et al. (2015a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

#### Platarsite PtAsS

**Origin:** Munni complex, west Pilbara block, Western Australia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented grain in a polished section using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was between 1 and 10 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 427, 350s, 291, 283, 253, 214.

**Source:** Mernagh and Hoatson (1995).

**Comments:** The sample was characterized by electron microprobe analyses.

#### Platinum Pt

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** ~220, ~185, ~170, ~155.

**Source:** Vermaak (2005).

#### Plattnerite PbO<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a pressed disc using 632.8 nm laser radiation. The laser radiation power at the sample was 0.27 mW.

**Raman shifts (cm<sup>-1</sup>):** 424w, 515s, 653w.

**Source:** Burgio et al. (2001).

**Comments:** Plattnerite slowly decomposes under the laser beam. For the Raman spectrum of plattnerite see also Inguanta et al. (2008).

#### Plavnoite K<sub>0.8</sub>Mn<sub>0.6</sub>[(UO<sub>2</sub>)<sub>2</sub>O<sub>2</sub>(SO<sub>4</sub>)]:3.5H<sub>2</sub>O

**Origin:** Jáchymov, Krušné Hory (Ore Mts.), Bohemia, Czech Republic (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm diode laser radiation. The laser radiation power at the sample was about 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 3533, 3385w, 1630w, 1106, 1027, 817s, 502, 475, 435, 377w, 348w, 292, 267, 229, 164s, 129w, 106w.

**Source:** Plášil et al. (2017).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Plimerite**  $\text{ZnFe}^{3+}_4(\text{PO}_4)_3(\text{OH})_5$ 

**Origin:** Huber open pit, Huber stock, Krásno, Horní Slavkov, Karlovy Vary region, Bohemia, Czech Republic (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532.2 nm laser radiation. The nominal laser radiation power was 5 mW.

**Source:** Sejkora et al. (2011).

**Raman shifts (cm<sup>-1</sup>):** ~3590, 3228 (broad), 1600w, (1164), 1118s, (1098w), (1079), 1051s, 1014s, 993, 964, 930sh, 774w.

**Plombièrite**  $\text{Ca}_4\text{Si}_6\text{O}_{16}(\text{OH})_2(\text{H}_2\text{O})_2 \cdot (\text{Ca} \cdot 5\text{H}_2\text{O})$ 

**Origin:** Crestmore quarry, north of Riverside, Riverside Co., California, USA.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed in nearly backscattered geometry using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 1.5 mW.

**Raman shifts (cm<sup>-1</sup>):** 1057sh, 1025, 996, 680sh, 664s.

**Source:** Biagioni et al. (2013b).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Plumbogummite**  $\text{PbAl}_3(\text{PO}_4)(\text{PO}_3\text{OH})(\text{OH})_6$ 

**Origin:** Guochengmine, Yangshuo, Guangxi province, China.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3602sh, 3479, (3372), 3249, (3121), (1182w), 1106s, (1057), 1023s, (1002), 980s, (971w), (826w), (634w), 613, 579sh, 507, (494), 464, 388sh, 368, 281sh, 251s, 187, (163w), 145.

**Source:** Frost et al. (2013l).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Plumbojarosite**  $\text{Pb}_{0.5}\text{Fe}^{3+}_3(\text{SO}_4)_2(\text{OH})_6$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a sample diluted with KBr powder and compressed to form a disk. A 514.5 nm Ar<sup>+</sup> laser was used. The laser radiation power at the sample was 38 mW.

**Raman shifts (cm<sup>-1</sup>):** 1169w, 1120sh, 1108, 1015sh, 1002, 623, 583w, 452sh, 440s, 341w, 221.

**Source:** Sasaki et al. (1998).

**Comments:** The sample was characterized by powder X-ray diffraction data and chemical analyses. For the Raman spectra of plumbojarosite see also Frost et al. (2006r) and Spratt et al. (2013).

**Plumbophyllite**  $\text{Pb}_2\text{Si}_4\text{O}_{10}\cdot\text{H}_2\text{O}$ 

**Origin:** Blue Bell mine, Soda Mts, Silver Lake District, San Bernardino Co., California, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3567sh, 3494+3470 (unresolved doublet?), (3443), 3215w, 1153w, 1137w, 1095w, (1039), 1027s, 972, 956, 926, (657), 643s, (634), 506w, (500w), 485w, 438w, 409w, (398w), 381, (368w), 349sh, 332, 309, 253, 203sh, 182, (155), 147s, 112.

**Source:** Frost et al. (2014t).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

**Plumbotsumite**  $\text{Pb}_{13}(\text{CO}_3)_6(\text{Si}_{10}\text{O}_{27})\cdot 3\text{H}_2\text{O}$ 

**Origin:** St. Anthony deposit, Mammoth district, Pinal Co., Arizona, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 4620w, 3546, 3510w, 2950w, 2720w, 2674sh, 1744w, 1732sh, 1716w, (1709), 1685w, 1479, 1424, 1379, 1333sh, 1084w, 1060sh, 1055s, 1047, 844sh, 839, 772w, 729w, 697, 683, 673sh, 636w, 609, 581sh, 481, 458, 432w, 396, 346w, 288sh, 280w, 246, 227, 179, 154+143s (unresolved doublet?), 107+103 (unresolved doublet?).

**Source:** López et al. (2013a).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

**Poitevinite**  $\text{Cu}(\text{SO}_4)\cdot\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1204, 1097, 1043.5s, 1014s, 669, 620.5, 607, 515, 419, 345, 268, 244, 207.5, 130w, 105w.

**Source:** Fu et al. (2012).

**Pokrovskite**  $\text{Mg}_2(\text{CO}_3)(\text{OH})_2$ 

**Origin:** Lytton, Sonoma Co., California, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3556w, 3444, 1582, 1452, 1386, 1088s, 929, 734, 703w, 521w, 446w, 402, 282, 172, 143.

**Source:** Frost (2006).

**Comments:** No independent analytical data are provided for the sample used.

**Poldervaartite**  $\text{Ca}(\text{Ca,Mn})(\text{SiO}_3\text{OH})(\text{OH})$

**Origin:** N'Chwaning Ilmine, Kalahari manganese fields, South Africa (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3547, 3521sh, 3509, (3502w), 3487, 952, (943w), 917, (907), 900, (865), 852s, 807, 792sh, 528sh, 513, (498w), 485, 473sh, 245w, 239w, 213, 203, 163sh, 153s, (148), (145), (116), 109, 104.

**Source:** Frost et al. (2015g).

**Comments:** The sample was characterized by qualitative electron microprobe analysis which may correspond to olmiite.

**Pollucite**  $\text{Cs}(\text{Si}_2\text{Al})\text{O}_6 \cdot n\text{H}_2\text{O}$

**Origin:** Auburn, Androscoggin Co., Maine, USA.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using Nd-YAG laser radiation. The laser radiation power at the sample was 300 mW.

**Raman shifts (cm<sup>-1</sup>):** 1109, 478s, 393, 299.

**Source:** Mozgawa (2001).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Polycrase-(Y)**  $\text{Y}(\text{Ti,Nb})_2(\text{O,OH})_6$

**Origin:** No data.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** ~1480w, ~1420w, ~1130w, ~1080w, ~845, ~695, ~530w, ~400s, ~280s, ~225s.

**Source:** Tomašić et al. (2004).

**Comments:** The Raman shifts are given for an initially metamict sample heated at 1000°C to regain its crystal structure. The sample was characterized by powder X-ray diffraction data and chemical analyses.

**Polydymite**  $\text{Ni}^{2+}\text{Ni}^{3+}_2\text{S}_4$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on grains in a Ni-based composite after exposure to an H<sub>2</sub>S-containing fume 1514 nm laser radiation was used. The nominal laser radiation power was 40 mW.

**Raman shifts (cm<sup>-1</sup>):** 379, 337, 287s, 223.

**Source:** Cheng and Liu (2007).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

### Polyhalite $K_2Ca_2Mg(SO_4)_4 \cdot 2H_2O$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 3437, 3288w, 1181w, 1165, 1144w, 1130, 1094w, 1069, 1014s, 987s, 652w, 641w, 626, 620sh, 477sh, 464, 448, 436.

**Source:** Jentzsch et al. (2012a).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of polyhalite see also Jentzsch et al. (2013).

### Popovite $Cu_5O_2(AsO_4)_2$

**Origin:** Arsenatnaya fumarole, Tolbachik volcano, Kamchatka, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm laser radiation. The laser radiation power at the sample was ~9 mW.

**Raman shifts (cm<sup>-1</sup>):** 846s, 810s, 642, 547, 489, 478w, 427, 377w, 344, 281, 258w, 212, 128, 97s.

**Source:** Pekov et al. (2015b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### Portlandite $Ca(OH)_2$

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 3620s, ~680 (broad), 356s, 252.

**Source:** Schmid and Dariz (2015).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of portlandite see also Lutz et al. (1994).

### Posnjakite $Cu_4(SO_4)(OH)_6 \cdot H_2O$

**Origin:** Ozernyi district, Sallo-Kuolajarvi, Kola Peninsula, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 3587s, 3566s, 3400, 971s, 620sh, 607, 594, 508, 479, 449w, 418w, 387, 316w, 241w, 194w, 136, 88s.

**Source:** Voloshin et al. (2015b).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectra of posnjakite see also Martens et al. (2003a), Frost et al. (2004n), and Lepot et al. (2006).

**Potarite** PdHg

**Origin:** Munni Munni layered intrusion, West Pilbara Block, Western Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented grains in a polished section using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was between 1 and 10 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 362, 340s, 285, 254.

**Source:** Mernagh and Hoatson (1995).

**Comments:** The sample was characterized by electron microprobe analyses.

**Pottsite** (Pb<sub>3</sub>Bi)Bi(VO<sub>4</sub>)<sub>4</sub>·H<sub>2</sub>O

**Origin:** Las Tapias, Cordoba province, Argentina.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 2912w, 885, 874, 707, 643, 465, 413s, 404, 370, 348, 331, 264w, 204, 185.

**Source:** Frost et al. (2006i).

**Comments:** No independent analytical data are provided for the sample used.

**Poubaite** PbBi<sub>2</sub>(Se,Te,S)<sub>4</sub>

**Origin:** Ozernyi district, Salla-Kuolajarvi, Kola Peninsula, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 139, 102s, 59.

**Source:** Voloshin et al. (2015a).

**Comments:** The samples used were characterized by electron microprobe analyses.

**Poudretteite** KNa<sub>2</sub>(B<sub>3</sub>Si<sub>12</sub>)O<sub>30</sub>

**Origin:** Mogok valley, Shan State, Myanmar.

**Experimental details:** Raman scattering measurements have been performed on a fragment of a single crystal with the beamdirection parallel to the *c*-axis using 325 nm laser excitation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1799w, 1660w, 1556w, 1176s, 1147, 1045w, 1011, 928, 908w, 849w, 788, 696, 662, 594w, 552s, 490s, 429w.

**Source:** Smith et al. (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Poughite** Fe<sup>3+</sup><sub>2</sub>(Te<sup>4+</sup>O<sub>3</sub>)<sub>2</sub>(SO<sub>4</sub>)·3H<sub>2</sub>O

**Origin:** Wendy Pit, El Indio gold mine, Coquimbo, Chile.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts

have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3509, 3481, (3477w), 2330, 2231, 2155, 1926w, 1793, 1706, 1582, 1335, 1187w, 1152w, 1078, 1026s, (1022), (655), 653s, 561, 509, 485, 382, 347, 236s, (234), 163, (161).

**Source:** Frost and Keeffe (2008c).

**Comments:** No independent analytical data are provided for the sample used.

**Povondraite** NaFe<sup>3+</sup><sub>3</sub>(Fe<sup>3+</sup><sub>4</sub>Mg<sub>2</sub>)(Si<sub>6</sub>O<sub>18</sub>)(BO<sub>3</sub>)<sub>3</sub>(OH)<sub>3</sub>O

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed using 488 or 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 14 mW. Polarized Raman spectra were collected from raw crystal surfaces in the spectral range 15–4000 cm<sup>-1</sup> in -y(zz)y, -y(zx)y, and -y(xx)y scattering geometries.

**Raman shifts (cm<sup>-1</sup>):** ~3555, ~990, ~800w, ~670w, ~625w, ~545, ~460, ~430, ~400w, ~315, ~280s, ~230s, ~165, ~140w.

**Source:** Watenphul et al. (2016a, b).

**Comments:** The Raman shifts are given for the scattering geometry -y(zz)y.

**Powellite** Ca(MoO<sub>4</sub>)

**Origin:** Dundas, Tasmania, Australia.

**Experimental details:** Raman scattering measurements have been performed on crystals oriented to provide maximum intensity using a 785 nm Nd-YAG laser. The laser radiation power at the sample was 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 879, 847, 794, 513, 456, 403, 392, 324, 267.

**Source:** Frost et al. (2004c).

**Comments:** No independent analytical data are provided for the sample used.

**Prehnite** Ca<sub>2</sub>Al(Si<sub>3</sub>Al)O<sub>10</sub>(OH)<sub>2</sub>

**Origin:** Valtournanche, Aosta valley, Italy.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne or 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~1110w, ~1080w, 991, ~950, 931, ~640, ~600, 541, 520s, 388s, 318.

**Source:** Andò and Garzanti (2014).

**Comments:** No independent analytical data are provided for the sample used.

**Preiswerkite** KFe<sup>2+</sup><sub>3</sub>(AlSi<sub>3</sub>O<sub>10</sub>)(OH)<sub>2</sub>

**Origin:** Liset, Selje, Sognog Fjordane, Norway.

**Experimental details:** Raman scattering measurements have been performed on oriented samples using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. The spectra were recorded with the electric field polarized perpendicular to the cleavage plane.

**Raman shifts (cm<sup>-1</sup>):** 3628s, 3620, 916, 648s, 292s, 216s (Sample 8); 916, 679, 648s, 488, (400), (379), 330, 292s, (280), 216s, 156, 108 (Sample 9).

**Source:** Tlili et al. (1989).

**Comments:** The samples were characterized by electron microprobe analyses. For the Raman spectra of preiswerkite see also Tlili and Smith (2007) and Orozbaev et al. (2011).

### Pretulite Sc(PO<sub>4</sub>)

**Origin:** Saint-Aubin-des-Châteaux, Armorican Massif, France.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 3 mW.

**Raman shifts (cm<sup>-1</sup>):** 1079s, 1043, 1024s, 595w, 475, 326, 234, 186w.

**Source:** Moëlo et al. (2002).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. For the Raman spectrum of pretulite see also Giarola et al. (2011).

### Příbramite CuSbSe<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline film using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 226s, 200, 153, 114.

**Source:** Xue et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Priceite Ca<sub>2</sub>B<sub>5</sub>O<sub>7</sub>(OH)<sub>5</sub>·H<sub>2</sub>O

**Origin:** 20-Mule-Team Canyon, Furnace Creek district, California, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3669, 3579sh, 3555s, 3510sh, 3496, 3468sh, 3404, 3385sh, 3221w, 1211, 1169w, 1127, 1100w, 1071, 1019, 991, 974sh, 956, 927w, 894, 842, 826, 736, (697), 689s, 674s, (660), 634, 602, 563sh, 545s, 511w, 481sh, 471, 450w, 433w, 409w, 387w, 368, 353sh, 306, 287sh, 266sh, 253, 231, 217w, 195, (183), 173, 148sh, 138, 129sh, 109.

**Source:** Frost et al. (2015).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

### Pridelite Mg-analogue K<sub>2</sub>(Ti<sub>7</sub>Mg)O<sub>16</sub>

### Pridelite Al-analogue K<sub>2</sub>(Ti<sub>6</sub>Al<sub>2</sub>)O<sub>16</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on oriented single crystals using 488 and 514.5 nm Ar<sup>+</sup> laser radiations. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 840, 702, 690, 635, 610, 550, 505, 497, 460, 455, 370, 350, 344, 331, 260, 193, 144, 123 (for the priderite Al analogue); 840, 710, 700, 640, 623, 580, 511, 463, 461, 380, 375, 360, 350, 285, 210, 152, 131 (for the priderite Mg analogue).

**Source:** Ohsaka and Fujiki (1982).

**Comments:** The empirical formulae of the samples used are K<sub>1.6</sub>(Ti<sub>7.2</sub>Mg<sub>0.8</sub>)O<sub>16</sub> and K<sub>1.6</sub>(Ti<sub>6.4</sub>Al<sub>1.6</sub>)O<sub>16</sub>. The intensities are given for the  $\alpha_{zz}$  polarization.

### Pridelite Cr-analogue (K,Ba)<sub>2-x</sub>(Ti<sub>6</sub>Cr<sub>2</sub>)O<sub>16</sub>

**Origin:** Gföhl granulite, Bohemian massif, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented grain using 532 nm laser radiation. The laser radiation power at the sample was 1.4 mW.

**Raman shifts (cm<sup>-1</sup>):** 800sh, 685s, 620, 545w, 350, 277, 195w, 150.

**Source:** Naemura et al. (2015).

**Comments:** The sample was characterized by electron microprobe analyses.

### Prismatine (Mg,Al,Fe)<sub>6</sub>Al<sub>4</sub>(Si,Al)<sub>4</sub>(B,Si,Al)(O,OH,F)<sub>22</sub>

**Origin:** Madagascar.

**Experimental details:** Methods of sample preparation are not described. Micro-Raman scattering measurements have been performed on a single crystal using 514.5 nm Ar<sup>+</sup> laser radiation with the polarization direction parallel to the crystal elongation. The laser radiation power at the sample was 5 W. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3615w, 3556, 1120w, 1028s, 973s, 864, 803, 760w, 610, 537, 459, 384, 286, 260s.

**Source:** Wopenka et al. (1999).

**Comments:** The sample contains 0.86 boron atoms per formula unit.

### Proustite Ag<sub>3</sub>AsS<sub>3</sub>

**Origin:** Jáchymov, Krušné Hory (Ore Mts.), Bohemia, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on a polished crystal using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 1.7 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 364s, 337, 315sh, 274w.

**Source:** Kharbish et al. (2009).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectra of proustite see also Byer et al. (1973) and Makreski et al. (2004).

### Pseudoboleite Pb<sub>31</sub>Cu<sub>24</sub>Cl<sub>62</sub>(OH)<sub>48</sub>

**Origin:** Siklerton Barrier Range, New South Wales, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3467, 3434, 3350, 3330, 973w, 908w, 817w, ~680s, 584, 512, 449, (388), (236), (179), 148s, 137s.

**Source:** Frost and Williams (2004).

**Comments:** No independent analytical data are provided for the sample used.

### Pseudobrookite ( $\text{Fe}^{3+}_2\text{Ti}\text{O}_5$ )

**Origin:** Marion Island, Hawaiian archipelago.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was between 2.5 and 40 mW.

**Raman shifts (cm<sup>-1</sup>):** 1334, 660s, 507w, 411w, 340, 226s, 200s.

**Source:** Prinsloo et al. (2011).

**Comments:** For the Raman spectra of pseudobrookite see also Bersani et al. (2000) and Wang et al. (2016).

### Pseudocotunnite K<sub>2</sub>PbCl<sub>4</sub> (?)

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~230.

**Source:** Oyamada (1974).

### Pseudojohannite Cu<sub>3</sub>(OH)<sub>2</sub>[(UO<sub>2</sub>)<sub>4</sub>O<sub>4</sub>(SO<sub>4</sub>)<sub>2</sub>]·12H<sub>2</sub>O

**Origin:** Rovnosta shaft, Jáchymov uranium deposit, Krušné Hory (Ore Mts.), Western Bohemia, Czech Republic (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3483w, (3353), (3226), 1625w, 1554w, 1333w, 1100, 1017, 810+805s (unresolved doublet?), 755sh, 539sh, 496, 465, 423s, 279, 210, 162+151 (unresolved doublet?).

**Source:** Frost et al. (2009h).

**Comments:** The sample was characterized by electron microprobe analyses.

### Pseudolaueite Mn<sup>2+</sup>Fe<sup>3+</sup><sub>2</sub>(PO<sub>4</sub>)<sub>2</sub>(OH)<sub>2</sub>·7·8H<sub>2</sub>O

**Origin:** Hagendorf South pegmatite, Bavaria, Germany.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3593sh, 3485, 3376, 3209w, 3110sh, 1123s, 1066w, 1046, (1034), 1000+993s (unresolved doublet?), 976, 843, 643, 626sh, (565), 501, (485), 471s, 456sh, 435, 408, 373w, 332, 303, 286, 271, 249, 223, 215, 201s, 189, 183, 164.

**Source:** Frost et al. (2015ac).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

### Pseudomalachite Cu<sub>5</sub>(PO<sub>4</sub>)<sub>2</sub>(OH)<sub>4</sub>

**Origin:** Banská Bystrica, central Slovakia.

**Experimental details:** Raman scattering measurements have been performed on an oriented crystal using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 17 mW. A 180°-scattering geometry was employed. Polarized spectra were collected with  $E \parallel b$  and  $E \perp b$ .

**Raman shifts (cm<sup>-1</sup>):** 3414, 1137w, 1112w, 1083, 1055, 996sh, 971, 945sh, 861w, 801w, 750, (703w), (664w), 750, 703w, (664w), (639w), 606, 539sh, 515, 477s, 446s, 412, 297, 254w, 241, 214, 209, 174s, 131s, 109s, 86s (for  $E \perp b$ ).

**Source:** Kharbish et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectra of pseudomalachite see also Frost et al. (2002a, g), Bouchard and Smith (2003), Majzlan et al. (2015), and Ciesielczuk et al. (2016).

### Pseudowollastonite CaSiO<sub>3</sub>

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been using 488 or 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 500 mW.

**Raman shifts (cm<sup>-1</sup>):** 1075, 989s, 932, 714w, 580s, 558, 511, 428w, 373s, 341, 327, 315, 301, 217w, 193, 167.

**Source:** Richet et al. (1998).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Pucherite Bi(VO<sub>4</sub>)

**Origin:** Pucher shaft, Schneeberg, Germany (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1002, (881), 872s, 710w, 693w, 647w, 415, 372s, 346, 333s, 256, 224, 196, 188.

**Source:** Frost et al. (2006i).

**Comments:** No independent analytical data are provided for the sample used.

### Pumpellyite-(Al) Ca<sub>2</sub>Al<sub>3</sub>(Si<sub>2</sub>O<sub>7</sub>)(SiO<sub>4</sub>)O(OH)·H<sub>2</sub>O

**Origin:** New Caledonia.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 633 nm He-Ne or 325 nm He-Cd laser radiation. The laser radiation power at the sample was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 1092w, 1015, 1002, 984, 957w, 922, 865, 816, 764w, 696s, 646w, 610, 589, 535, 508s, 480, 459, 429s, 361, 322, 293, 227, 208, 187, 172, 154, 135.

**Source:** Krenn et al. (2004).

**Comments:** The sample was characterized by electron microprobe analyses.

### Pyrargyrite Ag<sub>3</sub>SbS<sub>3</sub>

**Origin:** Jáchymov, Krušné Hory (Ore Mts.), Bohemia, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on a polished crystal using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 1.7 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 323s, 300, 274sh, 252sh.

**Source:** Kharbish et al. (2009).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectra of pyrargyrite see also Byer et al. (1973), Nilges et al. (2002), and Makreski et al. (2004).

### Pyrite FeS<sub>2</sub>

**Origin:** Guinaoang, NW Luzon, Philippines (isotropic variety) and Pine Creek, Northern Territory, Australia (anisotropic variety).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was between 1 and 10 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 446, 387s, 353s (for the isotropic variety); 428, 377s, 342s (for the anisotropic variety).

**Source:** Mernagh and Trudu (1993).

**Comments:** The samples were characterized by electron microprobe analyses. For the Raman spectra of pyrite see also Kleppe and Jephcoat (2004), White (2009), Frezzotti et al. (2012), and Andò and Garzanti (2014).

### Pyroaurite Mg<sub>6</sub>Fe<sup>3+</sup><sub>2</sub>(CO<sub>3</sub>)(OH)<sub>16</sub>·4H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532.12 nm Nd-YAG laser radiation. The laser radiation power at the sample was about 40 mW.

**Raman shifts (cm<sup>-1</sup>):** See comments below.

**Source:** Rozov et al. (2010).

**Comments:** Raman spectra of the members of the hydrotalcite-pyroaurite series containing less than 1 Fe atom per formula unit contain bands at ~3500, ~1380, ~1060 and ~545 cm<sup>-1</sup>. In the spectrum of the sample with the approximate formula Mg<sub>6</sub>(AlFe<sup>3+</sup>)(CO<sub>3</sub>)(OH)<sub>16</sub>·4H<sub>2</sub>O, the only band at ~545 cm<sup>-1</sup> is observed. Measurements with greater Fe contents were precluded by fluorescence.

### Pyrochroite Mn<sup>2+</sup>(OH)<sub>2</sub>

**Origin:** A sediment-hosted Mn deposit, Mesoarchean Mozaan Group, Pongola Supergroup, South Africa.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 635, 330.

**Source:** Ossa et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

### Pyrolusite MnO<sub>2</sub>

**Origin:** Kisenge Mine, Zaire.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 244 nm laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 666w, 610, ~550s, ~525s, 482, 384.

**Source:** Kim and Stair (2004).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of pyrolusite see also Julien et al. (2004).

### Pyromorphite Pb<sub>5</sub>(PO<sub>4</sub>)<sub>3</sub>Cl

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using Nd-YAG laser radiation. The laser radiation power at the sample was 300 mW.

**Source:** Bajda et al. (2011).

**Raman shifts (cm<sup>-1</sup>):** 1047w, 1012w, 984w, 945s, 920s, 813s, 781w, 764sh, 577w, 553, (548), (434w), 411, 392, 334, 324sh.

**Comments:** The empirical formula of the sample used is Pb<sub>5</sub>[(PO<sub>4</sub>)<sub>2.4</sub>(AsO<sub>4</sub>)<sub>0.6</sub>]Cl. The bands in the ranges 750–820 and 320–350 cm<sup>-1</sup> correspond to arsenate groups. For the Raman spectra of pyromorphite see also Levitt and Condrate Sr (1970), Bartholomäi and Klee (1978), Botto et al. (1997), Bouchard and Smith (2003), and Coccato et al. (2016).

### Pyromorphite As-rich Pb<sub>5</sub>(PO<sub>4</sub>,AsO<sub>4</sub>)<sub>3</sub>Cl

**Origin:** Bunker Hill Mine, Kellogg, Idaho, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3444, 3378, 3325, 3291, 3256, 1014, 979, 944, 943, 920, 917, 825, 818, 815s, 776, 768, 573, 549, 433, 414, 409, 391, 388, 377, 344, 339, 318, 206, 186, 177, 152, 111, 105.

**Source:** Frost et al. (2007c).

**Comments:** No independent analytical data are provided for the sample used.

**Pyrope**  $Mg_3Al_2(SiO_4)_3$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a polycrystalline grain using  $Ar^+$  laser radiation. The laser radiation power at the sample was between 5 and 50 mW.**Raman shifts (cm<sup>-1</sup>):** 1064, 928s, 910sh, 868, ~690w, 648, 562, 512w, 492w, 382sh, 364, 340w, 320w, 218w, 210.**Source:** McMillan et al. (1989).**Comments:** The sample was characterized by  $^{27}Al$  MAS NMR spectroscopy. For the Raman spectra of pyrope see also Mingsheng et al. (1994), Kolesov and Geiger (1998), Bersani et al. (2009), Frezzotti et al. (2012), Andò and Garzanti (2014), Gilg and Gast (2015), and Du et al. (2017).**Pyrophanite**  $Mn^{2+}TiO_3$ **Origin:** Perkupa evaporite mine, Bódva valley, inner Western Carpathians, Hungary.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 12 mW.**Raman shifts (cm<sup>-1</sup>):** 684s, ~600w, 466, 360, 334, 263, 235w, 202, 164.**Source:** Zajzon et al. (2013).**Comments:** The sample was characterized by electron microprobe analyses.**Pyrophyllite**  $Al_2Si_4O_{10}(OH)_2$ **Origin:** York Spring, Pennsylvania, USA.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 3670s, 707s, 360, 261s, 193s.**Source:** Wang et al. (2015)**Comments:** Only the strongest Raman bands are indicated in the cited paper. The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectrum of pyrophyllite see also Wada and Kamitakahara (1991).**Pyrosmalite-(Fe)**  $Fe^{2+}_8Si_6O_{15}(OH)_{10}$ **Origin:** Cannington mine, McKinlay Shire, Queensland, Australia.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 1023s, 820, 767w, 740w, 663w, 614s, 468, 365w, 325, 193.**Source:** Dong and Pollard (1997).**Comments:** The sample was characterized by qualitative electron microprobe analysis.**Pyrosmalite-(Mn)**  $Mn^{2+}_8Si_6O_{15}(OH,Cl)_{10}$ **Origin:** A Zn-Pb-Ag sulfide deposit art Dugald River, NW Queensland, Australia.**Experimental details:** Micro-Raman scattering measurements have been performed on an inclusion in quartz using 514.5 nm  $Ar^+$  laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 615s, 696w, 803, 1020.**Source:** Xu (1998).**Comments:** No independent analytical data are provided for the sample used.

**Pyroxmangite** Mn<sup>2+</sup>SiO<sub>3</sub>**Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 532.2 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** ~995s, ~915w, ~810w, ~660s, ~535, ~390, ~307.**Source:** Wang et al. (2001a).**Comments:** No independent analytical data are provided for the sample used. Another sample shows a doublet 965+995 cm<sup>-1</sup>.**Pyrrhotite** Fe<sub>7</sub>S<sub>8</sub>**Origin:** A dolerite sill, Siberian Precambrian platform, eastern Siberia, Russia.**Experimental details:** Micro-Raman scattering measurements have been performed on arbitrarily oriented inclusions in halite using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 372–378s, 339–342.**Source:** Grishina et al. (1992).**Comments:** The samples were characterized by electron microprobe analyses. For the Raman spectrum of pyrrhotite see also Lanteigne et al. (2012).**Qandilite** (Mg,Fe<sup>3+</sup>)<sub>2</sub>(Ti,Fe<sup>3+</sup>,Al)O<sub>4</sub>**Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 20 mW.**Raman shifts (cm<sup>-1</sup>):** 730s, 605w, 517, 387, 325, 272sh, 235sh, 141w.**Source:** De Lima (2016).**Comments:** A Fe-free sample was used. The sample was characterized by powder X-ray diffraction data.**Qingheite** Na<sub>2</sub>MnMgAl(PO<sub>4</sub>)<sub>3</sub>**Origin:** Santa Ana Pegmatite, Totoral pegmatitic field, Coronel Pringles department, San Luis, Argentina.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 1136+1140w (unresolved doublet?), 1130w, 1106w, 1083, 1068w, 1058w, 1047w, 1021, 980s, 964sh, 945sh, 690w, 644w, 606, 572, 504w, 472w, 453w, 420w, 369w, 308w, 280w, 229w, 217w, 167sh, 152w, 143sh.**Source:** Frost et al. (2013d).**Comments:** The sample was characterized by electron microprobe analyses.

**Qingsongite BN****Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powdery sample using 244 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1304, 1055s.**Source:** Reich et al. (2005).**Comments:** The sample was produced from commercial hexagonal BN by nucleation under high pressure (4.2 GPa) and temperature (1800–1900 K) using a MgBN catalyst system.**Quadrividyne** [(Na,K)<sub>6</sub>Cl<sub>2</sub>][Ca<sub>2</sub>Cl<sub>2</sub>][(Si<sub>6</sub>Al<sub>6</sub>O<sub>24</sub>)]**Origin:** Monte Somma caldera, Somma-Vesuvius complex, Napoli, Campania, Italy (type locality).**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** See comments below.**Source:** Binon et al. (2004).**Comments:** In the cited paper only ranges of Raman bands are indicated (2400–3700, 1050–1100, and 980–990 cm<sup>-1</sup>). The precise Raman shifts of quadrividyne are (RRUFF R141084, cm<sup>-1</sup>): 1047s, 985w, 966w, ~757w, 657, 471s, 425, 286 ( $\lambda = 532$  nm).**Quartz** SiO<sub>2</sub>**Origin:** Spruce Claim, King Co., Washington, USA.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 150 mW.**Raman shifts (cm<sup>-1</sup>):** 1231w, 1160w, 1083w, 808w, 697w, 463s, 401w, 354, 263w, 205, 128.**Source:** Jasinevicius (2009).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of quartz see also Hemley (1987a, b), Lepot et al. (2006), Ling et al. (2011), Ciobotă et al. (2012), Frezzotti et al. (2012), and Karwowski et al. (2013).**Quenstedtite** Fe<sup>3+</sup><sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>·11H<sub>2</sub>O**Origin:** Allan Hills 77005 martian meteorite.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532.3 nm Nd-YAG laser radiation. The nominal laser radiation power was  $\leq 6$  mW.**Raman shifts (cm<sup>-1</sup>):** 1130, 1107, 1024s, 985, 614w, 600, 479s, 308, 275s, 247, 157.**Source:** Kuebler (2013b).**Comments:** No independent analytical data are provided for the sample used.**Quetzalcoatlite** Cu<sup>2+</sup><sub>3</sub>Zn<sub>6</sub>Te<sup>6+</sup><sub>2</sub>O<sub>12</sub>(OH)<sub>6</sub>(Ag,Pb,□)Cl**Origin:** Vlue Bell mine, Soda Mts., California, USA (?).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 754sh, 719+693s (unresolved doublet?), 606, 602sh, 477, 403sh, (364w), 319, (248), 197, 141s, 108s.

**Source:** Frost and Dickfos (2009).

**Comments:** No independent analytical data are provided for the sample used.

### Quintinite Mg<sub>4</sub>Al<sub>2</sub>(OH)<sub>12</sub>(CO<sub>3</sub>)·3H<sub>2</sub>O

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3545sh, 3465, 1586w, 1406sh, 1346s, 1061s, 1045sh, 974, 950, 859sh, 722s, 696w, 669, 627sh, 558, 483w, 179sh, 156s.

**Source:** Frost and Dickfos (2007b).

**Comments:** Questionable data: in Figure 2 of the cited paper the band at 1061 cm<sup>-1</sup> (a band of symmetric C–O-stretching vibrations that should be strong for a carbonate) is absent. No independent analytical data are provided for the sample used.

### Quintinite Mg<sub>4</sub>Al<sub>2</sub>(OH)<sub>12</sub>(CO<sub>3</sub>)·3H<sub>2</sub>O

**Origin:** Jacupiranga mine, Cajati, São Paulo, Brazil.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3485, 3334sh, 3078sh, 1698w, 1440w, 1346sh, 1062s, 1046sh, 973, 833w, 698, (684), 559s, 484w, 401w, 367w, 308w, 183sh, 155.

**Source:** Theiss et al. (2015a).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

### Rabejacite Ca<sub>2</sub>[(UO<sub>2</sub>)<sub>4</sub>O<sub>4</sub>(SO<sub>4</sub>)<sub>2</sub>](H<sub>2</sub>O)<sub>8</sub>

**Origin:** Ranger No. 1 deposit, Jabiru, Northern Territory, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3547+3465 (unresolved doublet), 1175w, 1123sh, 1086s, 1010s, 848, 832, ~672, ~620, ~492, ~415, ~245w, ~198, ~181.

**Source:** Frost et al. (2004g).

**Comments:** No independent analytical data are provided for the sample used.

### Raguinitite TlFeS<sub>2</sub>

**Origin:** Crven Dol, Allchar, Roszdan, Republic of Macedonia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 1.9 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 395, 377s, 367, 321, 306, 275, 206w, 190, 166w, 137, 126w, 102w.

**Source:** Makreski et al. (2014).

**Comments:** The sample was characterized by electron microprobe analyses.

### Rajite CuTe<sup>4+</sup><sub>2</sub>O<sub>5</sub>

**Origin:** Lone Pine mine, Catron Co., New Mexico, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** (775), 754s, 731s, 661sh, 652s, 603, 540, 459w, 430, 393w, 318, 299, 267w, 237, 204, 187s, 162, 146s, 127, or 740, 676, 592, 438s, 370, 347, 212.

**Source:** Frost et al. (2008h).

**Comments:** Questionable data. No independent analytical data are provided for the sample used. Two widely different Raman spectra are provided for rajite from New Mexico in the cited paper.

### Ramanite-(Cs) CsB<sub>5</sub>O<sub>6</sub>(OH)<sub>4</sub>·2H<sub>2</sub>O

**Origin:** Island of Elba, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented inclusion in quartz using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was about 30 mW.

**Raman shifts (cm<sup>-1</sup>):** 907, 768, 548s, 462, 293, 98.

**Source:** Thomas et al. (2008).

**Comments:** The sample was characterized by electron microprobe analyses. The peak at 462 cm<sup>-1</sup> is influenced by a strong Raman band of the quartz matrix. For the Raman spectrum of ramanite-(Cs) see also Frezzotti et al. (2012).

### Ramanite-(Rb) RbB<sub>5</sub>O<sub>6</sub>(OH)<sub>4</sub>·2H<sub>2</sub>O

**Origin:** Island of Elba, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented inclusion in quartz using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was about 30 mW.

**Raman shifts (cm<sup>-1</sup>):** 914, 765, 554s, 508, 101.

**Source:** Thomas et al. (2008).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectrum of ramanite-(Rb) see also Frezzotti et al. (2012).

### Rambergite MnS

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation output power was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 473s, 288w, 221.

**Source:** Fernandez et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Rameauite $K_2CaO_8(UO_2)_6 \cdot 9H_2O$

**Origin:** Margnac mine, Compreignac, Haute-Vienne, Limousin, France.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 633 nm He-Ne laser radiation. The laser radiation power at the sample was about 4.5 mW.

**Raman shifts (cm<sup>-1</sup>):** 3450w (broad), 1635w, 813s, 791, 732sh, 578, 453, 363sh, 331, 298, 274, 260sh, 215w, 188, 139, 115w, 78.

**Source:** Plášil et al. (2016b).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data. The crystal structure is solved.

### Ramikite-(Y) $Li_4(Na,Ca)_{12}(Y,Ca,REE)_6Zr_6(PO_4)_{12}(CO_3)_4O_4[(OH),F]_4$

**Origin:** Poudrette (Demix) quarry, Mont Saint-Hilaire, Rouville RCM (Rouville Co.), Montérégie, Québec, Canada (type locality).

**Experimental details:** Raman scattering measurements have been performed from a face of single crystal using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3659w, 1117sh, 1088s, 1042sh, 1000s, 623, 568, 494, 405sh, 370s, 260, 183, 139w.

**Source:** McDonald et al. (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

### Ramsdellite $MnO_2$

**Origin:** An unknown locality in New Mexico, USA.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 12.5 mW. 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 775, 650s, 576s, 523s, 490, 392.

**Source:** Bernard et al. (1993a).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of ramsdellite see also Julien et al. (2004) and Kim and Stair (2004).

### Ranciéite $(Ca,Mn^{2+})_{0.2}(Mn^{4+},Mn^{3+})O_2 \cdot 0.6H_2O$

**Origin:** Xiangguang Mn-Ag deposit, northern China.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 645s, 370w, 304w.

**Source:** Fan et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Rankamaite**  $(\text{Na},\text{K})_3(\text{Ta},\text{Nb},\text{Al})_{11}(\text{O},\text{OH})_{31}$

**Origin:** Urubu pegmatite, Itinga, Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 948w, 876w, 805w, 633s, 328, 275, 239.

**Source:** Atencio et al. (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Rankinite**  $\text{Ca}_3\text{Si}_2\text{O}_7$

**Origin:** Upper Chegem caldera, Kabardino-Balkaria, Northern Caucasus, Russia.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation output power was between 30 and 50 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1048w, 1007, 971, 960, 947w, 891s, 671, 552, 507w, 472w, 450w, 347, 319w, 275w, 245w, 212w, 187, 140w.

**Source:** Galuskin et al. (2011c).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Rapidcreekite**  $\text{Ca}_2(\text{SO}_4)(\text{CO}_3)\cdot 4\text{H}_2\text{O}$

**Origin:** Bahariya depression, Western Desert, Egypt.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was between 20 and 200 mW.

**Raman shifts (cm<sup>-1</sup>):** 1129, 1080s, 1003s, 664, 482, 411.

**Source:** Ciobotă et al. (2012).

**Comments:** No independent analytical data are provided for the sample used.

**Raspite**  $\text{Pb}(\text{WO}_4)$

**Origin:** Broken Hill, Yancowinna Co., New South Wales, Australia.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 6 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 870s, 747, 667w, 645w, 523w, 494w, 395, 300, 282w, 205w, 196sh, 184w.

**Source:** Bastians et al. (2004).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of raspite see also Frost et al. (2004d) and Andrade et al. (2014).

**Rasvumite** KFe<sub>2</sub>S<sub>3</sub>

**Origin:** Miller Range 03346 nakhlite meteorite.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample in a thin section using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 474, 221, 154.

**Source:** Ling and Wang (2015).

**Comments:** The sample was characterized by optical reflectance.

**Ravatite** C<sub>14</sub>H<sub>10</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a single crystal. No other data are provided.

**Raman shifts (cm<sup>-1</sup>):** 3088, 3082, 3071, 3055, 3047, 3033, 3024, 3015, 3003, 1684w, 1660w, 1622, 1613, 1600, 1591, 1570, 1523, 1500w, 1491w, 1481w, 1456w, 1440s, 1429, 1418, 1404, 1377, 1363, 1348s, 1336, 1318, 1303, 1295, 1280, 1244, 1224, 1200, 1170, 1164, 1153, 1140, 1092, 1072w, 1035s, 1000, 972, 968, 950, 944, 875, 860, 829, 817, 791, 760, 753, 734, 713, 710s, 616, 547, 536, 498, 442, 428, 410s, 397, 282, 248s, 234.

**Source:** Godec and Colombo (1976).

**Comments:** For the Raman spectra of raratite see also Witt and Mecke (1967), and Nasdala and Pekov (1993).

**Raygrantite** Pb<sub>10</sub>Zn(SO<sub>4</sub>)<sub>6</sub>(SiO<sub>4</sub>)<sub>2</sub>(OH)<sub>2</sub>

**Origin:** Big Horn Mts., Maricopa Co., Arizona, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm solid-state laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3515, 1075, 1011, 971s, 964s, 907, 876, 838, 832, 613, 597, 463, 452, 437, 325, 250, 231.

**Source:** Yang et al. (2016a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Realgar** AsS

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 647.1 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 376w, 370w, 355s, 345, 341sh, 330w, 222s, 214w, 210w, 196s, 184s, 173w, 167w, 144, 67w, 61, 57, 52, 48, 41w, 28.

**Source:** Muniz-Miranda et al. (1996). For the Raman spectra of realgar see also Forneris (1969), Trentelman et al. (1996), Burgio and Clark (2001), and Frost et al. (2010c).

**Rebulite** Tl<sub>5</sub>Sb<sub>5</sub>As<sub>8</sub>S<sub>22</sub>

**Origin:** Crven Dol, Allchar, Roszdan, Republic of Macedonia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 1.9 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 395, 377s, 321, 306, 275, 206w, 190, 166w, 137, 126w, 102w.

**Source:** Makreski et al. (2014).

**Comments:** The sample was characterized by electron microprobe analyses.

**Reedmergnerite** NaBSi<sub>3</sub>O<sub>8</sub>

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 10 W.

**Raman shifts (cm<sup>-1</sup>):** 584s, 540, 517, 505, 464, 314, 261, 237, 224, 162, 142, 129.

**Source:** Kimata (1993).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of Reedmergnerite see also Manara et al. (2009).

**Reevesite** Ni<sub>6</sub>Fe<sup>3+</sup><sub>2</sub>(CO<sub>3</sub>)(OH)<sub>16</sub>·4H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3598, 3451sh, (3250), 1382, 1163w, 1074s, 832w, 676+621 (broad, unresolved doublet), 550sh, 526, 423, 308, 162sh, 145,

**Source:** Frost et al. (2010d).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of reevesite see also Frost et al. (2003h).

**Reichenbachite** Cu<sub>5</sub>(PO<sub>4</sub>)<sub>2</sub>(OH)<sub>4</sub>

**Origin:** Banská Bystrica, central Slovakia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 17 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3428, 3380, 1120sh, 1083, 1055, 1027w, 998, 971, (951sh), 863, 804, 752, 700w, (636sh), 607, (572sh), 540, 515, 480s, 453, 412sh, 365, 298, 255, 214, 188sh, 175s, 135, 110s, 89.

**Source:** Kharbish et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectra of reichenbachite see also Frost et al. (2002a, 2003a).

**Reinerite**  $\text{Zn}_3(\text{AsO}_3)_2$ 

**Origin:** Tsumeb mine, Tsumeb, Otavi district, Oshikoto, Namibia (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 804, 772, 752s, 722, 658, 297w, 279w, 240w, 219w, 188w, 176w, 152w, 141, 135s.

**Source:** Frost and Bahfenne (2010d).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of reinerite see also Bahfenne (2011).

**Reinhardbraunsite**  $\text{Ca}_5(\text{SiO}_4)_2(\text{OH})_2$ 

**Origin:** Upper Chegem volcanic structure, Northern Caucasus, Kabardino-Balkaria, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented grain using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was below 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 3562, 3532w, 3480, 924, (834sh), 821s, 554, 421, 409sh, 310w, 280w, 253w.

**Source:** Galuskin et al. (2009).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Rengeite**  $\text{Sr}_4\text{Ti}_4\text{ZrO}_8(\text{Si}_2\text{O}_7)_2$ 

**Origin:** Itoigawa region, central Japan.

**Experimental details:** Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 660, 265, 239.

**Source:** Ogawara et al. (2010).

**Retgersite**  $\text{Ni}(\text{SO}_4)\cdot 6\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** (1090w), 983s, 616.

**Source:** Petrova et al. (2012).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of retgersite see also Krishnamurti (1958), Jain et al. (1974), Cancela et al. (1983), and Aramendia et al. (2014).

**Reyerite**  $\text{Na}_2\text{Ca}_{14}\text{Al}_2\text{Si}_{22}\text{O}_{58}(\text{OH})_8\cdot 6\text{H}_2\text{O}$ 

**Origin:** No data.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 488 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was about 25 mW.

**Raman shifts (cm<sup>-1</sup>):** 1172, 1095w, 1078w, 1050, 1021, 907w, 752, 613s, 569s, 352, 300sh, 280s, 202, 169w.

**Source:** De Ferri et al. (2012).

**Comments:** No independent analytical data are provided for the sample used. The Raman shifts were determined by us based on spectral curve analysis of the published spectrum.

### Rhabdophane-(Ce) Ce(PO<sub>4</sub>)·H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was between 5 and 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1088, 1057, 977s, 642, 624, 571, 469s, 417.

**Source:** Assaaoudi et al. (2001).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Rhabdophane-(Nd) Nd(PO<sub>4</sub>)·H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was between 5 and 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1094, 1057, 1033, 983s, 630, 582, 546, 470s, 419.

**Source:** Assaaoudi et al. (2001).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Rheniite ReS<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 633 nm laser radiation. The laser radiation power at the sample was 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 438w, 419w, 407, 378w, 369, 349w, 325, 321, 311w, 308w, 284w, 278w, 237, 217s, 164, 153s, 146, 140w.

**Source:** Feng et al. (2015c).

**Comments:** For the Raman spectrum of rheniite see also Tongay et al. (2014).

### Rhodizite KBe<sub>4</sub>Al<sub>4</sub>(B<sub>11</sub>Be)O<sub>28</sub>

**Origin:** Antsongombato pegmatite, Central Madagascar.

**Experimental details:** Raman spectra were obtained on the dodecahedral and tetrahedral faces. Characteristics of the laser radiation are not indicated.

**Raman shifts (cm<sup>-1</sup>):** 857, 803, 651, 544, 470s, 430s, 294.

**Source:** Laurs et al. (2002).

**Comments:** The sample was characterized by electron microprobe analyses. It contains zones corresponding to rhodizite and londonite. For the Raman spectrum of rhodizite see also Frost et al. (2014a).

**Rhodochrosite** Mn(CO<sub>3</sub>)

**Origin:** Kohlenbachvalley, Eiserfeld, Siegerland, North Rhine-Westphalia, Germany.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1752w, 1439w, 1094s, 726, 293.

**Source:** Buzgar and Apopei (2009).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of rhodochrosite see also Rutt and Nicola (1974), Frezzotti et al. (2012), and Capitani et al. (2014).

**Rhodonite** Mn<sup>2+</sup>SiO<sub>3</sub>

**Origin:** Sverdlovsk region, Urals, Russia.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1038, 996s, 973s, 939w, 910w, 878, 714w, 667s, 557w, 510, 417, 385w, 347sh, 327, 265, 250.

**Source:** Buzatu and Buzgar (2010).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of rhodonite see also Mills et al. (2005), Makreski et al. (2006b), and Can et al. (2011).

**Rhombooclase** (H<sub>5</sub>O<sub>2</sub>)Fe<sup>3+</sup>(SO<sub>4</sub>)<sub>2</sub>·2H<sub>2</sub>O

**Origin:** Coranda-Hondol open pit, Certej Au-Ag deposit, Romania.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 2775w, 2661w, 1456w, 1181, 1081sh, 1028sh, 1014s, 763w, 650sh, 622sh, 603, 472sh, 454, 381, 265sh, 242.

**Source:** Apopei et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of rhombooclase see also Ling and Wang (2010).

**Rhönite** Ca<sub>4</sub>[Mg<sub>8</sub>Fe<sup>3+</sup><sub>2</sub>Ti<sub>2</sub>]O<sub>4</sub>[Si<sub>6</sub>Al<sub>6</sub>O<sub>36</sub>]

**Origin:** Eifel, Germany.

**Experimental details:** Raman scattering measurements have been performed on a arbitrarily oriented grains using 785 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 980, 840, 705, 655s, 535s, 470.

**Source:** Treiman (2008).

**Comments:** No independent analytical data are provided for the sample used.

**Richelsdorffite**  $\text{Ca}_2\text{Cu}_5\text{Sb}^{5+}(\text{AsO}_4)_4(\text{OH})_6\text{Cl}\cdot 6\text{H}_2\text{O}$ 

**Origin:** Wilhelm mine, Bauhaus, Richelsdorf District, Hesse, Germany (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1564w, 1376w, 1082w, 988w, 910sh, 849s, (835), (792), 546, 498sh, 415w, 344, 268sh, 185sh, 144s.

**Source:** Frost et al. (2011c).

**Comments:** No independent analytical data are provided for the sample used.

**Richterite**  $\text{Na}(\text{NaCa})\text{Mg}_5\text{Si}_8\text{O}_{22}(\text{OH})_2$ 

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed in the range from 3500 to 3800 cm<sup>-1</sup> in backscattering geometry, using a 514.5 nm Ar<sup>+</sup> laser. The laser radiation power is not indicated.

**Source:** Leissner et al. (2015).

**Raman shifts (cm<sup>-1</sup>):** 3730, 3712sh.

**Comments:** The sample was characterized by EMPA and ICP-MS.

**Riebeckite**  $\square\text{Na}_2(\text{Fe}^{2+}_3\text{Fe}^{3+}_2)\text{Si}_8\text{O}_{22}(\text{OH})_2$ 

**Origin:** Iacobdeal, Dobrogea, Romania.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1084, 980sh, 966s, 885, 666s, 576, 537s, 431w, 363, 325, 244w, 222sh, 198s, 171s, 140.

**Source:** Apopei et al. (2011).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of riebeckite see also Apopei and Buzgar (2010).

**Riebeckite (Crocidolite)**  $\square\text{Na}_2(\text{Fe}^{2+}_3\text{Fe}^{3+}_2)\text{Si}_8\text{O}_{22}(\text{OH})_2$ 

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an unoriented fibrous aggregate using 632.8 nm He-Ne laser radiation. The laser radiation power was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 1082s, 1030, 967s, 889, 771w, 733w, 664s, 577s, 537, 506sh, 470sh, 428, 374, 360sh, 331, 300, 272, 246, 211, 195, 162s.

**Source:** Rinaudo et al. (2004).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectra of crocidolite see also Petry et al. (2006) and Croce et al. (2013).

**Rimkorolgite** BaMg<sub>5</sub>(PO<sub>4</sub>)<sub>4</sub>·8H<sub>2</sub>O

**Origin:** Zheleznyi (Iron) mine, Kovdor massif, Kola Peninsula, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** (3444), 3272 (broad), (2991), 2913, 2859, 1492sh, 1480, 1467, 1455, 1436, 1236, 1135, 1105, 1073sh, 1052, (1035), 1016, (992), 975+964s (unresolved doublet?), (951), 930, 653sh, 622sh, 599, 570, 511, (485), 472, 439, 426, 373, 279, 262+252 (unresolved doublet?), 222, 195w, 159+146 (unresolved doublet?), 109.

**Source:** Frost et al. (2014h).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

**Ringwoodite** Mg<sub>2</sub>(SiO<sub>4</sub>)

**Origin:** Grove Mountains 052049 meteorite.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented grains in polished sections using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 841–849, 783–796, 285–296.

**Source:** Feng et al. (2011).

**Comments:** The samples were characterized by electron microprobe analyses. As the fayalite content increases from 27.8 to 81.6 mol %, the bands at 783–796 and 285–296 cm<sup>-1</sup> shift towards lower frequencies, whereas the band at 841–849 cm<sup>-1</sup> does not show significant correlation with the fayalite content. For the Raman spectrum of ringwoodite see also Akaogi et al. (1984).

**Rinkite** TiNa<sub>2</sub>Ca<sub>4</sub>REE(Si<sub>2</sub>O<sub>7</sub>)<sub>2</sub>OF<sub>3</sub>

**Origin:** Khibiny massif, Kola Peninsula, Russia.

**Experimental details:** Raman scattering measurements have been performed on an annealed metamict sample using 632.8 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~960, ~460.

**Source:** Zubko et al. (2013).

**Riomarinaite** Bi(SO<sub>4</sub>)(OH)·H<sub>2</sub>O

**Origin:** No data.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** ~1190w, ~1160w, ~1095w, ~1002, ~960s, ~630, ~525, ~402w, ~198s.

**Source:** Capitani et al. (2014).

**Comments:** No independent analytical data are provided for the sample used.

**Robertsrite** Ca<sub>2</sub>Mn<sup>3+</sup><sub>3</sub>O<sub>2</sub>(PO<sub>4</sub>)<sub>3</sub>·3H<sub>2</sub>O

**Origin:** Tip Top mine, Custer Co., South Dakota, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~1187s, 1036, 947, 625s, 552, 497, 385, 289s.

**Source:** Andrade et al. (2012).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data. The crystal structure is solved.

### Robinsonite Pb<sub>4</sub>Sb<sub>6</sub>S<sub>13</sub>

**Origin:** Zlatá Baňa, Slanské Vrchy Mts., central Slovakia.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample in the spectral region from 10 to 600 cm<sup>-1</sup> using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 337sh, 328, 314, 308, 249sh, 228sh, 209s, 188sh, 168, 149, 133, 111sh, 101, 91sh, 75w.

**Source:** Kharbish and Jeleň (2016).

**Comments:** The sample was characterized by electron microprobe analyses. The empirical formula of the sample used is Pb<sub>4.01</sub>Sb<sub>5.99</sub>S<sub>13.00</sub>.

### Rockbridgeite Fe<sup>2+</sup>Fe<sup>3+</sup><sub>4</sub>(PO<sub>4</sub>)<sub>3</sub>(OH)<sub>5</sub>

**Origin:** Galileia region, Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on a radiated aggregate using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 1186, 1137, 1061s, 981, 937, 638, 616, 576, 463, 382, 333s, 299, 241.

**Source:** Faulstich et al. (2013).

**Comments:** The sample was characterized by electron microprobe analyses.

### Rodalquilarite H<sub>3</sub>Fe<sup>3+</sup><sub>2</sub>(Te<sup>4+</sup>O<sub>3</sub>)<sub>4</sub>Cl

**Origin:** Grand Central Mines, Tombstone, Cochise Co., Arizona, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** (2998), 2870+2796 (unresolved doublet?), 2341, 781, 756sh, 725, 660sh, 641s, 612s, (599), 473, 449, 412, 400sh, 345s, 321s, (312), 233, 191, 179, 142, 110.

**Source:** Frost and Keeffe (2009i).

**Comments:** No independent analytical data are provided for the sample used.

### Rodolicoite Fe<sup>3+</sup>(PO<sub>4</sub>)

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 150 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1018s, 436, 415, 390, 336, 280, 199, 161.

**Source:** Murli et al. (1997).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of rodolicoite see also Bhalerao et al. (2012).

### Rokühnite $\text{FeCl}_2 \cdot 2\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed at 10 K on a single crystal using 514.5 nm  $\text{Ar}^+$  laser radiation, with the incident beam parallel to the *c*-axis. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 747w, 717w, 661sh, 640.5s, 594s, 552w, 501, 375, 202s, 196s, 146, 141w, 33.7, 30.6s.

**Source:** Graf and Schaack (1976).

**Comments:** For the Raman spectrum of rokühnite see also Graf (1978).

### Romanèchite $(\text{Ba},\text{H}_2\text{O})_2(\text{Mn}^{4+},\text{Mn}^{3+})_5\text{O}_{10}$

**Origin:** Bahariya depression, Western Desert, Egypt.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily sample using a 532 nm Nd-YAG laser. The laser radiation power at the sample was 20 to 200  $\mu\text{W}$ .

**Source:** Ciobotă et al. (2012).

**Raman shifts (cm<sup>-1</sup>):** ~1300, ~1100w, 644sh, 583s, ~500sh, ~390.

**Comments:** No independent analytical data are given for the sample used. For the Raman spectra of romanèchite see also Julien et al. (2003, 2004).

### Romanorlovite $\text{K}_8\text{Cu}_6\text{Cl}_{17}(\text{OH})_3$

**Origin:** Second scoria cone, Northern Breakthrough of the Great Tolbachik Fissure Eruption, Tolbachik, Kamchatka, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 532 nm laser radiation. The laser radiation output was 3 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3512w, 3440w, 931w, 879w, 548, 477, 264s, 178s.

**Source:** Pekov et al. (2016b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### Romarchite $\text{SnO}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a arbitrarily oriented particles using 785 nm laser radiation. The laser radiation power at the sample was ~200 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 210, 240.

**Source:** Chen and Grandbois (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Römerite**  $\text{Fe}^{2+}\text{Fe}^{3+}_2(\text{SO}_4)_4 \cdot 14\text{H}_2\text{O}$ 

**Origin:** Medvedza lens, Košice-Bankov magnesite deposit, Slovak Republic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3465sh, 3340, 3235, 3029, 1642w, 1164, 1117, 1058, 1035s, 1012s, 999, 733w, 650, 608, 472, 447, 399, 278+264 (unresolved doublet?), 231, 173, 145.

**Source:** Frost et al. (2011f).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Rondorfite**  $\text{Ca}_8\text{Mg}(\text{SiO}_4)_4\text{Cl}_2$ 

**Origin:** Upper Chegem caldera, Kabardino-Balkaria, Northern Caucasus, Russia.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation output power was between 30 and 50 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** ~1000w, ~975, ~950w, ~920w, ~862s, ~820, ~570, ~520, ~415w, ~385, ~330w, ~263.

**Source:** Galuskin et al. (2013a).

**Comments:** The sample was characterized by electron microprobe analyses.

**Rongibbsite**  $\text{Pb}_2(\text{Si}_4\text{Al})\text{O}_{11}(\text{OH})$ 

**Origin:** Big Horn Mts., Maricopa Co., Arizona, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3525s, 3430s, 962, 630sh, 602, 488, 453, 422, 372, 283, 258, 196s.

**Source:** Yang et al. (2013a).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Ronneburgite**  $\text{K}_2\text{MnV}_4\text{O}_{12}$ 

**Origin:** Ronneburg, Thuringia, Germany (type locality).

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 676 nm Kr<sup>+</sup> laser radiation. The laser radiation power was 1.5 mW.

**Raman shifts (cm<sup>-1</sup>):** 952s, 911, 878, 830, 658w, 461, 350, 336, 261.

**Source:** Witzke et al. (2001).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Rooseveltite** Bi(AsO<sub>4</sub>)**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 514.5 nm Ar<sup>+</sup> laser radiation.**Raman shifts (cm<sup>-1</sup>):** 841s, 795, 768, 425, 413, 386, 346s, 333sh, 276, 221.**Source:** Roncaglia et al. (1993).**Comments:** The sample was obtained by slow addition of diluted arsenic acid to a diluted stoichiometric Bi(NO<sub>3</sub>)<sub>3</sub>·5H<sub>2</sub>O solution and subsequent heating of the precipitated material at 600 °C during 12 h. The purity was checked by chemical analysis and powder X-ray diffractometry.**Roquesite** CuInS<sub>2</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 340sh, 298, 240sh.**Source:** Dutková et al. (2016).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of roquesite see also Ho et al. (2012).**Rosasite** CuZn(CO<sub>3</sub>)(OH)<sub>2</sub>**Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 632.8 nm He-Ne laser 30 mW. The laser radiation power at source reduced considerably by various filters.**Raman shifts (cm<sup>-1</sup>):** 3470, 3422w, 3232, 1540, 1514, 1453, 1086s, 1060, 843, 833w, 702, 508, 482w, 409, 390w, 332, 308w, 231, 208w, 193s, 146s, 126.**Source:** Bouchard and Smith (2003).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of rosasite see also Frost (2006) and Rotondo et al. (2012).**Roselite** Ca<sub>2</sub>Co(AsO<sub>4</sub>)<sub>2</sub>·2H<sub>2</sub>O**Origin:** Bou Azzer, Morocco.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3450, 3208, (3121), 3042, 1688, 1611, 1118, 976, 909, 864, (800), 798, 719, 659, 653, 540, 463, 440, 399, 373, 338, 307, 264, 243, 211, 197, 179, 155, 117.**Source:** Frost (2009a).**Comments:** No independent analytical data are provided for the sample used. Intensities of the bands are not indicated.

**Rosiaite** PbSb<sub>2</sub>O<sub>6</sub>**Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Diffusion Raman scattering measurements have been performed using 488 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 600 mW.**Raman shifts (cm<sup>-1</sup>):** 670s, 510, 498w, 318, 278w, 211.**Source:** Vandeborre et al. (1980).**Comments:** The sample was characterized by powder X-ray diffraction data.**Rostite** Al(SO<sub>4</sub>)(OH)·5H<sub>2</sub>O**Origin:** Le Cetine mine, Rosia, Chiusdino, Siena, Italy.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3295sh, (3222), 3155, 3082, (2948), (2764), 1692, 1605w, 1390w, 1312, 1227, (1145w), 1131, (1093w), 1083, (1070w), (998), 991s, (986), 939w, 874w, 854sh, 632, 620, 590, 570, 530w, 504, 434sh, 420, 340w, 319sh, 307sh, 295, 281sh, 216, 203sh, 169.**Source:** Frost et al. (2015x).**Comments:** The sample was characterized by qualitative electron microprobe analysis.**Rouaite** Cu<sub>2</sub>(NO<sub>3</sub>)(OH)<sub>3</sub>**Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 785 nm laser radiation. The laser radiation was 3 mW.**Raman shifts (cm<sup>-1</sup>):** 1423, 1321, 1047s, 714, 500.5, 456, 408, 331, 255.**Source:** Nytko et al. (2008).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of rouaite see also Nytko (2008).**Roumaite** (Nb,Ti)(Ca,Na, $\square$ )<sub>3</sub>(Ca,*REE*)<sub>4</sub>(Si<sub>2</sub>O<sub>7</sub>)<sub>2</sub>(OH)F<sub>3</sub>**Origin:** Rouma Island, Los Archipelago, Guinea (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated. A nearly 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 1582w (broad).**Source:** Biagioni et al. (2010).**Comments:** The Raman spectrum shows important contributions of fluorescence effects related to the presence of *REE*, which does not allow an accurate study of the region above 3000 cm<sup>-1</sup>. No data on the Raman spectrum below 1582 cm<sup>-1</sup> are provided.

**Rowleyite**  $[\text{Na}(\text{NH}_4,\text{K})_9\text{Cl}_4][(\text{V}^{5+},\text{V}^{4+})_2(\text{P},\text{As})\text{O}_8]_6 \cdot n[\text{H}_2\text{O},\text{Na},\text{NH}_4,\text{K},\text{Cl}]$ 

**Origin:** Rowley mine, about 100 km SW of Phoenix, Arizona, USA (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The nominal laser radiation power was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** ~1340, 1065w, 1002, 980, 825s, 683w, 565w, 460w, 325s, 280s, 180.

**Source:** Kampf et al. (2017b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Roxbyite** Cu<sub>9</sub>S<sub>5</sub>

**Origin:** Synthetic.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 466s, 259w.

**Source:** Kumar and Nagarajan (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Rozenite** Fe<sup>2+</sup>(SO<sub>4</sub>)·4H<sub>2</sub>O

**Origin:** Coranda-Hondol open pit, Certej Au-Ag deposit, Romania.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 3388, 3329sh, 3261sh, 1594w, 1176sh, 1149w, 1098sh, 1073w, 992s, 658sh, 612w, 480, 461sh, 383w, 284w, 239sh.

**Source:** Apopei et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectra of rozenite see also Chio et al. (2007), Buzatu et al. (2012, 2016), Jentzsch et al. (2013), Aramendia et al. (2014), and Kompanchenko et al. (2016).

**Ruffite** Ca<sub>2</sub>Cu(AsO<sub>4</sub>)<sub>2</sub>·2H<sub>2</sub>O

**Origin:** Maria Catalina mine, Tierra Amarilla, Chile (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 532 nm solid-state laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3335w (broad), 3147w (broad), 866w, 839s, 803w, 715w, 485w, 451w, 426w, 335, 294.

**Source:** Yang et al. (2011a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Rucklidgeite** PbBi<sub>2</sub>Te<sub>4</sub>

**Origin:** Ozernyi district, Salla-Kuolajarvi, Kola Peninsula, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 127, 102s, 57.

**Source:** Voloshin et al. (2015a).

**Comments:** The sample was characterized by electron microprobe analyses.

**Rudashevskyite** (Fe,Zn)S

**Origin:** Indarch meteorite (an EH4 enstatite chondrite).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented grains using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 1.2 mW.

**Raman shifts (cm<sup>-1</sup>):** ~460w, ~317s.

**Source:** Ma et al. (2012a).

**Comments:** No independent analytical data are provided for the sample used.

**Ruizite** Ca<sub>2</sub>Mn<sup>3+</sup><sub>2</sub>Si<sub>4</sub>O<sub>11</sub>(OH)<sub>4</sub>·2H<sub>2</sub>O

**Origin:** Wessels mine, Hotazel, Kalahari Manganese Field, Northern Cape Province, South Africa.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was 150 mW.

**Raman shifts (cm<sup>-1</sup>):** ~3578, ~3355w, ~3235w, ~2942, 924s, 727w, 639, 571s, 506w, 477, 433, 411, 364, 288, 256, 220, 180.

**Source:** Fendrich et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Rusinovite** Ca<sub>10</sub>(Si<sub>2</sub>O<sub>7</sub>)<sub>3</sub>Cl<sub>2</sub>

**Origin:** Upper Chegem caldera, Kabardino-Balkaria, northern Caucasus, Russia (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation output power was between 30 and 50 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1074w, 1036, 994w, 968w, 900s, 869, 830w, 652, 635, 568w, 549w, 528w, 430w, 409w, 365, 325w, 295w, 282w, 232w, 125w.

**Source:** Galuskin et al. (2011c).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Russellite** Bi<sub>2</sub>WO<sub>6</sub>

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 785 nm Nd-YAG laser. The laser radiation power at the sample was 1 mW.

**Raman shifts (cm<sup>-1</sup>):** 844, 795, 716, 667, 405, 349, 324, 284, 263

**Source:** Frost et al. (2004d).

**Comments:** No independent analytical data are provided for the sample used.

**Rustumite**  $\text{Ca}_{10}(\text{Si}_2\text{O}_7)_2(\text{SiO}_4)(\text{OH})_2\text{Cl}_2$

**Origin:** Upper Chegem Caldera, Northern Caucasus, Russia.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation output power was between 30 and 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 3632w, 3585, 1056w, 1004, 914s, 868w, 812, 648, 556w, 538w, 381, 335w.

**Source:** Gfeller et al. (2013).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Rutherfordine**  $(\text{UO}_2)(\text{CO}_3)$

**Origin:** Sierra Albarrana, Córdoba, Spain.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632.8 nm He-Ne laser radiation. The laser radiation output power was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 1120, 889s, 833, 789w, 220w, 162, 142.

**Source:** Bonales et al. (2015).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectra of rutherfordine see also Frost and Čejka (2009b) and Bonales et al. (2016).

**Rutile**  $\text{TiO}_2$

**Origin:** Santa Benedetta, Canavese, Italy.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne or 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 611s, 441s, 242, 142w.

**Source:** Andò and Garzanti (2014).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of rutile see also Balachandran and Eror (1982).

**Rynersonite**  $\text{CaTa}_2\text{O}_6$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a single crystal fiber using 633 nm He-Ne laser radiation. The laser radiation power at the sample was 6 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 690s, 654, 632w, 556w, 475, 342, 285, 243, 236, 175, 167, 151, 88s (with laser beam parallel to the fiber).

**Source:** Almeida et al. (2014).

**Sabugalite**  $\text{HAl}(\text{UO}_2)_4(\text{PO}_4)_4 \cdot 16\text{H}_2\text{O}$ **Origin:** No data.**Experimental details:** Raman scattering measurements have been performed at different temperatures on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 1008, 984, 970, 848, 826s, 806 (for the spectrum obtained at 40°C).**Source:** Frost et al. (2005k).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of sabugalite see also Frost and Weier (2004c).**Sahlinite**  $\text{Pb}_{14}\text{O}_9(\text{AsO}_4)_2\text{Cl}_4$ **Origin:** Långban, near Pajsberg and Filipstad, Värmland, Sweden (type locality).**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 20 mW.**Raman shifts (cm<sup>-1</sup>):** 3526w, 819s, 806s.**Source:** Jonsson (2003).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.**Sailaufite**  $(\text{Ca},\text{Na},\square)_2\text{Mn}^{3+}_3\text{O}_2(\text{AsO}_4)_2(\text{CO}_3)\cdot 3\text{H}_2\text{O}$ **Origin:** Hartkoppe hill, Ober-Sailauf, Spessart Mts., Germany (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 633 nm He-Ne laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** See comment below.**Source:** Wildner et al. (2003).**Comments:** The authors of the cited paper write: “Bands or band components observed in the IR- or Raman spectra around 730, 880, 1120, and 1420 cm<sup>-1</sup> can be assigned to . . . vibrational modes of the two different CO<sub>3</sub> groups.” However these bands could be assigned only to a single CO<sub>3</sub> group. Moreover, Raman spectrum of sailaufite is not given by Wildner et al. (2003). The bands at 730, 880, and 1420 cm<sup>-1</sup> can correspond to admixed Mn-bearing dolomite that is present in association with sailaufite.**Sakhaite**  $\text{Ca}_{48}\text{Mg}_{16}\text{Al}(\text{SiO}_3\text{OH})_4(\text{CO}_3)_{16}(\text{BO}_3)_{28}\cdot(\text{H}_2\text{O})_3(\text{HCl})_3$ **Origin:** Titovskoe, Sakha (Yakutia) Republic, Russia (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3546, 3391, 2897, 1727, 1703w, 1560w, 1524w, 1479, 1349w, 1312w, 1218, 1167sh, 1134+1123s (unresolved doublet?), 968s, 950sh, 855w, 737sh, 725, 651, 627, 396w, 310, 211, 156, (132).**Source:** Frost and Xi (2012j).**Comments:** No independent analytical data are provided for the sample used.

**Salammoniac** NH<sub>4</sub>Cl

**Origin:** Burning coal wastepile materials, Douro coalfield, Portugal.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** ~3120s, ~3050s, ~2807, (~2500 broad), (~2020 broad), ~1760, ~1705, ~1500, ~1400.

**Source:** Ribeiro et al. (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data to

**Saléeite** Mg(UO<sub>2</sub>)<sub>2</sub>(PO<sub>4</sub>)<sub>2</sub>·10H<sub>2</sub>O

**Origin:** East Alligator River, Northern Territory, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using 647.1 nm Kr<sup>+</sup> and 785 diode laser radiations. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 999s, 837s, 405, 284w, 194.

**Source:** Faulques et al. (2015a, b).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of saléeite see also Frost (2004b) and Frost and Weier (2004c).

**Samarskite-(Y)** (Y,Ce,U,Fe,Nb)(Nb,Ta,Ti)O<sub>4</sub>

**Origin:** Beinmyr pegmatite, Landås, Iveland, Aust-Agder, Norway.

**Experimental details:** Raman scattering measurements have been performed on a metamict sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** ~785s (broad), ~620 (broad), ~230sh (for a metamict sample); ~795, ~670s, ~535, ~417, ~360s, ~335s, ~230s, ~190s, ~115 (for a sample recrystallised in air at 1000°C.)

**Source:** Tomašić et al. (2010).

**Comments:** The sample was characterized by electron microprobe analyses.

**Sampleite** NaCaCu<sub>5</sub>(PO<sub>4</sub>)<sub>4</sub>Cl·5H<sub>2</sub>O

**Origin:** Northparkes mine, Goonumbla, New South Wales, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1269, 1152, 1088, (1016), 997s, 962s, 924sh, 643s, 604, 591, 557, 455s, 356, 282, 224, 190, 172.

**Source:** Frost et al. (2007m).

**Comments:** No independent analytical data are provided for the sample used.

**Sanderite** Mg(SO<sub>4</sub>)·2H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 15 mW.

**Raman shifts (cm<sup>-1</sup>):** 3539, 3446s, 1647, 1164, 1034s, 630w, 597w, 492w, 447, 266.

**Source:** Wang et al. (2006a).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of sanderite see also Frezzotti et al. (2012) and Brotton and Kaiser (2013).

### Sanguite KCuCl<sub>3</sub>

**Origin:** Glavnaya Tenoritovaya fumarole, Second scoria cone, Tolbachik volcano, Kamchatka, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power at the sample was 3 mW.

**Raman shifts (cm<sup>-1</sup>):** 547, 296sh, 272, 192s, 137, 117.

**Source:** Pekov et al. (2015a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. For the Raman spectrum of sanguite see also Choi et al. (2005).

### Sanidine K(AlSi<sub>3</sub>O<sub>8</sub>)

**Origin:** Zvegor, Republic of Macedonia.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 1117w, 1040w, 515s, 473, 450w, 406w, 379w, 338w, 283, 264w, 225w, 198w, 160, 122w, 108w.

**Source:** Makreski et al. (2009).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis. For the Raman spectra of sanidine see also Matson et al. (1986), Edwards et al. (2004), and Frezzotti et al. (2012).

### Sanjuanite Al<sub>2</sub>(PO<sub>4</sub>)(SO<sub>4</sub>)(OH)·9H<sub>2</sub>O

**Origin:** Chica de Zonda, San Juan province, Argentina (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3575, 3509, 3406, (3330), 3152+3090 (unresolved doublet?), 1457w, 1438, 1305w, 1148w, 1102, 1037, 984s, 609, 523w, 466, 430, 400w, 365sh, 351, 337sh, 218w, 197+184 (unresolved doublet?), (152), 142, 108.

**Source:** Frost and Palmer (2011h).

**Comments:** No independent analytical data are provided for the sample used.

### Sanmartinite Zn(WO<sub>4</sub>)

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 904s, ~180, 705, 675, ~540, ~510w, ~340, 273, ~180.

**Source:** Kloprogge et al. (2004b).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of sanmartinite see also Errandonea et al. (2008).

**Santabarbaraite**  $\text{Fe}^{3+}_3(\text{PO}_4)_2(\text{OH})_3 \cdot 5\text{H}_2\text{O}$

**Origin:** Santa Barbara mine, Tuscany, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** (3541), 3435, 3266sh, 1634, (1549), 1095sh, 1007s, 630sh, 592, 561sh, 478, 431sh, (318), 272, 221sh, (197), (159), 145, 111.

**Source:** Frost et al. (2016c).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

**Santarosaite**  $\text{CuB}_2\text{O}_4$

**Origin:** Santa Rosa mine, Atacama desert, Chile (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~1110, ~1010, ~872s, ~775, ~745w, ~702, ~472, ~320, ~170w, (~70), (~60), (~30).

**Source:** Schlüter et al. (2008).

**Comments:** The sample was characterized by powder X-ray diffraction data, electron microprobe analyses and electron energy loss spectroscopy.

**Santite**  $\text{KB}_5\text{O}_6(\text{OH})_4 \cdot 2\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 918s, 780–785w, 765–766, 556–557s, 510, 457, 369w, 296–299.

**Source:** Asensio et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Saponite**  $(\text{Ca},\text{Na})_{0.3}(\text{Mg},\text{Fe})_3(\text{Si},\text{Al})_4\text{O}_{10}(\text{OH})_2 \cdot 4\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdery sample using 1064 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1082, 1051w, 998, 918w, 778, 683s, (660), 464–550, 432, 360s, 340sh, 288, 265w, 229w, 202.

**Source:** Kloprogge and Frost (2000c).

**Comments:** The Raman shifts are given for a Na-saturated sample. For the Raman spectrum of saponite see also Wang et al. (1999).

**Sarcopside**  $\text{Fe}^{2+}_3(\text{PO}_4)_2$ 

**Origin:** Sowie Góry Mts., Lower Silesia, southwestern Poland.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1109w, 1078, 1039, 1021w, 974s, 930s, 624, 606w, 553, 478, 400, 284w.

**Source:** Łodziński and Sitarz (2009).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectrum of sarcopside see also Schneider et al. (2013).

**Sarkinite**  $\text{Mn}^{2+}_2(\text{AsO}_4)(\text{OH})$ 

**Origin:** Långban deposit, Bergslagen ore region, Filipstad district, Värmland, Sweden.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3550, 3535, 3528, 3519, 888, 839s, 826sh, 475, 380, 325.

**Source:** Makreski et al. (2013a).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of sarkinite see also Hålenius and Westlund (1998).

**Sarmientite**  $\text{Fe}^{3+}_2(\text{AsO}_4)(\text{SO}_4)(\text{OH}) \cdot 5\text{H}_2\text{O}$ 

**Origin:** Santa Elena mine, San Juan province, Argentina (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3482w, 3336sh, 3184w, 1614w, 1130sh, 1118w, 1081, 998s, 889, 868, 818s, 638w, (590), 570, 477, 444, 405, 370, 322, 294, 259, 202, 191.

**Source:** Colombo et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Sartorite**  $\text{PbAs}_2\text{S}_4$ 

**Origin:** Binntal, Switzerland.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed in the spectral region from 50 to 600 cm<sup>-1</sup> using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 375sh, 363s, 352sh, 336, 318sh, 300s, 281sh, 259sh, 229, 204w, 178, 167sh, 123w, 101w, 91, 85w, 75sh.

**Source:** Kharbish (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Sassolite**  $\text{B}(\text{OH})_3$ **Origin:** Synthetic.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** ~1160w, 880s, 499, ~205.**Source:** Peretyazhko et al. (2000).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of sassolite see also Thomas (2002), Michel et al. (2007), Thomas and Davidson (2010), and Frezzotti et al. (2012).**Scacchite**  $\text{MnCl}_2$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a single crystal with laser beam directed along the *c* axis of the crystal and the scattered light at approximately 90° with respect to the incident beam. 488 and 514.5 nm Ar<sup>+</sup>/Kr<sup>+</sup> laser radiations were used. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 234s, 144.**Source:** Piseri and Pollini (1984).**Comments:** No independent analytical data are provided for the sample used.**Schafarzikite**  $\text{Fe}^{2+}(\text{Sb}^{3+})_2\text{O}_4$ **Origin:** Pernek, Malé Karpaty Mts., Slovak Republic (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 633 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** (709w), 668s, 617sh, 558w, 526, (479w), 465, 403w, 353, (345w), 295, 249w, 219, 186w, 159, 132w, 119, 107.**Source:** Bahfenne (2011).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of schafarzikite see also Sejkora et al. (2007) and Kharbish (2012).**Scheelite**  $\text{Ca}(\text{WO}_4)$ **Origin:** Lodrino, Riviera, Ticino (Tessin), Switzerland.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne or 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 913s, 841w, 799w, 399, 332, 210.**Source:** Andò and Garzanti (2014).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of scheelite see also Frost et al. (2004d) and Kloprogge et al. (2004b).**Schiavinatoite**  $\text{Nb}(\text{BO}_4)$ **Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 488 and 514.5 nm Ar<sup>+</sup> laser radiations. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 986, 956s, 880, 815, 710w, 544s, 433, ~310w, 252, 235s.

**Source:** Heyns et al. (1990).

**Comments:** No independent analytical data are provided for the sample used.

**Schlossmacherite**  $(\text{H}_3\text{O})\text{Al}_3(\text{SO}_4)_2(\text{OH})_6$

**Origin:** Emma Luisa Au, Guanaco district, Antofagasta, Chile (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power at the sample was 0.1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3537, 3449w, 3410, (3382), (3363), 2918, 1868, (2850), 1651sh, 1590w, 1458 +1442 (unresolved doublet?), 1304w, 1139w, 1082w, 1031w, 1000w, 938sh, 915, 864s, 819+809s (unresolved doublet?), 601w, 513, 459sh, 437s, 392, 358, 338sh, 312, 297, 263, 224, 203, 184sh, 147.

**Source:** Frost et al. (2012c).

**Comments:** No independent analytical data are provided for the sample used.

**Schmiederite**  $\text{Cu}_2\text{Pb}_2(\text{Se}^{4+}\text{O}_3)(\text{Se}^{6+}\text{O}_4)(\text{OH})_4$

**Origin:** El Dragon mine, Potosí, Bolivia (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3428, (1919w), 1852w, 1604, 1576, 1457w, 1418, 1349w, 1095s, 934, 834, 764, 739w, 538w, 398s, 281, 247s, 178, 153, 139s.

**Source:** Frost and Keeffe (2008a).

**Comments:** No independent analytical data are provided for the sample used.

**Schmitterite**  $(\text{UO}_2)(\text{Te}^{4+}\text{O}_3)$

**Origin:** Ozernyi district, Salla-Kuolajarvi, Kola Peninsula, Russia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser power was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 1102, 1091, 882s, 849, 796, 406sh, 391, 323, 304w, 204w, 176w, 141, 122w, 111.

**Source:** Voloshin et al. (2015b).

**Comments:** The sample was characterized electron microprobe analyses. For the Raman spectrum of schmitterite see also Frost et al. (2006b).

**Schneiderhöhnite**  $\text{Fe}^{2+}\text{Fe}^{3+}_3\text{As}^{3+}_5\text{O}_{13}$

**Origin:** Urucum mine, Doce River, Galileia, Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts

have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 382w, 370w, 353sh, 345, 318, 295s, 279, 259sh, 247s, 219sh, 214w, 198, (193), 184s, 164, 148, 141, 122w, 117.

**Source:** Bahfenne and Frost (2009).

**Comments:** No independent analytical data are provided for the sample used.

### Schoenfliesite MgSn(OH)<sub>6</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 632.8 nm He-Ne laser radiation. The laser power was varied between 1.94 and 0.07 mW.

**Raman shifts (cm<sup>-1</sup>):** 980, 602s, ~460w, ~365w, 289.

**Source:** Barchiche et al. (2008).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Schoepite (UO<sub>2</sub>)<sub>8</sub>O<sub>2</sub>(OH)<sub>12</sub>·12H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm diode laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 829s, 805sh, 746w, 551, 454, 438, 337, 260, 208.

**Source:** Stefaniak et al. (2008).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of schoepite see also Amme et al. (2002) and Frost et al. (2007h).

### Scholzite CaZn<sub>2</sub>(PO<sub>4</sub>)<sub>2</sub>·2H<sub>2</sub>O

**Origin:** Reaphook Hill, Martins Well, South Flinders Ranges, South Australia, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power at the sample was 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3437, 3343, 3283, 3185sh, 1171, 1115, 1088w, 1053w, 1026w, 1000s, (935), 923.

**Source:** Frost (2004a).

**Comments:** No independent analytical data are provided for the sample used. Raman shifts below 900 cm<sup>-1</sup> are not indicated.

### Schorl NaFe<sup>2+</sup><sub>3</sub>Al<sub>6</sub>(Si<sub>6</sub>O<sub>18</sub>)(BO<sub>3</sub>)<sub>3</sub>(OH)<sub>3</sub>(OH)

**Origin:** Bonče, Prilep municipality, Republic of Macedonia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1066s, 980, 806, 784, 770, 705, 672, 536w, 369s, 314w, 239s, 217.

**Source:** Makreski and Jovanovski (2009).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectra of schorl see also Ertl et al. (2015) and Watenphul et al. (2016a, b).

**Schorlomite**  $\text{Ca}_3\text{Ti}_2(\text{SiFe}^{3+})_2\text{O}_{12}$

**Origin:** Wiluy River, Sakha-Yakutia, Russia.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 946–952, 785–786, 728–739, 639–641w, 508–510s, 431–435, 340–350s, 295sh, 253–256, 212–219w, 157w.

**Source:** Galuskina et al. (2005).

**Comments:** A schorlomite variety enriched in Zr and Sc was used. The sample was characterized by electron microprobe analyses.

**Schreibersite** (Fe,Ni)<sub>3</sub>P

**Origin:** Almahatta Sitta meteorite.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 22.5 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** ~650s, ~510, ~410s, ~395s, ~300s, ~220.

**Source:** Kaliwoda et al. (2013).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectrum of schreibersite see also La Cruz (2015).

**Schreyerite**  $\text{V}^{3+}{}_2\text{Ti}^{4+}{}_3\text{O}_9$

**Origin:** Vihanti, Northern Ostrobothnia region, Finland.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 633 nm He-Ne laser radiation. The nominal laser radiation power was 2 or 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 810s, 705s, 653s, 593, 532w, 468, 426, 358w, 308, 175s, 90.

**Source:** Voloshin et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Schröckingerite**  $\text{NaCa}_3(\text{UO}_2)(\text{SO}_4)(\text{CO}_3)_3\text{F}\cdot 10\text{H}_2\text{O}$

**Origin:** Wheal Edward, St. Just, Cornwall, UK.

**Experimental details:** Methods of sample preparation are not indicated. Raman scattering measurements have been performed using 785 nm laser radiation. The nominal laser power at the source was ~370 mW.

**Raman shifts(cm<sup>-1</sup>):** 1093, 1009, ~980, 815s, ~745, ~620w, ~470w, ~305w, ~250w.

**Source:** Driscoll et al. (2014).

**Comments:** The sample was characterized by electron microprobe analysis. For the Raman spectrum of schröckingerite see also Frost et al. (2007d).

**Schuetteite**  $\text{Hg}_3\text{O}_2(\text{SO}_4)$ **Origin:** Synthetic.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** ~1090, ~1060, ~975s, ~620w, ~600w, ~520w, ~455, ~425, ~220s.**Source:** Schofield (2004).**Comments:** The sample was characterized by powder X-ray diffraction data.**Schultenite**  $\text{Pb}(\text{AsO}_3\text{OH})$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 827s, 799sh, 467, 357, 149, 93s, (73).**Source:** Petzelt (1977).**Comments:** No independent analytical data are provided for the sample used. The Raman shifts are given for the scattering geometry  $y(p_1)-y$ . For the Raman spectrum of schultenite see also Mlynarska et al. (2014).**Schumacherite**  $\text{Bi}_3\text{O}(\text{VO}_4)_2(\text{OH})$ **Origin:** Wombat Hole Prospect, Morass Creek gorge, near Benambra, Victoria, Australia.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3616w, 3589w, 1557, 1041, 943, 809, 672s, 641, 498w, 410s, 341, 248, 197.**Source:** Frost et al. (2006i).**Comments:** No independent analytical data are provided for the sample used.**Schwertmannite**  $\text{Fe}^{3+} \cdot {}_{16}\text{O}_{16}(\text{OH},\text{SO}_4)_{12-13} \cdot 10\text{H}_2\text{O}$  (?)**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using He-Ne laser. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1120w, 981, 715, 580sh, 544, 421s, 350, 318, 294sh.**Source:** Mazzetti and Thistlethwaite (2002).**Comments:** The sample was characterized by powder X-ray diffraction data.**Scolecite**  $\text{Ca}(\text{Si}_3\text{Al}_2\text{O}_{10}) \cdot 3\text{H}_2\text{O}$ **Origin:** Nasik, Maharashtra, India.**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser power at the sample was 10 mW.**Raman shifts (cm<sup>-1</sup>):** 3536, 3472, 3405, 3212, 3182, 3087+3080, 1105, 1088, 1049+1044, 941, 718, 535s, 496, 480+472, 447s, 437, 426s, 354, 328+318, (301), 295s, 283+276+255, 245+241+224, 179, 171, 158, 146.

**Source:** Wopenka et al. (1998).

**Comments:** Bands whose intensities are significantly dependent upon polarization are indicated in the cited paper. For the Raman spectra of scolecite see also Pechar (1984) and Mozgawa (2001).

**Scorodite**  $\text{Fe}^{3+}(\text{AsO}_4)\cdot 2\text{H}_2\text{O}$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 785 nm solid-state laser radiation. The laser radiation power at the sample was about 0.3 mW or some what more.

**Raman shifts (cm<sup>-1</sup>):** 886s, 796s, 444, 416, 376, 333, 287, 254, 176s, 128.

**Source:** Das and Hendry (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of scorodite see also Gomez et al. (2010a, 2011), Frost et al. (2015w), Culka et al. (2016b), and Kloporgge and Wood (2017).

**Scotlandite**  $\text{Pb}(\text{S}^{4+}\text{O}_3)$

**Origin:** Leadhills, Scotland (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The elaser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 975sh, 935s, 880sh, 622, 474s, 190, 144.

**Source:** Frost and Keeffe (2009d).

**Comments:** No independent analytical data are provided for the sample used.

**Scottytite**  $\text{BaCu}_2\text{Si}_2\text{O}_7$

**Origin:** Wessels mine, Kalahari Manganese Fields, South Africa (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1019w, 958w, 896s, 866w, 675s, 612, 578, 560, 459s.

**Source:** Yang et al. (2013b).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. For the Raman spectrum of scottytite see also Xia et al. (2014).

**Scrutinyite**  $\text{PbO}_2$

**Origin:** Synthetic.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 534w, 366w, 269, 133s, 80w,

**Source:** Inguanta et al. (2008).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Sederholmite** NiSe**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on hollow nanospheres using 532 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1075s, 539, 389, 207w.**Source:** Shi et al. (2013).**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts of a bulk sample are (cm<sup>-1</sup>): 1060s, 524, 374, 192w.**Segnitite** PbFe<sup>3+</sup><sub>3</sub>(AsO<sub>4</sub>)(AsO<sub>3</sub>OH)(OH)<sub>6</sub>**Origin:** Broken Hill, New South Wales, Australia.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** (3467w), 3440sh, 3217, 2982sh, 1417w, 1231w, 1128w, 998w, 931sh, 860 +848s (unresolved doublet?), 811sh, 746sh, 689w, 572, 481s, (465), 441, 419sh, 370, (342), 318, 300, 250, 202, (195).**Source:** Frost et al. (2005l).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.**Seinäjokite** FeSb<sub>2</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** ~1060, ~700sh, ~660s, ~525.**Source:** Xie et al. (2011).**Comments:** The sample was characterized by powder X-ray diffraction data.**Sejkoraite-(Y)** Y<sub>2</sub>[(UO<sub>2</sub>)<sub>8</sub>O<sub>6</sub>(SO<sub>4</sub>)<sub>4</sub>(OH)<sub>2</sub>]·26H<sub>2</sub>O**Origin:** Červená vein, Jáchymov ore district, Western Bohemia, Czech Republic (type locality).**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 732 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1537w, 1222w, 1157w, 1095w, 1014, 896w, 829s, 798sh, 670w, 546sh, 477sh, 461, 438sh, 404s, 369sh, 326w, 274, 262, 237sh, 211.**Source:** Plášil et al. (2011a).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Sekaninaite**  $\text{Fe}^{2+} \text{Al}_4\text{Si}_5\text{O}_{18}$ 

**Origin:** A miarolitic pegmatite at Zimník, Strzegom-Sobótka massif, Sudetes, Poland.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 30 mW.

**Raman shifts (cm<sup>-1</sup>):** 3630sh, 3597, 3579, 1158w, 1049w, 1004w, 989, 917w, 667, 599, 569s, 552s, 477w, 420, 296, 253, 152.

**Source:** Gadas et al. (2016).

**Comments:** The sample was characterized by electron microprobe analyses and LA-ICP-MS. For the Raman spectrum of sekaninaite see also Radica et al. (2013).

**Selenium** Se

**Origin:** Synthetic.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 237 + 234s (unresolved doublet?), 140.

**Source:** Campos et al. (2004a).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of selenium see also Campos et al. (2004b).

**Seligmannite** CuPbAsS<sub>3</sub>

**Origin:** Binntal, Switzerland.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed in the spectral region from 50 to 600 cm<sup>-1</sup> using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** (363), 354s, 344sh, 334, 324, 311sh, 288, 231, 215sh, 202, 189sh, 172h, 155w, 121w, 106sh, 97s, 90s, 70s.

**Source:** Kharbish (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analysis.

**Sellaite** MgF<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a single crystal in different scattering geometries, using 488 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was ~75 mW. A 90°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 515w, 410s, 295, 92.

**Source:** Porto et al. (1967).

**Comments:** The band intensities are indicated for the sum of spectra obtained in different scattering geometries. For the Raman spectrum of sellaite see also Krishnan and Katiyar (1965).

**Sénarmontite** Sb<sub>2</sub>O<sub>3</sub>**Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The laser radiation power was below 1 mW.**Raman shifts (cm<sup>-1</sup>):** 451, 373w, 253s, 189, 115w.**Source:** Makreski et al. (2013b).**Comments:** The sample was characterized by thermal analysis. For the Raman spectra of Sénarmontite see also Cody et al. (1979), Voit et al. (2009), and Orman (2010).**Senegalite** Al<sub>2</sub>(PO<sub>4</sub>)(OH)<sub>3</sub>·H<sub>2</sub>O**Origin:** Jangada mine, Quadrilátero Ferrífero, municipality of Brumadinho, Minas Gerais, Brazil.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3614sh, 3610s, 3606sh, 3507–3505s, 3429sh, 3374sh, 3339, 3270w, 3206sh, 3099w, 2975w, 1753w, 1679w, (1587w), (1425w), 1377w, 1206w, 1179w, 1154, 1110w, 1071, 1029, (1026), 892w, 829w, 708, 677w, 635, 616sh, 581w, 559sh, 545, 501sh, 480, 462sh, 444, 417, 375, 364sh, 329sh, 318sh, (312w), 303, 237, 202sh, 193, 178, 166, (154w), 136 + 133 (unresolved doublet?), 102.**Source:** Frost et al. (2013g).**Comments:** The sample was characterized by qualitative electron microprobe analysis.**Sepiolite** Mg<sub>4</sub>Si<sub>6</sub>O<sub>15</sub>(OH)<sub>2</sub>·6H<sub>2</sub>O**Origin:** Durango, Mexico.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on randomly oriented crystals in back-scattering geometry, using 1064 nm Nd-YAG laser radiation. The nominal laser radiation power was 900 mW.**Raman shifts (cm<sup>-1</sup>):** ~1080, ~780, ~675s, ~380, ~335, ~290, ~265, ~230w, ~200s, ~170.**Source:** McKeown et al. (2002).**Comments:** The sample was characterized by powder X-ray diffraction data.**Sérandite** NaMn<sup>2+</sup><sub>2</sub>Si<sub>3</sub>O<sub>8</sub>(OH)**Origin:** Poudrette quarry, Saint-Hilaire Mt., Montérégie (Rouville) Co., Québec, Canada (type locality).**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 638 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1026s, 903, 666s, 422, 304, 168.**Source:** Haring and McDonald (2014a).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of sérandite see also Origlieri et al. (2017).

**Serendibite**  $\text{Ca}_4[\text{Mg}_6\text{Al}_6]\text{O}_4[\text{Si}_6\text{B}_3\text{Al}_3\text{O}_{36}]$ **Origin:** Ratnapura area, Sri Lanka.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 325 or 514.5 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 997, 895, 756, 681, 635, 572, 530, 470, 405, 364, 310.**Source:** Schmetzer et al. (2002).**Comments:** The sample was characterized by electron microprobe analyses.**Serpierite**  $\text{Ca}(\text{Cu},\text{Zn})_4(\text{SO}_4)_2(\text{OH})_6 \cdot 3\text{H}_2\text{O}$ **Origin:** Carchia, NW Italy.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power at the sample was 4 mW.**Raman shifts (cm<sup>-1</sup>):** 3616w, 3570w, 1168w, 1132, 1115sh, 1085w, 991s, 651w, 605w, 474sh, 445, 426, 415, 338w, 244w, 218w.**Source:** Coccato et al. (2016).**Comments:** No independent analytical data are provided for the sample used.**Shattuckite**  $\text{Cu}_5(\text{SiO}_3)_4(\text{OH})_2$ **Origin:** Navojoa, Sonora, Mexico.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3602, (3567w), 3424sh, 3367w, (3153w), 1564w, 1107w, 1054, (1000w), 981, 953sh, 887, 865w, 832w, 781, 739w, 667s, 549, 498, 439, 394, 349sh, 340, 326, 306sh, 255, 238, 211s, 191sh, (160w), 152, 135–139 sh, (117w), 113, (107w).**Source:** Frost and Xi (2012b).**Comments:** No independent analytical data are provided for the sample used.**Shcherbinaite**  $\text{V}_2\text{O}_5$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a sample in rotated tube using 488 and 514.5 nm Ar<sup>+</sup>, as well as 647.1 nm Kr<sup>+</sup> laser radiations. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 993, 703, 528.5, 483, 476, 405, 305, 285s, 198, 147s, 105.**Source:** Sanchez et al. (1982).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of shcherbinaite see also Menezes et al. (2009).

**Shchurovskyite**  $K_2CaCu_6O_2(AsO_4)_4$ 

**Origin:** Arsenatnaya fumarole, Tolbachik volcano, Kamchatka, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 840s, 630, 486, 304, 135, 100.

**Source:** Pekov et al. (2015d).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Shortite**  $Na_2Ca_2(CO_3)_3$ 

**Origin:** No data.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 1523, 1470, 1440, 1407, 1387, 1091s, 1071s, 730, 719, 715, 695, 265s, 201, 171, 141.

**Source:** Shatskiy et al. (2015).

**Comments:** For the Raman spectra of shortite see also Frost and Dickfos (2007b, 2008).

**Shuangfengite**  $IrTe_2$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed in a nearly back-scattering (xx) geometry on an oriented crystal, from the surface parallel to the (ab) plane using 532 nm solid-state laser radiation. The nominal laser radiation power was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 166, 126.

**Source:** Glamazda et al. (2014).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of shuangfengite see also Lazarević et al. (2014).

**Shulamitite**  $Ca_3TiFe^{3+}AlO_8$ 

**Origin:** Central part of the Hatrurim Basin, Israel (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample in a polished section using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation output power was between 30 and 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 1501 (broad), 802sh, 742s, 561, 498sh, 388, 290, 238, 145w, 110w.

**Source:** Sharygin et al. (2013a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Siderite**  $Fe(CO_3)$ 

**Origin:** Minas Gerais, Brazil.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 488 and 514.5 nm Ar<sup>+</sup> laser radiations. The nominal laser radiation power was in the range from 100 to 500 mW.

**Raman shifts (cm<sup>-1</sup>):** 1738, 1088s, 731, 299, 194w.

**Source:** Rutt and Nicola (1974).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of siderite see also Buzgar and Apopei (2009), Das and Hendry (2011), Saheb et al. (2011), Frezzotti et al. (2012), Zhao and Guo (2014), and Andò and Garzanti (2014).

**Sideronatrite** Na<sub>2</sub>Fe<sup>3+</sup>(SO<sub>4</sub>)<sub>2</sub>(OH)·3H<sub>2</sub>O

**Origin:** Sierra Gorda, Chile.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was 2.5 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1646, 1223, 1189, 1159, 1117sh, 1106, 1024, 1013s, 996s, 624, 614sh, 600w, 536, 469, 458sh, 391, 259sh, 246s, 216sh, 203, 170, 115.

**Source:** Rouchon et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Sidorenkite** Na<sub>3</sub>Mn(PO<sub>4</sub>)(CO<sub>3</sub>)

**Origin:** Alluaiv Mt., Lovozero massif, Kola Peninsula, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1074, 1044s, 1035sh, 1012s, 1004sh, 966sh, 959s, (953), 625w, 579, 469w, 414w, 297w, 252w, 202, 179w, 159, 129w.

**Source:** Frost et al. (2015c).

**Comments:** The sample was characterized by quqlitative electron microprobe analyses.

**Sidwillite** MoO<sub>3</sub>·2H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 488 and 514.5 nm Ar<sup>+</sup> laser radiations. The laser radiation power at the sample was 10–50 mW.

**Raman shifts (cm<sup>-1</sup>):** 934, 771sh, 729s, 627, 418w, 386w, 353w, 331, 272s, 247, 216, 184, 168, 119, 95, 65.

**Source:** Seguin et al. (1995).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of sidwillite see also Philip et al. (1988).

**Siegenite** CoNi<sub>2</sub>S<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Raman spectrum was measured in argon atmosphere. Characteristics of laser radiation are not indicated.

**Raman shifts (cm<sup>-1</sup>):** 373s, 342s, 301, 239, 150.

**Source:** Xia et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Sigloite** Fe<sup>3+</sup>Al<sub>2</sub>(PO<sub>4</sub>)<sub>2</sub>(OH)<sub>3</sub>·7H<sub>2</sub>O

**Origin:** Siglo XX (Llallagua) mine, Andes Mts., Bustillo province, Potosí, Bolivia (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3615, 3552, 3493s, 3449s, 3422sh, 3356sh, 3118s, (2988), 1631w, (1532w), 1235–1231sh, 1228, 1167, 1099 + 1086 (unresolved doublet?), 1009s, 993sh, 888, 816, 693w, 659sh, 619sh, 596, 571, 550sh, 528, (506), (489), 453, 427, 401, 338sh, 308, 277, (267), 253, 241, 191, 177, 169sh, 140sh, 129, 112.

**Source:** Frost et al. (2013aa).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

**Siidraite** Pb<sub>2</sub>Cu(OH)<sub>2</sub>I<sub>3</sub>

**Origin:** Broken Hill Cu-Zn-Pb ore deposit, Yancowinna Co., New South Wales, Australia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 532 nm laser radiation. The laser radiation power at the sample was 1.8 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3455, 3443, 743w, 370, 332, 313sh, 277, ~248sh, ~217w, ~140sh, 128s, 116, 97.

**Source:** Welch et al. (2016).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Silicocarnotite** Ca<sub>5</sub>[(PO<sub>4</sub>)(SiO<sub>4</sub>)](PO<sub>4</sub>)

**Origin:** Hatrurim basin, Negev Desert, Israel (type locality).

**Experimental details:** The laser radiation wavelength is not indicated. The laser radiation power at the sample was 44 mW.

**Raman shifts (cm<sup>-1</sup>):** 1085, 1056, 1014 + 1004 (unresolved doublet?), 967s, (939w), 904sh, 893, 878, 850s, 788w, 734w, 711w, 693w, 671w, 640, 626, 584, 557, 474, 448, (418), 397, 318sh, 302, 275, 258, 234, 190sh, 153w.

**Source:** Galuskin et al. (2015a).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. For the Raman spectra of silicocarnotite see also Serena et al. (2014, 2015).

**Silicon Si**

**Origin:** Dhofar 280 lunar highland meteorite.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented samples using 532 nm laser radiation. The laser radiation power at the samples was no more than 5 mW.

**Raman shifts (cm<sup>-1</sup>):** ~950w, 504–515s, ~280w.

**Source:** Nazarov et al. (2012).

**Comments:** The samples were characterized by electron microprobe analyses. The strongest band of synthetic crystalline Si is observed at 520 cm<sup>-1</sup>.

**Sillénite Bi<sub>12</sub>SiO<sub>20</sub>**

**Origin:** Synthetic.

**Description:** Synthesized from the stoichiometric mixture of oxides at 700 °C for 48 h. Cubic, space group *I23*.

**Source:** Betsch and White (1978).

**Raman shifts (cm<sup>-1</sup>):** 621w, 538s, 458w, 328, 276s, 249sh, 205, 165, 143, 129s, 95sh, 87s, 66, 57s, 43w.

**Sillimanite Al<sub>2</sub>SiO<sub>5</sub>**

**Origin:** Premosello Chiovenda, Ossola valley, Verbano-Cusio-Ossola province, Piedmont, Italy.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~1125, ~970, ~955, 870, ~707, ~596, ~480, 456, ~412, ~395, 309s, 235s, 142.

**Source:** Andò and Garzanti (2014).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of sillimanite see also Mernagh and Liu (1991) and Frezzotti et al. (2012).

**Simonkolleite Zn<sub>5</sub>(OH)<sub>8</sub>Cl<sub>2</sub>·H<sub>2</sub>O**

**Origin:** Artificial (a product of Zn corrosion in NaCl solution).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 40 mW.

**Raman shifts (cm<sup>-1</sup>):** 3580, 3480s, 3450, 1030, 910, 730, 390s, 260s, 210.

**Source:** Bernard et al. (1993b).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of simonkolleite see also Khamlich et al. (2013).

**Sinhalite MgAl(BO<sub>4</sub>)**

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 864, 554w, 488, 376.

**Source:** Ross (1972).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of sinhalite see also Hayward et al. (1994).

**Sinjarite**  $\text{CaCl}_2 \cdot 2\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3486, 3452s, 3216w, 1638s, 1620w (at 21 °C); 3545w, 3491, 3475, 3437s, 3388, 3215w, 3211w, 1635s, 1630, 1616 (at -172 °C).**Source:** Uriarte et al. (2015).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of sinjarite see also Baumgartner and Bakker (2010).**Sinoite**  $\text{Si}_2\text{N}_2\text{O}$ **Origin:** Zakłodzie meteorite.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power at the sample was 1.2 mW.**Raman shifts (cm<sup>-1</sup>):** 1142w, 983w, 941w, 891w, 730w, 544, 496w, 455w, 373w, 328w, 217w, 185s.**Source:** Ma et al. (2012a).**Comments:** The mineral was identified by electron back-scatter diffraction. For the Raman spectrum of sinoite see also Sekine et al. (2006).**Skinnerite**  $\text{Cu}_3\text{SbS}_3$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on nanocrystals using 514 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 354.**Source:** Qiu et al. (2013).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.**Skippenite**  $\text{Bi}_2\text{Se}_2\text{Te}$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a thin film. Characteristics of laser radiation are not indicated.**Raman shifts (cm<sup>-1</sup>):** 165, 147, 117s.**Source:** Gopal et al. (2015).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectrum of skippenite see also Voloshin et al. (2015a).

**Sklodowskite**  $\text{Mg}(\text{UO}_2)_2(\text{SiO}_3\text{OH})_2 \cdot 6\text{H}_2\text{O}$ 

**Origin:** Eva mine, Northern Territory, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3506, 3420sh, 3316w, 1640w, 1528w, 1413w, 1312w, 1244w, 1150w, (986), 970, (957), 934w, 897w, 853w, 827w, 801, 777s, (756w), 549, 474, 414, 393sh, 318sh, 305, 282, 264, 217sh, 200 + 197s (unresolved doublet?), 156, 137, (127), 113.

**Source:** Frost et al. (2006e).

**Comments:** No independent analytical data are provided for the sample used.

**Skorpionite**  $\text{Ca}_3\text{Zn}_2(\text{PO}_4)_2(\text{CO}_3)(\text{OH})_2 \cdot \text{H}_2\text{O}$ 

**Origin:** Skorpion Zn mine, Lüderitz district, Karas region, Namibia (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 488, 514.5 or 632.8 nm laser radiation. The nominal laser radiation power was 20 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3566s, 1633w, 1505, 1398, 1102, 1075s, 1054, 1016, 972s, 702, 639, 575, 468, 423, 384, 322, 276, 237.

**Source:** Krause et al. (2008).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Smirnite**  $\text{Bi}^{3+}_2\text{Te}^{4+}\text{O}_5$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an oriented single crystal using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 50 mW. A 90°-scattering geometry was employed.

**Raman shifts (for the y(xx)z scattering geometry, cm<sup>-1</sup>):** 768s, 740, 721sh, 625, 382w, 347, 282w, 254w, 239, 206w, 193w, 164w, 153w, 114, 102s, 89s, 64, 57s, 44w.

**Source:** Domoratskii et al. (2000).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of smirnite see also Klein et al. (1998).

**Smithite**  $\text{AgAsS}_2$ 

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 362s, 324s, 301, 279w, 239, 207w, 176, 141, 120w.

**Source:** Minceva-Sukarova et al. (2003).

**Comments:** No independent analytical data are provided for the sample used.

**Smithsonite** Zn(CO<sub>3</sub>)**Origin:** Lavrion, Greece.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 488 and 514.5 nm Ar<sup>+</sup> laser radiations. The nominal laser radiation power was in the range from 100 to 500 mW.**Raman shifts (cm<sup>-1</sup>):** 1735, 1406, 1090s, 726, 302, 194.**Source:** Rutt and Nicola (1974).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of smithsonite see also Bouchard and Smith (2003) and Frezzotti et al. (2012).**Smythite** (Fe,Ni)<sub>3+x</sub>S<sub>4</sub> ( $x \approx 0\text{--}0.3$ )**Origin:** Harrodsburg, Bloomington, Indiana, USA.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 394, 358, 329, 326, 267, 262.**Source:** Bon and Rakovan (2012).**Comments:** The sample was characterized by single-crystal X-ray diffraction data. The crystal structure is solved.**Sobolevskite** PdB<sub>i</sub>**Origin:** Southern Sopchinskoe deposit, Monchegorsk district, Kola Peninsula, Russia.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser power was 50 mW.**Raman shifts (cm<sup>-1</sup>):** 236w, 106w, 82, 63s.**Source:** Voloshin et al. (2015a).**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectrum of sobolevskite see also Bakker (2014).**Sodalite** Na<sub>4</sub>(Si<sub>3</sub>Al<sub>3</sub>)O<sub>12</sub>Cl**Origin:** Mogok, Myanmar.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 1057–1062, 986–987, 973, 914, 463–464s, 451s, 263s.**Source:** Culka et al. (2016a).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of sodalite see also Balassone et al. (2012), Hettmann et al. (2012), and Zahoransky et al. (2016).**Soddyite** (UO<sub>2</sub>)<sub>2</sub>(SiO<sub>4</sub>)·2H<sub>2</sub>O**Origin:** Sierra Albarrana, Córdoba, Spain.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632.8 nm He-Ne laser radiation. The laser radiation output power was 20 mW.**Raman shifts (cm<sup>-1</sup>):** 832s, 463, 404, 312, 293, 225, 195, 107.**Source:** Bonales et al. (2015).**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectra of soddyite see also Biwer et al. (1990), Giammar and Hering (2002), Frost et al. (2006d, h), and Amme et al. (2002).

**Söhngeite**  $\text{Ga(OH)}_3$ 

**Origin:** Tsumeb mine, Namibia (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 473 nm laser radiation. The nominal laser radiation power was 50 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3334, 3240, 3189sh, 3100, 3000, 923, 455w, 327s, 273w, 256, 185w.

**Source:** Welch and Kleppe (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Sonolite**  $\text{Mn}^{2+} \cdot {}_9(\text{SiO}_4)_4(\text{OH})_2$ 

**Origin:** Franklin, Sussex Co., New Jersey, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3555sh, 3544w, 3532sh, 948, 906, 848s, (838), 832sh, 814, 668, 638.

**Source:** Frost et al. (2007k).

**Comments:** The sample was characterized by electron microprobe analysis.

**Sonoraita**  $\text{Fe}^{3+}(\text{Te}^{4+}\text{O}_3)(\text{OH}) \cdot \text{H}_2\text{O}$ 

**Origin:** Tombstone, Tombstone district, Cochise Co., Arizona, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3450 + 3423 (unresolved doublet?), 3350sh, 3223sh, 3000sh, 994w, 911w, (804w), 779s, (714), 666s, 638sh, 521sh, 468, 425, 387, (374), 312, 267s, 253s, 234, 209, 159.

**Source:** Frost and Keeffe (2009c).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of sonoraita see also Frost et al. (2015b).

**Spangolite**  $\text{Cu}_6\text{Al}(\text{SO}_4)(\text{OH})_{12}\text{Cl} \cdot 3\text{H}_2\text{O}$ 

**Origin:** Monte Fucinaia, central Western Italy.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power at the sample was 4 mW.

**Raman shifts (cm<sup>-1</sup>):** 968s, 615w, 520s, 410, 168.

**Source:** Coccato et al. (2016).

**Comments:** No independent analytical data are provided for the sample used.

**Spencerite**  $\text{Zn}_4(\text{PO}_4)_2(\text{OH})_2 \cdot 3\text{H}_2\text{O}$ **Origin:** Salmo, British Columbia, Canada.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power at the sample was 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3516, 1095w, 1019w, 999s, 989w, 952w.**Source:** Frost (2004a).**Comments:** No independent analytical data are provided for the sample used.**Sperrylite**  $\text{PtAs}_2$ **Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 18794.59 cm<sup>-1</sup> laser radiation. The laser radiation power at the sample was between 1 and 2 mW.**Raman shifts (cm<sup>-1</sup>):** 293w, 279, 226, 216s.**Source:** Bakker (2014).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of sperrylite see also Müller and Lutz (1991) and Mernagh and Hoatson (1995).**Spertiniite**  $\text{Cu}(\text{OH})_2$ **Origin:** Artificial (a product of brass corrosion).**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power at the sample was 74  $\mu\text{W}$ .**Raman shifts (cm<sup>-1</sup>):** ~3555s, ~3305, ~950w, ~840w, ~495s, ~450, ~293.**Source:** Schmutzler et al. (2016).**Comments:** No independent analytical data are provided for the sample used.**Spessartine**  $\text{Mn}^{2+} \text{Al}_2(\text{SiO}_4)_3$ **Origin:** Lojane, municipality of Lipkovo, Republic of Macedonia.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 1064 nm Nd-YAG laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1025sh, 976, 901s, 838, 632w, 607w, 557, 496, 454w, 413w, 377sh, 354, 293, 228, 183.**Source:** Makreski et al. (2005b).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of spessartine see also Mingsheng et al. (1994), Kolesov and Geiger (1998), Bersani et al. (2009), Jovanovski et al. (2009), Frezzotti et al. (2012), and Andò and Garzanti (2014).**Sphalerite**  $\text{ZnS}$ **Origin:** Rio Tinto, Spain.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was between 1 and 10 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 447, 420, 407, 397, 350s, 336, 287, 275s, 237, 219, 208, 178, 156, 144, 117.  
**Source:** Mernagh and Trudu (1993).

**Comments:** The Raman shifts are given for Fe-bearing sphalerite. No independent quantitative analytical data are provided for the sample used. For the Raman spectra of sphalerite see also White (2009), Frezzotti et al. (2012), and Andò and Garzanti (2014).

### Spherocobaltite Co(CO<sub>3</sub>)

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1090s, 725w, 302, ~194.

**Source:** Chariton et al. (2017).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data. For the Raman spectrum of spherocobaltite see also Rutt and Nicola (1974).

### Spinel MgAl<sub>2</sub>O<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 632.8 nm He-Ne and 473.1 nm Nd-YAG laser radiations. The laser radiation power at the sample was <1 mW.

**Raman shifts (cm<sup>-1</sup>):** 768, 720w, 670, 562w, 493w, 408s, 375sh, 308.

**Source:** D'Ippolito et al. (2015).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectra of spinel see also Shoval et al. (2001), Jasinevicius (2009), Kojitani et al. (2013), Culka et al. (2016a, b), and Dongre et al. (2016).

### Spionkopite Cu<sub>39</sub>S<sub>28</sub>

**Origin:** Synthetic.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 474s.

**Source:** Parker et al. (2008).

**Comments:** The sharp band at 474 cm<sup>-1</sup> corresponds to S-S pairs.

### Spiroffite Mn<sup>2+</sup><sub>2</sub>Te<sup>4+</sup><sub>3</sub>O<sub>8</sub>

**Origin:** Moctezuma mine, Sonora, Mexico (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** (773w), 743s, 721, 650sh, 466s, 394, 346s, 226, 148.

**Source:** Frost et al. (2009g).

**Comments:** No independent analytical data are provided for the sample used. The IR spectrum of presumed spiroffite given in the cited paper corresponds to quartz.

**Spodumene**  $\text{LiAlSi}_2\text{O}_6$ 

**Origin:** Conțu-Negovanu pegmatite field, Lotru-Cibin Mts., Sibiu Co., Romania.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal. Experimental details are not described.

**Raman shifts (cm<sup>-1</sup>):** 1098, 1070s, 1017, 783, 705s, 582, 522, 438, 393, 355s, 296, 249.

**Source:** Buzatu and Buzgar (2010).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of spodumene see also Anderson et al. (2001) and Jasinevicius (2009).

**Spurrite**  $\text{Ca}_5(\text{SiO}_4)_2(\text{CO}_3)$ 

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 1080s, 948w, 932w, 864, 852, 704, 547w, 520w, 404w, 389w.

**Source:** Gastaldi et al. (2008).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Šreinite**  $\text{Pb}(\text{UO}_2)_4(\text{BiO})_3(\text{PO}_4)_2(\text{OH})_7 \cdot 4\text{H}_2\text{O}$ 

**Origin:** Horní Halže, Krušné Hory (Ore Mts.), Czech Republic (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm laser radiation. The laser radiation power at the sample was 4 mW.

**Raman shifts (cm<sup>-1</sup>):** 1361w, 1060w, 1023w, 975w, 871sh, 839sh, 797s, 678w, 595w, 507w, 457w, 449w, 334.

**Source:** Sejkora and Čejka (2007).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Srilankite**  $(\text{Ti},\text{Zr})\text{O}_2$ 

**Origin:** Xiuyan meteorite crater, Xiuyan Co., Liaoning province, NE China.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented Zr-free sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 825w, 610, 572, 533, 442sh, 428s, 412sh, 357, 340w, 315, 287, 175s, 151.

**Source:** Chen et al. (2013a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectrum of srilankite see also Mammone et al. (1981).

**Stanfieldite**  $\text{Ca}_4\text{Mg}_5(\text{PO}_4)_6$ 

**Origin:** Artificial (a product of pyrometamorphic substitution of apatite in slag).

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power at the sample was between 1 and 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 1293w, 1228w, 1158w, 1124w, 1075, 983sh, 974s, 968s, 753, 620, 611sh, 533, 514, 468, 402, 348, 293w, 176w.

**Source:** Schneider et al. (2013).

**Comments:** The sample was characterized by electron microprobe analyses.

### Stanleyite V<sup>4+</sup>O(SO<sub>4</sub>)·6H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was between 10 and 40 mW.

**Raman shifts (cm<sup>-1</sup>):** 1078, 1028, 1006, 630, 450, 310.

**Source:** Hardcastle and Wachs (1991).

**Comments:** No independent analytical data are provided for the sample used. Band intensities are not indicated.

### Stannite Cu<sub>2</sub>FeSnS<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. A nearly 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 350w, 318s, 286.

**Source:** Himmrich and Haeuseler (1991).

**Comments:** For the Raman spectra of stannite see also Fontané et al. (2012) and Evrard et al. (2015).

### Starkeyite Mg(SO<sub>4</sub>)·4H<sub>2</sub>O

**Origin:** Calingasta, San Juan province, Argentina.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~1156, ~1120, ~1102s, ~1085w, ~615, ~560w, ~475.

**Source:** Peterson (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of starkeyite see also Wang et al. (2006a) and Frezzotti et al. (2012).

### Starovaite KCu<sub>5</sub>O(VO<sub>4</sub>)<sub>3</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed at 250 K in a quasi-back-scattering geometry, from the surface parallel to the *a*-axis of a microtwinned crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** ~953s, ~908, ~860, ~834w.

**Source:** Choi et al. (2004).

**Staurolite**  $\text{Fe}^{2+}_2\text{Al}_9\text{Si}_4\text{O}_{23}(\text{OH})$ 

**Origin:** Štavica, municipality of Prilep, Republic of Macedonia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 1064 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3675, 3622w, 3571w, 3520sh, 3451sh, 3426s, 1022, 970s, 938sh, 898sh, 847sh, 684w, 640sh, 593, 543, 525sh, 487, 432, 399w.

**Source:** Makreski et al. (2005b).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of staurolite see also Andò and Garzanti (2014).

**Steedeite**  $\text{NaMn}_2[\text{Si}_3\text{BO}_9](\text{OH})_2$ 

**Origin:** Poudrette quarry, Montérégie (Rouville) Co., Québec, Canada (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3443, 3317w, 1700, 1368, 1030, 1000s, 874, 836, 696, 636s, 431, 330, 264, 197w, 120.

**Source:** Haring and McDonald (2014a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Steenstrupine-(Ce)**  $\text{Na}_{14}\text{Ce}_6\text{Mn}^{2+}_2\text{Fe}^{3+}_2\text{Zr}(\text{PO}_4)_7\text{Si}_{12}\text{O}_{36}(\text{OH})_2 \cdot 3\text{H}_2\text{O}$ 

**Origin:** Karnasurt Mt., Lovozero alkaline massif, Kola Peninsula, Russia.

**Experimental details:** Raman scattering measurements have been performed on a partly metamict sample annealed at 500 °C using 632.8 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~957s, ~880sh, ~756, ~600 (broad).

**Source:** Kusz et al. (2010).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Stephanite**  $\text{Ag}_5\text{SbS}_4$ 

**Origin:** Bohemia, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an oriented crystal with the laser polarization parallel to the *a*-, *b*- and *c*-axes. 785 nm solid-state laser radiation was used. The nominal laser radiation power was 1.7 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 335s, 317w, 306w, 301, 233, 204w, 178w.

**Source:** Kharbish et al. (2009).

**Comments:** The sample was characterized by electron microprobe analyses. The Raman shifts are given as the sum of the spectra of all scattering geometries.

**Štěpite**  $\text{U}(\text{AsO}_3\text{OH})_2 \cdot 4\text{H}_2\text{O}$ 

**Origin:** Geschieber vein, Jáchymov ore district, Western Bohemia, Czech Republic (type locality).

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 3552, 3484, 1641w (broad), 896s, 844s, 811s, 760s, 420, 401, 377, 368, 351, 322, 312, 287, 262, 235, 180, 160, 139, 115, 107.

**Source:** Plášil et al. (2013b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Stercorite**  $(\text{NH}_4)\text{Na}(\text{PO}_3\text{OH}) \cdot 4\text{H}_2\text{O}$ 

**Origin:** Petrogale Cave, Madura, Western Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3158, 3024sh, 2900sh, 920s, 577, 476, 450sh, 396w, 345, 326sh, 216sh, 197 + 185 (unresolved doublet), (155), 143s, 110.

**Source:** Frost et al. (2011u).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Steropesite**  $\text{Tl}_3\text{BiCl}_6$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 1036 nm Nd-YAG laser radiation. The nominal laser radiation power was between 30 and 300 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 261s, 218, 117s.

**Source:** Beck and Benz (2010).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and X-ray absorption spectrum.

**Stetindite**  $\text{Ce}(\text{SiO}_4)$ 

**Origin:** Stetind pegmatite, Tysfjord, Nordland, Norway (type locality).

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** See comment below.

**Source:** Schlüter et al. (2009).

**Comments:** Raman micro-spectroscopy shows weak OH bands in the frequency range between 3200 and 3700 cm<sup>-1</sup> corresponding to vibrations of OH groups. No other data on the Raman spectrum of stetindite are given in the cited paper.

**Stibarsen** SbAs

**Origin:** Synthetic.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 216 (calculated).

**Source:** Zhang et al. (2016a).

**Stibiconite**  $\text{Sb}^{3+}\text{Sb}^{5+}_2\text{O}_6(\text{OH})$ 

**Origin:** Yucunani Mine, Tejocotes, Oaxaca, Mexico.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3603sh, 3424 + 3225 (unresolved doublet?), 3018sh, 2755w, 855sh, 827w, 736w, 609, 564w, (537w), 522, (508), 461, 409 + 400 (unresolved doublet?), 261, (250), 220sh, 199s, 146, 109w.

**Source:** Bahfenne and Frost (2010e).

**Comments:** No independent analytical data are provided for the sample used.

**Stibioclaudetite**  $\text{AsSbO}_3$ 

**Origin:** Tsumeb mine, Tsumeb, Namibia (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 817w, 766w, 726w, 631w, 620w, 517w, 477, 468, 430sh, 414s, 342, 323w, 298w, 273, 232, 210, 202, 183, 171s, 155s, 125w, 115w.

**Source:** Origlieri et al. (2009).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. For the Raman spectrum of Stibioclaudetite see also Origlieri (2005).

**Stibiocolumbite**  $\text{SbNbO}_4$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 200 mW.

**Raman shifts (cm<sup>-1</sup>):** 913, 740w, 718, 620s (broad), 542, 448, 397, 377s, 350, 292, 269s, 239, 232, 192s, 168s, 128s, 87s, 75s, 54w, 37.

**Source:** Ayyub et al. (1986).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of stibiocolumbite see also Ayyub et al. (1987).

**Stibiopalladinite**  $\text{Pd}_5\text{Sb}_2$ 

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 18794.59 cm<sup>-1</sup> laser radiation. The laser radiation power at the sample was between 1 and 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 187w, 169, 108s.

**Source:** Bakker (2014).

**Comments:** No independent analytical data are provided for the sample used.

**Stibnite**  $\text{Sb}_2\text{S}_3$ 

**Origin:** Schlaining, Oberwart, Burgenland, Austria.

**Experimental details:** Raman scattering measurements have been performed on an oriented crystal with the laser polarization parallel and perpendicular to the cleavage and elongation of kermesite. 632.8 nm He-Ne laser radiations were used. The nominal laser radiation power was 1.7 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 310, 300, 281s, (254w), 237s, (225w), 207, 189, (180w), 156w, 125, 99, 71, 59s, 50, 39.

**Source:** Kharbish et al. (2009).

**Comments:** The sample was characterized by electron microprobe analysis. The Raman shifts are given as the sum of the spectra of all scattering geometries. For the Raman spectra of stibnite see also Mernagh and Trudu (1993), Minceva-Sukarova et al. (2003), Roy et al. (2008), Frost et al. (2010c), and Makreski et al. (2013b).

**Stichtite**  $\text{Mg}_6\text{Cr}_2(\text{CO}_3)(\text{OH})_{16}\cdot 4\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1087s, 1067sh, 539s, (531), 458, (446), 366w, 328w, 317w, 292w, 248w, 215w, 153.

**Source:** Frost and Erickson (2004).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of stichtite see also Mills et al. (2011b).

**Stilbite-Ca**  $\text{NaCa}_4(\text{Si}_{27}\text{Al}_9)\text{O}_{72}\cdot 28\text{H}_2\text{O}$ 

**Origin:** Berufjördur, Sudur-Múlasýsla, Eastern Region, Iceland.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 785 nm diode laser radiation. The maximum output power of 300 mW could be filtered to diminish the power at the sample.

**Raman shifts (cm<sup>-1</sup>):** 794, 644w, 497s, 459w, 410s, 320w.

**Source:** Jehlička et al. (2012).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of stilbite-Ca see also Mozgawa (2001), Makreski et al. (2009), Jehlička and Vandenabeele (2015), and Ma et al. (2016b).

**Stilbite-Na**  $\text{Na}_9(\text{Si}_{27}\text{Al}_9)\text{O}_{72}\cdot 28\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 1.5 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1133, 801, 618, 499s, 458, 411s, 152.

**Source:** Ma et al. (2016b).

**Comments:** The sample was characterized by powder X-ray diffraction data. The crystal structure is solved by the Rietveld method.

**Stilleite** ZnSe**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a thin film using 532 Nd-YAG laser radiation. The laser radiation power at the sample was 0.1 mW.**Raman shifts (cm<sup>-1</sup>):** 500, 252s, 202w.**Source:** Perna et al. (2006).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of stilleite see also Yang et al. (1999).**Stilpnomelane** (K,Ca,Na)(Fe,Mg,Al)<sub>8</sub>(Si,Al)<sub>12</sub>(O,OH)<sub>36</sub>·*n*H<sub>2</sub>O**Origin:** Martian meteorite MIL 03346.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532.3 nm Nd-YAG laser radiation. The nominal laser radiation power was 14.5 mW.**Raman shifts (cm<sup>-1</sup>):** 3579w, 3568w, 1156, 897, 820w, 588s, 501, 379, 291.**Source:** Kuebler (2013a).**Comments:** The sample was characterized by electron microprobe analyses.**Stishovite** SiO<sub>2</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 16 mW. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 960, 750s, 584, 228.**Source:** Liu and El Gorsev (2007). For the Raman spectra of stishovite see also Hemley (1987a, b), Von Czarnowski and Hübner (1987), Holtstam et al. (2003), Miyahara et al. (2013), and Spektor et al. (2016).**Stoiberite** Cu<sub>5</sub>O<sub>2</sub>(VO<sub>4</sub>)<sub>2</sub>**Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532.1 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** ~950, ~900s, ~800s, ~560w, ~505w, ~410, ~330w.**Source:** Kawada et al. (2015).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of stoiberite see also Newhouse et al. (2016).**Stolzite** Pb(WO<sub>4</sub>)**Origin:** Vysoká hill, near Havlíčkův Brod, Czech Republic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation output power was 4 mW.**Raman shifts (cm<sup>-1</sup>):** 905s, 766, 752, 357, 328, 324s, 192w, 178, 90, 77w, 71w, 64, 56.**Source:** Pauliš et al. (2016).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of stolzite see also Frost et al. (2004d), Kloprogge et al. (2004b), and Andrade et al. (2014).

**Stoppaniite**  $\text{Fe}^{3+}_2\text{Be}_3\text{Si}_6\text{O}_{18}\cdot\text{H}_2\text{O}$ 

**Origin:** Capranica, Vico volcanic complex, Latium, Italy (type locality).

**Experimental details:** No data in the cited paper.

**Raman shifts (cm<sup>-1</sup>):** 3595–3588.

**Source:** Della Ventura et al. (2000).

**Stottite**  $\text{Fe}^{2+}\text{Ge(OH)}_6$ 

**Origin:** Tsumeb mine, Tsumeb, Namibia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was below 80 mW. A 135°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3352, 3240, 3159, 3064, 636s, 418, 297, 266.

**Source:** Kleppe et al. (2012).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data.

**Strashimirite**  $\text{Cu}_4(\text{AsO}_4)_2(\text{OH})_2\cdot2.5\text{H}_2\text{O}$ 

**Origin:** Zálesí deposit, Rychlebské Hory Mts., northern Moravia, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3585w, 3488w, 3450w, 852s, 831sh, 554sh, 526sh, 497, 467sh, 393w, 337, 294s, 239sh, 220, 172sh, 152s.

**Source:** Frost et al. (2009i).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Strengite**  $\text{Fe}^{3+}(\text{PO}_4)\cdot2\text{H}_2\text{O}$ 

**Origin:** Iron Monarch, Middleback Ranges, South Australia, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1357, 1250, 1158, 1137, 1005, 985s, 744, 694, 560, 487, 447, 434, 398, 317, 303, 249, 204, 172s, 153, 135.

**Source:** Frost et al. (2004l).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of strengite see also Kloprogge and Wood (2017).

**Stringhamite** CaCu(SiO<sub>4</sub>)·H<sub>2</sub>O**Origin:** Christmas mine, Gila Co., Arizona, USA.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power at the sample was 0.1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3239sh, 3193, 1371w, 1147w, 1061, (1027w), (997w), 980sh, 956s, 908, 848s, 825, 799, 764w, 693w, 626w, 570s, 519, 505, 431w, 396, 369, 341w, 326w, 303.**Source:** Frost and Xi (2012f).**Comments:** No independent analytical data are provided for the sample used.**Stromeyerite** CuAgS**Origin:** Artificial (a product of Ag-Cu alloy corrosion).**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 266–280 (broad).**Source:** De Caro et al. (2016).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.**Stronadelphite** Sr<sub>5</sub>(PO<sub>4</sub>)<sub>3</sub>F**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powder sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1055, 1042, 1029, 952s, 606sh, 595, 582, 575, 445, 423, 305w, 241, 208w, 196w, 186w, 174w.**Source:** Zhai et al. (2015).**Comments:** The sample was characterized by powder X-ray diffraction data.**Strontianite** Sr(CO<sub>3</sub>)**Origin:** Drensteinfurt, Münsterland, North Rhine-Westphalia, Germany.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.**Raman shifts (cm<sup>-1</sup>):** 1543w, 1445, 1069s, 700, 242.**Source:** Buzgar and Apopei (2009).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of strontianite see also Frezzotti et al. (2012).**Strontiofluorite** SrF<sub>2</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a single crystal using 253.65 nm Hg radiation.**Raman shifts (cm<sup>-1</sup>):** 285.**Source:** Warrier and Krishnan (1964).

**Strontiohurlbutite**  $\text{SrBe}_2(\text{PO}_4)_2$ 

**Origin:** Nanping No. 31 pegmatite, Fujian province, SE China (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single-crystal sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 1178, 1135, 1022s, 587, 575, 550, 494, 442, 421, 343, 204, 176.

**Source:** Rao et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Strontiojoaquinite**  $(\text{Na},\text{Fe})_2\text{Ba}_2\text{Sr}_2\text{Ti}_2(\text{SiO}_3)_8(\text{O},\text{OH})_2 \cdot \text{H}_2\text{O}$ 

**Origin:** Junilla Claim, San Benito Co., California, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3599w, 3587sh, 3519 + 3511 (unresolved doublet?), 3485sh, 1123s, 1062, 1031, 971s, 912, 892, 738w, 682 + 679 (unresolved doublet?), 621s, 602sh, 511, 468+437 (unresolved doublet?), 387–386, 357sh, 339, 284, 267, 193sh, 173, 159, 145.

**Source:** Frost and Pinto (2007).

**Comments:** The sample was characterized by electron microprobe analysis.

**Strunzite**  $\text{Mn}^{2+}\text{Fe}^{3+}_2(\text{PO}_4)_2(\text{OH})_2 \cdot 6\text{H}_2\text{O}$ 

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3483, 3410, 3340, 3120, 1120, 1048, 1000s, 975, 639, 567, 513, 469s, 433, 406, 329, 301, 281sh, 248, 199, 183, 168.

**Source:** Frost et al. (2002c).

**Comments:** The sample was characterized by powder X-ray diffraction data and qualitative electron microprobe analysis.

**Struvite-(K)**  $\text{KMg}(\text{PO}_4) \cdot 6\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 1064 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1075w, 1015w, 1005w, 985w, 946s, 569s, 470w, 430, and a series of bands in the range from 250 to 400 cm<sup>-1</sup>.

**Source:** Stefov et al. (2004).

**Comments:** No independent analytical data are provided for the sample used.

**Struvite**  $(\text{NH}_4)\text{Mg}(\text{PO}_4) \cdot 6\text{H}_2\text{O}$ **Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3239sh, 3115, 2921sh, (2903sh), 2368w, 1077, 1013w, 950s, (942), 890, 564, 463w, 428, 300, 242, 229, 206.**Source:** Frost et al. (2005j).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of struvite see also García et al. (2013).**Studtite**  $(\text{UO}_2)(\text{O}_2)(\text{H}_2\text{O})_2 \cdot 2\text{H}_2\text{O}$ **Origin:** Menzenschwand, Schwarzwald (Black Forest Mts.), Germany.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 6 mW. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 3473w, 3145, 1712w, 1685, 865s, 838sh, 819s, 810sh, 408w, 352w, 294w, 266w, 230w.**Source:** Bastians et al. (2004).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of studtite see also Amme et al. (2002) and Colmenero et al. (2017).**Sturmanite**  $\text{Ca}_6\text{Fe}^{3+} \cdot 2(\text{SO}_4)_2[\text{B}(\text{OH})_4](\text{OH})_{11}\text{O} \cdot 25\text{H}_2\text{O}$ **Origin:** Black Rock mine, Kuruman Manganese Fields, Kalahari, South Africa (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3677sh, 3622 + 3600 (unresolved doublet?), 3479, (3401), 3276sh, 1776w, 1697, 1636sh, 1117w, 1069, 995sh, 990s, 981sh, 959w, 760w, 623w, 579s, 530, 501, 455, 383sh, 355, 268sh, (232), 205.**Source:** Frost et al. (2014ag).**Comments:** The sample was characterized by electron microprobe analysis.**Stützite**  $\text{Ag}_{5-x}\text{Te}_3$  ( $x = 0.24\text{--}0.36$ )**Origin:** Coranda-Hondol open pit, Certej Au-Ag deposit, South Apuseni Mts., Romania.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented grain in a polished section using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 147s, 80sh, 64.**Source:** Apopei et al. (2014b).**Comments:** The sample was characterized by electron microprobe analyses.

**Sudoite**  $Mg_2Al_3(Si_3Al)O_{10}(OH)_8$ **Origin:** Semail ophiolite, Oman.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> or 532 nm solid-state laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3696, 3692, 3666, 3646, 1109, 1080, 1045, 1005, 733, 702, 665, 616, 559s, 549, 477, 403, 388, 365, 259s, 211, 190, 94.**Source:** Reynard et al. (2015).**Comments:** The empirical formula of the sample used is  $(Mg_{1.7}Fe_{0.3}Al_4)(Si_3Al)O_{10}(OH)_8$ .**Sudovikovite** PtSe<sub>2</sub>**Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The nominal laser radiation power was 10 mW.**Raman shifts (cm<sup>-1</sup>):** 206, 177.**Source:** Altamura et al. (2014).**Comments:** The sample was characterized by powder X-ray diffraction data.**Sulphohalite** Na<sub>6</sub>(SO<sub>4</sub>)<sub>2</sub>ClF**Origin:** Searles Lake, San Bernardino Co., California, USA (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** (1132sh), 1128, (1120sh), 1021w, (1010sh), 1003s, (997sh), 986sh, 635, 624sh, (481sh), 472, 467sh, 159 + 146 (unresolved doublet?), 117 + 109 (unresolved doublet?).**Source:** Frost et al. (2014z).**Comments:** No independent analytical data are provided for the sample used. The sample was characterized by qualitative electron microprobe analysis.**Sulfur** S**Origin:** Mariana Arc.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The laser radiation output power was 100 mW.**Raman shifts (cm<sup>-1</sup>):** 472s, 437, 246, 219s, 186w, 153.**Source:** White (2009).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of sulfur see also Venkateswarlu (1940), Mycroft et al. (1990), Turcotte and Benner (1993), Munce et al. (2007), and Frezzotti et al. (2012).

**Sulvanite** Cu<sub>3</sub>VS<sub>4</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using Ar<sup>+</sup> or Kr<sup>+</sup> laser radiation. The laser radiation power at the sample was below 50 mW.**Raman shifts (cm<sup>-1</sup>):** 448sh, 440s, 376s, 301w, 201s, 147.**Source:** Petritis et al. (1981).**Comments:** The sample was characterized by powder X-ray diffraction data.**Suredaite** PbSnS<sub>3</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on nanorods using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 625, 442, 309s, 201, (143s).**Source:** Wang et al. (2001b).**Comments:** The sample was characterized by powder X-ray diffraction data.**Sursassite** Mn<sup>2+</sup><sub>2</sub>Al<sub>3</sub>(SiO<sub>4</sub>)(Si<sub>2</sub>O<sub>7</sub>)(OH)<sub>3</sub>**Origin:** Strategic Manganese Mine, near Woodstock, New Brunswick, Canada.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 633 nm He-Ne laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3452, 3335, 3230, 2998sh, 1086w, 1026w, 925s, 866, 822, 705, 618, 554s, 491sh, 353, 283, (213), 151.**Source:** Reddy and Frost (2007).**Comments:** The sample was characterized by powder X-ray diffraction data. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Susannite** Pb<sub>4</sub>(SO<sub>4</sub>)(CO<sub>3</sub>)<sub>2</sub>(OH)<sub>2</sub>**Origin:** Herzog Julius Shaft, Astfeld, Schlackental, Harz Mts., Germany.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3630, 3550, 3513, 3447, 3377, 3307, 3241, 3179, 1154, 1105, 1048, 1026, 1011, 964s, 628, 602, 497, 470, 450, 427, 393, 363, 239, 203.**Source:** Frost et al. (2003e).**Comments:** Questionable data: bands of symmetric stretching vibrations of carbonate groups are unusually weak. No independent analytical data are provided for the sample used.

**Suseinargiuite**  $(\text{Na}_{0.5}\text{Bi}_{0.5})(\text{MoO}_4)$ 

**Origin:** Su Seinargiu, Sardinia, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 1.5 mW.

**Raman shifts (cm<sup>-1</sup>):** 876s, 772, 376, 319s, 188, 131w.

**Source:** Orlandi et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Svanbergite**  $\text{SrAl}_3(\text{SO}_4)(\text{PO}_4)(\text{OH})_6$ 

**Origin:** Mt. Brusilof mine, Radium, British Columbia, Canada.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3518sh, 3467, 3415sh, 3319sh, (3215sh), 3151w, 3064sh, 1098, 1034sh, 1022s, 998, 981sh, 896, 654, 633, 616s, 602sh, 588sh, 572sh, 522, 486, 474sh, 392, 369sh, 280w, 246, 179.

**Source:** Frost and Palmer (2011b).

**Comments:** No independent analytical data are provided for the sample used.

**Švenekite**  $\text{Ca}[\text{AsO}_2(\text{OH})_2]_2$ 

**Origin:** Geschieber vein, Jáchymov ore district, Western Bohemia, Czech Republic (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was 3 mW.

**Raman shifts (cm<sup>-1</sup>):** 3368, 2917w, 2385w, 929, 901, 871s, 840, 753s, 726, 541w, 498w, 417, 393, 358, 330, 289, 268, 223, 172w.

**Source:** Ondruš et al. (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Svornostite**  $\text{K}_2\text{Mg}[(\text{UO}_2)(\text{SO}_4)_2]_2 \cdot 8\text{H}_2\text{O}$ 

**Origin:** Geschieber vein, Jáchymov ore district, Western Bohemia, Czech Republic (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm solid-state laser radiation. The nominal laser radiation power was 2.5 mW.

**Raman shifts (cm<sup>-1</sup>):** 3622w, 3545, 3496, 1220w, 1200, 1155, 1110w, 1028, 989, 951w, 854s, 725w, 643, 610w, 458, 438, 322w, 268w, 207sh, 186, 132, 75.

**Source:** Plášil et al. (2015b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Swedenborgite**  $\text{NaBe}_4\text{Sb}^{5+}\text{O}_7$ 

**Origin:** Långban, near Pajsberg and Filipstad, Värmland, Sweden (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 633 nm laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 906w, 797s, 767, ~740, 575, 427s.

**Source:** Gaft et al. (2013).

**Comments:** The Raman spectrum agrees well to that from the RRUFF database.

**Symplesite-(Fe)**  $\text{Fe}^{2+}_3(\text{AsO}_4)_2 \cdot 8\text{H}_2\text{O}$ 

**Origin:** Laubach mine, Laufdorf, Wetzlar, Hesse, Germany.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3448w, 892, 841s, 803, 768s, 520sh, 498s, 442, 373, 319w, 281, 249, 225sh, 207, 189w, 172w, 137w, 113w.

**Source:** Makreski et al. (2015b).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Synchysite-(Ce)**  $\text{CaCe}(\text{CO}_3)_2\text{F}$ 

**Origin:** Soultz-sous-Forêts, Rhine Graben, France.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was about 14 mW.

**Raman shifts (cm<sup>-1</sup>):** 1101s, 1083s, 758w, 742, 515, 477, 454w, 276.

**Source:** Middleton et al. (2013).

**Comments:** The sample was characterized by electron microprobe analyses.

**Syngenite**  $\text{K}_2\text{Ca}(\text{SO}_4)_2 \cdot \text{H}_2\text{O}$ 

**Origin:** Kalush mine, western Ukraine.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 3306, 1167, 1143, 1120w, 1084w, 1007s, 982s, 663w, 641, 495, 472sh, 442, 240w.

**Source:** Buzgar et al. (2009).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of syngenite see also Frezzotti et al. (2012) and Jentzsch et al. (2012a, 2013).

**Szaibélyite**  $\text{MgBO}_2(\text{OH})$ 

**Origin:** Vysoká-Zlatno Cu-Au porphyry-skarn deposit, Štiavnica Neogene strato volcano, Western Carpathians, Slovakia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3567, 3559s, 1516w, 1463, 1284, 1186, 988, 915w, 836s, 661, 627, 611, 529, 493, 345, 321, 296, 184, 161.

**Source:** Bilohuščin et al. (2017).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectra of szaibélyite see also Frost et al. (2015aa) and Galuskina et al. (2008).

#### Szenicsite Cu<sub>3</sub>(MoO<sub>4</sub>)(OH)<sub>4</sub>

**Origin:** Jardinera No 1 Mine, Inca de Oro, Chile (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 785 nm Nd-YAG laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3559, 3518, 3506w, 3503w, 3500w, 928, (903sh), 898s, (895sh), 827, 801w, 687w, 476, 408s, 349, 308, 280, 211, 147, 105.

**Source:** Frost et al. (2007a).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of szenicsite see also Yang et al. (2012).

#### Szmikite Mn(SO<sub>4</sub>)·H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1188, 1089, 1021s, 654w, 623, 493, 426, 263w.

**Source:** Buzgar et al. (2009).

**Comments:** No independent analytical data are provided for the sample used.

#### Szomolnokite Fe(SO<sub>4</sub>)·H<sub>2</sub>O

**Origin:** Baia Sprie mining area, Romania.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632 nm Nd-YAG laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 1191, 1091, 1020s, 667w, 623, 492, 427.

**Source:** Buzatu et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of szomolnokite see also Chio et al. (2007), Jentzsch et al. (2013), Rull et al. (2014), and Apopei et al. (2015).

#### Takedaite Ca<sub>3</sub>B<sub>2</sub>O<sub>6</sub>

**Origin:** Fuka mine, Okayama prefecture, Japan (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** (1087s) (with shoulders), 929w, 911w, (715 + 712) (unresolved doublet?), 585w, 330w, (~282), 217w, (159 + 154) (unresolved doublet?).

**Source:** Frost et al. (2014n).

**Comments:** Questionable data. The sample was characterized by qualitative electron microprobe analysis (only Ca, O, and C have been found). The bands at 1087, 715 + 712, ~282, and 159 + 154 cm<sup>-1</sup> correspond to calcite that is the main component in the sample used.

### Takovite Ni<sub>6</sub>Al<sub>2</sub>(CO<sub>3</sub>)(OH)<sub>16</sub>·4H<sub>2</sub>O

**Origin:** Kambalda, Western Australia, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3461, 2855, 2615, 1543, 1060s, 1042, 992, 697, 558s, 533, 492, 403, 324, 253, 225, 218.

**Source:** Frost et al. (2003h).

**Comments:** No independent analytical data are provided for the sample used.

### Talc Mg<sub>3</sub>Si<sub>4</sub>O<sub>10</sub>(OH)<sub>2</sub>

**Origin:** Greiner, Zillertal, Austria.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 257 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was below 3 mW.

**Raman shifts (cm<sup>-1</sup>):** 3675s, 3660, 1051w, 793, 707, 676s, 469, 434, 363, 333w.

**Source:** Petry et al. (2006).

**Comments:** The sample was characterized by electron microprobe analyses. For Raman spectra of talc see also Blaha and Rosasco (1978), Rosasco and Blaha (1980), Wada and Kamitakahara (1991), and Frezzotti et al. (2012).

### Talmessite Ca<sub>2</sub>Mg(AsO<sub>4</sub>)<sub>2</sub>·2H<sub>2</sub>O

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 2882, 2376, 931, 905, 877, 836s, 814, 783, 455s, 445, 388, 363, 357, 305, 276, 212, 196, 173.

**Source:** Frost and Klopdroge (2003).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of talmessite see also Frost (2009a).

**Tangdanite**  $\text{Ca}_2\text{Cu}_9(\text{AsO}_4)_4(\text{SO}_4)_{0.5}(\text{OH})_9 \cdot 9\text{H}_2\text{O}$ **Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3489, 3403, 1136, 1007, 883, 841s, 802, 669, 618, 505, 493, 462, 414, 385, 359, 314, 260, 210, 179.**Source:** Frost and Klopdroge (2003).**Comments:** No independent analytical data are provided for the sample used. In the cited paper tangdanite was described with the old name clinotyrolite. For the Raman spectrum of tangdanite see also Frost et al. (2012n, 2015z).**Tangeite**  $\text{CaCu}(\text{AsO}_4)(\text{OH})$ **Origin:** Tange gorge, Tyuya-Mayun, Kyrgyzstan (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** (3242), 3118, (868w), 842s, 823, 798, 768w, (715w), 507w, 482, 463, 392w, 367, 321s, 284, 264, 208, 184, 165, 145, 135.**Source:** Martens et al. (2003c).**Comments:** No independent analytical data are provided for the sample used.**Tantalite-(Fe)**  $\text{Fe}^{2+}\text{Ta}_2\text{O}_6$ **Origin:** Suzhou granite, Suzhou City, southern Jiangsu, China.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 700 mW.**Raman shifts (cm<sup>-1</sup>):** 880.**Source:** Wang et al. (1997).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.**Tantalite-(Mg)**  $\text{MgTa}_2\text{O}_6$ **Origin:** Synthetic.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 740sh, 712s, 662, 568w, 540w, 473, 425, 356w, 334, 253s, 185s.**Source:** Husson et al. (1979).**Comments:** No independent analytical data are provided for the sample used.

**Tantalite-(Mn)** Mn<sup>2+</sup>Ta<sub>2</sub>O<sub>6</sub>

**Origin:** Alto do Giz pegmatite, Borborema pegmatite province, northeastern Brazil.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 14 mW.

**Raman shifts (cm<sup>-1</sup>):** 887s, 621, 547, 526, 324, 282, 238, 202, 121.

**Source:** Thomas et al. (2011a).

**Comments:** The sample was characterized by qualitative electron microprobe analyses.

**Tantite orthorhombic polymorph** Ta<sub>2</sub>O<sub>5</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 981, 948, 903, 844, 762, 711, 642, 612s, 562, 494, 458, 377, 338, 269, 245s, 196, 139, 106s, 78.

**Source:** Joseph et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of Ta<sub>2</sub>O<sub>5</sub> see also Dobal et al. (2000) and Meng et al. (1997).

**Taranakite** K<sub>3</sub>Al<sub>5</sub>(PO<sub>3</sub>OH)<sub>6</sub>(PO<sub>4</sub>)<sub>2</sub>·18H<sub>2</sub>O

**Origin:** Jenolan Caves, New South Wales, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1149, 1126s, 1116sh, 1100sh, 1064w, 1026, 1010sh, (991), 962s, (946sh), (922sh), 811, 656, 648, 636, 615sh, 595, (580), 572sh, 560s, 547, (537sh), 529sh, 505sh, 489, 464, 444, 416s, (404), 396s, (388sh), 348w, 328, 304, 271, 260sh, 248, (237sh), 223, 202, 188s, 165, 155.

**Source:** Frost et al. (2011v).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Tarapacáite** K<sub>2</sub>(CrO<sub>4</sub>)

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 457.9 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was between 5 and 30 mW.

**Raman shifts (cm<sup>-1</sup>):** 906, 886, 883, 873, 859s, 395, 390, 388, 354s, 351s.

**Source:** Serghiou and Guillaume (2004).

**Comments:** For the Raman spectra of tarapacáite see also Kiefer and Bernstein (1972) and Huang and Butler (1990).

**Tarbuttite**  $\text{Zn}_2(\text{PO}_4)(\text{OH})$ **Origin:** Broken Hill, Zambia.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power at the sample was 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3446, 1069, 1051, 1011, 965s.**Source:** Frost (2004a).**Comments:** No independent analytical data are provided for the sample used.**Tausonite**  $\text{SrTiO}_3$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using the conventional 14358-Å mercury *e* line. The radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1030, 720, 675, 620..., 360s, 310s, 250, 80.**Source:** Perry et al. (1967).**Comments:** No independent analytical data are provided for the sample used.**Tazheranite**  $(\text{Zr,Ti,Ca})(\text{O},\square)_2$ **Origin:** Synthetic (stabilized cubic  $\text{ZrO}_2$ ).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 625s, 480, 360, 250, 150.**Source:** Phillipi and Mazdiyasni (1971).**Comments:** For the Raman spectrum of tazheranite see also Galuskina et al. (2013a).**Tazzoliite**  $\text{Ba}_2\text{CaSr}_{0.5}\text{Na}_{0.5}\text{Ti}_2\text{Nb}_3\text{SiO}_{17}[\text{PO}_2(\text{OH})_2]_{0.5}$ **Origin:** Euganei Hills, Padova, Italy (type locality).**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was between 10 and 50 mW.**Raman shifts (cm<sup>-1</sup>):** 3516w, 1062w, 981w, 961w, 869w, 754s, 563s, 540, 328, 261s, 229s.**Source:** Cámara et al. (2012a).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.**Teepleite**  $\text{Na}_2\text{B}(\text{OH})_4\text{Cl}$ **Origin:** No data.**Experimental details:** Polarized Raman scattering measurements have been performed on a single crystal using Ar<sup>+</sup> laser radiation.**Raman shifts (cm<sup>-1</sup>):** 3555, 3535, 3525, 1195, 1185, 946, 854, 770, 743, 660, 505, 499, 429, 373, 185, 143, 135, 113.**Source:** Devarajan et al. (1974).**Comments:** No independent analytical data are provided for the sample used.

**Teineite** Cu<sup>2+</sup>(Te<sup>4+</sup>O<sub>3</sub>)·2H<sub>2</sub>O**Origin:** Moctezuma Mine, Mexico.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3495, (3139), 3040, 2854sh, (2641w), 2286w, 778sh, 739s, 701, 667, 509s, 458sh, 384sh, 347, 319, 250sh, 235, 175, 131.**Source:** Frost and Keeffe (2009b).**Comments:** No independent analytical data are provided for the sample used.**Tellurantimony** Sb<sub>2</sub>Te<sub>3</sub>**Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was below 3 mW. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 164.5, 111, 68s.**Source:** Chis et al. (2012).**Comments:** No independent analytical data are provided for the sample used.**Tellurium** Te**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a thin film using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 136, 116s.**Source:** Russo et al. (2008).**Comments:** For the Raman spectrum of tellurium see also Pine and Dresselhaus (1971).**Tellurobismuthite** Bi<sub>2</sub>Te<sub>3</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a thin film using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was <<2 mW.**Raman shifts (cm<sup>-1</sup>):** 133, 101s, 60, 38.**Source:** Xu et al. (2015a).**Comments:** For the Raman spectra of tellurobismuthite see also Richter et al. (1977) and Chis et al. (2012).**Tengerite-(Y)** Y<sub>2</sub>(CO<sub>3</sub>)<sub>3</sub>·2–3H<sub>2</sub>O**Origin:** Paratoo copper mine, Yunta, Olary Province, South Australia, Australia.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3621w, 3367sh, 3281, 3241sh, 3047, 2920, 2789sh, 2657, 1689w, (1637), 1618, 1592sh, 1392w, 1334, 1114sh, 1100s, 1091sh, 1067, (1062), 1038w, 1006w, 775 + 765 (unresolved doublet?), 689 + 674 (unresolved doublet?), 611sh, 589, 553+544 (unresolved doublet?), 508, 479, 474, 417w, 408, 398, 355w.

**Source:** Frost et al. (2015s).

**Comments:** No independent analytical data are provided for the sample used. IR spectra of presumed tengerite presented in Figs. 1b, 2b, and 4b of the cited paper are wrong. Actually, they are IR spectra of a silicate with minor admixture of quartz. IR bands of the silicate and quartz are erroneously assigned to vibrations of carbonate groups.

**Tennantite** Cu<sub>6</sub>[Cu<sub>4</sub>(Fe,Zn)<sub>2</sub>]As<sub>4</sub>S<sub>13</sub>

**Origin:** Tsumeb mine, Tsumeb, Namibia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was between 1 and 10 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 377s, 344.

**Source:** Mernagh and Trudu (1993).

**Comments:** The sample was characterized by electron microprobe analyses. For the IR spectrum of tennantite see also Kharbishi et al. (2009).

**Tenorite** CuO

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a thin film using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 631, 346, 296s.

**Source:** Debbichi et al. (2012).

**Comments:** The sample was characterized by X-ray diffraction data.

**Tephroite** Mn<sup>2+</sup><sub>2</sub>(SiO<sub>4</sub>)

**Origin:** Franklin, New Jersey, USA.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 933, 892, 840s, 806s, 516w, 387, 306w, 278w, 243.

**Source:** Welsh (2008).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectra of tephroite see also Stidham et al. (1976), Piriou and McMillan (1983), and Mouri and Enami (2008).

**Tetrahedrite** Cu<sub>6</sub>[Cu<sub>4</sub>(Fe,Zn)<sub>2</sub>]Sb<sub>4</sub>S<sub>13</sub>

**Origin:** Kremnice, Slovakia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 4.25 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 379sh, 366s, 356s, 331, 298, 258w.

**Source:** Kharbishi et al. (2009).

**Comments:** The sample was characterized by electron microprobe analyses. The atomic ratio Sb:As is 3:1. For the Raman spectra of tetrahedrite see also Mernagh and Trudu (1993) and Rath et al. (2015).

**Tetrawickmanite** Mn<sup>2+</sup>Sn<sup>4+</sup>(OH)<sub>6</sub>

**Origin:** Långban, near Pajsberg and Filipstad, Värmland, Sweden.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 3374w, 3253, 3145, 3062sh.

**Source:** Lafuente et al. (2015).

**Comments:** The Raman spectrum was obtained only in the range of O–H-stretching vibrations.

**Thaumasite** Ca<sub>3</sub>Si(OH)<sub>6</sub>(CO<sub>3</sub>)(SO<sub>4</sub>)·12H<sub>2</sub>O

**Origin:** Black Rock mine, Kuruman, Kalahari, Northen Cape Province, South Africa.

**Experimental details:** Raman scattering measurements have been performed on a single crystal using 458 nm solid-state diode source laser radiation, with the laser beam parallel to [100] and at the 180° polarization counterclockwise from [001]. The laser radiation power at the sample was 40 mW.

**Raman shifts (cm<sup>-1</sup>):** ~3500, ~3440, ~3370, ~3100sh, 1685, 1112, 1066s, 983s, 887w, 658, 588w, 455w, 418w, 250w, 193w, 143w, 120w, 92.

**Source:** Gatta et al. (2012b).

**Comments:** In the cited paper, Raman spectra of thaumasite have been obtained in different scattering geometries. For the Raman spectrum of thaumasite see also Goryainov (2016).

**Thecotrichite** Ca<sub>3</sub>(CH<sub>3</sub>COO)<sub>3</sub>Cl(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O

**Origin:** Artificial (efflorescent salt occurring on surfaces of porous calcareous objects stored in wooden cabinets).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 0.9 mW.

**Raman shifts (cm<sup>-1</sup>):** 3470w, 3372w, 3011w, 2986w, 2956w, 2928, 1472s, 1431, 1349, 1058s, 1046s, 968s, 961s, 749, 710w, 667.

**Source:** Wahlberg et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data. The crystal structure is solved.

**Theophrastite** Ni(OH)<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 3601w, 3571, 450, 315.

**Source:** Gourrier et al. (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Thermonatrite** Na<sub>2</sub>(CO<sub>3</sub>)·H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented particle using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 3404w, 3278w, 2977w, 1535w, 1433w, 1394w, 1067s, 700w, 683w, 652w.

**Source:** Bouchard and Smith (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of thermonatrite see also Frezzotti et al. (2012).

**Thometzekite**  $\text{PbCu}^{2+}_2(\text{AsO}_4)_2 \cdot 2\text{H}_2\text{O}$

**Origin:** Tsumeb mine, Tsumeb, Namibia (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3519w, 3282w, 2821w, 2345sh, 984w, 841s, 790sh, 728w, 499s, 428, 401, 356s, 322, 239w.

**Source:** Frost and Weier (2004e).

**Comments:** No independent analytical data are provided for the sample used.

**Thomsonite-Ca**  $\text{NaCa}_2(\text{Al}_5\text{Si}_5)\text{O}_{20} \cdot 6\text{H}_2\text{O}$

**Origin:** Dobrna, Děčín, Bohemia, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 Nd-YAG or 785 nm diode laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 1071, 990, 968, 930w, 608, 536s, 494w, 474w, 443, 391w, 341w, 310w, 268w, 258w, 220w, 197w, 180, 167w, 156w, 120w.

**Source:** Jehlička et al. (2012).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of thomsonite-Ca see also Wopenka et al. (1998), Mozgawa (2001), and Jehlička and Vandenabeele (2015).

**Thorianite**  $\text{ThO}_2$

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was between 30 and 150 mW.

**Raman shifts (cm<sup>-1</sup>):** 1033w, 885w, 467s.

**Source:** Jayaraman et al. (1988).

**Comments:** The spectrum was obtained at 0.8 GPa.

**Thorikosite**  $\text{Pb}_3\text{O}_3\text{Sb}^{3+}(\text{OH})\text{Cl}_2$

**Origin:** Lavrion, Greece (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3602w, 3541sh, 3508+3504s (unresolved doublet?), (3488sh), 1085w, 730, (657), 596, 325s, 275 + 269s (unresolved doublet?), (155), 133s, 112, 105w.

**Source:** Frost and Bahfenne (2011b).

**Comments:** No independent analytical data are provided for the sample used.

### Thorite Th(SiO<sub>4</sub>)

**Origin:** Synthetic.

**Experimental details:** Polarized Raman scattering measurements have been performed on a single crystal, using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 250 mW. A 90°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 920, 894, 855, 596, 517, 439, 312, 293, 264, 194, 129, 126.

**Source:** Syme et al. (1977).

**Comments:** For Raman spectra of thorite see also Lahalle et al. (1986) and Costin et al. (2012).

### Thorneite Pb<sub>6</sub>(Te<sub>2</sub>O<sub>10</sub>)(CO<sub>3</sub>)Cl<sub>2</sub>(H<sub>2</sub>O)

**Origin:** Otto Mt., near Baker, San Bernardino Co., California, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation, with the light propagating parallel to the *c* axis of a single crystal. The nominal laser radiation power was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** ~3300 (broad), 1630w, 1056 (sharp), and a series of strong peaks below 900 cm<sup>-1</sup>.

**Source:** Kampf et al. (2010a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### Thortveitite Sc<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a pulverized crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 4 W.

**Raman shifts (cm<sup>-1</sup>):** 949, 932s, 688w, 543, 510, 445, 435s, 392s, 347, 280w, 253, 205, 194.

**Source:** Bretheau-Raynal et al. (1979).

**Comments:** The sample was characterized by electron microprobe analyses.

### Thorutite (Th,U,Ca)Ti<sub>2</sub>(O,OH)<sub>6</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powder sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** The strongest Raman peaks are observed at 760, 620, and 195 cm<sup>-1</sup>.

**Source:** Zhang et al. (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Threadgoldite**  $\text{Al}(\text{UO}_2)_2(\text{PO}_4)_2(\text{OH}) \cdot 8\text{H}_2\text{O}$ 

**Origin:** South Alligator River, West Arnhem region, Northern Territory, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3576w, 3411w, 3158w, 1655w, 1107w, 1057w, 1026 + 1019s (unresolved doublet?), 999, 974s, 953w, (840w), 827s, (817), 612, 533, 451, 419, 398s, 391, 329, 292, 201s, 188, 146, 114.

**Source:** Frost et al. (2006a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Tiemannite** HgSe

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed at 90 K on a cleaved (111) plane, in a—z(x,x)z polarization using 514.5 nm Ar<sup>+</sup> laser radiation.

**Raman shifts (cm<sup>-1</sup>):** 133, 43.

**Source:** Szuszkiewicz et al. (1999).

**Tilasite** CaMg(AsO<sub>4</sub>)F

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1518w, 1318w, 1107w, 1056w, 820, 659w, 611, 493, 410s, 297, 245.

**Source:** Frost and Kloprogge (2003).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of tilasite see also Downs et al. (2012).

**Tilleyite** Ca<sub>5</sub>Si<sub>2</sub>O<sub>7</sub>(CO<sub>3</sub>)<sub>2</sub>

**Origin:** Kushiro, Hiba-gun, Hiroshima prefecture, Honshu Island, Japan.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** (3638sh), 3635w, (3629sh), 3594w, (3578w), 3574w, 1748w, 1738w, 1501w, 1436w, 1412w, 1093, 1086s, 1080sh, 1067w, 1047, (1018w), 1010, (999w), 986, 966w, 572, 546, 528, 505sh, 493, 483sh, 456, 450sh, 424sh, 413, 396, 380sh, 366, 353, 329, 321sh, 302sh, 282s, (273), 260sh, 242sh, 234, 204sh, 197, 176, 155, 143.

**Source:** Frost et al. (2015e).

**Comments:** The sample was characterized by qualitative electron microprobe analysis. Bands between 600 and 900 cm<sup>-1</sup> are not indicated. The bands in the range from 3500 to 3700 cm<sup>-1</sup> may correspond to an impurity.

**Tiragalloite** Mn<sup>2+</sup><sub>4</sub>As<sup>5+</sup>Si<sub>3</sub>O<sub>12</sub>(OH)

**Origin:** Valletta mine, Maira Valley, Cuneo province, Piedmont, Italy.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation output power of 80 mW was attenuated by means of a series of density filters.

**Raman shifts (cm<sup>-1</sup>):** 1004, 975, 960s, 902s, 869s, 863, 803, 785, 661s, 647s, 549, 508, 481, 398, 364, 320, 286w, 218w, 181w, 153w.

**Source:** Cámara et al. (2015).

**Comments:** The sample was characterized by electron microprobe analyses.

**Tissintite** (Ca,Na, $\square$ )AlSi<sub>2</sub>O<sub>6</sub>

**Origin:** Tissint Martian meteorite (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented grain in a polished section using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 997 (broad), 693s, 573, 523, 417sh, 377s, 203.

**Source:** Ma et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Tistarite** Ti<sub>2</sub>O<sub>3</sub>

**Origin:** Allende meteorite (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented grain in a polished section using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** Only a figure of the Raman spectrum of tistarite is given in the cited paper. The strongest peak is observed at ~250 cm<sup>-1</sup>.

**Source:** Ma and Rossman (2009a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Titanite** CaTi(SiO<sub>4</sub>)O

**Origin:** Village of Dunje, Municipality of Prilep, Republic of Macedonia.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 nm Ar<sup>+</sup> or 1064 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 912, 872, 856, 608s, 548, 467s, 425, 333w, 316, 286sh, 253, 233w, 208sh, 164, 146w.

**Source:** Makreski et al. (2005b).

**Comments:** For the Raman spectra of titanite see also Meyer et al. (1996), Jasinevicius (2009), Andò and Garzanti (2014), and Gaft et al. (2015).

**Titanoholtite**  $(\text{Ti}_{0.75}\square_{0.25})\text{Al}_6\text{BSi}_3\text{O}_{18}$ 

**Origin:** Szklary pegmatite, Lower Silesia, Poland (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was ~5.5 mW.

**Raman shifts (cm<sup>-1</sup>):** 1055, 935s, 885, 624, 561s, 507s, 466s, 407s, 362s, 286, 211.

**Source:** Pieczka et al. (2013).

**Comments:** The sample was characterized by electron diffraction data and electron microprobe analyses.

**Tlapallite**  $\text{H}_6(\text{Ca},\text{Pb})_2(\text{Cu},\text{Zn})_3\text{O}_2(\text{SO}_4)(\text{Te}^{4+}\text{O}_3)_4(\text{Te}^{6+}\text{O}_4)$ 

**Origin:** Mina Bambollita, Moctezuma, Sonora, Mexico (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 2926w, 2867w, 2754w, 2594w, 2320w, 2206w, 1957w, 1571w, 1474sh, 1104, 1062w, 973s, 796 + 788s (unresolved doublet?), 744sh, 708, 691sh, 610sh, (523), 509, 474, 438s, 419sh, 383sh, 353sh, 314, 291, 258, 229, 189, 168, 146, 121s.

**Source:** Frost (2009b).

**Comments:** No independent analytical data are provided for the sample used.

**Tobermorite**  $\text{Ca}_4\text{Si}_6\text{O}_{17}(\text{H}_2\text{O})_2 \cdot (\text{Ca} \cdot 3\text{H}_2\text{O})$ 

**Origin:** N'Chwaning II mine, Kalahari Manganese Fields, Republic of South Africa.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed in nearly back-scattered geometry using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3525, 1145w, 1013, 682s, 619, 530w, 475w, 447w, 425w, 366w, 321w.

**Source:** Biagioni et al. (2012).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data. The crystal structure is solved. For the Raman spectrum of tobermorite see also Biagioni et al. (2013b).

**Todorokite**  $(\text{Na},\text{Ca},\text{K},\text{Ba},\text{Sr})_{1-x}(\text{Mn},\text{Mg},\text{Al})_6\text{O}_{12} \cdot 3-4\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample (pressed as a pellet) using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 2.5 mW.

**Raman shifts (cm<sup>-1</sup>):** 643s, 359, 295.

**Source:** Feng et al. (2004).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of todorokite see also Julien et al. (2004).

**Tokyoite**  $\text{Ba}_2\text{Mn}^{3+}(\text{VO}_4)_2(\text{OH})$ **Origin:** Postmasburg Manganese Field, South Africa.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 935, 906s, 846, 830s, 720, 464, 420, 406, 390, 340, 305, 241.**Source:** Costin et al. (2014).**Comments:** As-rich variety. The sample was characterized by electron microprobe analyses.**Tolbachite** CuCl<sub>2</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 or 785.5 nm laser radiation.**Raman shifts (cm<sup>-1</sup>):** 562, 290s, 234.**Source:** Aceto et al. (2006).**Comments:** For the Raman spectrum of tolbachite see also Burgio and Clark (2001).**Tondiite** Cu<sub>3</sub>MgCl<sub>2</sub>(OH)<sub>6</sub>**Origin:** Vesuvius volcano, Italy (type locality).**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 647 nm Kr<sup>+</sup> laser radiation. The laser radiation power at the sample was 6 mW. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 942, 695, 503s, 395, 363s.**Source:** Malcherek et al. (2014).**Comments:** The sample was characterized by electron microprobe analyses. The crystal structure is solved.**Tooeleite** Fe<sup>3+</sup><sub>6</sub>(AsO<sub>3</sub>)<sub>4</sub>(SO<sub>4</sub>)(OH)<sub>4</sub>·4H<sub>2</sub>O**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 514 nm diode laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 1597sh, 1554, 1522, 1422, 1287s, 1085, 983, 870sh, 803, (758), 661sh, 604s, 508, 438sh, 464, 284.**Source:** Liu et al. (2013).**Comments:** The sample was characterized by powder X-ray diffraction data. The assignment of the strong band at 1287 cm<sup>-1</sup> to asymmetric stretching vibrations of SO<sub>4</sub><sup>2-</sup> given in the cited paper is questionable.

**Topaz**  $\text{Al}_2\text{SiO}_4\text{F}_2$ **Origin:** Topaz Mountain, Thomas Range, Utah, USA.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 1167, 1079, 1008, 985, 927s, 854, 643, 559, 545, 454, 400, 370, 325, 314, 284s, 265s, 237s.**Source:** Kloprogge and Frost (2000a).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of topaz see also Bradbury and Williams (2003), Jasinevicius (2009), and Andò and Garzanti (2014).**Torbernite**  $\text{Cu}(\text{UO}_2)_2(\text{PO}_4)_2 \cdot 12\text{H}_2\text{O}$ **Origin:** Mount Painter, 9 km N of Arkaroola, South Australia.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power at the sample was 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3359, 3197, 3032sh, 1004sh, (995), 988, 957, 900w, 826s, 808sh, 629, 464, 439, 406, 399, 290, 222.**Source:** Frost (2004b).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of torbernite see also Frost and Weier (2004c, d) and Driscoll et al. (2014).**Toturite**  $\text{Ca}_3\text{Sn}_2(\text{SiFe}^{3+})_2\text{O}_{12}$ **Origin:** Upper Chegem structure, Northern Caucasus, Kabardino-Balkaria, Russia (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented grain in polished section using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation output power was 40–60 mW. A 0°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 930w, 879w, 810w, 784w, 734, 678sh, 575, 527sh, 497 + 494s (unresolved doublet?), 413w, 345sh, 301s, (266), 244, 185w, 156w, 148.**Source:** Galuskina et al. (2010c).**Comments:** The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis. The sample was characterized by backscatter electron diffraction data and electron microprobe analyses.**Trabzonite**  $\text{Ca}_4[\text{Si}_3\text{O}_9(\text{OH})]\text{OH}$ **Origin:** Upper Chegem caldera, Northern Caucasus, Kabardino-Balkaria, Russia.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented grain in polished section using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation output power was 30–50 mW. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 3602, 3576, 1020sh, 1006, 957s, 902, 872, 660s.**Source:** Armbruster et al. (2012).**Comments:** The sample was characterized by electron microprobe analyses. The crystal structure is solved.

**Tremolite**  $\square \text{Ca}_2(\text{Mg}_{5.0-4.5}\text{Fe}^{2+}_{0.0-0.5})\text{Si}_8\text{O}_{22}(\text{OH})_2$ **Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 20 mW.**Raman shifts (cm<sup>-1</sup>):** 1062, 1031, 950w, 932, 751w, 676s, 531w, 516w, 438w, 418, 396, 373, 355, 254, 234s, 225, 180, 162.**Source:** Rinaudo et al. (2004).**Comments:** The sample was characterized by selected areaelectron diffraction and electron microprobe analyses. For the Raman spectra of tremolite see also Blaha and Rosasco (1978), Petry et al. (2006), Makreski et al. (2006a), Apopei and Buzgar (2010), Apopei et al. (2011), Weber et al. (2012), Andò and Garzanti (2014), Bersani et al. (2014), and Leissner et al. (2015).**Trevorite**  $\text{NiFe}^{3+}_2\text{O}_4$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 647 nm Kr<sup>+</sup> laser radiation. The laser radiation output power was 5 mW (0.5 mW at the sample).**Raman shifts (cm<sup>-1</sup>):** 704s, 663sh, 590, 568, 487s, 456sh, 333, 211, 189w.**Source:** Hosterman (2011).**Comments:** The sample was characterized by powder X-ray diffraction data.**Tridymite** SiO<sub>2</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a poedered sample using 476.5 nm laser radiation. The nominal laser radiation power was 400 mW.**Raman shifts (cm<sup>-1</sup>):** 1086w, 786, 456, 426s, 407s, 468s, 336w, 293, 205, 152, 100w.**Source:** Etchepare et al. (1978).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of tridymite see also Ilieva et al. (2007), Knyazev et al. (2012), and Wilson (2014).**Trilithionite**  $\text{KLi}_{1.5}\text{Al}_{1.5}(\text{Si}_3\text{Al})\text{O}_{10}\text{F}_2$ **Origin:** Eranair, Finland.**Experimental details:** Raman scattering measurements have been performed with the electric field polarized perpendicular to the cleavage plane using 514.5 or 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3691w, 1128, 1094, (750), 707s, (650), 561, (405), (300), 260, 244, 182s, 94s.**Source:** Tlili et al. (1989).**Comments:** A Fe- and Mn-rich variety. The sample was characterized by electron microprobe analyses.

**Trinepheline** NaAlSiO<sub>4</sub>

**Origin:** Jadeite deposit of Tawmaw-Hpakant, Myanmar (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The nominal laser radiation power was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 1031w, 676, 572w, 518w, 494s, 487sh, 453s, 406, 375w, 359w, 347w, 311, 304w, 264w, 223, 203, 153w.

**Source:** Ferraris et al. (2014).

**Comments:** The sample was characterized by electron microprobe analyses. The crystal structure is solved.

**Triplite** (Mn<sup>2+</sup>,Fe<sup>2+</sup>)<sub>2</sub>(PO<sub>4</sub>)F

**Origin:** Codera valley, Sondrio province, Central Alps, Italy.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632.8 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3498w, 1120w, 1072w, 1036, 980.5s, 808w, 680w, 610.5, 605, 598, 573w, 468.5w, 450w, 429.5sh, 421, 398.5sh, 277.5w, 242.5w, 218.5w, 192.5w, 179.5w, 161w, 137.5w.

**Source:** Vignola et al. (2014).

**Comments:** The sample was characterized by electron microprobe analyses. The crystal structure is solved. For the Raman spectra of triplite see also Frezzotti et al. (2012) and Frost et al. (2014aj).

**Trippkeite** Cu<sup>2+</sup>As<sup>3+</sup><sub>2</sub>O<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 633 nm He-Ne laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 810sh, 780s, 657, 539, 496, (463sh), 446, 421w, 371s, 306w, 285, 235, 203, 193, 182, 141sh, 134s.

**Source:** Bahfenne (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data. For Raman spectra of trippkeite see also Bahfenne et al. (2011a) and Kharbish (2012).

**Tripuhite** Fe<sup>3+</sup>Sb<sup>5+</sup>O<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Micro-Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 20 μW.

**Raman shifts (cm<sup>-1</sup>):** 740, 652s, 500, 420 (Sample 1); 767w, 652s, 465 (Sample 2).

**Source:** Bolanz (2014).

**Comments:** The samples were characterized by powder X-ray diffraction data.

**Trotalite** CoSe<sub>2</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powder sample using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was below 0.5 mW.**Raman shifts (cm<sup>-1</sup>):** 188.**Source:** Zhu et al. (2010).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of trotalite see also Zhang et al. (2014).**Troilite** FeS**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 2 mW.**Raman shifts (cm<sup>-1</sup>):** 360, 310s, 160.**Source:** Avril et al. (2013).**Comments:** For the Raman spectra of troilite see also Ma et al. (2012a) and Kaliwoda et al. (2013).**Trona** Na<sub>3</sub>(HCO<sub>3</sub>)(CO<sub>3</sub>)·2H<sub>2</sub>O**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented individual particles using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 2 mW.**Raman shifts (cm<sup>-1</sup>):** 3440, 3059w, 2436w, 1720w, 1561w, 1430, 1058s, 846w, 697w, 639w.**Source:** Jentzsch et al. (2013).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of trona see also Frezzotti et al. (2012).**Tscher migite** (NH<sub>4</sub>)Al(SO<sub>4</sub>)<sub>2</sub>·12H<sub>2</sub>O**Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3364w, 3114w, 2982w, 2892w, 1680w, 1630w, 1132, 1102w, 991 + 983s (unresolved doublet?), 619s, 542sh, 507 + 499 (unresolved doublet?), 456s, 387, 330.**Source:** Frost and Kloprogge (2001).**Comments:** No independent analytical data are provided for the sample used.**Tsumcorite** PbZn<sub>2</sub>(AsO<sub>4</sub>)<sub>2</sub>·2H<sub>2</sub>O**Origin:** Tsumeb mine, Tsumeb, Namibia (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3503w, 3245w, 2925sh, 927, (868sh), 834s, 746, 521sh, 493s, 439, 400, 361, (340sh), 293, 242w, 197.

**Source:** Frost and Xi (2012a).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of tsumcorite see also Frost and Weier (2004e).

#### Tsumebite Pb<sub>2</sub>Cu(PO<sub>4</sub>)(SO<sub>4</sub>)(OH)

**Origin:** Blue Bell mine, near Baker, San Bernardino Co., California, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3648w, (3446sh), 3397, 3335, 3239sh, 1097w, 1061w, 971s, 935, (923sh), (852sh), 827, 606, 598sh, 554, 540w, 482sh, 468, 442s, 389, 358sh, 339, 321.

**Source:** Frost and Palmer (2011e).

**Comments:** No independent analytical data are provided for the sample used.

#### Tsumoite BiTe

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a thin film using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 117, (91), 88s, ~56.

**Source:** Russo et al. (2008).

**Comments:** The sample was characterized by powder X-ray diffraction data.

#### Tugarinovite MoO<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The nominal laser radiation power was between 0.7 and 7 mW.

**Raman shifts (cm<sup>-1</sup>):** 744s, 571, 496s, 464w, 363s, 230, 204s.

**Source:** Solferino and Anderson (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of tugarinovite see also Srivastava and Chase (1972).

#### Tuite Ca<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>

**Origin:** Suizhou chondrite, China (type locality).

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 1095w, 997, 975s, 640w, 578, 411, 192.

**Source:** Xie et al. (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectra of tuite see also Zhai et al. (2010, 2014) and Xie et al. (2016).

**Tululite** Ca<sub>14</sub>(Fe<sup>3+</sup>,Al)(Al,Zn,Fe<sup>3+</sup>,Si,P,Mn,Mg)<sub>15</sub>O<sub>36</sub>

**Origin:** Tulul Al Hammam area, Siwaqa complex, Mottled Zone Formation, Dead Sea region, Jordan (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented grain using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 17 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 934w, 831w, 817w, 754sh, 636s, 550sh, 522, 456, 295sh, 260, 199w.

**Source:** Khouri et al. (2016a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Tunellite** SrB<sub>6</sub>O<sub>9</sub>(OH)<sub>2</sub>·3H<sub>2</sub>O

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3614s, 3567s, (3526sh), 3430sh, 3383 + 3369s (unresolved doublet?), (3324), 3282, 3243sh, 1113sh, 1082, (1063), 1043, 994s, (979sh), 954sh, 901, 879w, 861w, 819, 790w, 737, 715sh, 677sh, 664sh, 639s, 601w, 568, 523, 480sh, 464s, 445sh, 426sh, 371, (350), 332s, 317sh, 297w, 289w, 270sh, 256, 243sh, 210sh, 192, (159), 150s, (141), 114 + 109 (unresolved doublet?).

**Source:** Frost et al. (2014e).

**Comments:** No independent analytical data are provided for the sample used.

**Tungstenite** WS<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a powder sample using 532 laser radiation. The nominal laser radiation power was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 419, 350.

**Source:** Nuvoli et al. (2014).

**Comments:** For the Raman spectrum of tungstenite see also Štengl et al. (2015).

**Tungstite** WO<sub>3</sub>·H<sub>2</sub>O

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was between 0.06 and 0.15 mW.

**Raman shifts (cm<sup>-1</sup>):** ~949s, ~650s, ~377w, ~237.

**Source:** Tarassov et al. (2002).

**Comments:** No independent analytical data are provided for the sample used.

**Tunisite**  $\text{NaCa}_2\text{Al}_4(\text{CO}_3)_4(\text{OH})_8\text{Cl}$ 

**Origin:** Condorcet, Nyons, Drôme, Rhône-Alpes, France.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power at the sample was about 0.1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3561sh, 3482s, 3419, 1945w, 1703w, 1683w, 1542sh, 1522, 1499sh, 1127s, 854, 842 + 838w (unresolved doublet?), 731, 676w, 534, 441sh, (425), 417, (408), 387sh, 350w, 325w, 293, 279w, 234sh, 221, 200sh, 188sh, 177, 164, 151sh, 132w, 115.

**Source:** Frost et al. (2015d).

**Comments:** The sample was characterized by qualitative electron microprobe analysis. For the Raman spectrum of tunisite see also Frost and Dickfos (2007b).

**Turquoise**  $\text{CuAl}_6(\text{PO}_4)_4(\text{OH})_8 \cdot 4\text{H}_2\text{O}$ 

**Origin:** Kouroudaiko mine, Falemeriver, Senegal.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3506, 3471s, 3453sh, 3290, 3092sh, 1614w, 1184sh, 1161, 1104, 1064sh, 1041s, (1031), 991sh, 935w, (836sh), 815, 642, 592, 571, 548, 511, 483, 469, 437sh, 423, (417sh), 385, 335, (320sh), 301sh, 277sh, 259w, 244sh, 231, (218sh), 210, 196sh, 175, 152w.

**Source:** Čejka et al. (2015).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectra of turquoise see also Guo et al. (2010) and Bernardino et al. (2016).

**Tuzlaite**  $\text{NaCaB}_5\text{O}_8(\text{OH})_2 \cdot 3\text{H}_2\text{O}$ 

**Origin:** Tuzla evaporite deposit, Bosnia and Herzegovina (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 100 mW. A 90°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3615, 3475s, 3434s, 3328w, 3228w, 3165w, 1247w, 1072w, 1027sh, 866, 827, 761, 704w, 663, 589, 546, 468, 447w, 366w, 340, 323w, 282w.

**Source:** Bermanec et al. (2003).

**Comments:** The sample was characterized by powder X-ray diffraction data.

**Tychite**  $\text{Na}_6\text{Mg}_2(\text{CO}_3)_4(\text{SO}_4)$ 

**Origin:** Searles Lake, San Bernardino Co., California, USA (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1137s, 1103s, 1049, 995s, 970.

**Source:** Palaich et al. (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of tychite see also Schmidt et al. (2006).

**Tyrolite**  $\text{Ca}_2\text{Cu}_9(\text{AsO}_4)_4(\text{CO}_3)(\text{OH})_8 \cdot 11\text{H}_2\text{O}$ **Origin:** Brixlegg, Tyrol, Austria.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3545, 3438, 3379, 3303, 3204, 1667, 1635, 1498, 1463, 1431, 1370, 1088, 1058, 855, 830 (broad), 795, 755s, 717s, 598, 570, 534, 524, 503, 480, 433s, 355, 301, 262, 217, 202, 179.**Source:** Klopdroge and Frost (2000b).**Comments:** No independent analytical data are provided for the sample used.**Tyuyamunite**  $\text{Ca}(\text{UO}_2)_2(\text{VO}_4)_2 \cdot 5\text{H}_2\text{O}$ **Origin:** Chihuahua, Mexico.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 975, 827, 747s, 644, 608, 582, 525, 470, 404, 369s, 345, 304, 239, 186, 155.**Source:** Frost et al. (2005c).**Comments:** No independent analytical data are provided for the sample used.**Ulexite**  $\text{NaCaB}_5\text{O}_6(\text{OH})_6 \cdot 5\text{H}_2\text{O}$ **Origin:** An unknown locality in Morocco.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3490, (3433w), 3401, 1133, 1111sh, 1005s, 745w, 668w, 639w, 617w, 602w, 551w, 491, (475), 421sh, 412, 367, 305, 250, 200, 166.**Source:** Klopdroge and Frost (1999a).**Comments:** Questionable data: the strong band at 1005 cm<sup>-1</sup> may correspond to a sulfate. No independent analytical data are provided for the sample used.**Ulrichite**  $\text{CaCu}(\text{UO}_2)(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ **Origin:** Lake Boga granite quarry, Northwest Victoria, Australia (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using 785 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** (1077), 1028, (1009), 975, 812s, (458w).**Source:** Faulques et al. (2015a, b).

**Ulvöspinel**  $\text{Fe}^{2+}\text{TiO}_4$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed at 1 GPa on an arbitrarily oriented sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was 10 mW.**Raman shifts (cm<sup>-1</sup>):** 681s, 493.**Source:** Kyono et al. (2011).**Comments:** The sample was characterized by electron microprobe analyses.**Umangite**  $\text{Cu}_3\text{Se}_2$ **Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power at the sample was 10 mW.**Raman shifts (cm<sup>-1</sup>):** 58sh, 49.**Source:** Izquierdo-Roca et al. (2009).**Comments:** No independent analytical data are provided for the sample used.**Umbite**  $\text{K}_2\text{ZrSi}_3\text{O}_9 \cdot \text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed using 1064 nm Nd-YAG laser radiation with a resolution of 1 cm<sup>-1</sup>. No other data are provided.**Raman shifts (cm<sup>-1</sup>):** ~970, ~930, ~910.**Source:** Lin and Rocha (2005).**Comments:** In the cited paper, Raman spectrum of umbite below 900 cm<sup>-1</sup> is given as a figure, without indication of Raman shifts. The sample was characterized by powder X-ray diffraction data.**Umbrianite**  $\text{K}_7\text{Na}_2\text{Ca}_2[\text{Al}_3\text{Si}_{10}\text{O}_{29}]\text{F}_2\text{Cl}_2$ **Origin:** Pian di Celle volcano, Umbria, Italy (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented grain in a polished section using 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was 50 mW. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 3120, 2970, 2810, 1142, 1036s, 735s, 646, 593s, 525s, 491, 400, 324, 256.**Source:** Sharygin et al. (2013b).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Ungemachite**  $K_3Na_8Fe^{3+}(SO_4)_6(NO_3)_2 \cdot 6H_2O$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was 2 mW.**Raman shifts (cm<sup>-1</sup>):** 3420, 3370sh, 1711w, 1663w, 1383, 1192, 1163, 1144, 1047s, 1035, 1011, 952, 721, 655, 645sh, 619, 600w, 534w, 472, 464w, 446.**Source:** Jentzsch et al. (2012b).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of ungemachite see also Jentzsch et al. (2013).**Uraninite**  $UO_2$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powder sample using 514.5 nm Ar<sup>+</sup> laser and 785 nm diode laser radiations. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1149s, 598 (broad), 445 (514.5 nm); 1343w, 1149w, 618w, 445s, 230w (785 nm).**Source:** Stefaniak et al. (2008).**Comments:** The sample was characterized by powder X-ray diffraction data.**Uranophane- $\alpha$**   $Ca(UO_2)_2(SiO_3OH)_2 \cdot 5H_2O$ **Origin:** Dieresis uranium mine, Sierra Albarrana, Córdoba, Spain.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 20 mW.**Raman shifts (cm<sup>-1</sup>):** 967, 798s, ~548w, ~400w, ~292w, ~210.**Source:** Bonales et al. (2015).**Comments:** The sample was characterized by qualitative electron microprobe analysis. For the Raman spectra of uranophane see also Biwer et al. (1990), Amme et al. (2002), Frost et al. (2006e), and Driscoll et al. (2014).**Uranopilite**  $(UO_2)_6(SO_4)O_2(OH)_6 \cdot 14H_2O$ **Origin:** South Alligator River, Northern Territory, Australia.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3547, 3470, 1143w, 1117w, 1098w, 1011, 842s, (832sh), 547, 406, 320, 294, 253.**Source:** Frost et al. (2005b).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of uranopilite see also Frost et al. (2007i).

**Uranosphaerite**  $\text{Bi}(\text{UO}_2)\text{O}_2(\text{OH})$ 

**Origin:** Horní Halže, Krušné Hory (Czech Ore Mts.), Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 633 nm laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 3404, 884w, 794s, 600s, 524, 475, 387, 378, 348, 305, 278, 263, 245, 227, 184, 138.

**Source:** Sejkora et al. (2008).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Urea solution**  $\text{CO}(\text{NH}_2)_2 \cdot \text{aq}$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3435, 3357, 3323, 3242, 1649, 1581, 1047, 1012, ~548, ~379w.

**Source:** Frost et al. (2000).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of urea in aqueous solution see also Spinner (1959).

**Ushkovite**  $\text{MgFe}^{3+}(\text{PO}_4)_2(\text{OH})_2 \cdot 8\text{H}_2\text{O}$ 

**Origin:** Linópolis, Divino das Laranjeiras, Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3517, 3495, (3449), 3343, 3286, (3225), 1611w, 1140sh, 1121, 1097, 1068, 1041, 1012sh, 991 + 984s (unresolved doublet?), 959sh, 835sh, 810w, 780w, (650), 637, 610 + 606w (unresolved doublet?), 583, 563, 548sh, 506, 492w, 469w, 442, (421sh), 410, 386, 321 + 313w (unresolved doublet?), 283sh, 274w, 261, 239sh, 216, 206, 183, 173sh, 156sh, 144, 132sh, 115sh, 109w.

**Source:** López et al. (2015b).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

**Usturite**  $\text{Ca}_3(\text{SbZr})(\text{FeO}_4)_3$ 

**Origin:** Upper Chegem volcanic structure, Kabardino-Balkaria, Northern Caucasus, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented grain in a polished section using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation output power was between 40 and 60 mW. A 0°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 815, 789, 751, 733sh, (615), 591, 565sh, 498s, 411w, 303 + 294s (unresolved doublet?), 262 + 244 (unresolved doublet?), 218sh, 187w, 161w, 149.

**Source:** Galuskina et al. (2010a).

**Comments:** The sample was characterized by single-crystal electron back-scatter diffraction, powder X-ray diffraction data and electron microprobe analyses.

### Uvarovite Ca<sub>3</sub>Cr<sub>2</sub>(SiO<sub>4</sub>)<sub>3</sub>

**Origin:** Sweden (?).

**Experimental details:** Polarized Raman scattering measurements have been performed on a single crystal in different scattering geometries using 488 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 894, 828, ~618w, ~590w, 526, ~510w, 370s, ~272, ~242, 176.

**Source:** Kolesov and Geiger (1998).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of uvarovite see also Mingsheng et al. (1994), Bersani et al. (2009), Makreski et al. (2011), Frezzotti et al. (2012), and Andò and Garzanti (2014).

### Uvite CaMg<sub>3</sub>(Al<sub>5</sub>Mg)(Si<sub>6</sub>O<sub>18</sub>)(BO<sub>3</sub>)<sub>3</sub>(OH)<sub>3</sub>(OH)

**Origin:** Brumado district, Bahia, Brazil.

**Experimental details:** Polarized micro-Raman scattering measurements have been performed using 488 and 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3636w, 3592, (3554w), (3518w), ~705, ~670, ~372s, ~244, ~215.

**Source:** Fantini et al. (2014).

**Comments:** The sample was characterized electron microprobe analyses. For the Raman spectrum of uvite see also Hoang et al. (2011).

### Vaesite NiS<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 15 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 515w, 468s, 414w, 274, 263, 235w.

**Source:** Bishop et al. (2000).

**Comments:** The sample was characterized by powder X-ray diffraction data.

### Vajdakite (Mo<sup>6+</sup>O<sub>2</sub>)<sub>2</sub>As<sup>3+</sup><sub>2</sub>O<sub>5</sub>·3H<sub>2</sub>O

**Origin:** Jáchymov uranium deposit, Krušné Hory (Ore Mts.), Western Bohemia, Czech Republic (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3481, 3417, (3144sh), 3112w, 953-951s, 910sh, 898, (876w), 804, (799), 760, 720w, 604w, 560, 549, 521, 480, (473), 386s, 369, 333, 282w, 238sh, 227 + 224 (unresolved doublet?), 179, 157, 138w, 128.

**Source:** Čejka et al. (2010a).

**Comments:** Holotype sample was used.

### Valentinite Sb<sub>2</sub>O<sub>3</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 300 mW. A 90°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 690w, 602w, 502, 449w, 294s, 269sh, 223s, 194, 100s, 103w, 71.

**Source:** Cody et al. (1979).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of valentinite see also Orman (2010).

### Vanackerite Pb<sub>4</sub>Cd(AsO<sub>4</sub>)<sub>3</sub>(Cl,OH)

**Origin:** Tsumeb mine, Tsumeb, Namibia (type locality).

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** ~830s, ~792, ~770, ~457, ~353.

**Source:** Schlüter et al. (2016).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### Vanadinite Pb<sub>5</sub>(VO<sub>4</sub>)<sub>3</sub>Cl

**Origin:** Mibladen, Morocco.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 827s, 811, 365, 323, 291.

**Source:** Frost et al. (2003a).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of vanadinite see also Levitt and Condrate, Sr (1970), Adams and Gardner (1974), and Bartholomäi and Klee (1978).

### Vandendriesscheite Pb<sub>1.6</sub>(UO<sub>2</sub>)<sub>10</sub>O<sub>6</sub>(OH)<sub>11</sub>·11H<sub>2</sub>O

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3530sh, 3475, 3262sh, (2904w), (2853w), 1624w, 1395, 854 + 852 (unresolved doublet?), 841s, (832), 819sh, 779, 703, 548, (503), 456, (425w), 404, (355), 332, 303, 273sh, 248, 218, 193.

**Source:** Frost et al. (2007h).

**Comments:** No independent analytical data are provided for the sample used.

**Vanmeerscheite** U(UO<sub>2</sub>)<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>(OH)<sub>6</sub>·4H<sub>2</sub>O

**Origin:** Kobokobo, Kivu, Democratic Republic of Congo (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** ~3390, 1208sh, 1153, 1110s, (1086sh), 1017 + 1013s (unresolved doublet?), 939sh, 860w, 650w, 624, 571, 453sh, 442s, 363, 290, 226s.

**Source:** Frost et al. (2009d).

**Comments:** No independent analytical data are provided for the sample used.

**Vantasselite** Al<sub>4</sub>(PO<sub>4</sub>)<sub>3</sub>(OH)<sub>3</sub>·9H<sub>2</sub>O

**Origin:** Bihain, Vielsalm, Stavelot massif, Luxembourg province, Belgium (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3608sh, 3570sh, 3502s, (3436), 3399s, 3369sh, 3327sh, 3211sh, 2943sh, 1703sh, 1656sh, 1622sh, 1595, 1456w, 1299w, 1232w, 1200w, 1146, 1128sh, 1106sh, 1090s, (1076), 1051s, 1027sh, 1013s, 949, 930, 833sh, 813w, 715w, 649, 593, 557, 522 + 515, 494, 451 + 437 + 423 (unresolved triplet?), 374, 334sh, 317s.

**Source:** Frost et al. (2015v).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

**Vanthoffite** Na<sub>6</sub>Mg(SO<sub>4</sub>)<sub>4</sub>

**Origin:** Synthetic (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was about 2 mW.

**Raman shifts (cm<sup>-1</sup>):** 1195w, 1178w, 1154w, 1129w, 1096w, 1076w, 1012s, 1002s, 643, 637, 629, 622, 613w, 603w, 473, 458, 452.

**Source:** Jentzsch et al. (2011).

**Comments:** No independent analytical data are provided for the sample used.

**Vapnikite**  $\text{Ca}_3\text{UO}_6$ 

**Origin:** Jabel Harmun, Palestinian Autonomy, Israel (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented grain in a polished section using 488 nm  $\text{Ar}^+$  laser radiation. The laser radiation power at the sample was below 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 1446w, 725s, 474w, 391, 248w.

**Source:** Galuskin et al. (2014).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Variscite**  $\text{Al}(\text{PO}_4) \cdot 2\text{H}_2\text{O}$ 

**Origin:** Cioclovina cave, 40 km SE of Hunedoara, Şureanu Mts., Romania.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 1064 nm Nd-YAG laser radiation. The laser radiation output power was 350 mW.

**Raman shifts (cm<sup>-1</sup>):** 3400–3100 (broad), 1634, 1079sh, 1055, 1026, 605w, 562w, 434s, 225, 168, 144.

**Source:** Onac et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectra of variscite see also Frost et al. (2004) and Litvinenko et al. (2016).

**Västmanlandite-(Ce)**  $\text{Ce}_3\text{CaMg}_2\text{Al}_2\text{Si}_5\text{O}_{19}(\text{OH})_2\text{F}$ 

**Origin:** Västmanl and Co., Bergslagen region, Sweden (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 633 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3671sh, ~3586, 3517s, ~3446, ~3317s, ~3201, ~2545w, ~2142w, ~1058, 1034, 1004, 968, ~944, 920, 900s, ~690, ~675, ~633, 574, 555, 501, 464, ~436, 412, 387, 361, 341, 329, 287, 234, 224, ~200.

**Source:** Holtstam et al. (2005).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Vaterite**  $\text{Ca}(\text{CO}_3)$ 

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1555w, 1542w, 1480w, 1460w, 1441w, 1421w, 1091s, 1085.5sh, 1081, 1075s, 881 + 878 + 874w, 751w, 743.5w, 738w, 685, 674, 667, 333sh, 302s, 268, 210, 175, 151, 120s, 106s.

**Source:** Wehrmeister et al. (2010).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of vaterite see also Behrens et al. (1995), Frezzotti et al. (2012), Kristova et al. (2014), and Sánchez-Pastor et al. (2016).

**Vauquelinite** CuPb<sub>2</sub>(CrO<sub>4</sub>)(PO<sub>4</sub>)(OH)

**Origin:** Kintore Open Cut, Broken Hill, New South Wales, Australia.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 785 nm Nd-YAG laser. The laser radiation power at the sample was 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** (843), 827s, 375, 348s, 332sh.

**Source:** Frost (2004c).

**Comments:** No independent analytical data are provided for the sample used.

**Vauxite** Fe<sup>2+</sup>Al<sub>2</sub>(PO<sub>4</sub>)<sub>2</sub>(OH)<sub>2</sub>·6H<sub>2</sub>O

**Origin:** Siglo XX mine (Llallagua), Bustillo province, Potosí department, Bolivia (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3648s, 3555, 3402, 3328 (broad), 3103s, 2918sh, 1696sh, 1633w, 1601w, 1567sh, 1370w, 1309sh, 1150sh, 1134 + 1122, 1105sh, 1075sh, 1059sh, 1046sh, 1027s, 1009s, 1000sh, 978s, (954sh), 918sh, 910w, 900sh, 535, 502 + 498w (unresolved doublet?), 478sh, 470, 461sh, 451sh, 418, 412sh, 399sh, 393, 370 + 364 (unresolved doublet?), (341sh), 332, 320sh, 284, 273sh, 267sh, 238, 230sh, 208, 181, 154 + 148 (unresolved doublet?), 132 + 127 (unresolved doublet?), 112 + 109 (unresolved doublet?).

**Source:** Scholz et al. (2015).

**Comments:** The sample was characterized by electron microprobe analysis.

**Väyrynenite** BeMn<sup>2+</sup>(PO<sub>4</sub>)(OH)

**Origin:** Viitaniemi pegmatite, Eräjärvi area, Orivesi, Finland (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3473sh, 3388sh, 3315w, (3249sh), 3219s, 3154sh, 1802sh, 1768w, 1660w, 1186sh, 1139sh, 1126, 1074, 1044, 1009 + 1004s (unresolved doublet?), 986, 936w, 898w, 800, 769w, 741, 707w, 642w, 619, 599, 573w, 538w, 518 + 506 (unresolved doublet?), 463, 404, 381, 353, 334, 287w, 266w, 238sh, 232, 220, 189 + 184 (unresolved doublet?), (171), 163, 129 + 123 (unresolved doublet?), 114sh.

**Source:** Frost et al. (2014m).

**Comments:** The sample was characterized by electron microprobe analyses.

**Velikite** Cu<sub>2</sub>HgSnS<sub>4</sub>**Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 318s, 283.**Source:** Himmrich and Haeuseler (1991).**Comments:** The sample was characterized by powder X-ray diffraction data.**Versiliaite** (Fe<sup>2+</sup><sub>2</sub>Fe<sup>3+</sup><sub>2</sub>)(Fe<sup>3+</sup><sub>2</sub>Sb<sup>3+</sup><sub>6</sub>)O<sub>16</sub>S**Origin:** An abandoned mine in the Karrantza valley, western area of the Basque Co., Spain.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 20 mW.**Raman shifts (cm<sup>-1</sup>):** 612, 505, 410s, 293s, 246, 226s.**Source:** Goienaga et al. (2011).**Comments:** The sample was characterized by X-ray fluorescence spectroscopy.**Vésigniéite** Cu<sub>3</sub>Ba(VO<sub>4</sub>)<sub>2</sub>(OH)<sub>2</sub>**Origin:** Vrančice deposit, central Bohemia, Czech Republic.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3463sh, 2896w, 2609sh, 1960w, 1636sh, 1559w, 1052w, 856s, 821s, 750, 511w, 466, (371sh), 355sh, 332, 307s, 185sh, 175, 162sh, 112w.**Source:** Frost et al. (2011e).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectrum of Vésigniéite see also Wulferding et al. (2012).**Vesuvianite** (Ca,Na)<sub>19</sub>(Al,Mg,Fe)<sub>13</sub>(SiO<sub>4</sub>)<sub>10</sub>(Si<sub>2</sub>O<sub>7</sub>)<sub>4</sub>(OH,F,O)<sub>10</sub>**Origin:** Dosso degli Areti, Italy.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 930s, 868, 696, 640, 410, 226.**Source:** Andò and Garzanti (2014).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of vesuvianite in the OH region see Galuskin et al. (2007a).**Veszelyite** (Cu,Zn)<sub>2</sub>Zn(PO<sub>4</sub>)(OH)<sub>3</sub>·2H<sub>2</sub>O**Origin:** Zdravo Vrelo, near Kreševo, Bosnia and Herzegovina.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 3566 (sharp), 3555sh, (3497sh), 3425, 2290sh, (3302sh), 3286, (3184sh), 2852w, 2662sh (weak), 2233, 2042, 1970, 1805, 1632, 1587, 1379, 1108w, 1045w, 1025w, 967, 951, 929, 882, 833, 624, 607, 556, 539, 486, 470, 439.

**Source:** Danisi et al. (2013).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data. The crystal structure is solved. No data on band intensities below 2662 cm<sup>-1</sup> are provided in the cited paper. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

### Villamanínite CuS<sub>2</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline aggregate using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 512s, 264, 207.

**Source:** Anastassakis and Perry (1976).

**Comments:** No independent analytical data are provided for the sample used.

### Vivianite Fe<sup>2+</sup><sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>·8H<sub>2</sub>O

**Origin:** Catavi Mine, Llallagua, Bolivia.

**Experimental details:** Raman scattering measurements have been performed on a cleavage plain using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sampling objective was 50 mW.

**Raman shifts (cm<sup>-1</sup>):** 1050, 986, 947s, 867m, 828w, 568, 532, 453, 422, 342w, 303w, 270w, 235, 227, 196, 162w, 126.

**Source:** Rodgers et al. (1993).

**Comments:** The sample was characterized Mössbauer spectroscopy and electron microprobe analyses. For the Raman spectra of vivianite see also Piriou and Poullen (1984), Frost et al. (2002f), and Hsu et al. (2014).

### Vladimirivanovite Na<sub>6</sub>Ca<sub>2</sub>[Al<sub>6</sub>Si<sub>6</sub>O<sub>24</sub>]·(SO<sub>4</sub>,S<sub>3</sub>,S<sub>2</sub>,Cl)<sub>2</sub>·H<sub>2</sub>O

**Origin:** Tultuilazurite deposit, Baikal Lake region, Russia (type locality).

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 3124 (broad), 1189, (1183), 992, 799s, 726sh, 544 (sharp), 428, 353.

**Source:** Sapozhnikov et al. (2012).

**Comments:** The sample was characterized by powder X-ray diffraction, thermal data, and electron microprobe analyses. The crystal structure is solved.

### Vladykinite Na<sub>3</sub>Sr<sub>4</sub>(Fe<sup>2+</sup>Fe<sup>3+</sup>)Si<sub>8</sub>O<sub>24</sub>

**Origin:** Murun complex, eastern Siberia, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1039w, 991, 968, 915, 681w, 465s, 401 (very strong), 348, 264w, 203s, 167w, 129w.

**Source:** Chakhmouradian et al. (2014).

**Comments:** The sample was characterized by powder X-ray diffraction data, Mössbauer spectroscopy and electron microprobe analyses. The crystal structure is solved.

**Voglite**  $\text{Ca}_2\text{Cu}(\text{UO}_2)(\text{CO}_3)_4 \cdot 6\text{H}_2\text{O}$ 

**Origin:** White Canyon No. 1 mine, Frey Point, San Juan Co., Utah, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3535 + 3391w (broad; unresolved doublet?), 2939w, 1369, 1094, 836s, 749w, (261), 223, 148.

**Source:** Frost et al. (2008b).

**Comments:** No independent analytical data are provided for the sample used.

**Volaschioite**  $\text{Fe}_4(\text{SO}_4)\text{O}_2(\text{OH})_6 \cdot 2\text{H}_2\text{O}$ 

**Origin:** Fornovolasco, Apuan Alps, Tuscany, Italy (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated. A nearly 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1530w, 1178, 1055, 1005, 941w, 527, 453s, 408s, 319s, 250.

**Source:** Biagioni et al. (2011b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Volborthite**  $\text{Cu}_3\text{V}_2\text{O}_7(\text{OH})_2 \cdot 2\text{H}_2\text{O}$ 

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 894s, 820, 758, 476, 438w, 342, 236, 164w.

**Source:** Ni et al. (2010a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectra of volborthite see also Frost et al. (2011e) and Wulferding et al. (2012).

**Vonsenite**  $\text{Fe}^{2+} \text{Fe}^{3+} \text{O}_2(\text{BO}_3)$ 

**Origin:** Brosso mine, Torino, Italy.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1605w, 1462 + 1443 (unresolved doublet?), 1347sh, 1304, 1284sh, 1059, 997, 728sh, (687), 642, 529, 381s, 315, 324s, (315), 249s, (232), 158+145 (unresolved doublet?), 114.

**Source:** Frost et al. (2014ac).

**Comments:** The sample was characterized by electron microprobe analysis.

**Vorlanite** CaUO<sub>4</sub>

**Origin:** Upper Chegem caldera, Kabardino-Balkaria, Northern Caucasus, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed from crystal cross-section approximately perpendicular to basal pinacoid in thin section using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation output power was between 40 and 60 mW. A 0°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** 1370, 683s, 524, 450w, 371w, 226.

**Source:** Galuskin et al. (2011a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. For the Raman spectra of vorlanite see also Galuskin et al. (2012a, 2013b, 2014).

**Vrbaite** Hg<sub>3</sub>Tl<sub>4</sub>As<sub>8</sub>Sb<sub>2</sub>S<sub>20</sub>

**Origin:** Allchar, Republic of Macedonia.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation output power was 0.46 mW.

**Raman shifts (cm<sup>-1</sup>):** 397, 383sh, 378, 370, 357, 346w, 322s, 306s, 244, 236, 195, 187w, 171w, 162w, 151, 130, 122w, 111, 103.

**Source:** Makreski et al. (2014).

**Comments:** The sample was characterized by electron microprobe analyses.

**Vuorelainenite** Mn<sup>2+</sup>V<sup>3+</sup><sub>2</sub>O<sub>4</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on a single crystal in different scattering geometries using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was about 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 585s, 479s, ~300, 178.

**Source:** Takubo et al. (2011).

**Comments:** No independent analytical data are provided for the sample used.

**Vysokýite** U<sup>4+</sup>[AsO<sub>2</sub>(OH)<sub>2</sub>]<sub>4</sub>·4H<sub>2</sub>O

**Origin:** Geschieber vein, Jáchymov ore district, Western Bohemia, Czech Republic (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using a 780 nm diode-pumped solid-state laser. The nominal laser radiation power was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 2750w, 2230w (broad), 1545, 1425, 902s, 816s, 769sh, 595, 559, 427, 368, 324, 200 + 184 (unresolved doublet?), 99w, 61w.

**Source:** Plášil et al. (2013d).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Vysotskite** (Pd,Ni)S**Origin:** Synthetic (Ni-free).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented grains in a polished section using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation output power was 500 mW.**Raman shifts (cm<sup>-1</sup>):** 392, 368, 353w, 348, 326s.**Source:** Pikl et al. (1999).**Comments:** No independent analytical data are provided for the sample used.**Wadeite** K<sub>2</sub>ZrSi<sub>3</sub>O<sub>9</sub>**Origin:** Saima alkaline complex, Liaodong Peninsula, northeastern China.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1057w, 990s, 930s, 734w, 629, 561s, 490s, 433, 370, 342, 191s, 153.**Source:** Wu et al. (2015).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectrum of wadeite see also Geisinger et al. (1987).**Wadsleyite** Mg<sub>2</sub>(SiO<sub>4</sub>)**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 488 or 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was between 100 and 200 mW.**Raman shifts (cm<sup>-1</sup>):** 940, 919, 898, 850s, 836s, 588, 570, 528, 460, 408, 307, 280, 213.**Source:** Akaogi et al. (1984).**Comments:** The sample was characterized by powder X-ray diffraction and optical data. For Raman spectra of wadsleyite see also Kleppe et al. (2001, 2006) and Mao et al. (2011).**Wagnerite-Ma5bc** Mg<sub>2</sub>(PO<sub>4</sub>)F**Origin:** Larsemann Hills, Prydz Bay, East Antarctica.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 5 mW.**Raman shifts (cm<sup>-1</sup>):** 3570 (other values are not indicated: only a figure is given in the cited paper).**Source:** Ren et al. (2003).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Waimirite-(Y)  $\text{YF}_3$** **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power is not indicated. A 90°-scattering geometry was employed.**Raman shifts ( $\text{cm}^{-1}$ ):** 533 (broad), 444, 389, 366s, 349s, 342sh, 293, 262, 244, 220w, 189s, 171, 147w, 111, 75.**Source:** Wilmarth et al. (1988).**Comments:** For the Raman spectrum of waimirite-(Y) see also Lage et al. (2004).**Wakabayashilite  $(\text{As},\text{Sb})_6\text{As}_4\text{S}_{14}$** **Origin:** Jas Roux, Hautes-Alpes, France.**Experimental details:** Raman scattering measurements have been performed on a single crystal with the laser beam perpendicular to the fiber axis (*c* axis) using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 2 mW.**Raman shifts ( $\text{cm}^{-1}$ ):** 398s, 382, 356s, 337s, 328, 315, 304, 227–229, 205s, 191, 167, 137, 131sh, 108, 87, 67sh, 60s.**Source:** Bindi et al. (2014).**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses.**Wakefieldite-(Ce)  $\text{CeVO}_4$** **Origin:** Synthetic.**Experimental details:** No data.**Raman shifts ( $\text{cm}^{-1}$ ):** 1012w, 482, 244, 202, 148s, 120s.**Source:** Au et al. (1996).**Comments:** The sample was characterized by powder X-ray diffraction data.**Wakefieldite-(La)  $\text{LaVO}_4$** **Origin:** Synthetic.**Experimental details:** No data.**Raman shifts ( $\text{cm}^{-1}$ ):** 1000, 862s, 705w, 528w, 410w, 290w, 150s, 122.**Source:** Au et al. (1996).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of wakefieldite-(La) see also Sun et al. (2010b) and Xie et al. (2012).**Wakefieldite-(Nd)  $\text{NdVO}_4$** **Origin:** Synthetic.**Experimental details:** No data.**Raman shifts ( $\text{cm}^{-1}$ ):** 1000, 874s, 812, 700, 528, 482, 412w, 310, 290, 150s, 122s.**Source:** Au et al. (1996).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of wakefieldite-(Nd) see also Au and Zhang (1997) and Moriyama et al. (2011).

**Wakefieldite-(Y) YVO<sub>4</sub>****Origin:** Synthetic.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 1090, 896, 842w, 820w, 662w, 494, 422, 398s, 320s, 280s, 150w, 122.**Source:** Au et al. (1996).**Comments:** The sample was characterized by powder X-ray diffraction data.**Walpurgite Bi<sub>4</sub>O<sub>4</sub>(UO<sub>2</sub>)(AsO<sub>4</sub>)<sub>2</sub>·2H<sub>2</sub>O****Origin:** Weisser Hirsch Mine, Schneeberg, Saxony, Germany (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3515w, 3375w, 1597w, 1323w, 1003w, 948w, 892w, 836s, (823), (795), 790s, 771sh, 615, 546, 513s, 491sh, 432, 398, 365, 331, 296, (278), 242, 208, (199), 154.**Source:** Frost et al. (2006l).**Comments:** No independent analytical data are provided for the sample used.**Walstromite BaCa<sub>2</sub>Si<sub>3</sub>O<sub>9</sub>****Origin:** Big Creek deposit, Fresno Co., California, USA (type locality).**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 633 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1071, 1037, 988s, 650s, 501, 473w, 378, 291, 153, 124.**Source:** Gaft et al. (2013).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of walstromite see also Zedgenizov et al. (2014).**Wardite NaAl<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>(OH)<sub>4</sub>·2H<sub>2</sub>O****Origin:** Lavrada Ilha, Minas Gerais, Brazil.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 785 nm laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3607s, 3588, 3542s, 3383, 3282w, 1579w, 1319w, 1178w, 1133, (1103), 1079, 1047s, 1029sh, 1013sh, 992s, 681, 609, 580sh, 486, 403sh, 392, 340w, 334, 323sh.**Source:** Frost et al. (2014l).**Comments:** The sample was characterized by qualitative electron microprobe analysis. For the Raman spectrum of wardite see also Kampf et al. (2014a).

**Waterhouseite** Mn<sub>7</sub>(PO<sub>4</sub>)<sub>2</sub>(OH)<sub>8</sub>

**Origin:** Iron Monarch deposit, Middleback Ranges, South Australia, Australia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single crystal using 518 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 3555sh, 3510, 3439s, 3411sh, 1612w, 1076s, ~1050, ~1018, 984, 929s, 809s, 667, ~595sh, 571s, ~540sh, ~513s, 433, ~342, ~321, ~267, 174, ~137.

**Source:** Pring et al. (2005).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Wavellite** Al<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>(OH)<sub>3</sub>·5H<sub>2</sub>O

**Origin:** Zbirow, Bohemia, Czech Republic.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 632.8 nm He-Ne laser radiation. The laser radiation output power was 18 mW.

**Raman shifts (cm<sup>-1</sup>):** 3490, 3406w, 3198sh, 3078, 1145w, 1061sh, 1017s, 950w, 920w, 633, 559sh, 540, 408s, 311, 274, 213w.

**Source:** Capitelli et al. (2014).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Waylandite** BiAl<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>(OH)<sub>6</sub>

**Origin:** Leucamp, Montsalvy, Cantal, Auvergne-Rhône-Alpes, France.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 25 mW.

**Raman shifts (cm<sup>-1</sup>):** 3170w, 1112w, 1021sh, 1012 (broad), 791s, 725, 612s, 706, 602w, 523, 470w, 450w, 415, 400sh, 306s, 280, 257, 226, 191w, 156, 139, 119, 95sh.

**Source:** Gama (2000).

**Comments:** The sample was characterized by electron microprobe analyses.

**Weddellite** Ca(C<sub>2</sub>O<sub>4</sub>)·2H<sub>2</sub>O

**Origin:** Synthetic.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was between 50 and 100 mW.

**Raman shifts (cm<sup>-1</sup>):** 3500–3200 (broad), 2941, 2855w, 1640, 1476s, 911s, 870w, 597w (broad), 506s, 188.

**Source:** Conti et al. (2015).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of weddellite see also Frost and Weier (2003) and Frost (2004d).

**Weeksite**  $K_2(UO_2)_2(Si_5O_{13}) \cdot 4H_2O$ **Origin:** Anderson's Mine, Yavapai Co., Arizona, USA.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3610sh, 3548, 3497sh, 3356sh, 1637, 1154, 1008, 962, 939, 814 + 810s (unresolved doublet?), 800, 765, 744, 574, 521, 480, 349, 333, 301, 266, 210s, 167.5, 113.**Source:** Frost et al. (2006d, h).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of weeksite see also Biwer et al. (1990).**Wegscheiderite**  $Na_5H_3(CO_3)_4$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3120w (broad), 2930w (broad), 2500w (broad), 1910w (broad), 1700w, 1675sh, 1560w, 1450sh, 1429, 1391, 1355w (broad), 1270w (broad), 1057s, 1038s, 1022s, 841w, 699, 686, 654, 240, 224, 186, 153s, 118, 105s, 96w, 89, 72s, 55.**Source:** Bertoluzza et al. (1981).**Comments:** No independent analytical data are provided for the sample used.**Weissbergite**  $TlSbS_2$ **Origin:** Synthetic.**Experimental details:** Polarized Raman scattering measurements have been performed on a single crystal in different configurations using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 17 mW.**Raman shifts (cm<sup>-1</sup>):** 334sh, 321s, 310s, 293sh, 275sh, ~250w, 178w, 162w, 145w, 127, 106, 94, 81, 62, 51, 41 (for *E* parallel to the *a-c* plane).**Source:** Kharbish (2011).**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. For the Raman spectra of weissbergite see also Minceva-Sukarova et al. (2003) and Makreski et al. (2013b, 2014).**Weloganite**  $Na_2Sr_3Zr(CO_3)_6 \cdot 3H_2O$ **Origin:** Francon quarry, Québec province, Canada (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** (3444), 3403, 3376sh, 3329, (3325), 1740w, 1732sh, 1712w, 1700w, 1681, 1622, 1563w, 1548w, 1526w, 1417, 1385w, 1371w, 1350, 1082s, 1073sh, 1061sh, 870w, 762, 749, 736, 728, 696w, 682sh, 679, (657w), 550w, 424w, 372sh, 354, 326w, 312sh

**Source:** Frost et al. (2013ab).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of weloganite see also Vard and Williams-Jones (1993).

### Wendwilsonite Ca<sub>2</sub>Mg(AsO<sub>4</sub>)<sub>2</sub>·2H<sub>2</sub>O

**Origin:** Bou Azzer district, Morocco.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3332w, 3119w, (3001), 1724w, 1624sh, 1098w, 970w, 871, 832s, 800, 714w, 669w, (626w), 478sh, 454, 425, 361, 341, 306, 286w, 244w, 212sh, 191, 164, (140w), 127w.

**Source:** Frost et al. (2014v).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

### Wernerkrauseite Ca(Fe<sup>3+</sup>,Mn<sup>3+</sup>)<sub>2</sub>Mn<sup>4+</sup>O<sub>6</sub>

**Origin:** Bellerberg volcano, Eifel, Germany (type locality).

**Experimental details:** Raman scattering measurements have been performed on a grain in a polished section using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was between 10 and 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 1239w, 670sh, 622s, (558), 495, 408sh, (332w), 294, 169, 117sh.

**Source:** Galuskin et al. (2016b).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

### Wetherillite Na<sub>2</sub>Mg(UO<sub>2</sub>)<sub>2</sub>(SO<sub>4</sub>)<sub>4</sub>·18H<sub>2</sub>O

**Origin:** Blue Lizard mine, San Juan Co., Utah, USA (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** ~3600–3000, 1610, 1230, 1180, 1120, 1105, 1080, 1010s, 995, 922w, 890sh, ~830s, 815sh, 700w, 640, 615sh, 580sh, 506, 445, 385, ~240.

**Source:** Kampf et al. (2015b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Wheatleyite**  $\text{Na}_2\text{Cu}(\text{C}_2\text{O}_4)_2 \cdot 2\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3519, 3448, 3359w, 1733s, 1714w, 1674, 1651sh, 1470, 1434s, 1262, 1066, 904, 860, 798, 585, 565+560s (ubresolved doublet?), 387, 277, 243, 210, 173s, 139sh, 127.**Source:** Frost et al. (2008k).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of wheatleyite see also Palacios et al. (2011).**Whelanite**  $\text{Cu}_2\text{Ca}_6[\text{Si}_6\text{O}_{17}(\text{OH})](\text{CO}_3)(\text{OH})_3(\text{H}_2\text{O})_2$ **Origin:** Bawanamine, Milford, Utah, USA (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented single crystals using 532 nm laser radiation. The laser radiation power is not indicated. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 3599sh, 3558s, 3222w, 2954, 2917sh, 1600w, 1542w, 1471, 1085, 1012, 850, 715sh, 671s, 530w, 481, 458, 400+381 (unresolved doublet?), 254w, 217 + 201 (unresolved doublet?), 165 + 151 (unresolved doublet?), 106.**Source:** Kampf et al. (2012).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved. For the Raman spectrum of whelanite see also Frost and Xi (2012e).**Whewellite**  $\text{Ca}(\text{C}_2\text{O}_4) \cdot \text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 532 nm Nd-YAG laser radiation. The laser radiation power at the sample was between 50 and 100 mW.**Raman shifts (cm<sup>-1</sup>):** 3486, 3426, 3340, 3256, 3056, 2972w, 2919w, 1629, 1490s, 1463s, 896, 503, 140, and several bands between 160 and 250 cm<sup>-1</sup>.**Source:** Conti et al. (2015).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of whewellite see also Frost and Weier (2003), Frost et al. (2003k), Frost (2004d), Jehlička and Edwards (2008), and Conti et al. (2014).**Whitecapsite**  $\text{H}_{16}\text{Fe}^{2+}_5\text{Fe}^{3+}_{14}\text{Sb}^{3+}_6(\text{AsO}_4)_{18}\text{O}_{16} \cdot 120\text{H}_2\text{O}$ **Origin:** White Caps mine, Manhattan district, Nye Co., Nevada, USA (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented grain using 632.8 nm laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 3400 (broad), 3250, 2930sh, 2350w, 1655w, 1380w, 1165w, 1095w, 870s, 790sh, 585, 531s, 466, 318, 268, 202s, 175s, 120s.**Source:** Pekov et al. (2014b).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Whiteite [possibly, whiteite-(CaMnMg)]**  $\text{CaMn}^{2+}\text{Mg}_2\text{Al}_2(\text{PO}_4)_4(\text{OH})_2 \cdot 8\text{H}_2\text{O}$  (?)

**Origin:** No data.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3552sh, 3496s, 3426, 3220, 2939, 1692w, 1607 + 1586 (unresolved doublet?), 1368 + 1334 (unresolved doublet?), 1266sh, 1173, 1076, 978 + 972 + 960s (unresolved triplet?), 630, 586 + 571 (unresolved doublet?), 553sh, 500sh, 479, (457), 432, 363, 303sh, 282, 238, 176sh, 150, 109.

**Source:** Frost et al. (2014ab).

**Comments:** No independent analytical data are provided for the sample used.

**Whitlockite**  $\text{Ca}_9\text{Mg}(\text{PO}_3\text{OH})(\text{PO}_4)_6$

**Origin:** Sixiangkot chondrite.

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 1107w, 1084, 1030, 1015w, 976s, 959s, 855w, 820w, 668, 622, 605, 595, 553, 480, 450, 410, 328, 236, 179.

**Source:** Chen et al. (1995).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of whitlockite see also Jolliff et al. (2006) and Tait et al. (2011).

**Whitmoreite**  $\text{Fe}^{2+}\text{Fe}^{3+}_2(\text{PO}_4)_2(\text{OH})_2 \cdot 4\text{H}_2\text{O}$

**Origin:** Hagendorf-South (Hagendorf-Süd) pegmatite, Bavaria, Germany.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 1910w, 1157sh, 1144, 1032, 973s, 937s, 915, (617), 593, 565, 546sh, 474sh, 433, 305, 276, 243s, 190, 152 + 150 (unresolved doublet?).

**Source:** Frost et al. (2003b).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

**Widenmannite**  $\text{Pb}_2(\text{OH})_2[(\text{UO}_2)(\text{CO}_3)_2]$

**Origin:** Synthetic (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 3592sh, 3568, 3078, 1509w, 1470w, 1381, 1348w, 1122, 1068, 1058w, 849s, 736w, 725, 355, 268, 246, 225, 211w, 191, 128w, 115w.

**Source:** Plášil et al. (2010b).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Willemite**  $\text{Zn}_2\text{SiO}_4$ **Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm  $\text{Ar}^+$  laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 951w, 911, 875s.**Source:** Lin and Shen (1994).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of willemite see also Annen and Davis (1993).**Willemseite**  $\text{Ni}_3\text{Si}_4\text{O}_{10}(\text{OH})_2$ **Origin:** Scotia talc mine, Bon Accord area, Barberton district, South Africa.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was 0.5 mW.**Raman shifts (cm<sup>-1</sup>):** 3660s, 3645s, 3622s, 1043, 789, 671s, 410, 383s, 296s, 185s, 109.**Source:** Villanova-de-Benavent et al. (2014).**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.**Winstanleyite**  $\text{TiTe}^{4+} \text{O}_8$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powdery sample using 632.8 nm He-Ne laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 859w, 650, 475s, 385.**Source:** Ghribi et al. (2015).**Comments:** The sample was characterized by powder X-ray diffraction data.**Witherite**  $\text{Ba}(\text{CO}_3)_2$ **Origin:** Alston Moor, England (type locality).**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 488 or 514.5 nm  $\text{Ar}^+$  laser radiation. The nominal laser radiation power was 200 mW.**Raman shifts (cm<sup>-1</sup>):** 1423w, 1060s, 700w, 690, 222, 178w, 151s, 133s, 99w, 90, 78.**Source:** Scheetz and White (1977).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of witherite see also Buzgar and Apopei (2009) and Frezzotti et al. (2012).**Wittichenite**  $\text{Cu}_3\text{BiS}_3$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on nanocrystals using  $\text{Ar}^+$  laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 459, 355w, 153s, 116s.**Source:** Zhong et al. (2012).**Comments:** The sample was characterized by powder X-ray diffraction data and qualitative electron microprobe analysis. For the Raman spectrum of wittichenite see also Yan et al. (2013).

**Wollastonite** CaSiO<sub>3</sub>

**Origin:** Willsboro mine, Willsboro, Essex Co., New York, USA.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 or 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 500 mW.

**Raman shifts (cm<sup>-1</sup>):** 1153w, 1063sh, 1046, 1023w, 999w, 972s, 852, 668sh, 637, 622sh, 583w, 469w, 414, 339, 323, 306w, 282w, 251, 239, 229, 217w, 193, 163.

**Source:** Richet et al. (1998).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of wollastonite see also Buzatu and Buzgar (2010).

**Woodhouseite** CaAl<sub>3</sub>(SO<sub>4</sub>)(PO<sub>4</sub>)(OH)<sub>6</sub>

**Origin:** Champion mine, White Mountains, Mono Co., California, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3460, 3401sh, 3122, 3001sh, 1778w, 1168w, 1151w, 1096, 1032 + 1028s (unresolved doublet?), 1004, 988, 974sh, 666sh, 653, 618, 590, 534, 485+475 (unresolved doublet?), 408s, 364w, (258), 249, 230sh, 181, 142, 118.

**Source:** Frost et al. (2011s).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectrum of woodhouseite see also Maubec et al. (2012).

**Wopmayite** Ca<sub>6</sub>Na<sub>3</sub>□Mn(PO<sub>4</sub>)<sub>3</sub>(PO<sub>3</sub>OH)<sub>4</sub>

**Origin:** Tanco Mine, Bernic Lake, Manitoba, Canada (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal laser radiation power was between 5 and 12.5 mW. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** No data: only a figure of the Raman spectrum of wopmayite is presented in the cited paper. The strongest band is observed at ~960 cm<sup>-1</sup>.

**Source:** Cooper et al. (2013b).

**Wulfenite** PbMoO<sub>4</sub>

**Origin:** Synthetic (commercial reactant).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm laser radiation. The laser radiation power at the sample was 0.3 mW.

**Raman shifts (cm<sup>-1</sup>):** 868s, 765, 742, 347w, 315s, 189w, 168w.

**Source:** Bayne and Butler (2014).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of wulfenite see also Frost et al. (2004c), Nitta et al. (2006), and Rotondo et al. (2012).

**Wupatkiite**  $\text{CoAl}_2(\text{SO}_4)_4 \cdot 22\text{H}_2\text{O}$ **Origin:** Cloncurry, Queensland, Australia.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power at the sample was 1 mW. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3479sh, 3296, 2987sh, 1134, 1069, 1009, 995s, 976, 882, 779, 622, 601, 517, 468, 426, 390w, 287sh, 213.**Source:** Locke et al. (2007).**Comments:** The sample was characterized by electron microprobe analysis which corresponds to an intermediate member of the wupatkiite–halotrichite solid-solution series.**Wurtzite** ZnS**Origin:** Manus Spreading Centre, Bismarck Sea.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was between 1 and 10 mW. A 180°-scattering geometry was employed.**Raman shifts (cm<sup>-1</sup>):** 402 (broad), 350s, 327sh, 297s, 245w, 233w, 222, 173, 158.**Source:** Mernagh and Trudu (1993).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectra of wurtzite see also White (2009) and Ma et al. (2012a).**Wüstite** FeO**Origin:** Synthetic (type locality).**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 632.8 nm He-Ne laser radiation. The laser radiation power at the sample was 0.7 mW.**Raman shifts (cm<sup>-1</sup>):** 652.**Source:** De Faria et al. (1997).**Comments:** The sample was characterized by powder X-ray diffraction data.**Xenotime-(Y)** Y(PO<sub>4</sub>)**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented acicular crystals using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 25 mW.**Raman shifts (cm<sup>-1</sup>):** 1056s, 1023, 997s, 578w, 481, 330, 292.**Source:** Richman (1966).**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of xenotime-(Y) see also Liu et al. (2008), Qiong et al. (2008), Bracco et al. (2012), Frezzotti et al. (2012), Andò and Garzanti (2014), and Švecová et al. (2016).

**Xieite** FeCr<sub>2</sub>O<sub>4</sub>

**Origin:** Suizhou meteorite (type locality).

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 665sh, 605.

**Source:** Chen et al. (2008a).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Xocolatlite** Ca<sub>2</sub>Mn<sup>4+</sup><sub>2</sub>Te<sup>6+</sup><sub>2</sub>O<sub>12</sub>·H<sub>2</sub>O

**Origin:** Moctezuma deposit, Sonora, Mexico (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 699, 630s, 520, 390, 246w.

**Source:** Grundler et al. (2008).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Xocomecatlite** Cu<sub>3</sub>(Te<sup>6+</sup>O<sub>4</sub>)(OH)<sub>4</sub>

**Origin:** Mina Bambollita, Moctezuma, Sonora, Mexico.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 2926s, 2867, 2754, 2594, 2326, 2206, 1957, 1602, (1544), 1368w, 1314w, 1121w, 974, 796, 763, 710s, 680sh, 600sh, 509, 470, 438, 407sh, 291, 259, 231, 189, 161, 149.

**Source:** Frost and Keeffe (2009g).

**Comments:** The sample was characterized by chemical data.

**Xonotlite** Ca<sub>6</sub>Si<sub>6</sub>O<sub>17</sub>(OH)<sub>2</sub>

**Origin:** Point Sal, near Vandenberg Air Force Base, Santa Barbara Co., California, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** (3665), 3627, 3611w, (3578), (3528), 3303sh, 2909w, (1660w), (1603w), (1488 + 1423w) (unresolved doublet?), 1070, 1042s, 1015w, 980, 961s, (953), 862s, 816sh, 777, 695s, 626, 593s, 524, 505, 445, 421, 393, 369, 335, 304, 271w, 259w, 234, 205, 158, 135, 105.

**Source:** Frost et al. (2012b).

**Comments:** No independent analytical data are provided for the sample used.

**Yarrowite** Cu<sub>9</sub>S<sub>8</sub>**Origin:** Synthetic.**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 470s, 263.**Source:** Kumar and Nagarajan (2011).**Comments:** The sample was characterized by powder X-ray diffraction data.**Ye'elmitte** Ca<sub>4</sub>Al<sub>6</sub>O<sub>12</sub>(SO<sub>4</sub>)**Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was 20 mW.**Raman shifts (cm<sup>-1</sup>):** 991s, 616w, 521.**Source:** Gastaldi et al. (2008).**Comments:** The sample was characterized by powder X-ray diffraction data.**Yecorite** Fe<sup>3+</sup><sub>3</sub>Bi<sub>5</sub>O<sub>9</sub>(Te<sup>4+</sup>O<sub>3</sub>)(Te<sup>6+</sup>O<sub>4</sub>)<sub>2</sub>·9H<sub>2</sub>O**Origin:** Marie Elena mine, Yecora, Sonora, Mexico (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3400sh, 3180w, 2936w, 2878sh, 979w, 808, 796w, 699 + 690 (unresolved doublet?), 640sh, 578, 470 + 465s (unresolved doublet?), (396), 390, 355, 301, 265, 206, 145, 128.**Source:** Frost and Keeffe (2009h).**Comments:** No independent analytical data are provided for the sample used.**Yimengite** K(Cr,Ti,Fe,Mg)<sub>12</sub>O<sub>19</sub>**Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 632.8 nm He-Ne laser radiation. The nominal laser radiation power was between 4 and 8 mW.**Raman shifts (cm<sup>-1</sup>):** 695s, 629s, 545, 471, 285w.**Source:** Konzett et al. (2005).**Comments:** The sample was characterized by X-ray diffraction data and electron microprobe analyses.**Yingjiangite** K<sub>2</sub>Ca(UO<sub>2</sub>)<sub>7</sub>(PO<sub>4</sub>)<sub>4</sub>(OH)<sub>6</sub>·6H<sub>2</sub>O**Origin:** Xiaozhuang U deposit, China.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3510w, 3375sh, 3180w, 1047, 1004, 841 + 836s (unresolved doublet?), 817sh, 567, 531, 437, 393, 269sh, 204s, 147s.

**Source:** Frost et al. (2008a).

**Comments:** No independent analytical data are provided for the sample used.

### Yttriaite-(Y) Y<sub>2</sub>O<sub>3</sub>

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 2.5 mW.

**Raman shifts (cm<sup>-1</sup>):** The strongest peak is observed at 378 cm<sup>-1</sup>. Raman shifts of other bands are not indicated.

**Source:** Mills et al. (2011c).

**Comments:** Raman spectrum of natural yttriaite-(Y) given in the cited paper as a figure differs significantly from that of synthetic Y<sub>2</sub>O<sub>3</sub>.

### Yukonite Ca<sub>2</sub>Fe<sup>3+</sup><sub>3</sub>(AsO<sub>4</sub>)<sub>3</sub>(OH)<sub>4</sub>·4H<sub>2</sub>O

**Origin:** No data.

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 785 nm diode laser radiation. The laser radiation power at the sample was >0.3 mW.

**Raman shifts (cm<sup>-1</sup>):** 1059s, 992s, 929, 854s, 633, 527, 449, 387s, 237, 137.

**Source:** Das and Hendry (2011).

**Comments:** The sample was characterized by powder X-ray diffraction data. The strong bands at 1059 and 992 cm<sup>-1</sup> may correspond to impurities (a carbonate and a sulfate). For the Raman spectra of yukonite see also Gomez et al. (2010a, b) and Gómez and Lee (2012).

### Yuksporite K<sub>4</sub>(Ca,Na)<sub>14</sub>(Sr,Ba)<sub>2</sub>(□,Mn,Fe)(Ti,Nb)<sub>4</sub>(O,OH)<sub>4</sub>(Si<sub>6</sub>O<sub>17</sub>)<sub>2</sub>(Si<sub>2</sub>O<sub>7</sub>)<sub>3</sub>(H<sub>2</sub>O,OH)<sub>3</sub>

**Origin:** Hackman valley, Yukspor Mt., Khibiny massif, Kola Peninsula, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3668w (sharp), 3628sh, 3562w, 3460w, 3298sh, 2908w, 1103sh, 1078s, 1074sh, 1045, 1008w, 979, 954, 929sh, 891sh, 870s, 845sh, 815 + 803 (unresolved doublet?), 764, 723, 670s, 656sh, 641s, 588, 542, 525, 473+463 (unresolved doublet?), 437sh, 426, 395, 370, 348sh, 307, 288, 262sh, 241, 211, 141.

**Source:** Frost et al. (2015j).

**Comments:** The sample was characterized by qualitative electron microprobe analysis.

### Yurmarinite Na<sub>7</sub>(Fe<sup>3+</sup>,Mg,Cu)<sub>4</sub>(AsO<sub>4</sub>)<sub>6</sub>

**Origin:** Arsenatnaya fumarole, Tolbachik volcano, Kamchatka, Russia (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 532 nm laser radiation. The nominal radiation power at the sample was about 30 mW.

**Raman shifts (cm<sup>-1</sup>):** 931sh, 859s, 831, 794s, 481, 409s, 331, 288, 187, 162, 111sh.

**Source:** Pekov et al. (2014d).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### **Yushkinite** (Mg,Al)(OH)<sub>2</sub>VS<sub>2</sub>

**Origin:** Silova-Yakha River, Pai-Khoi Anticlinorium (type locality).

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 762, 570, 373s, 345, 301w.

**Source:** Koval'chuk, and Makeev (2007).

**Comments:** The sample was characterized by electron microprobe analyses.

### **Yvonite** Cu(AsO<sub>3</sub>OH)·2H<sub>2</sub>O

**Origin:** Salsigne mine, north of Carcassonne, Aude, France (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3485, 3314, 3061, 2831, 953, 897, 863, 842, 824, 795, 756, 637, 559, 546, 490, 473, 360, 342.

**Source:** Frost et al. (2015w).

**Comments:** No independent analytical data are provided for the sample used. Band intensities are not indicated.

### **Żabińskiite** Ca[Al<sub>0.5</sub>(Ta,Nb)<sub>0.5</sub>](SiO<sub>4</sub>)O

**Origin:** Piława Góra pegmatite, Góry Sowie Block, Poland (type locality).

**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power at the sample was 5 mW.

**Raman shifts (cm<sup>-1</sup>):** 997, 835, 642w, 581, 487, 431w, 341s.

**Source:** Pieczka et al. (2016a).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

### **Zadovite** BaCa<sub>6</sub>[(SiO<sub>4</sub>)(PO<sub>4</sub>)](PO<sub>4</sub>)<sub>2</sub>F

**Origin:** Hatrurim Basin, Negev Desert, Israel (type locality).

**Experimental details:** No data.

**Raman shifts (cm<sup>-1</sup>):** 1031, 992w, 969s, 881s, 839sh, 627w, 589, 520w, 430, 389, 342sh, 299w, 222.

**Source:** Galuskin et al. (2015e).

**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. The crystal structure is solved.

**Zálesíite**  $\text{CaCu}_6(\text{AsO}_4)_2(\text{AsO}_3\text{OH})(\text{OH})_6 \cdot 3\text{H}_2\text{O}$ 

**Origin:** Zálesí U deposit, Rychlebské Hory Mts., northern Moravia, Czech Republic (type locality).

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3457sh, 3361w, 3124w, (3106w), 1102, 912sh, 873s, 839s, (806), 623 + 520 (unresolved doublet?), 534s, 489, 433, 378sh, 354, 278, 239, 214sh, 170sh, 155 + 143s (unresolved doublet?).

**Source:** Čejka et al. (2011c).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Zanazziite**  $\text{Ca}_2\text{Be}_4\text{Mg}_5(\text{PO}_4)_6(\text{OH})_4 \cdot 6\text{H}_2\text{O}$ 

**Origin:** Ponte do Piauimine, Piaui valley, municipality of Itinga, Minas Gerais, Brazil.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3447 + 3437s (unresolved doublet?), 3256sh, (3098), 1644w, 1569w, 1466w, 1096, 1064, 1047, 1007, 970 + 964s (unresolved doublet?), 756, 589, 568, 559, 487, 457, 419, (404), 371, 294sh, 264, 236, 182, 166, 145, 132sh, 117.

**Source:** Frost et al. (2013ae).

**Comments:** The sample was characterized by electron microprobe analyses.

**Zaratite**  $\text{Ni}_3(\text{CO}_3)(\text{OH})_4 \cdot 4\text{H}_2\text{O}$ 

**Origin:** Cape Ortegal, Galicia, Spain (type locality).

**Experimental details:** Raman scattering measurements have been performed on a massive sample using 532 nm laser radiation. The nominal laser radiation power was 10 mW.

**Raman shifts (cm<sup>-1</sup>):** 3604, 3428w, 3328w, 3217sh, 3110w, 2983w, 2935, 2867w, 2753w, 1609, 1366s, 1073s, 972, 941, 788w, 685w, 536w, 458.

**Source:** Garcia-Guinea et al. (2013).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses. For the Raman spectra of zaratite see also Frost et al. (2008l) and LaIglesia et al. (2014).

**Zdeněkite**  $\text{NaPbCu}_5(\text{AsO}_4)_4\text{Cl} \cdot 5\text{H}_2\text{O}$ 

**Origin:** Cap Garonne Mine, near le Pradet, France.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** (1109w), (936w), 850s, 795s, 537s, 486s, 445, 339s, 278, 247.

**Source:** Frost et al. (2007m).

**Comments:** No independent analytical data are provided for the sample used.

**Zellerite**  $\text{Ca}(\text{UO}_2)(\text{CO}_3)_2 \cdot 5\text{H}_2\text{O}$ 

**Origin:** White Canyon No. 1 Mine, Frey Point, Utah, USA.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.

**Raman shifts (cm<sup>-1</sup>):** 3514w, 3375sh, 2945w, 1374w, 1091, 854s, 758, 363w, 233, 147.

**Source:** Frost et al. (2008f).

**Comments:** Questionable data. No independent analytical data are provided for the sample used. In the figures given in the cited paper the mineral is named “Zellerite/Liebegite.” The IR spectrum of the sample used corresponds to a sulfate.

**Zemannite**  $\text{Mg}_{0.5}\text{ZnFe}^{3+}(\text{TeO}_3)_3 \cdot 4.5\text{H}_2\text{O}$ 

**Origin:** Mina Bambollita, Moctezuma, Sonora, Mexico.

**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 740s, 650, 460s, 375, 213, 136.

**Source:** Frost et al. (2008i).

**Comments:** No independent analytical data are provided for the sample used.

**Zemkorite**  $\text{Na}_2\text{Ca}(\text{CO}_3)_2$ 

**Origin:** Product of heating of natural nyerereite to 400 °C.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 1078s, 993w, 710.

**Source:** Golovin et al. (2014).

**Comments:** The sample was characterized by electron microprobe analyses.

**Zhangpeishanite** BaFCl

**Origin:** Synthetic.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented crystal using 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 255, 215s, 165, 145.

**Source:** Sundarakannan et al. (2002).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of zhangpeishanite see also Scott (1968) and Sundarakannan and Kesavamoorthy (1998).

**Ziesite** Cu<sub>2</sub>V<sup>5+</sup><sub>2</sub>O<sub>7</sub>**Origin:** Synthetic.**Experimental details:** Methods of sample preparation are not described. Raman scattering measurements have been performed using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 950sh, 912s, 855, 786w, 389, 259, 192w.**Source:** De Waal and Hutter (1994).**Comments:** No independent analytical data are provided for the sample used.**Zincite** ZnO**Origin:** Franklin or Sterling Hill, New Jersey, USA**Experimental details:** No data.**Raman shifts (cm<sup>-1</sup>):** 1603 (broad), 1080, 1004sh, 569, 522s, 486, 478, 438, 378w, 331w, 252w.**Source:** Welsh (2008).**Comments:** The sample was characterized by EDS analyses. For the Raman spectra of zincite see also Bouchard and Smith (2003) and Kunert et al. (2006).**Zincochromite** ZnCr<sub>2</sub>O<sub>4</sub>**Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed from the (100) face of a single crystal using unpolarized 488 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 692s, 610, 515, 457w, 166.**Source:** Lutz et al. (1991).**Comments:** In the cited paper also polarized Raman spectra of zincochromite are given. For the Raman spectrum of zincochromite see also D'Ippolito et al. (2015).**Zincociapite** ZnFe<sup>3+</sup><sub>4</sub>(SO<sub>4</sub>)<sub>6</sub>(OH)<sub>2</sub>·20H<sub>2</sub>O**Origin:** Les Valettes, Wallis, Switzerland.**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 1231, 1162, 1159sh, 1099, 1021s, 1005s, 987sh, 893w, 860w, 738w, 624, (613sh), 565, 485, 450, 424, 302, 267s, 218.**Source:** Frost (2011c).**Comments:** No independent analytical data are provided for the sample used.

**Zincospiroffite**  $\text{Zn}_2\text{Te}_3\text{O}_8$ 

**Origin:** Zhongshangou Au deposit, Chongli Co., Hebei Province, China (type locality).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 514.5 nm Ar<sup>+</sup> laser radiation. The nominal laser radiation power was 20 mW.

**Raman shifts (cm<sup>-1</sup>):** 748, 725s, 646, 578w, 536w, 407w, 344, 304w, 233w, 181, 123.

**Source:** Zhang et al. (2004).

**Comments:** The sample was characterized by powder X-ray diffraction data and electron microprobe analyses.

**Zinkenite**  $\text{Pb}_9\text{Sb}_{22}\text{S}_{42}$ 

**Origin:** Zlatá Baňa, Slanské Vrchy Mts., central Slovakia.

**Experimental details:** Raman scattering measurements have been performed on a polycrystalline sample using 532 nm Nd-YAG laser radiation. Exciting radiation with the power density of  $8.5 \times 10^{-3}$  Å mW mm<sup>-2</sup> was used. A 180°-scattering geometry was employed.

**Raman shifts (cm<sup>-1</sup>):** (335sh), 312s, (302sh), 282s, (271sh), 238, 204sh, 192, 156, 130w, 119w, 103, 75sh, 69, 58.

**Source:** Kharbish and Jeleň (2016).

**Comments:** The sample was characterized by electron microprobe analyses. For the Raman spectrum of zinkenite see also Goienaga et al. (2011).

**Zippeite**  $\text{K}_3(\text{UO}_2)_4(\text{SO}_4)_2\text{O}_3(\text{OH}) \cdot 3\text{H}_2\text{O}$ 

**Origin:** Abandoned uranium mine at Pecs, Hungary.

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1233w, 1091, 1012, 842s, 740, 398, 192.

**Source:** Stefaniak et al. (2009).

**Comments:** The sample was characterized by qualitative electron microprobe analysis. For the Raman spectra of zippeite see also Frost et al. (2005i) and Plášil et al. (2010a).

**Zircon**  $\text{ZrSiO}_4$ 

**Origin:** Kozjak Mt., Kozjačija, Macedonia.

**Experimental details:** Raman scattering measurements have been performed on a powdered sample using 1064 nm Nd-YAG laser radiation. The laser radiation power is not indicated.

**Raman shifts (cm<sup>-1</sup>):** 1008s, 973, 769, 438, 394w, 356s, 224, 200w, 180w.

**Source:** Makreski et al. (2005b).

**Comments:** No independent analytical data are provided for the sample used. For the Raman spectra of zircon see also Nicola and Rutt (1974), Syme et al. (1977), Geisler et al. (2003), Gucsik et al. (2004), Jasinevicius (2009), Frezzotti et al. (2012), Nhlabathi (2012), Andò and Garzanti (2014), and Grüneberger et al. (2016).

**Zoisite**  $\text{Ca}_2\text{Al}_3[\text{Si}_2\text{O}_7][\text{SiO}_4]\text{O}(\text{OH})$ **Origin:** No data.**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented single-crystal platelet using 532 nm laser radiation. The nominal laser radiation power was 150 mW.**Raman shifts (cm<sup>-1</sup>):** 3150w, 1092s, 1018s, 983, 946w, 928, 909, 889, 872, 860, 778w, 727w, 678, 623, 597, 574, 530, 493s, 456, 435, 420, 395, 337, 312w, 287, 280, 261, 215, 192.**Source:** Mao et al. (2007).**Comments:** The sample was characterized by single-crystal X-ray diffraction data and electron microprobe analyses. For the Raman spectra of zoisite see also Jasinevicius (2009), Andò and Garzanti (2014), and Weis et al. (2016).**Zorite**  $\text{Na}_6\text{Ti}_5\text{Si}_{12}\text{O}_{34}(\text{O},\text{OH})_5 \cdot 11\text{H}_2\text{O}$ **Origin:** Synthetic.**Experimental details:** Raman scattering measurements have been performed on a powdery sample using 1064 nm Nd-YAG laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 1050w, 940, 905, 870sh, 755s, and a series of bands between 200 and 550 cm<sup>-1</sup>.**Source:** Craveiro and Lin (2012).**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of zorite see also Ferdov et al. (2008).**Zuktamrurite**  $\text{FeP}_2$ **Origin:** Synthetic.**Experimental details:** Polarized Raman scattering measurements have been performed on a cluster of needle-like crystals by the back-scattering technique, in different scattering geometries, using 514.5 nm Ar<sup>+</sup> laser radiation. The laser radiation power is not indicated.**Raman shifts (cm<sup>-1</sup>):** 448, 386–388, 323–326s.**Source:** Lutz and Müller (1991).**Comments:** No independent analytical data are provided for the sample used.**Zunyite**  $\text{Al}_{13}\text{Si}_5\text{O}_{20}(\text{OH},\text{F})_{18}\text{Cl}$ **Origin:** Zuni mine, San Juan Co., Colorado, USA (type locality).**Experimental details:** Raman scattering measurements have been performed on arbitrarily oriented crystals using a 633 nm He-Ne laser. The laser radiation power is not indicated. The Raman shifts have been determined for the maxima of individual peaks obtained as a result of the spectral curve analysis.**Raman shifts (cm<sup>-1</sup>):** 3635, 3431, 3369, 3352, 3335, 3317, 3304, 1295, 1239, 1207, 1176, 1141, 1126, 1101, 1067, 994, 950s, 930s, 701, 612, 467, 444, 397s, 374sh, 360s, 334, 313, 271, 250, 213, 202s.**Source:** Klopogge and Frost (1999d).**Comments:** No independent analytical data are provided for the sample used.

**Zýkaite**  $\text{Fe}^{3+}_4(\text{AsO}_4)_3(\text{SO}_4)(\text{OH}) \cdot 15\text{H}_2\text{O}$

**Origin:** Kaňk, near Kutná Hora, Czech Republic (?).

**Experimental details:** Raman scattering measurements have been performed on an arbitrarily oriented sample using 785 nm laser radiation. The nominal laser radiation power was between 60 and 120 mW.

**Raman shifts (cm<sup>-1</sup>):** 1113w, 1063w, 998, 895, 883, 835–815 (broad), 472sh, 442, 412sh, 306sh, 285s, 217.

**Source:** Culka et al. (2016b).

**Comments:** The sample was characterized by powder X-ray diffraction data. For the Raman spectrum of zýkaite see also Frost et al. (2011m).

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# Index

**A**

- Abellaite, 95, 741  
Abelsonite, 741  
Aburite, 742  
Acanthite, 742  
Acetamide solution, 742  
Actinolite, 742, 743  
Adachiite, 743  
Adamite, 743  
Adelite, 743  
Admontite, 71, 744  
Adolpaterite, 744  
Aegirine, 744  
Aegirine-augite, 267  
Aegirine Li analogue, 744  
Aerinite, 745  
Aeschynite-(Y), 745  
Afmite, 745  
Aflatellite, 745  
Agakhanovite-(Y), 746  
Agardite-(Ce), 629, 746  
Agardite-(La), 746  
Agardite-(Nd), 630  
Agardite-(Y), 746  
Agricolaite, 747  
Ahlfeldite, 747  
Ahrensite, 747  
Aikinite, 747  
Ajoite, 748  
Akaganeite, 748  
Åkermanite, 245, 748  
Åkermanite Sr analogue, 748  
Akimotoite, 321, 749  
Aklimaita, 749  
Alabandite, 749  
Alacránite, 749  
Alamosite, 749  
Alamosite polymorph, 266  
Alarsite, 750  
Albertiniite, 750  
Albite, 750  
Aleksite, 750  
Alforsite, 431  
Alforsite F-analogue, 431  
Alforsite OH-analogue, 751  
Alforsite vanadate analogue, 578  
Alfredopetrovite, 661  
Allactite, 617, 751  
Allanite (Ce), 751  
Allanite-(Nd), 751  
Allanpringite, 752  
Allendeite, 752  
Allophane, 752  
Almandine, 752  
Almarudite, 753  
Alpersite, 501  
Alstonite, 753  
Altaite, 753  
Althausite, 458, 753  
Alum-(K), 754  
Aluminite, 754  
Aluminium acid selenite hydrate, 639  
Aluminium decavanadate hydrate, 556  
Aluminium niobate, 125  
Aluminium phosphate hydrate, 355  
Aluminium selenite hydrate, 640  
Aluminocerite-(Ce), 754  
Aluminociapite, 501, 755  
Alumohydrocalcite, 755  
Alumovesuvianite, 251  
Alunite, 755  
Alunogen, 517, 755  
Alwilkinsite-(Y), 755  
Amakinite, 210  
Amarantite, 756  
Amarillite, 502  
Amblygonite, 756  
Ambrinoite, 756  
Ameghinite, 756  
Amesite, 757  
Ammoniojarosite, 757  
Ammoniozippeite, 532  
Ammonium bicarbonate, 80  
Ammonium calcium borate, 43  
Ammonium cuprooxopolymolybdate  
     $(\text{NH}_4)_4[\text{H}_6\text{CuMo}_6\text{O}_{24}] \cdot 4\text{H}_2\text{O}$ , 665  
Ammonium dichromate, 590  
Ammonium heptamolybdate, 666

- Ammonium iron(II) phosphate hydrate, 357  
 Ammonium magnesium phosphate, 357  
 Ammonium manganese(II) borophosphate, 393  
 Ammonium nickel molybdate ( $\text{NH}_4\text{Ni}_2(\text{HMnO}_4)(\text{MoO}_4)_2$ , 666  
 Ammonium paratungstate tetrahydrate, 707  
 Ammonium pentaborate, 41  
 Ammonium sulfate tellurate, 536  
 Ammonium titanophosphate, 358  
 Ammonium uranyl vanadate hydrate, 556  
 Ammonium vanadyl compound ( $\text{NH}_4_{0.5}\text{V}_2\text{O}_5 \cdot n\text{H}_2\text{O}$ , 557  
 Ammonium vanadyl pyrophosphate, 355  
 Ammonium zirconofluoride, 226  
 Analcime, 757  
 Anapaite, 758  
 Anatase, 758  
 Aencylite-(Ce), 758  
 Andalusite, 759  
 Andersonite, 759  
 Andradite, 759  
 Andychristyite, 760  
 Angastonite, 760  
 Anglesite, 760  
 Anhydrite, 8, 760  
 Anilite, 761  
 Ankerite, 761  
 Ankoleite, 432  
 Annabergite, 761  
 Annite, 761  
 Annite Cl-analogue, 761  
 Anorpiment, 762  
 Anorthite, 762  
 Antarcticite, 762  
 Anthophyllite, 763  
 Anthraxolite, 763  
 Antigorite, 763, 764  
 Antimonelite, 764  
 Antimony, 764  
 Antimony(III) phosphate, 359  
 Antimony(V) oxophosphate, 359  
 Antlerite, 764  
 Antofagastaite, 474  
 Apachite, 765  
 Aphthitalite, 765  
 Apjohnite, 765  
 Apuanite, 765  
 Aradite, 766  
 Aragonite, 8, 731, 766  
 Arangasite, 535  
 Arapovite-related silicate, 766  
 Aravaipaite, 767  
 Arcanite, 767  
 Archerite, 767  
 Ardealite, 535, 767  
 Ardennite-(As), 768  
 Arfvedsonite, 768  
 Argentojarosite, 768  
 Argutite, 768  
 Arhbarite, 617  
 Arisite (Ce), 769  
 Armalcolite, 769  
 Arrojadite-(KFe), 769  
 Arsenbrackebuschite, 769  
 Arsendscloisite Sr-analogue, 770  
 Arseniosiderite, 770  
 Arsenogorceixite, 770  
 Arsenolamprite, 770  
 Arsenolite, 770  
 Arsenopyrite, 771  
 Arsentsumebite, 771  
 Arsenuranylite, 771  
 Arthurite, 772  
 Artinite, 772  
 Arzakite, 772  
 Asbolane, 772, 773  
 Aspedamite, 773  
 Asselbornite, 773  
 Atacamite, 773  
 Atelestite, 774  
 Atelisite (Y), 774  
 Athabascaite, 774  
 Atokite, 774  
 Augelite, 775  
 Augite, 775  
 Aurichalcite, 775  
 Aurostibite, 776  
 Austinite, 776  
 Autunite, 776  
 Avicennite, 776  
 Avogadrite, 776  
 Awaruite, 777  
 Axinite-(Fe), 777  
 Azurite, 777
- B**
- Bacalite, 104  
 Backite, 777  
 Badalovite, 632  
 Baddeleyite, 778  
 Bafertisite, 778  
 Baghdadite, 778  
 Bahianite, 778  
 Bairdite, 779  
 Balestraita, 779  
 Balkanite, 779  
 Bambollaite Te analogue, 779  
 Baotite, 780  
 Barahonaite-(Al), 780  
 Barahonaite-(Fe), 780  
 Bararite, 780  
 Barberite, 781  
 Barbosalite, 781  
 Barentsite, 84  
 Bariandite Al-free analogue, 781  
 Barićite, 781  
 Barioferrite, 782  
 Barioperovskite, 782  
 Barium borate, 42

- Barium bromide dihydrate, 664  
Barium calcium diborate, 43  
Barium calcium tellurate, 680  
Barium cerium tantalite, 126  
Barium chromium pyrophosphate, 361  
Barium cobalt antimonate, 127  
Barium cobaltate, 127  
Barium cobalt selenite hydrate, 640  
Barium cobalt tellurate, 680  
Barium copper tellurate tellurite, 681  
Barium formate, 98  
Barium lanthanum thorium orthovanadate, 558  
Barium magnesium fluoride, 227  
Barium manganese fluoride, 227  
Barium nickel oxide BaNiO<sub>2</sub>, 128  
Barium nickel oxide BaNiO<sub>3</sub>, 129  
Barium nickel tellurate, 682  
Barium niobate, 129  
Barium sodium cyclotriphosphate hydrate, 361  
Barium strontium orthoborate fluoride, 21  
Barium titanate, 130  
Barium titanium sulfide, 481  
Barium vanadyl phosphate, 362  
Barium vanadyl vanadate, 558  
Barium zinc tellurate, 682  
Barium zirconium orthoborate, 22  
Barnesite, 782  
Barringtonite, 782  
Barrydawsonite-(Y), 782  
Bartelkeite, 783  
Barylite, 783  
Barysilite, 246  
Baryte, 783  
Baryte selenate analogue, 641  
Barytocalcite, 784  
Bassanite, 784  
Bassoite, 784  
Bastnäsite-(Ce), 784  
Batievaite-(Y), 340  
Batiferrite co-bearing, 785  
Baumhauerite, 785  
Bavenite, 785  
Bayerite, 785  
Bayldonite, 786  
Bayleyite, 90, 786  
Baylissite NH<sub>4</sub>-analogue, 786  
Bazhenovite, 786  
Bazirite, 341, 787  
Bazzite, 787  
Mereheadite, 77  
Beaverite-(Cu), 787  
Beaverite-(Zn), 529  
Becquerelite, 787  
Behierite, 788  
Behoite, 788  
Běhounekite, 788  
Belakovskite, 788  
Bellidoite, 789  
Bendadaite, 789  
Benitoite, 789  
Benstonite, 789  
Beraunite, 351, 353, 789  
Berborite, 40  
Berdesinskiite, 790  
Bergenite, 790  
Berlinite, 790  
Berlineite tetragonal polymorph, 791  
Bermanite, 791  
Bernalite, 791  
Berndtite, 791  
Berthierite, 791  
Bertrandite, 792  
Beryl, 792  
Beryl Cs-bearing, 792  
Beryllonite, 793  
Berzeliite, 793  
Berzeliite polymorph alluaudite-type, 793  
Betalomonosovite, 344, 345, 793  
Bettertonite, 618  
Beudantite, 794  
Beusite, 794  
Beyerite, 794  
Bianchite/Goslarite, 794  
Bikitaite, 795  
Billietite, 795  
Biotite, 795  
Biphosphamite, 795  
Birnessite, 795, 796  
Bischofite, 796  
Bismite, 174, 796  
Bismoclite, 796  
Bismuth, 796  
Bismuth(III) aluminite Bi<sub>2</sub>Al<sub>4</sub>O<sub>9</sub>, 131  
Bismuth(III) aluminoferrite Bi<sub>2</sub>Fe<sub>3</sub>AlO<sub>9</sub>, 132  
Bismuth(III) calcium oxophosphate, 363  
Bismuth copper sulfate tellurite, 482  
Bismuth ferrite, 135  
Bismuth(III) ferrite dimolybdate, 667  
Bismuthinite, 797  
Bismuth(III) magnesium oxovanadate, 560  
Bismuth(III) magnesium oxovanadate BiMg(VO<sub>4</sub>)O, 559  
Bismuth molybdate, 668  
Bismuth(III) nickel oxophosphate BiNi(PO<sub>4</sub>)O, 364  
Bismuth(III) stannate pyrochlore-type, 133  
Bismuth sulfate, 483  
Bismuth(III) tantalate Bi<sub>7</sub>Ta<sub>3</sub>O<sub>18</sub>, 133  
Bismuth(III) tellurite selenate, 642  
Bismuth(III) titanate Bi<sub>4</sub>Ti<sub>3</sub>O<sub>12</sub>, 134  
Bismuth tungstate, 708  
Bismuthyl sulfate, 483  
Bismutite, 797  
Bismutocolumbite, 175, 797  
Bismutoferrite, 797  
Bismutotantalite, 798  
Bismutotantalite triclinic dimorph, 176  
Bitikleite, 798  
Bityite, 327  
Bixbyite, 798

- Blatterite, 798  
 Blödite, 799  
 Bluebellite, 799  
 Bluelizardite, 799  
 Bobcookite, 471, 799  
 Bobdownsite, 800  
 Bobierrite, 800  
 Bobshannonite, 800  
 Bohdanowiczite, 800  
 Böhmite, 801  
 Boleite, 801  
 Boltwoodite, 801  
 Bonaccordite, 801  
 Bonattite, 802  
 Bonazziite, 802  
 Boracite, 802  
 Borax, 803  
 Bornite, 803  
 Boron arsenate, 599  
 Boron phosphate, 365  
 Bosiite, 803  
 Botallackite, 803  
 Botryogen, 803  
 Bottinoite, 804  
 Boulangerite, 804  
 Bouronite, 804  
 Boussingaultite, 804, 805  
 Bowieite, 805  
 Braccoite, 805  
 Bracewellite, 805  
 Brackebuschite, 806  
 Bradaczekite, 626  
 Bradleyite, 806  
 Braggite, 806  
 Brandholzite, 806  
 Brannerite, 807  
 Brannockite, 807  
 Brassite, 807  
 Braunita, 176, 807  
 Brazilianite, 808  
 Bredigite, 808  
 Breithauptite, 808  
 Brewsterite-Sr, 808  
 Brianyoungite, 809  
 Briartite, 809  
 Bridgmanite, 321  
 Bridgmanite trigonal polymorph, 322  
 Britvinite, 15, 16, 809  
 Brizziite, 809  
 Brizzite polymorph, 177  
 Brochantite, 810  
 Bromargyrite, 810  
 Bromellite, 178, 810  
 Brookite, 178, 811  
 Browneite, 811  
 Brownleeite, 811  
 Brownmillerite, 811  
 Brucite, 2, 12, 812  
 Brucite Co-analogue, 179  
 Brüggenite, 812  
 Brugnatellite, 812  
 Brunogeierte, 597  
 Brushite, 812  
 Buchwaldite, 813  
 Buchwaldite dimorph, 450  
 Bukovskyite, 813  
 Bulgakite, 345  
 Bunnoite, 813  
 Bunsenite, 813  
 Burangaite, 814  
 Burbankite, 814  
 Burckhardite, 814  
 Burgessite, 815  
 Burkeite, 815  
 Buseckite, 815  
 Bustamite, 815  
 Butlerite, 816  
 Buttgenbachite, 816  
 Byströmite, 816
- C**
- Cabalzarite, 816  
 Cabvinita, 817  
 Cacoxenite, 817  
 Cadmium formatedihydrate, 98  
 Cadmium molybdate, 668  
 Cadmium oxalate trihydrate, 99  
 Cadmium stannate, 136  
 Cadmium tungstate, 708  
 Cadmoindite, 817  
 Cadmoselite, 817  
 Cafarsite, 818  
 Cafetite, 818  
 Cahnite, 818  
 Cairncrossite, 818  
 Calamaite, 476  
 Calaverite, 819  
 Calciborite, 819  
 Calcioaravaipaite, 819  
 Calciojohillerite, 634  
 Calciolangbeinite, 820  
 Calcio-olivine, 819  
 Calcipetersite, 820  
 Calcite, 8, 731, 820  
 Calcium antimonite, 138  
 Calcium arsenate  $\text{CaAs}_2\text{O}_6$ , 602  
 Calcium borate, 45  
 Calcium chlorarsenate, 601  
 Calcium chlorophosphate ("chlor-spodiosite"), 368  
 Calcium copper titanate  $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ , 139  
 Calcium dihydrophosphate monohydrate, 369  
 Calcium hydroxychloride, 540  
 Calcium indium oxide  $\text{Ca}_2\text{InO}_4$ , 135  
 Calcium iron(III) tin orthophosphate, 432  
 Calcium magnesium lanthanum phosphate, 370  
 Calcium magnesium yttrium phosphate, 370  
 Calcium niobate columbite-type, 139  
 Calcium orthoarsenate trigonal polymorph, 603

- Calcium orthoborate fluoride, 23  
Calcium orthophosphate orthosilicate, 347  
Calcium orthovanadate trigonal polymorph, 560  
Calcium plumbate, 140  
Calcium samarium thorium arsenate, 603  
Calcium strontium orthophosphate whitlockite-type, 422  
Calcium tellurite monohydrate, 683  
Calcium tetraborate, 45  
Calcmolite, 821  
Calderite, 821  
Calderónite, 821  
Caledonite, 821  
Callaghanite, 822  
Calomel, 822  
Calumetite, 822  
Camaronesite, 822  
Camerolite, 823  
Campostriniite, 503  
Canavesite, 823  
Cancrinite, 727, 823  
Cancrinite Ca-free analogue, 306  
Cancrinite  $\text{CO}_3$ -deficient, 301  
Cancrinite  $\text{NO}_3$ -analogue, 304  
Cancrinite  $\text{NO}_3$ -analogue low-hydrous, 305  
Cancrinite  $\text{SO}_4$ -rich, 823  
Canfieldite, 824  
Cannonite, 824  
Canosioite, 619  
Canutite, 637  
Caoxite, 104, 105  
Carbocernaite, 824  
Carbonatecyanotrichite, 824  
Carletonite, 825  
Carlfrancisite, 825  
Carlfriesite, 825  
Carlhintzeite, 226  
Carlinite, 825  
Carlosturanite, 826  
Carlsbergite, 826  
Carlsonite, 515  
Carminite, 826  
Carnallite, 826  
Carnegieite, 826  
Carnegieite (high), 306  
Carnegieite (low), 307  
Carnotite, 827  
Carpathite, 827  
Capholite, 827  
Carboydite, 827  
Carrollite, 828  
Caryopilitite, 828  
Cassiterite, 828  
Castellarite, 597, 828  
Caswellsilverite, 829  
Catalanoite, 829  
Catapleite, 829  
Catapleite heating product, 346  
Cattierite, 829  
Cavansite, 829  
Cebaite (Ce), 830  
Čejkaite, 830  
Celadonite, 830  
Celestine, 830  
Celsian, 831  
Centennialite, 545  
Cerianite-(Ce), 831  
Cerium metaphosphate trihydrate, 372  
Cerium(III) polyphosphate, 372  
Cerium(IV) pyrophosphate, 371  
Černýite, 831  
Ceruleite, 831  
Cerussite, 16, 832  
Cervantite, 832  
Cesanite, 832  
Cesárolite, 118  
Cesium acid (pentahydrogen) arsenate, 600  
Cesium acid arsenate selenate, 642  
Cesium acid (pentahydrogen) phosphate, 366  
Cesium antimony chloride, 539  
Cesium beryllium orthoborate, 22  
Cesium borosilicate pollucite-type, 330  
Cesium calcium borate, 44  
Cesium copper chloride, 537  
Cesium fluoromolybdate  $\text{CsMoO}_2\text{F}_3$ , 669  
Cesium hexafluorophosphate, 228, 229  
Cesium iron arsenate  $\text{Cs}_7\text{Fe}_7\text{O}_2(\text{AsO}_4)_8$ , 601  
Cesium iron sulfate, 484  
Cesium magnesium chloride, 538  
Cesium manganese(II) pyrophosphate, 367  
Cesium sodium stibiochloride, 539  
Cesium stibiofluoride, 229  
Cesium thorium molybdate, 670  
Cesium uranyl niobate  $\text{Cs}_2(\text{UO}_2)_2(\text{Nb}_2\text{O}_8)$ , 137  
Cesium uranyl niobate  
     $\text{Cs}_9[(\text{UO}_2)_4\text{O}_4(\text{NbO}_5)(\text{Nb}_2\text{O}_8)_2]$ , 137  
Cesium uranyl oxophosphate, 368  
Cesium uranyl tungstate  
     $\text{Cs}_4[(\text{UO}_2)_4(\text{WO}_5)(\text{W}_2\text{O}_8)\text{O}_2]$ , 709  
Cesium uranyl tungstate  $\text{Cs}_4[(\text{UO}_2)_7(\text{WO}_5)_3\text{O}_3]$ , 710  
Cesium uranyl tungstate  $\text{Cs}_8(\text{UO}_2)_4(\text{WO}_4)_4(\text{WO}_5)_2$ , 710  
Chabazite-Ca, 832  
Chalcanthite, 832  
Chalcoalumite, 833  
Chalcocite, 833  
Chalcocyanite, 833  
Chalcomenite, 833  
Chalconatronite, 834  
Chalcophanite, 834  
Chalcophyllite, 834  
Chalcopyrite, 834  
Chalcosiderite, 835  
Chalcostibite, 835  
Challacolloite, 835  
Chambersite, 835  
Chamosite, 836  
Changbaiite, 836  
Changoite, 522, 836  
Changoite (slightly deuterated), 503

- Chapmanite, 836  
 Charlesite, 521  
 Charoite, 836  
 Chegemite, 837  
 Chekhovichite, 837  
 Chenevixite, 837  
 Cheralite, 837  
 Cheralite La-bearing, 620  
 Cheremnykhite trigonal dimorph, 585  
 Chernikovite, 838  
 Chernovite-(Y), 838  
 Chervetite, 838  
 Chiavennite, 327, 838  
 Chibaite, 207, 839  
 Childrenite, 839  
 Chiolite, 839  
 Chloraluminite, 839  
 Chlorapatite, 840  
 Chlorargyrite, 840  
 Chlorellastadite, 335  
 Chloritoid, 840  
 Chlorkyuygenite, 840  
 Chlormayenite, 180, 840  
 Chlorocalcite, 841  
 Chloromagnesite, 841  
 Chlorophoenicite, 630  
 Chloroxiphite, 841  
 Chondrodite, 841  
 Chromatite, 842  
 Chromite, 842  
 Chromium disilicide, 320  
 Chromium iron(III) orthovanadate, 561  
 Chromium uranium oxide  $\text{Cr}_2\text{UO}_6$ , 141  
 Chromium vanadate  $\text{Cr}_2\text{V}_4\text{O}_{13}$ , 562  
 Chrysoberyl, 181, 842  
 Chrysocolla, 843  
 Chrysotallite, 843  
 Chrysotile, 9, 843  
 Chudobaite, 599  
 Chukanovite, 85, 843  
 Chukhrovite (Ca), 843  
 Churchite-(Nd), 844  
 Churchite-(Y), 844  
 Cinnabar, 844  
 Claringbullite, 844  
 Clarkeite, 210  
 Claudetite, 845  
 Clausthalite, 845  
 Clinoatacamite, 845  
 Clinobisvanite, 579, 846  
 Clinocervantite, 224, 846  
 Clinochalcomenite, 846  
 Clinochlore, 846  
 Clinoclase, 847  
 Clinoenstatite, 847  
 Clinohedrite, 847  
 Clinometaborite, 847  
 Clinoptilolite (Na), 848  
 Clinotobermorite-like mineral, 848  
 Clinozoisite, 848  
 Clintonite, 848  
 Coahuilite, 106  
 Coalingite, 94, 849  
 Cobaltarthurite, 849  
 Cobaltaustinite, 849  
 Cobalt dinickel orthoborate, 39  
 Cobalt ferrite spinel-type, 142  
 Cobaltkoritnigite, 849  
 Cobaltomenite, 661, 850  
 Cobaltpentlandite, 850  
 Cobalt selenite, 662  
 Cobalt selenite hydrate, 663  
 Cobalt zinc tellurium oxide, 141  
 Coccinitite, 850  
 Cochromite, 850  
 Cochromite Ni-bearing, 182  
 Coconinoite, 851  
 Coesite, 851  
 Coffinite, 851  
 Colemanite, 851  
 Colimaite, 852  
 Colinowensite, 279, 852  
 Coloradoite, 852  
 Columbite-(Mg), 852  
 Columbite-(Mn), 183, 853  
 Comancheite, 545, 853  
 Combeite, 853  
 Compreignacite, 853  
 Conichalcite, 853  
 Connellite, 854  
 Cookeite, 292, 297  
 Cooperite, 854  
 Copiapite, 504, 854  
 Copper acid diperiodate hydrate, 702  
 Copper(II) carbonate, 81  
 Copper chromate, 590  
 Copper divanadate hydroxide hydrate, 562  
 Copper(II) hydroxide, 142  
 Copper iodate, 699, 700  
 Copper molybdate selenite, 644  
 Copper oxychloride hydrate, 541  
 Copper strontium formate, 100  
 Copper tinanium oxyphosphate, 373  
 Coquandite, 855  
 Coquimbite, 855  
 Corderoite, 855  
 Cordierite, 855  
 Cordylite (Ce), 856  
 Corkite, 856  
 Cornetite, 856  
 Cornubite, 856  
 Cornwallite, 857  
 Coronadite, 857  
 Correianevesite, 857  
 Corundum, 183, 858  
 Cosalite, 858  
 Cotunnite, 858  
 Coulsonite, 858

- Covellite, 858  
Crandallite, 859  
Cranswickite, 859  
Creaseyite, 859  
Crednerite, 859  
Creelite, 860  
Cristobalite, 860  
Crocoite, 860  
Cryptohalite, 861  
Cryptomelane, 861  
Cu,Al-hydroxyphosphate, 459  
Cubanite, 861  
Cuboargyrite, 861  
Cumengeite, 549, 861  
Cummingtonite, 862  
Cuprite, 862  
Cuprocopiapite, 862  
Cuproiridsite, 862  
Cupromolybdite, 863  
Cuprorthosite, 863  
Cuprorivaita, 863  
Cuproskłodowskite, 863  
Cuprospinel, 864  
Cuprotungstite, 864  
Curienite, 864  
Curite, 864  
Cuspidine, 244, 865  
Cyanochroite, 865  
Cyanotrichite, 865  
Cymrite, 865  
Cyprine, 250  
Cyrilovite, 866  
Czochralskiite, 866
- D**
- Dachiardite (Na), 866  
Dalnegorskite, 269  
Danalite, 329  
Danburite, 866  
Daqingshanite-(Ce), 456  
Darapskite, 867  
Darrellhenryite, 332, 333, 867  
Dashkovite, 867  
Datolite, 867  
Daubréelite, 868  
Davidite-(La), 868  
Davidlloydite, 868  
Davinciite, 282  
Davisite, 868  
Dawsonite, 869  
Decrespignyite-(Y), 869  
Delafoseite Al analogue, 184  
Delafoseite, 869  
Delhayelite, 869  
Deliensite, 870  
Dellaite, 870  
Deltalumite, 122  
Delvauxite, 870  
Demartinite, 871  
Demesmaekerite, 871  
Demicheleite-(Br), 871  
Demicheleite-(Cl), 871  
Demicheleite-(I), 871  
Denningite, 696, 872  
Depmeierite, 302  
Derriksite, 872  
Desautelsite, 872  
Dessauite-(Y), 872  
Destinezite, 873  
Deveroite-(Ce), 106, 110  
Devilline, 873  
Devitoite, 873  
Devitrite, 873  
Dewindtite, 874  
Diaboleite, 874  
Diadochite, 874  
Diamond, 874  
Diaoyudaite, 220  
Diaspore, 875  
Dicalcium hexaborate monohydrate, 46  
Dickinsonite-(KMnNa), 875  
Dickite, 875  
Digenite, 875  
Dimorphite, 876  
Diomignite, 876  
Diopside, 876  
Dioprase, 876  
Dipotassium sodium zinc pentaborate, 47  
Dissakisite-(La), 877  
Dixenite, 877  
Djerfisherite, 877  
Dmisokolovite, 877  
Dmisteinbergite, 313, 878  
Dolomite, 878  
Domerockite, 878  
Donnayite-(Y), 878  
Dorallcharite, 879  
Dorfmanite, 879  
Dorrite, 267  
Double perovskite  $\text{KBa}(\text{XeNaO}_6)$ , 704  
Double perovskite  $\text{KCa}(\text{XeNaO}_6)$ , 704  
Double perovskite  $\text{KSr}(\text{XeNaO}_6)$ , 705  
Double-ring borate  $(\text{Na,K})_3\text{Sr}(\text{B}_5\text{O}_{10})$ , 47  
Dovyrenite, 879  
Downeyite, 879  
Doyleite, 880  
Dravite, 880  
Dreyerite, 880  
Drugmanite, 467  
Drysdallite, 880  
Dualite, 283  
Dufrénoysite, 881  
Duftite, 881  
Dumontite, 881  
Dumortierite, 881  
Dundasite, 882  
Durangite, 882  
Dussertite, 882

- Duttonite, 211  
 Dwornikite, 882  
 Dypingite, 883  
 Dysprosium copper hydroxysulfate  
 $\text{Dy}_2\text{Cu}(\text{SO}_4)_2(\text{OH})_4$ , 485  
 Dysprosium decavanadate hydrate, 563  
 Dzhalindite, 883  
 Dzhuluite, 883  
 Dzierżanowskite, 883
- E**  
 Eakerite, 884  
 Eastonite, 884  
 Ecandrewsite, 884  
 Ecdemite, 885  
 Eckhardtite, 885  
 Edgrewite, 885  
 Edingtonite, 885  
 Edoyerite, 886  
 Effenbergerite, 886  
 Eitelite, 886  
 Ekanite, 886  
 Ekplexite, 887  
 Elbaite, 887  
 Elbrusite, 888  
 Eleomelanite, 470  
 Eleonorite, 888  
 Elpasolite, 888  
 Eltyubyuite, 888  
 Embreyite, 595  
 Emmonsite, 889  
 Enargite, 889  
 Enstatite, 889  
 Eosphorite, 890  
 Epidote, 890  
 Epidote-(Sr), 257  
 Epistilbite, 890  
 Epsomite, 890, 891  
 Ericlaxmanite, 891  
 Erikapohlite, 891  
 Eringaite, 891  
 Eriochalcite, 892  
 Erionite-Ca, 892  
 Erionite-K, 313  
 Erlichmanite, 892  
 Ernstburkeite, 892  
 Erythrite, 893  
 Erythrosiderite, 893  
 Eskebornite, 893  
 Eskolaite, 894  
 Esperite, 894  
 Ettringite, 731, 894  
 Euchroite, 894  
 Euclase, 895  
 Eucryptite- $\beta$ , 895  
 Eugsterite, 895  
 Eulytine, 896  
 Euxenite-(Y), 896  
 Evansite, 896
- Eveite, 896  
 Evenkite, 897  
 Ezcurrite, 897
- F**  
 Fabriesite, 897  
 Fairfieldite, 897  
 Falcondoite, 286, 898  
 Falottaite, 898  
 Fangite, 898  
 Farringtonite, 898  
 Fassinaite, 899  
 Faujasite-Ca, 316  
 Faujasite-Na, 899  
 Favreauite, 899  
 Fayalite, 899  
 Feitknechtite, 900  
 Felsőbányaite, 900  
 Ferberite, 900  
 Fergusonite-(Ce)- $\beta$ , 900  
 Fergusonite-(La)- $\beta$ , 901  
 Fergusonite-(Nd)- $\beta$ , 901  
 Fergusonite-(Y), 901, 902  
 Fergusonite-(Y)- $\beta$ , 901  
 Fermiite, 902  
 Feroxyhyte, 902  
 Ferriakasakaite-(La), 258  
 Ferriallanite-(Ce), 902  
 Ferricopiapite, 505, 903  
 Ferricoronadite, 117  
 Ferri-eckermannite, 903  
 Ferrierite-K, 903  
 Ferrierite-Na, 903  
 Ferrierite-NH<sub>4</sub>, 319  
 Ferri-fluoro-katophorite, 277  
 Ferri-fluoro-leakeite, 274  
 Ferrihollandite, 118  
 Ferrihydrite, 904  
 Ferri-kaersutite, 904  
 Ferri-leakeite, 274  
 Ferrillotharmeyerite, 904  
 Ferrimolybdite, 905  
 Ferrinatrile, 473, 905  
 Ferrisaponite, 300  
 Ferrisepiolite, 297  
 Ferristrunzite, 905  
 Ferrivauxite, 434  
 Ferro-actinolite, 905  
 Ferrocapholite, 906  
 Ferroceladonite, 906  
 Ferro-ferriferro-fluoro-leakeite, 273  
 Ferro-ferrikerphorite, 271  
 Ferro-ferrinybōite, 272  
 Ferro-glaucophane, 906  
 Ferrohögbomite, 907  
 Ferro-hornblende, 906  
 Ferrokésterite, 907  
 Ferronigerite-2N1S, 215  
 Ferro-pargasite, 271

- Ferrorhodonite, 265  
Ferroselite, 907  
Ferrosilite, 907  
Ferrostrunzite, 908  
Ferrovesuvianite, 251, 256  
Ferruccite, 908  
Fersmite, 908  
Feruvite, 908  
Fervanite (?), 586  
Fetiasite, 620  
Fibroferrite, 519  
Fichtelite, 909  
Fiedlerite, 909  
Fiedlerite-1A, 550  
Finnemanite, 909  
Flamite, 909  
Flinteite, 910  
Florencite-(La), 910  
Florencite-(Nd), 452  
Fluellite, 910  
Fluocerite-(Ce), 911  
Fluocerite-(La), 911  
Fluorapatite As-rich, 911  
Fluorapatite, 911  
Fluorapophyllite-(K), 735, 736, 912  
Fluorbarytolamprophyllite, 336  
Fluor-buergerite, 912  
Fluorcalciorbitolite, 912  
Fluorcalciomicrolite, 185, 912  
Fluorcalcipyrochlore, 215  
Fluorcalcioroméite, 913  
Fluorcaphite, 913  
Fluorcarmoite-(BaNa), 451  
Fluorchegemite, 238  
Fluor-dravite, 334  
Fluor-elbaite, 913  
Fluorite, 914  
Fluorkyuygenite, 914  
Fluorlamprophyllite, 914  
Fluormayenite, 915  
Fluormayenite-related garnet, 914  
Fluornatropyrochlore, 185  
Fluorocronite, 915  
Fluoro-edenite, 915  
Fluoro-pargasite, 278  
Fluorwardite, 916  
Fluor-schorl, 913  
Fluor-uvite, 916  
Fluorvesuvianite, 257  
Fluorwavelite, 439, 916  
Fogoite-(Y), 341  
Foitite, 916  
Fontarnauite, 71  
Foordite, 917  
Forêtite, 917  
Formanite-(Y), 917  
Formicaite, 917  
Fornacite, 918  
Forsterite, 918  
Fougèrite, 918  
Fowlerite, 264  
Fraipontite, 918  
Francevillite, 919  
Francisite, 919  
Franckeite, 919  
Françoisite-(Nd), 919  
Franconite, 920  
Frankdicksonite, 920  
Franklinite, 173, 920  
Freboldite, 920  
Fredrikssonite, 921  
Fresnoite, 921  
Friedrichbeckeite, 921  
Frohbergite, 921  
Frolovite, 922  
Frondelite, 922  
Fulgurite (a high-silicon glass), 922  
Fupingquite, 465
- G**
- Gadolinite-(Nd), 922  
Gadolinite-(Y), 326  
Gahnite, 923  
Gaidonnayite, 923  
Galaxite, 923  
Galeite, 523  
Galena, 923  
Galileiite, 924  
Gallite, 924  
Gallium hydroxyde hydrate  $\text{Ga(OH)}_3 \cdot n\text{H}_2\text{O}$ , 186  
Gallium(III) oxide, 124  
 $\beta$ -Gallium(III)-oxide, 131  
Gallium sulfide, 924  
Gallium(III) oxyhydroxide, 124  
Galloplumbogummite, 924  
Galuskinite, 925  
Gamagarite, 925  
Gamma-alumina, 180  
Gananite, 235, 925  
Ganomalite, 253, 926  
Ganterite, 926  
Garavellite, 926  
Garnet, 926  
Gartrellite, 927  
Garutite, 927  
Gaspéite, 927  
Gaudefroyite, 927  
Gauthierite, 209  
Gaylussite, 928  
Gazeevite, 928  
Gearsutite, 928  
Geffroyite, 928  
Gehlenite, 929  
Geikielite, 929  
Geminite, 929  
Gerdtremmelite, 631  
Gerénite-(Y), 279  
Gerhardtite, 929

- Gerstleyite, 930  
 Geschieberite (?), 505  
 Geschieberite, 930  
 Ghiaiaite, 930  
 Gianellaite, 506  
 Gibbsite, 930  
 Gilalite, 931  
 Gillardite, 931  
 Gillespite, 931  
 Giniite, 932  
 Gismondine, 932  
 Glass, 300  
 Glauberite, 932  
 Glaucoberinitite, 932  
 Glauconite, 932  
 Glaucomphane, 933  
 Glaukosphaerite, 933  
 Glushinskite, 933  
 Gmelinite-Na, 934  
 Goethite, 934  
 Goldfieldite, 934  
 Goldmanite, 934  
 Gonnardite, 934  
 Goosecreekite, 935  
 Gorceixite, 935  
 Gordaite, 507  
 Görgeyite, 935  
 Gormanite, 935  
 Goryainovite, 441, 936  
 Goslarite, 936  
 Götzenite, 936  
 Goudeyite, 936  
 Gowerite, 937  
 Goyazite, 937  
 Graemite, 937  
 Graeserite, 937  
 Graftonite, 938  
 Gramaccioliite-(Y), 938  
 Grandaitte, 938  
 Grandidierite, 938  
 Graphite, 729, 939  
 Gratonite, 939  
 Greenockite, 939  
 Gregoryite, 939  
 Greigite, 940  
 Griceite, 940  
 Grimaldiite, 940  
 Grimselite, 941  
 Grossite, 941  
 Grossular, 941  
 Groutite, 941  
 Grumiplucite, 942  
 Grunerite, 757, 942  
 Guanacoite, 942  
 Guanine, 943  
 Gudmundite, 943  
 Gugiaite, 328  
 Guilleminite, 943  
 Guimaraesite, 466  
 Gunningite, 943  
 Gurimite, 944  
 Gwihabaite, 944  
 Gypsum, 944  
 Gyrolite, 944  
**H**  
 Hafnon, 945  
 Häggite, 212  
 Haidingerite, 945  
 Haiweeite, 945  
 Hakite, 945  
 Halite, 732, 946  
 Halloysite-10Å, 946  
 Halotrichite, 946  
 Hambergite, 946  
 Hanjiangite, 947  
 Hanksite, 947  
 Hannayite, 947  
 Hannebachite, 947  
 Hansesmarkite, 948  
 Haradaite, 269  
 Hardystonite, 246, 948  
 Harmotome, 948  
 Harmunite, 948  
 Harmunite cubic polymorph, 187  
 Harmunite Mn<sup>4+</sup>-bearing, 949  
 Hartite, 949  
 Hashemite, 949  
 Hatchetine, 949  
 Hatrurite triclinic polymorph, 239  
 Hatrurite, 950  
 Hauerite, 950  
 Hausmannite, 187, 950  
 Häyüne, 951  
 Hawleyite, 951  
 Hawthorneite, 951  
 Haynesite, 951  
 Hazenite, 952  
 Heazlewoodite, 952  
 Hectorite, 952  
 Hedenbergite, 952  
 Hedyphane, 953  
 Heisenbergite, 953  
 Heklaite, 236  
 Heliophyllite, 953  
 Hellyerite, 953  
 Hematite, 954  
 Hemihedrite, 954  
 Hemimorphite, 954  
 Hemleyite, 955  
 Hemusite, 955  
 Hendricksite, 955  
 Henmilite, 955  
 Henritermierite, 956  
 Henryite, 956  
 Herbertsmithite, 956  
 Hercynite, 956  
 Herderite, 957

- Herzenbergite, 957  
Hessite, 957  
Hetaerolite, 957  
Heterogenite, 958  
Heterosite, 958  
Heulandite, 958  
Hexaamminenickel(II) nitrate, 111  
Hexacelsian, 308, 958  
Hexaferrum, 959  
Hexahydrite, 959  
Hexahydroborite, 959  
Hiärneite, 959  
Hibonite, 960  
Hibonite-(Fe), 960  
Hidalgoite, 960  
Hieratite, 960  
Hilarionite, 961  
Hingganite-(Y), 326, 961  
Hinsdalite, 961  
Hiortdahlite, 961  
Hisingerite, 961  
Hochelagaite, 962  
Hoelite, 962  
Hoganite, 962  
Hogarthite, 962  
Hohmannite, 963  
Holdawayite, 963  
Holfertite, 963  
Hollandite, 963  
Hollingworthite, 964  
Holmquistite, 964  
Honessite, 964  
Hopeite, 964, 965  
Hörnesite, 965  
Hsianghualite, 965  
Huanghaiite-(Ce), 965  
Huanzalaite, 717, 966  
Hubeite, 966  
Hübnerite, 966  
Hughesite, 966  
Huizingite-(Al), 516  
Humberstonite, 967  
Humboldtine, 967  
Humite, 967, 968  
Hummerite, 968  
Hungchaoite, 968  
Huntite, 968  
Hureaulite, 969  
Hurlbutite, 969  
Hyalite, 223  
Hydrobiotite, 296  
Hydroboracite, 969  
Hydrocalumite, 222, 546, 969  
Hydrocerussite, 15–17, 970  
Hydrochamosite-1M, 299  
Hydrodelhayelite-related compound, 970  
Hydrogarnet  $\text{Sr}_3\text{Al}_2(\text{OH})_{12}$ , 164  
Hydrohalite, 553, 971  
Hydrohonesite, 971  
Hydrokenomicrolite, 188  
Hydromagnesite, 971  
Hydronaujakasite, 298  
Hydroniumjarosite, 971, 972  
Hydronium jarosite Pb,As-bearing, 512  
Hydronium jarosite Pb,Cu-bearing, 513  
Hydronium jarosite Pb,Zn-bearing, 514  
Hydromoromite, 216, 972  
Hydrotalcite, 972  
Hydrotalcite-2H, 972  
Hydroterskite, 343  
Hydrotungstate, 706, 973  
Hydrovesuvianite, 261  
Hydroxyapophyllite-(K), 973  
Hydroxycalciobetafite, 973  
Hydroxycalcimicrolite, 974  
Hydroxycalcipyrochlore, 974  
Hydroxycalcioroméite, 974  
Hydroxycancrinite (?), 301  
Hydroxyferroroméite, 974  
Hydroxykenoelsmoreite, 975  
Hydroxylapatite, 975  
Hydroxylbastnäsite-(Ce), 975  
Hydroxylchondrodite, 976  
Hydroxylclinohumite, 976  
Hydroxyle gedgewite, 976  
Hydroxylellstadite, 977  
Hydroxylgadolinite-(Y), 325  
Hydroxylgugiaite, 324  
Hydroxylherderite, 977  
Hydrozincite, 977  
Hydrucerussite-like mineral 9–40, 87  
Hypersthene, 978
- I**
- Ianbruceite, 978  
Iangreyite, 978  
Ice, 978  
Idaite, 979  
Idrialite, 979  
Ikaite, 95, 979  
Ilesite, 980  
Ilmenite, 980  
Ilsemannite, 189  
Ilvaite, 980  
Imogolite, 287, 980  
Inderite, 981  
Indite, 981  
Indium oxide, 143  
Indium vanadate selenite  $\text{In}(\text{VSe}_2\text{O}_8)$ , 644  
Indium vanadate tellurite  $\text{In}(\text{VTe}_2\text{O}_8)$ , 684  
Indium zinc selenite  $\text{In}_2\text{Zn}(\text{SeO}_3)_4$ , 645  
Inesite, 981  
Innsbruckite, 981  
Insizwaite, 982  
Inyoite, 982  
Iodargyrite, 982  
Iowaite, 983  
Iranite, 596, 983

- Irarsite, 983  
 Iriginitite, 984  
 Irinarassite, 984  
 Iron, 984  
 Iron(II) acid phosphate hydrate, 376  
 Iron(III) basic sulfate, 485, 486  
 Iron dimolybdate selenite hydrate  
 $\text{Fe}_2(\text{Mo}_2\text{O}_7)(\text{SeO}_3)_2 \cdot \text{H}_2\text{O}$ , 646  
 Iseite, 984  
 Ishikawaite, 224  
 Isocubanite, 985  
 Isokite, 985  
 Isomertieite, 985  
 Ivanyukite-Cs, 342  
 Ivsite, 507, 985  
 Iwakiite-hausmannite intermediate member, 189  
 Iwateite, 985  
 Iyoite, 986
- J**  
 Jáchymovite, 986  
 Jacobsite, 986  
 Jadeite, 986  
 Jakobssonite, 987  
 Jalpaite, 987  
 Jamborite, 987  
 Jamesonite, 987  
 Janchevite, 589  
 Jarosite, 988  
 Jeffbenite, 988  
 Jennite, 988  
 Ježekite, 989  
 Jianshuiite, 212  
 Jixianite, 989  
 Joaquinite-(Ce), 989  
 Joegoldsteinite, 508, 989  
 Joëlbruggerite, 990  
 Johachidolite, 990  
 Johannite, 990  
 Johnbaumite, 991  
 Johnbaumite Sr-analogue, 621  
 Johnnnesite, 991  
 Jordisite, 991  
 Jörgkellerite, 433  
 Joteite, 992  
 Jouravskite, 530  
 Juansilvaite, 638  
 Junitoite, 249  
 Jurbanite, 529
- K**  
 Kaatialaite, 622  
 Kaersutite, 992  
 Kainite, 992  
 Kalgoorlieite, 992  
 Kaliborate, 993  
 Kalicinite, 993  
 Kalininite, 508, 993  
 Kalinite, 993  
 Kaliophilite, 994  
 Kalsilite, 312, 994  
 Kamacite, 994  
 Kamarizaite, 628  
 Kamiokite, 679  
 Kamotoite-(Y), 994  
 Kampelite, 994  
 Kamphaugite-(Y), 995  
 Kanemite, 288  
 Kangite, 995  
 Kaňkite, 995  
 Kanoite, 996  
 Kaolinite, 2, 996  
 Kapellasite, 996  
 Kapundaite, 996  
 Karelianite, 997  
 Karpenkoite, 997  
 Karrooite, 997  
 Kashimite, 997  
 Kasolite, 998  
 Kassite, 998  
 Katayamalite, 998  
 Katerinopoulosite, 520  
 Katiersite, 622  
 Katoite, 998  
 Kawazulite, 999  
 Kazanskyite, 999  
 Keilite, 999  
 Keiviite-(Yb), 247, 1000  
 Kemmlitzite, 1000  
 Kempite, 1000  
 Kentbrooksite, 895  
 Kentrolite, 1000  
 Kenyaite, 1001  
 Kerimasite, 1001  
 Kermesite, 1001  
 Keyite, 1001  
 Khademite, 1002  
 Khatyrkite, 1002  
 Khesinite, 263, 1002  
 Khvorovite, 1002  
 Kiddcreekite, 1003  
 Kidwellite, 1003  
 Kieftite, 1003  
 Kieserite, 1003  
 Kilchoanite, 1003  
 Killalaite, 1004  
 Kimzeyite, 1004  
 Kinoite, 1004  
 Kinoshitalite, 1005  
 Kintoreite, 1005  
 Kipushite, 1005  
 Kirschsteinite, 241, 1005  
 Kladnoite, 1006  
 Klaprothite, 1006  
 Klebelsbergite, 1006  
 Klockmannite, 1006  
 Knorrtingite, 1007  
 Kobokoboite, 1007

- Koechlinite, 1007  
Kojonenite, 1007  
Kokchetavite, 1007  
Koktaite, 1008  
Kolskyite, 1008  
Kolwezite, 1008  
Konyaite, 1008  
Koritnigite, 1009  
Kornelite, 1009  
Kornerupine, 1009  
Kosmochlor, 1010  
Kosnarite NH<sub>4</sub>-analogue, 435  
Kosnarite NH<sub>4</sub>-analogue cubic polymorph, 435  
Kosnarite, 1010  
Kotoite, 1010  
Kottenheimite dimorph, 471  
Köttigite, 1010  
Kotulskite, 1011  
Kovdorskite, 1011  
Kozyrevskite, 1011  
Krásnoite, 437  
Kremersite, 1011  
Krieselite, 1012  
Kröhnikite, 1012  
KröhnikiteMn analogue, 508  
Krotite, 1012  
Krut'aite, 1012  
Kryzhanovskite, 1013  
Ktenasite, 523, 1013  
Kuksite, 1013  
Kuksite trigonal dimorph, 459  
Kuksite trigonal Mg analogue, 460  
Kulanite, 1013  
Kuliginite, 551  
Kullerudite, 1014  
Kumdykolite, 1014  
Kummerite, 436  
Kumtyubeite, 1014  
Kuramite, 1014  
Kuranakhite, 1015  
Kuratite, 1015  
Kurnakovite, 1015  
Kusachiite, 217, 1015  
Kushiroite, 1016  
Kutnohorite, 1016  
Kuzminite, 1016  
Kyanite, 1016  
Kyawthuite, 190, 1017
- L**  
Laachite, 733, 1017  
Lacroixite, 1017  
Lafossaitte, 1017  
Laihunite, 242, 1018  
Lakargiite, 1018  
Lamprophyllite, 1018  
Lanarkite, 1019  
Långbanite, 1019  
Langbeinite, 1019  
Langite, 1019  
Lanmchangite, 1020  
Lansfordite, 1020  
Lantanum nitrate hexahydrate, 112  
Lanthanite-(Nd), 1020  
Lanthanum aluminum oxide, 144  
Lanthanum calcium oxophosphate, 374  
Lanthanum iron(III) oxide, 144  
Lanthanum molybdate, 670  
Lanthanum orthoborate, 24  
Lanthanum orthosilicate, 238  
Lanthanum oxosulfate, 487  
Lanthanum selenite, 646, 647  
Lanthanum strontium oxophosphate, 375  
Lanthanum uranyl orthovanadate divanadate, 564  
Lapeyreite, 1020  
Larnite, 1021  
Laueite, 1021  
Laumontite, 1021  
Laurentianite, 1021  
Laurionite, 1022  
Laurionite Ba-analogue, 547  
Laurionite I-analogue, 703  
Laurite, 1022  
Lausenite, 1022  
Lautarite, 1023  
Lavendulan, 1023  
Lavenite Fe-analogue, 338  
Lavinskyite, 1023  
Lawrencite, 1023  
Lawsonite, 247, 1024  
Layered perovskite BaBi<sub>2</sub>Ta<sub>2</sub>O<sub>9</sub>, 191  
Layered perovskite CaBi<sub>2</sub>Ta<sub>2</sub>O<sub>9</sub>, 191  
Layered perovskite K<sub>4</sub>Xe<sub>3</sub>O<sub>12</sub>, 706  
Layered perovskite SrBi<sub>2</sub>Ta<sub>2</sub>O<sub>9</sub>, 192  
Lazaridisite, 524, 1024  
Lazulite, 1024  
Lazurite, 1024  
Lead, 1025  
Lead aluminium orthoborate fluoride Pb<sub>6</sub>Al(BO<sub>3</sub>)<sub>2</sub>OF<sub>7</sub>, 24  
Lead beryllium phosphate hurlbutite-type, 376  
Lead bismuth orthoborate, 25  
Lead borate Pb<sub>6</sub>B<sub>11</sub>O<sub>18</sub>(OH)<sub>9</sub>, 48  
Lead borate PbB<sub>4</sub>O<sub>7</sub>, 49  
Lead cadmium orthoborate, 26  
Lead copper orthoborate, 26  
Lead copper tellurate tellurite, 684  
Lead iron(III) phosphate, 377  
Lead iron(III) trivanadate, 564  
Lead orthoborate chromate, 591  
Lead orthoborate molybdate, 671  
Lead orthoborate tungstate, 27, 29  
Lead(II) oxalate, 100  
Lead(II) oxysulfate, 487  
Lead phosphate nitrate hydrate, 378  
Lead phosphate sulfate, 378  
Lead selenate, 643  
Lead silver phosphate apatite-type, 379  
Lead sodium calcium phosphate apatite-type, 380

- Lead(II) stannate  $Pb_2SnO_4$ , 145  
 Lead tin oxide  $Pb^{2+}_4Pb^{4+}Sn^{4+}O_8$ , 146  
 Lead uranyl divanadate, 565  
 Leadhillite, 533, 534, 1025  
 Lechatelierite, 1025  
 Lecoqite-(Y), 85  
 Leguernite, 1025  
 Leifite, 329  
 Leightonite, 1025  
 Leiteite, 1026  
 Lemanskite, 623, 624, 1026  
 Lemoynite, 1026  
 Leogangite, 1027  
 Leószilárdite, 1027  
 Lepidocrocite, 200, 1027  
 Lesukite Cu-bearing variety, 121  
 Letovicite, 1027  
 Leucite, 1028  
 Leucophosphite, 1028  
 Lévyne-Ca, 1028  
 Leydetite, 1028  
 Libethenite, 1029  
 Liebenbergite, 1029  
 Liebigite, 1029  
 Likasite, 1030  
 Lime, 1030  
 Linarite, 1030  
 Lindbergite, 1030, 1031  
 Lindgrenite, 1031  
 Lindsleyite, 1031  
 Línekite, 90  
 Lingunite, 1031  
 Lingunite K-analogue, 1031  
 Linnaeite, 1032  
 Linzhiite, 1032  
 Liroconite, 1032  
 Lishizhenite, 509  
 Liskeardite, 1032  
 Litharge, 1033  
 Lithiophilite, 1033  
 Lithiophorite, 1033  
 Lithiophosphate, 1033  
 Lithiotantite, 1034  
 Lithium aluminate  $LiAl_5O_8$ , 146  
 Lithium aluminate  $LiAlO_2$ -beta, 147  
 Lithium aluminate  $LiAlO_2$ -gamma, 148  
 Lithium aluminium orthoborate, 28  
 Lithium aluminium oxide-alpha, 148  
 Lithium aluminium oxide-gamma, 149  
 Lithium aluminoborate, 49  
 Lithium cesium borate  $Li_4Cs_3B_7O_{14}$ , 50  
 Lithium chromium pyrophosphate, 380  
 Lithium cobalt(III) iron(III) oxide delafossite-type, 149  
 Lithium copper tungstate, 712  
 Lithium cyclo-hexaphosphate trihydrate, 383  
 Lithium dimolybdate selenite, 672  
 Lithium ferrite  $LiFe^{3+}_5O_8$ , 150  
 Lithium hexafluorosilicate, 230  
 Lithium iron(III) oxide, 151  
 Lithiumiron(III) pyrophosphate, 381  
 Lithium iron(II) sulfate fluoride tavorite-type, 488  
 Lithium iron(III) tungstate wolframite-type, 711  
 Lithium magnesium manganese(IV) oxide spinel-type, 151  
 Lithium magnesium phosphate olivine-type, 382  
 Lithium manganese oxide spinel-type, 152  
 Lithium metasilicate, 265  
 Lithium molybdate tellurite, 672  
 Lithium nickel phosphate triphylite-type, 382  
 Lithium nickel tungstate, 713  
 Lithium nickel vanadate, 566  
 Lithium niobateilmenite-type, 153  
 Lithium sodium borate  $LiNaB_4O_7$ , 51  
 Lithium strontium borate  $Li_2Sr_4B_{12}O_{23}$ , 52  
 Lithium strontium orthoborate, 29  
 Lithium strontium orthophosphate, 384  
 Lithium tetraborate, 53  
 Lithium trivanadate, 566  
 Lithium tungstate tellurite, 685  
 Lithium tungstate vanadate brannerite-type, 567  
 Lithium vanadyl phosphate, 384–386  
 Lithium zinc niobium oxide spinel-type, 153  
 Lithium zinc phosphate monohydrate, 386  
 Lithium zinc selenite  $Li_2Zn_3(SeO_3)_4 \cdot 2H_2O$ , 648  
 Lithium zirconium arsenate, 604, 605  
 Liversidgeite, 1034  
 Livingstonite, 1034  
 Lizardite, 1034  
 Löllingite, 1035  
 Lomonosovite, 1035  
 Lonecreekite, 1035  
 Lonsdaleite, 1035  
 Lópezite, 1036  
 Lorándite, 1036  
 Lorenzenite, 1036  
 Löweite, 1036  
 Luanshiweiite, 284  
 Luddenite, 1037  
 Ludjibaite, 1037  
 Ludlamite, 1037  
 Ludlockite, 627, 1037  
 Ludwigite, 1038  
 Lueshite, 193, 1038  
 Luinaite-(OH), 334  
 Lulzacite, 453, 1038  
 Lüneburgite, 41, 1038  
 Luobusaite, 322  
 Luogufengite, 1039  
 Lusernaite-(Y), 1039
- M**  
 Macedonite, 1039  
 Mackayite, 1039  
 Mackinawite, 1040  
 Macquartite, 1040  
 Magadiite, 1040  
 Magbasite, 1040  
 Maghemite, 1041

- Magnesio-arfvedsonite, 1041  
Magnesioaubertite, 474  
Magnesiocanutite, 636  
Magnesiocarpholite, 734, 1041  
Magnesiochloritoid, 236, 1041  
Magnesiochromite, 1042  
Magnesiocopiapite, 509, 1042  
Magnesio-ferri-hornblende, 270  
Magnesioferrite, 1042  
Magnesio-foitite, 1042  
Magnesiohögbonite-2N3S, 122, 219  
Magnesiohögbonite-2N4S, 222, 1043  
Magnesio-hornblende, 1043  
Magnesiokoritnigite, 598  
Magnesiopascoite, 580  
Magnesiotaaffeite-2N'2S, 1043  
Magnesiotaaffeite-6N'3S, 1043  
Magnesiovesuvianite, 253  
Magnesiovoltaita, 480  
Magnesite, 1043  
Magnesium acid phosphate hydrate, 387  
Magnesium borophosphate, 365  
Magnesium chromate, 592  
Magnesium hydroxychlorite atacamite-type, 551  
Magnesium hydroxysulfate hydrate, 489  
Magnesium orthoborate fluoride, 30  
Magnesium oxychloride hydrate  $Mg_3Cl_2(OH)_4 \cdot 4H_2O$ , 541  
Magnesium strontium diorthoborate, 54  
Magnesium sulfate hydroxide  
     $Mg_6(SO_4)(OH)_{10} \cdot 7H_2O$ , 490  
Magnesium tellurite  $MgTe_2O_5$ , 686  
Magnesium vanadate  $Mg_7V_4O_{16}(OH)_2 \cdot H_2O$ , 568  
Magnetite, 1044  
Magnetoplumbite, 1044  
Majorite, 1044  
Makatite, 1044  
Malachite, 1045  
Malayaite, 1045  
Malladrite, 1045  
Mallardite, 1045  
Mallestigite, 1045  
Mandarinoite, 1046  
Manganese acid phosphate hydrate, 388  
Manganese(II) antimony(III) oxide, 154  
Manganese hydroxysulfate  $Mn_5(SO_4)(OH)_8$ , 489  
Manganese(II) titanium orthophosphate, 388  
Manganese(II) titanium phosphate  $MnTi_4(PO_4)_6$ , 389  
Mangangordonite, 457  
Manganite, 1046  
Manganlotharmeyerite, 1046  
Manganochromite, 1046  
Manganolangbeinite, 1047  
Manganosite, 1047  
Manitobaite, 354  
Manjiroite, 1047  
Marcasite, 1047  
Margarite, 289, 1047  
Margarosanite, 1048  
Marićite, 1048  
Markascherite, 1048  
Marokite, 1048  
Marthozite, 1048  
Martinandresite, 318  
Martyite, 735, 1049  
Maruyamaite, 1049  
Mascagnite, 1049  
Maskelynite, 1049  
Massicot, 1050  
Masuyite, 206  
Mathesiusite, 1050  
Mathiasite, 1050  
Matildite, 1050  
Matioliite, 1051  
Matlockite, 1051  
Mattagamite, 1051  
Matteuccite, 1051  
Maxwellite, 1051  
Mazzite-Na, 317  
Mbobomkulite, 1052  
Mcallisterite, 1052  
Mcalpineite, 1052  
Mcconnellite, 1052  
Mcguinnessite, 1053  
Megawite, 1053  
Meisserite, 1053  
Meixnerite, 1053  
Melanarsite, 738, 739, 1054  
Melanophlogite, 5–11, 1054  
Melaanterite, 1054  
Meliphanite, 1054  
Mellite, 1054  
Mellizinkalite, 1055  
Mendeleevite-(Nd), 322  
Mendipite, 1055  
Mercallite, 510, 1055  
Mercury(I) acid phosphate, 390  
Mercury(I) orthoarsenate, 605  
Mercury(II) orthoarsenate, 606  
Merelaniite, 1055  
Merenskyite, 1056  
Meridianiite, 1056  
Merlinoite, 314  
Merrillite, 1056  
Merrillite Na-free analogue, 1056  
Merwinite, 1056  
Mesolite, 1057  
Meta-ankoleite, 1057  
Meta-autunite, 1057  
Metacinnabar, 1057  
Metahewettite, 1058  
Metakirchheimerite, 1058  
Metalodèvite, 1058  
Metamunirite, 1058  
Metarauchite, 1058  
Metarossite, 1059  
Metasideronatrite, 476  
Metastibnite, 1059  
Metastudtite, 193, 1059

- Metathénardite, 479, 1059  
 Metatorbernite, 1060  
 Metatyuyamunite, 1060  
 Metauranocircite-I, 1060  
 Metauranospinite, 1060  
 Metavariscite, 1061  
 Metavivianite, 1061  
 Metazeunerite, 1061  
 Meurigite-Na, 1061  
 Meyerhofferite, 1062  
 Meymacite monoclinic analogue, 1062  
 Miargyrite, 1062  
 Microcline, 724, 1062  
 Miersite, 1062  
 Mikasaite, 1063  
 Milarite, 1063  
 Millerite, 1063  
 Millosevichite, 1063  
 Mimetite, 1064  
 Minguzzite, 1064  
 Minium, 194, 1064  
 Minjiangite, 360, 438, 469  
 Minnesotaite, 1064  
 Minyulite, 352, 1064  
 Mirabilite, 1065  
 Misakiite, 1065  
 Mitscherlichite, 1065  
 Mixite, 1065  
 Moctezumite, 1066  
 Mogánite, 1066  
 Mohite, 1066  
 Mohrite, 1066  
 Moissanite, 1066  
 Mojaveite, 1067  
 Molybdenite, 1067  
 Molybdite, 1067  
 Molybdoornacite, 1067  
 Molybdophyllite, 14, 15, 1068  
 Molybdyl phosphate, 390  
 Molysite, 1068  
 Monazite-(Ce), 1068  
 Monazite-(La), 1068  
 Monazite-(Nd), 1068  
 Monazite-(Sm), 1069  
 Moncheite, 1069  
 Monetite, 1069  
 Monipite, 1069  
 Monohydrocalcite, 1070  
 Montebrasite, 1070  
 Monteponite, 1070  
 Montgomeryite, 1070  
 Monticellite, 1070  
 Montmorillonite, 296, 1071  
 Montroseite, 1071  
 Montroydite, 217, 1071  
 Moolooite, 1071  
 Mopungite, 195, 1072  
 Moraskoite, 1072  
 Mordenite, 1072  
 Morenosite, 1072  
 Morimotoite, 237  
 Moschelite, 1073  
 Mosesite, 1073  
 Mottramite, 1073  
 Motukoreite-related mineral, 533  
 Mountkeithite, 1073  
 Moydite-(Y), 1073  
 Mukhinite, 1074  
 Mukhinite V-rich analogue, 1074  
 Mullite, 1074  
 Muscovite, 734, 1074  
 Mushistonite, 213
- N**
- Nabiasite, 1075  
 Nabimusite, 1075  
 Nacrite, 1075  
 Nadorite, 1075  
 Nafertisite, 1076  
 Nagelschmidtite, 1076  
 Nahcolite, 1076  
 Nahpoite, 1076  
 Nakaurite, 92, 93  
 Nalipoite, 451  
 Namibite, 1077  
 Nantokite, 1077  
 Naquite, 1077  
 Narsarsukite, 1077  
 Nasonite, 245  
 Natalyite, 1077  
 Natisite, 1078  
 Natrite, 1078  
 Natroalunite, 1078  
 Natrochalcite, 1078  
 Natrodufrénite, 351, 1079  
 Natrojarosite, 1079  
 Natrolemoynite, 1079  
 Natrolite, 1079  
 Natron, 1080  
 Natroniobite, 1080  
 Natropalermoite, 1080  
 Natrophilite, 461, 1080  
 Natrosilite, 1081  
 Natrouranospinite, 1081  
 Natroxalate, 1081  
 Natrozippeite, 1081  
 Naumannite, 1082  
 Nealite, 1082  
 Negevite, 1082  
 Neighborite, 1082  
 Nekoite, 1082  
 Nenadkevichite, 1083  
 Nepheline, 1083  
 Neptuniump(IV) oxalate hexahydrate, 101  
 Nesquehonite, 1083  
 Nestolaite, 1083  
 Newberryite, 1084  
 Nežilovite, 1084

- Nichromite, 195  
Nickel antimonate fluoride, 231  
Nickelaustinite, 1084  
Nickelbischofite, 1084  
Nickelboussingaultite, 1085  
Nickelhexahydrite, 1085  
Nickel hydroxychlorite atacamite-type, 552  
Nickel hydroxysulfate hydrate  
     $\text{Ni}_3(\text{SO}_4)_2(\text{OH})_2 \cdot 2\text{H}_2\text{O}$ , 491  
Nickeline, 1085  
Nickel manganese(IV) oxide, 155  
Nickel oxychloride hydrate  $\text{Ni}_3\text{Cl}_{2.1}(\text{OH})_{3.9} \cdot 4\text{H}_2\text{O}$ , 542  
Nickelpicromerite, 1085  
Nickel vanadyl phosphate hydrate, 391  
Nickenichite, 635  
Nierite hexagonal polyborph, 1086  
Nierite, 113  
Nifontovite, 1086  
Nomite, 1086  
Niningerite, 1086  
Niobium sulfide  $\text{NbS}_3$ , 491  
Nioboholtite, 1086  
Niobylphosphate, 392  
Niter, 1087  
Nitratine, 114, 1087  
Nitrobarite, 1087  
Nitrocalcite, 1087  
Nitromagnesite, 1088  
Nobleite, 1088  
Noelbensonite, 1088  
Nolanite, 1088  
Nolzeite, 331  
Nontronite, 1088  
Norbergite, 1089  
Nordenskiöldine, 1089  
Nordstrandite, 1089  
Normandite, 1089  
Norsethite, 1090  
Northupite, 1090  
Nosean, 1090  
Nováčekite-II, 1090  
Novgorodovaite, 1091  
Nsutite, 1091  
Nullaginite, 1091  
Nyerereite, 1091
- O**  
Offretite, 1092  
Okenite, 1092  
Okhotskite, 254  
Oldhamite, 1092  
Olgite, 1092  
Olivenite, 1093  
Olivine P-rich variety, 1093  
Olmiite, 1093  
Olshanskyite, 1093  
Omongwaite, 1094  
Omphacite, 1094  
Onoratoite, 1094
- Opal-A, 1094  
Opal-CT, 1094  
Ophirite, 1095  
Oppenheimerite, 1095  
Ordoñezite, 1095  
Orlandiite, 663  
Orpiment, 1095  
Orschallite, 1096  
Orthobrannerite, 214  
Orthoclase, 1096  
Orthojoaquinite-(Ce), 1096  
Osakaite, 521, 1096  
Osbornite, 114, 1097  
Oskarssonite, 1097  
Osumilite, 1097  
Otavite, 1097  
Ottemannite, 1098  
Ottensite, 1098  
Ottohahnite, 1098  
Otwayite, 1098  
Oxammite, 1099  
Oxo-magnesio-hastingsite, 276  
Oxybetafite-(Gd), 196  
Oxybetafite-(Sm), 196  
Oxybismuthobetafite, 197  
Oxybritholite thorium analogue, 243  
Oxycalcioroméite, 1099  
Oxy-dravite, 1099  
Oxykinoshitalite, 1099  
Oxynatromicrolite, 1100  
Oxyplumbboroméite, 1100  
Oxypyromorphite, 439  
Oyelite, 1100  
Ozokerite, 1100
- P**  
Pabstite, 280, 1100  
Padmaite, 1101  
Paganosite phosphate analogue, 461  
Pakhomovskyite, 1101  
Palermoite, 1101  
Palladinite, 1101  
Palladosilicide, 1102  
Palygorskite, 1102  
Panguite, 1102  
Panichiite, 1102  
Papagoite, 1102  
Parabutlerite, 477, 1103  
Paracquimbite, 1103  
Paragonite, 1103  
Paraguanajuatite, 1103  
Parahopeite, 1104  
Paramelaconite, 197  
Paramontroseite, 1104  
Paranatrolite, 1104  
Paraotwayite, 1104  
Parapierrrotite, 1105  
Pararealgar, 1105  
Pararobertsite, 1105

- Parascholzite, 1105  
 Parascorodite, 1105  
 Parasibirske, 1106  
 Parasymplesite, 1106  
 Paratacamite, 1106  
 Paratellurite, 1107  
 Paratooite-(La), 94, 1107  
 Paravauxite, 1107  
 Pargasite, 1107  
 Parisite-(Ce), 79, 1108  
 Parisite-(La), 78, 1108  
 Parnauite, 1108  
 Parsonsite, 1108  
 Parthéite, 1109  
 Partzite, 1109  
 Pašavaite, 1109  
 Pascoite, 1110  
 Patrónite, 1110  
 Pattersonite, 1110  
 Pauflerite, 1110  
 Pauflerite tetragonal dimorph, 517  
 Pauladamsite, 519  
 Paulingite-K, 1111  
 Paulmooreite, 1111  
 Pauloabibite, 1111  
 Paulscherrerite, 1111  
 Pavlovskyite, 1112  
 Pearlite, 323  
 Peatite-(Y), 1112  
 Pecoraite, 1112  
 Pectolite, 1112  
 Peisleyite, 1113  
 Pélidotite, 1113  
 Penberthycroftite, 624  
 Penkisite, 453  
 Penkvilksite- $2O$ , 1113  
 Penroseite, 1113  
 Pentagonite, 1114  
 Pentahydrite, 1114  
 Pentahydroborite, 1114  
 Pentlandite, 1114  
 Peretaite, 1115  
 Perhamite, 1115  
 Perite, 1115  
 Permingeatite, 1115  
 Perovskite, 1116  
 Pertsevite-(OH), 1116  
 Petalite, 1116  
 Petersite-(Ce), 1116  
 Petewilliamsite-related Cd diarsenate, 625  
 Petitjeanite, 455, 1117  
 Petrukite, 1117  
 Petterdite, 1117  
 Petzite, 1117  
 Pezzottaite, 1117  
 Pharmacolite, 1118  
 Pharmacosiderite, 1118  
 Pharmazincite, 1118  
 Phenakite, 1118  
 Philipsbornite, 1119  
 Philipsburgite, 1119  
 Phillipsite-K, 1119  
 Phillipsite-NH<sub>4</sub>, 315  
 Philolithite, 1119  
 Phlogopite, 734, 1120  
 Phoenicochroite, 1120  
 Phosgenite, 1120  
 Phosphammite, 1120  
 Phosphohedyphane, 1121  
 Phosphophyllite, 1121  
 Phosphorrösslerite, 462  
 Phosphosiderite, 1121  
 Phosphuranylite, 1121  
 Phurcalite, 1122  
 Pickeringite, 1122  
 Picromerite, 1122  
 Picromerite dimorph (?), 512  
 Picropharmacolite, 1122  
 Pieczkaite, 1123  
 Piemontite, 1123  
 Pigeonite, 1123  
 Pilawite-(Y), 240  
 Pilsenite, 1123, 1124  
 Pimelite, 1124  
 Pinakiolite, 1124  
 Pingguite, 696  
 Pinnoite, 1124  
 Pirssonite, 1125  
 Pittcrite, 1125  
 Plancheite, 1125  
 Plášilit, 511, 1125  
 Platarsite, 1126  
 Platinum, 1126  
 Plattnerite, 1126  
 Plavnoite, 1126  
 Plimerite, 1127  
 Plombièreite, 1127  
 Plumbogummite, 1127  
 Plumbojarosite, 1127  
 Plumbophyllite, 289, 1128  
 Plumbotellurite, 698  
 Plumbotsumite, 1128  
 Poitevinite, 1128  
 Pokrovskite, 1128  
 Poldervaartite, 1129  
 Pollucite, 1129  
 Polyakovite-(Ce), 336  
 Polycrase-(Y), 1129  
 Polydymite, 1129  
 Polyhalite, 1130  
 Popovite, 1130  
 Portlandite, 1130  
 Posnjakite, 1130  
 Potarite, 1131  
 Potassic-ferri-leakeite, 275  
 Potassic-ferro-pargasite, 276  
 Potassic-magnesio-fluoro-arfvedsonite, 273  
 Potassium acid phosphate, 394

- Potassium acid pyrophosphate hydrate, 394  
Potassium acid selenite, 648  
Potassium acid tellurate hydrate  
     $K_2[TeO_2(OH)_4] \cdot 3H_2O$ , 686  
Potassium aluminium molybdate, 673  
Potassium antimonate tungstate, 713  
Potassium antimony fluoride, 231  
Potassium antimony oxoarsenate, 607  
Potassium antimony oxophosphate, 396  
Potassium antimony(V) oxophosphate, 395  
Potassium arsenate tungstate  $K(As_2O_9)$ , 714  
Potassium barium borate  $KBaB_5O_9$ , 54  
Potassium bismuth(III) phosphate, 396  
Potassium bismuth(III) tungstate, 715  
Potassium borate  $KB_3O_3(OH)_4 \cdot H_2O$ , 73  
Potassium borate  $KB_3O_5 \cdot H_2O$ , 55  
Potassium borosilicate pollucite-type, 330  
Potassium borosulfate  $K_5[B(SO_4)_4]$ , 492  
Potassium calcium orthoborate, 31  
Potassium chloride borate perovskite-related  
     $K_3B_6O_{10}Cl$ , 56  
Potassium chromium divanadate, 568, 569  
Potassium decavanadate decahydrate, 570  
Potassium difluorophosphate, 397  
Potassium diuranate, 155  
Potassium hexavanadate hydrate, 570  
Potassium hydronium uranyl selenate hydrate, 649  
Potassium iron diarsenate (pyroarsenate), 608  
Potassium iron pyrophosphate, 398  
Potassium lead borophosphate, 398  
Potassium lead carbonate fluoride, 81  
Potassium lead phosphate, 399  
Potassium magnesium acid phosphate hydrate, 400  
Potassium magnesium acid pyrophosphate hydrate, 400  
Potassium magnesium arsenate hexahydrate, 608  
Potassium magnesium chromate hydrate, 592  
Potassium magnesium orthoborate, 31  
Potassium magnesium orthophosphate  $KMg_4(PO_4)_3$ , 401  
Potassium magnesium yttrium phosphate  
    (xenotime-type), 402  
Potassium manganese arsenate, 609  
Potassium manganese(III) fluoride, 232  
Potassium mercury chloride hydrate, 543  
Potassium monofluorophosphate, 402  
Potassium nickel chromate hydrate, 593  
Potassium niobate, 156  
Potassium niobate  $KNb_7O_{18}$ , 157  
Potassium niobate perovskite-type, 157  
Potassium niobium tungstate, 158  
Potassium niobium oxophosphate, 403  
Potassium pentaborate, 56  
Potassium peroxochromate, 593  
Potassium sodium iron arsenate  
     $Na_{2.77}K_{1.52}Fe_{2.57}(AsO_4)_4$ , 610  
Potassium sodium selenite, 650  
Potassium sodium vanadyl sulfate, 493  
Potassium sodium zinc borate  $K_2NaZnB_5O_{10}$ , 57  
Potassium strontium orthoborate, 32  
Potassium tantalate tungstate, 159  
Potassium tantalite perovskite-type, 159  
Potassium tin orthophosphate, 404  
Potassium titanium iodate, 701  
Potassium titanium oxophosphate, 404  
Potassium titanium silicate  $K_2TiSi_3O_9 \cdot H_2O$ , 338  
Potassium triborate, 58  
Potassium uranium(V) sorosilicate, 349  
Potassium uranyl fluoride, 232  
Potassium urinate, 160  
Potassiumvanadyl phosphate, 405  
Potassium ytterbium acid orthoborate acid  
    orthophosphate, 406  
Potassium ytterbium tungstate, 715  
Potassium yttrium selenite, 650  
Potassium zinc acid pyrophosphate hydrate, 406  
Potassium zinc cyclotriphosphate benitoite-type, 407  
Potassium zinc hydrogen phosphate, 463  
Potassium zinc selenite  $K_2Zn_3(SeO_3)_4$ , 651  
Potassium zinc sulfate chloride trihydrate, 493  
Potassium zinc sulfate hexahydrate, 494  
Potassium zirconium arsenate, 610  
Pottsite, 1131  
Poubaite, 1131  
Poudretteite, 1131  
Poughite, 697, 1131  
Povondraite, 1132  
Powellite, 1132  
Praseodymium chromate(V), 594  
Praseodymium cyclotriphosphatetrihydrate, 408  
Prehnite, 1132  
Preiswerkite, 1132  
Preutelite, 1133  
Příbramite, 1133  
Priceite, 76, 1133  
Priderite Al-analogue, 1133  
Priderite Cr-analogue, 1134  
Priderite Mg-analogue, 1133  
Prismatine, 1134  
Probertite, 76  
Proshchenkoite-(Y), 332  
Protoimogolite, 290  
Proustite, 1134  
Pseudoboleite, 1134  
Pseudobrookite, 1135  
Pseudocotunnite, 1135  
Pseudojohannite, 1135  
Pseudolaueite, 1135  
Pseudomalachite, 1136  
Pseudowollastonite, 1136  
Pucherite, 585, 1136  
Pumpellyite-(Al), 1136  
Pyracmonite, 525  
Pyrargyrite, 1137  
Pyrite, 1137  
Pyroaurite, 1137  
Pyrochroite, 214, 1137  
Pyrolusite, 1138  
Pyromorphite As-rich, 1138  
Pyromorphite, 1138

- Pyrope, 1139  
 Pyrophanite, 198, 1139  
 Pyrophyllite, 291, 1139  
 Pyrosmalite-(Fe), 1139  
 Pyrosmalite-(Mn), 1139  
 Pyroxmangite, 1140  
 Pyrrhotite, 1140
- Q**
- Qandilite, 1140  
 Qingheite, 1140  
 Qingsongite, 1141  
 Qingsongite (C-bearing), 115, 116  
 Quadridavyne, 1141  
 Quartz, 1141  
 Quenstedtite, 1141  
 Quetzalcoatlite, 1141  
 Quintinite, 1142  
 Quintinite-related hydroxyde carbonate  
      $Mg_4Cr_2(OH)_{12}(CO_3)\cdot nH_2O$ , 87  
 Quintinite-related hydroxyde carbonate  
      $Ni_4Cr_2(OH)_{12}(CO_3)\cdot nH_2O$ , 88
- R**
- Raadeite, 463  
 Rabejacite, 1142  
 Raguinite, 1142  
 Rajite, 1143  
 Ramanite-(Cs), 1143  
 Ramanite-(Rb), 1143  
 Rambergite, 1143  
 Rameautite, 1144  
 Ramikite-(Y), 1144  
 Ramsdellite, 1144  
 Ranciéite, 1144  
 Rankamaite, 1145  
 Rankinite, 1145  
 Rapidcreekite, 1145  
 Raspite, 1145  
 Rasvumite, 1146  
 Ravatite, 1146  
 Raygrantite, 1146  
 Realgar, 1146  
 Rebulite, 1147  
 Reedmergnerite, 1147  
 Reevesite, 1147  
 Refikite, 107  
 Reichenbachite, 1147  
 Reinerite, 1148  
 Reinhardbraunsite, 1148  
 Rengeite, 1148  
 Reppiaite, 582  
 Retgersite, 1148  
 Reyerite, 1148  
 Rhabdophane-(Ce), 1149  
 Rhabdophane-(Nd), 1149  
 Rheniite, 1149  
 Rhodium sulfate, 525
- Rhodium sulfate hydrate, 526  
 Rhodizite, 1149  
 Rhodochrosite, 1150  
 Rhodonite, 1150  
 Rhomboclase, 473, 1150  
 Rhönite, 1150  
 Richelsdorffite, 1151  
 Richterite, 1151  
 Riebeckite, 1151  
 Riebeckite (Crocidolite), 1151  
 Rimkorolgit, 1152  
 Ringwoodite, 1152  
 Rinkite, 1152  
 Riomarinaita, 1152  
 Riotintoite, 472  
 Rippite, 282  
 Robertsite, 1152  
 Robinsonite, 1153  
 Rockbridgeite, 444, 1153  
 Rodalquilarite, 1153  
 Rodolicoite, 1153  
 Roedderite Na-free analogue, 284  
 Rokühnrite, 1154  
 Romanéchite, 1154  
 Romanorlovite, 737, 1154  
 Romarchite, 218, 1154  
 Römerite, 475, 1155  
 Rondorfite, 1155  
 Rongibbsite, 319, 1155  
 Ronneburgite, 587, 1155  
 Rooseveltite, 1156  
 Roquesite, 1156  
 Rosasite, 1156  
 Roscherite, 467  
 Roselite, 1156  
 Rosiaite, 1157  
 Rostite, 1157  
 Rouaite, 1157  
 Roumaite, 1157  
 Rowlandite-like mineral, 249  
 Rowleyite, 1158  
 Roxbyite, 1158  
 Roymillerite, 97  
 Rozenite, 1158  
 Rruffite, 1158  
 Rubicline, 308  
 Rubidium beryllium sulfate hydrate, 495  
 Rubidium iron(III) pyrophosphate, 408  
 Rubidium vanadyl phosphate, 409  
 Rucklidgeite, 1159  
 Rudashevskyite, 1159  
 Ruizite, 1159  
 Rusinovite, 1159  
 Russellite, 1159  
 Rustumite, 1160  
 Rutherfordine, 1160  
 Rutile, 198, 1160  
 Rynersonite, 1160

**S**

- Sabugalite, 1161  
Sahlinite, 1161  
Sailaufite, 1161  
Sakhaite, 1161  
Salammoniac, 1162  
Saléeite, 1162  
Samarium metaphosphate, 410  
Samarium orthoborate, 33  
Samarium oxalate decahydrate, 102  
Samarskite-(Y), 208, 225, 1162  
Samarskite-(Yb), 208  
Sampleite, 1162  
Sanderite  $\text{Fe}^{2+}$  analogue, 526  
Sanderite, 1162  
Sanguite, 553, 1163  
Sanidine, 1163  
Sanjuanite, 1163  
Sanmartinite, 718, 1163  
Santabarbaraite, 1164  
Santarosite, 1164  
Santite, 1164  
Saponite, 1164  
Sapphirine, 323  
Sarcopside, 1165  
Sarkinite, 1165  
Sarmientite, 1165  
Sartorite, 1165  
Sassolite, 1166  
Satimolite, 75  
Sborgite, 73  
Scacchite, 1166  
Scandium arsenate monohydrate, 611  
Scandium lanthanum orthoborate, 33  
Scandium vanadate tellurite, 687  
Scandium vanadyl selenite, 652  
Scarbroite, 89  
Schafarzikite, 1166  
Schäferite, 555  
Schäferite Ni analogue, 584  
Schairerite, 527  
Scheelite, 1166  
Schiavinatoite, 1166  
Schlossmacherite, 1167  
Schmiederite, 1167  
Schmitterite, 1167  
Schneiderhöhnlite, 1167  
Schoenfliesite, 199, 1168  
Schoepite, 1168  
Scholzite, 1168  
Schorl, 1168  
Schorlomite, 1169  
Schreibersite, 1169  
Schreyerite, 1169  
Schröckingerite, 1169  
Schuetteite, 1170  
Schülerite-type mineral, 343  
Schultenite, 1170  
Schumacherite, 1170  
Schwartzembergite, 537  
Schwertmannite, 1170  
Scolecite, 1170  
Scorodite, 1171  
Scotlandite, 1171  
Scottyite, 248, 1171  
Scrutinyite, 1171  
Sederholmite, 1172  
Segnitite, 1172  
Seinäjokite, 1172  
Sejkoraite-(Y), 1172  
Sekaninaite, 1173  
Selenium, 1173  
Seligmannite, 1173  
Sellaite, 1173  
Sénarmontite, 1174  
Senegalite, 1174  
Sepiolite, 1174  
Sérandite, 1174  
Serendibite, 1175  
Serpierite, 1175  
Shannonite, 96  
Shattuckite, 1175  
Shcherbinaita, 1175  
Shchurovskyite, 1176  
Shortite, 1176  
Shuangfengite, 1176  
Shulamitite, 1176  
Shumwayite, 514  
Siderite, 1176  
Sideronatriite, 1177  
Sidorenkite, 1177  
Sidwillite, 1177  
Siegenite, 1177  
Sigloite, 1178  
Siidraite, 1178  
Silicocarnotite, 1178  
Silicon, 8, 1179  
Silinaite, 291  
Sillénite, 1179  
Sillimanite, 1179  
Silver indium sulfide  $\text{AgIn}_5\text{S}_8$ , 495  
Silver iron(III) pyrophosphate, 410  
Silver tantalum sulfide, 496  
Simojovelite, 108  
Simonkolleite, 547, 548, 1179  
Sinhalaite, 72, 1179  
Sinjarite, 1180  
Sinoite, 116, 1180  
Skinnerite, 1180  
Skippenite, 1180  
Sklodowskite, 1181  
Skorpionite, 1181  
Smirnite, 1181  
Smirnovskite, 440  
Smithite, 1181  
Smithsonite, 1182  
Smythite, 1182  
Sobolevskite, 1182

- Sodalite, 1182  
 Sodalite Ca-Al-Mo-analogue, 120  
 Sodalite Ca-Al-Mo-W-analogue, 119  
 Sodalite Ca-Al-Mo-W-analogue, 120  
 Sodalite nitrite analogue, 309  
 Soddyite, 1182  
 Sodium acid diarsenite tellurite, 688  
 Sodium acid pyrophosphate hydrate, 411  
 Sodium acid selenite, 653  
 Sodium acid tellurate  $\text{Na}_2[\text{TeO}_2(\text{OH})_4]$ , 688  
 Sodium aluminium molybdate, 674  
 Sodium aluminum borate  $\text{Na}_2\text{Al}_2\text{B}_2\text{O}_7$ , 58  
 Sodium barium borate  $\text{NaBaB}_5\text{O}_9$ , 59  
 Sodium bismuth molybdate scheelite-type, 674  
 Sodium borate  $\text{Na}_2\text{B}_5\text{O}_8(\text{OH})\cdot 2\text{H}_2\text{O}$ , 60  
 Sodium borophosphate  $\text{Na}_5(\text{B}_2\text{P}_3\text{O}_{13})$ , 60  
 Sodium borosulfate  $\text{Na}_5[\text{B}(\text{SO}_4)_4]$ , 61  
 Sodium cadmium selenate hydrate, 654  
 Sodium cadmium sulfate hydrate, 497  
 Sodium calcium orthoborate, 34, 35  
 Sodium calcium pentaborate  $\text{Na}_3\text{Ca}(\text{B}_5\text{O}_{10})$ , 62  
 Sodium calcium silicophosphate  $\text{Na}_2\text{Ca}_4(\text{PO}_4)_2\text{SiO}_4$   
     (apatite-type), 457  
 Sodium diuranate, 161  
 Sodium gadolinium oxophosphate, 412  
 Sodium indium arsenate (alluaudite-type), 612  
 Sodium iron(II) iron(III) phosphate alluaudite-type, 412  
 Sodium iron(II) pyrophosphate, 413  
 Sodium iron(III) pyrophosphate, 414  
 Sodium iron(III) tin orthophosphate, 441  
 Sodium lanthanum orthoborate, 35  
 Sodium lanthanum pyrophosphate, 414  
 Sodium lead neodymium arsenate chloride  
     (apatite-type), 613  
 Sodium lithium aluminosilicate  $\text{Na}_3\text{Li}_2(\text{AlSi}_2\text{O}_8)$ , 285  
 Sodium lithium gadolinium carbonate  $\text{Na}_2\text{LiGd}(\text{CO}_3)_3$ , 82  
 Sodium lithium selenate hydrate, 654  
 Sodium magnesium orthophosphate pyrophosphate  
      $\text{Na}_4\text{Mg}_3(\text{PO}_4)_2(\text{P}_2\text{O}_7)$ , 415  
 Sodium magnesium pentaborate  $\text{Na}_3\text{MgB}_5\text{O}_{10}$ , 63  
 Sodium manganese(II) iron(III) phosphate  
     alluaudite-type, 416  
 Sodium manganese(II) sulfate alluaudite-type, 497  
 Sodium molybdenum(VI) tellurite, 689  
 Sodium nickel iron(III) arsenate, 613  
 Sodium niobium oxophosphate, 416  
 Sodium samarium orthoborate, 36  
 Sodium scandium carbonate  $\text{Na}_5\text{Sc}(\text{CO}_3)_3\cdot 2\text{H}_2\text{O}$ , 83  
 Sodium stannate, 161  
 Sodium strontium aluminum borate  $\text{NaSr}_7\text{AlB}_{18}\text{O}_{36}$ , 64  
 Sodium strontium orthoborate, 37  
 Sodium tantalite perovskite-type, 162  
 Sodium tellurite tellurite hydrate  $\text{Na}_2\text{Te}_2\text{O}_6\cdot 1.5\text{H}_2\text{O}$ , 690  
 Sodium tellurite  $\beta\text{-Na}_2\text{Te}_4\text{O}_9$ , 690  
 Sodium thioborate  $\text{Na}_3\text{B}_3\text{S}_6$ , 498  
 Sodium thioborate  $\text{Na}_3\text{BS}_3$ , 499  
 Sodium tin orthophosphate, 417  
 Sodium tin phosphate, 442  
 Sodium titanate  $\text{Na}_2\text{Ti}_3\text{O}_7$ , 200  
 Sodium titanate  $\text{Na}_2\text{Ti}_6\text{O}_{13}$ , 207  
 Sodium titanium iodate, 702  
 Sodium titanium phosphate, 445  
 Sodium titanium silicate  $\text{Na}_2\text{TiSi}_2\text{O}_7\cdot 2\text{H}_2\text{O}$ , 339  
 Sodium tungsten tellurite, 691  
 Sodium uranate, 163  
 Sodium vanadyl borate  $\text{Na}_3(\text{VO}_2)\text{B}_6\text{O}_{11}$ , 64  
 Sodium vanadyl phosphate  $\text{Na}(\text{VO})\text{PO}_4$ , 418  
 Sodium vanadyl phosphate  $\text{Na}_2(\text{VO}_2)(\text{PO}_4)$ , 418  
 Sodium yttrium selenite, 655  
 Sodium yttrium tellurate borate  $\text{Na}_2\text{Y}_2(\text{Te}^{6+}\text{B}_2\text{O}_{10})$ , 65  
 Sodium yttrium titanate, 163  
 Sodium zinc orthophosphate, 419  
 Sodium zinc pentaborate  $\text{Na}_3\text{ZnB}_5\text{O}_{10}$ , 66  
 Sodium zinc pyrophosphate, 420  
 Sodium zinc selenite  $\text{Na}_2\text{Zn}_3(\text{SeO}_3)_4\cdot 2\text{H}_2\text{O}$ , 656  
 Sodium zirconium arsenate, 614, 615  
 Söhngeite, 1183  
 Somersetite, 86  
 Sonolite, 1183  
 Sonoraite, 1183  
 Spangolite, 1183  
 Spencerite, 1184  
 Sperrylite, 1184  
 Spertiniite, 201, 1184  
 Spessartine, 1184  
 Spessartine Ca-rich, 241  
 Sphaerobertrandite, 324  
 Sphaerobismoite, 202  
 Sphalerite, 1184  
 Spherocobaltite, 1185  
 Spinel, 1185  
 Spionkopite, 1185  
 Spiroffite, 1185  
 Spodumene, 1186  
 Spurrite, 1186  
 Šreinite, 1186  
 Srilankite, 1186  
 Stanfieldite, 1186  
 Stanleyite, 1187  
 Stannite, 1187  
 Starkeyite, 1187  
 Starovaite, 1187  
 Staurolite, 1188  
 Steedeite, 1188  
 Steenstrupine-(Ce), 1188  
 Stepanovite, 108  
 Stephanite, 522, 1188  
 Štěpite, 1189  
 Stercorite, 1189  
 Steropesite, 1189  
 Stetindite, 1189  
 Stevensite, 293  
 Stibarsen, 1189  
 Stibiconite, 1190  
 Stibioclaudetite, 1190  
 Stibiocolumbite, 1190  
 Stibiopalladinite, 1190  
 Stibnite, 1191

- Stichtite, 79, 1191  
Stilbite-Ca, 1191  
Stilbite-Na, 1191  
Stilleite, 1192  
Stilpnomelane, 1192  
Stishovite, 1192  
Stoiberite, 1192  
Stolzite, 1192  
Stoppaniite, 1193  
Stottite, 1193  
Strashimirite, 1193  
Strengite, 1193  
Stringhamite, 1194  
Stromeyerite, 1194  
Stronadelphite, 1194  
Strontianite, 1194  
Strontiofluorite, 1194  
Strontiohurlbutite, 445, 1195  
Strontiojoaquinite, 1195  
Strontium aluminum hydroxide, 164  
Strontium bismuth(III) selenite hydrate, 656  
Strontium borate chloride  $\text{Sr}_2\text{B}_5\text{O}_9\text{Cl}$ , 67  
Strontium borate  $\text{SrB}_2\text{O}_4$ , 67  
Strontium borate  $\text{SrB}_8\text{O}_{13}$ , 68  
Strontium boroarsenate  $\text{Sr}(\text{BAsO}_5)$ , 69  
Strontium cerium antimonate perovskite-type, 164  
Strontium copper tellurate tellurite, 692  
Strontium iron(III) oxycarbonate, 83  
Strontium iron phosphate whitlockite-related, 420  
Strontium magnesium niobate, 165  
Strontium magnesium pyrophosphate, 421  
Strontium selenate, 657  
Strontium tungstate, 716  
Strontium vanadyl vanadate, 571  
Strunzite, 1195  
Struvite, 1196  
Struvite Cd analogue, 356  
Struvite-(K), 1195  
Studtite, 1196  
Sturmanite, 1196  
Stützite, 1196  
Sudoite, 294, 1197  
Sudovikovite, 1197  
Sulfhydrlybystrite, 310  
Sulfur, 1197  
Sulphohalite, 1197  
Sulvanite, 1198  
Suredaite, 1198  
Sursassite, 1198  
Susannite, 1198  
Suseinargiuuite, 1199  
Svabite, 633  
Svanbergite, 1199  
Švenekite, 1199  
Svornostite, 1199  
Swamboite-(Nd), 349  
Swedenborgite, 1200  
Symplesite, 628, 1200  
Synchysite-(Ce), 1200  
Syngenite, 1200  
Szaibélyite, 1200  
Szenicsite, 1201  
Szmkite, 1201  
Szomolnokite, 478, 1201
- T**
- Takedaite, 1201  
Takovite, 1202  
Talc, 1202  
Talmessite, 1202  
Tangdanite, 1203  
Tangeite, 1203  
Tantalite-(Fe), 1203  
Tantalite-(Mg), 1203  
Tantalite-(Mn), 1204  
Tantalum oxyarsenate, 615  
Tantalum oxyphosphate, 422  
Tantalum oxyvanadate, 572  
Tantite, 202  
Tantite orthorhombic polymorph, 1204  
Taranakite, 1204  
Tarapacáite, 1204  
Tarbuttite, 1205  
Tausonite, 1205  
Tazheranite, 1205  
Tazzoliite, 1205  
Teepleite, 1205  
Teineite, 1206  
Tellurantimony, 1206  
Tellurite rhombohedral polymorph, 166  
Tellurium, 694, 1206  
Tellurium(IV) oxosulfate, 499  
Tellurium(IV) oxovanadate, 572  
Tellurium oxumolybdate, 675  
Tellurium(IV) oxyphosphate, 423  
Tellurium(IV) oxyseleenate, 658  
Tellurium oxyselenite, 658  
Tellurium(IV) tin oxide  $\text{Te}_3\text{SnO}_8$ , 166  
Tellurium(IV) titanium oxide  $\text{Te}_3\text{TiO}_8$ , 167  
Tellurium(IV) zirconium oxide  $\text{Te}_3\text{ZrO}_8$ , 168  
Tellurobismuthite, 1206  
Telluroperite, 555  
Tengerite-(Y), 1206  
Tennantite, 1207  
Tenorite, 1207  
Tephroite, 1207  
Terlinguacreekite, 549  
Tetraferrintronitrite, 295  
Tetrahedrite, 1207  
Tetrammine zinc borofluoride, 233  
Tetrawickmanite, 1208  
Thadeuite, 468  
Thallium feldspar, 311  
Thallium sodalite, 311  
Thallium tellurite, 692  
Thallium(I) selenite vanadate  $\text{TiSeVO}_5$ , 573  
Thallium(I) tellurite vanadate  $\text{TiTeVO}_5$ , 574  
Thaumasite, 732, 734, 1208

- Thecotrichite, 1208  
Theophrastite, 1208  
Thermonatrite, 1208  
Thometzekite, 1209  
Thomsonite-Ca, 1209  
Thorianite, 1209  
Thorikosite, 1209  
Thorite, 1210  
Thorium divanadate cubic polymorph, 574  
Thorium divanadate orthorhombic polymorph, 575  
Thorium hydrogenphosphate, 424  
Thorium tellurite, 693  
Thorneite, 1210  
Thortveitite, 1210  
Thorutite, 1210  
Threadgoldite, 1211  
Tiemannite, 1211  
Tilasite, 1211  
Tilleyite, 1211  
Tin(IV) hydroxide, 168  
Tin tetraborate, 69  
Tiragalloite, 1212  
Tissintite, 1212  
Tistarite, 203, 1212  
Titanite, 1212  
Titanium acid phosphate monohydrate, 425  
Titanium(III) orthophosphate, 424  
Titanium oxophosphate hydrate, 426  
Titanoholtite, 1213  
Tlapallite, 1213  
Tobelite hydrated variety, 286  
Tobermorite, 278, 1213  
Todorokite, 1213  
Tokyoite, 1214  
Tolbachite, 554, 1214  
Tondiite, 1214  
Tooeleite, 1214  
Topaz, 723, 725, 1215  
Torbernite, 1215  
Toturite, 1215  
Trabzonite, 1215  
Tremolite, 1216  
Trevorite, 1216  
Trevorite Co-analogue, 203  
Triammonium hydrogen disulfate, 500  
Triazolite, 110  
Tridymite, 1216  
Trilithionite, 1216  
Trinepheline, 1217  
Triphyllite Mg-analogue, 446  
Triplite, 1217  
Trippkeite, 1217  
Tripuhyte, 1217  
Trogtalite, 1218  
Troilite, 1218  
Trolleite, 454  
Trona, 1218  
Tschermigite, 1218  
Tsichernichite, 317  
Tsumcorite, 1218  
Tsumebite, 1219  
Tsumoite, 1219  
Tugarinovite, 1219  
Tuite, 1219  
Tululite, 1220  
Tunellite, 1220  
Tungstenite, 1220  
Tungsten(VI) oxyphosphate, 427  
Tungsten trioxide monoclinic, 169  
Tungsten trioxide orthorhombic, 170  
Tungsten trioxide triclinic, 170  
Tungstite, 1220  
Tunisite, 1221  
Turquoise, 1221  
Tuzlaite, 1221  
Tvrdýite, 352, 447  
Tychite, 1221  
Tyretskite (monoclinic polytype), 74  
Tyrolite, 1222  
Tyuyamunite, 1222
- U**
- Uedaite-(Ce), 254  
Ulexite, 1222  
Ulfanderssonite-(Ce), 243  
Ulrichite, 1222  
Ulvöspinel Zn-analogue, 204  
Ulvöspinel, 1223  
Umangite, 1223  
Umbite, 1223  
Umbrianite, 1223  
Ungemachite, 1224  
Uraninite, 1224  
Uranium(IV) oxalate fluoride hydrate, 102  
Uranophane- $\alpha$ , 1224  
Uranopilite, 1224  
Uranosphaerite, 1225  
Uranospinitite, 638  
Uranyl fluoride, 234  
Uranyl nitrate hexahydrate, 113  
Uranyl oxy-hydroxyphosphate, 427  
Uranyl perrhenate hydrate, 719  
Urea solution, 1225  
Ushkovite, 1225  
Usturite, 1225  
Uvarovite, 1226  
Uvite, 1226
- V**
- Vaesite, 1226  
Vajdakite, 1226  
Valentinite, 1227  
Vanackerite, 1227  
Vanadinite Sr,OH-analogue, 580  
Vanadinite, 1227  
Vanadium(III) antimony(V) selenite, 659  
Vanadium oxide bariandite-type, 171  
Vanadyl molybdate, 678

- $\beta$ -Vanadyl pyrophosphate, 363  
 $\gamma$ -Vanadyl pyrophosphate, 374  
Vanadyl selenite, 660  
Vanadyl sulfate, 517  
Vandenbrandeite, 204  
Vandenbrandeite hydrogen-free analogue, 205  
Vandendriesscheite, 1227  
Vanmeersscheite, 1228  
Vantasselite, 1228  
Vanthoffite, 1228  
Vapnikite, 1229  
Variscite, 1229  
Variscite-*4O*, 353  
Varulite, 455  
Västmanlandite-(Ce), 1229  
Vaterite, 1229  
Vauquelinite, 1230  
Vauxite, 1230  
Väyrynenite, 443, 1230  
Velikite, 1231  
Versiliaite, 1231  
Vésigniéite, 1231  
Vesuvianite, 2, 5, 259, 1231  
Vesuvianite B-bearing, 262, 263  
Vesuvianite Cr-bearing, 260  
Vesuvianite S-bearing, 260  
Veszelyite, 1231  
Villamanírite, 1232  
Vishnevite, 303  
Vishnevite CO<sub>3</sub>-bearing, 304  
Vishnevite potassium analogue, 302  
Vittingeite, 268  
Vivianite, 731, 1232  
Vladimirivanovite, 1232  
Vladykinitite, 1232  
Voglite, 1233  
Volaschioite, 1233  
Volborthite, 1233  
Vonsenite, 1233  
Vorlanite, 1234  
Vrbaite, 1234  
Vuorelainenite, 1234  
Vyacheslavite, 464  
Vyacheslavite anhydrous Th analogue, 464  
Vysokýite, 626, 1234  
Vysotskite, 1235
- W**  
Wadalite, 237  
Wadeite, 1235  
Wadeite dimorph, 280  
Wadeite Rb analogue, 281  
Wadsleyite, 1235  
Wagnerite-*Ma5bc*, 1235  
Waimirite-(Y), 1236  
Waimirite-(Yb), 235  
Wakabayashilite, 1236  
Wakefieldite-(Ce), 1236  
Wakefieldite-(La), 1236  
Wakefieldite-(Nd), 1236  
Wakefieldite-(Pr), 581  
Wakefieldite-(Y), 588, 1237  
Walpurgite, 1237  
Walstromite, 1237  
Wardite, 1237  
Waterhouseite, 1238  
Wavellite, 1238  
Wavellite-(OH), 443  
Waylandite, 1238  
Weddellite, 1238  
Weeksite, 1239  
Wegscheiderite, 1239  
Weissbergite, 1239  
Weloganite, 1239  
Wendwilsonite, 1240  
Wermlandite carbonate analogue, 91  
Wernerbaurite, 584  
Wernerkrauseite, 1240  
Wesselsite, 298  
Wetherillite, 1240  
Wheatleyite, 1241  
Whelanite, 1241  
Whewellite, 1241  
Whitecapsite, 1241  
Whiteite [possibly, whiteite-(CaMnMg)], 1242  
Whitlockite, 1242  
Whitmoreite, 1242  
Widenmannite, 1242  
Wiklundite, 348  
Wilhelmgümbelite, 448  
Willemite, 1243  
Willemseite, 1243  
Wiluite, 252, 255  
Windhoekite Na-bearing variety, 293  
Winstanleyite, 1243  
Witherite, 1243  
Wittichenite, 1243  
Wollastonite, 1244  
Wölsendorfite, 221  
Woodallite, 123  
Woodhouseite, 1244  
Wopmayite, 1244  
Wulfenite, 1244  
Wupatkiite, 1245  
Wurtzite, 1245  
Wüstite, 1245
- X**  
Xanthoxenite, 438  
Xenotime-(Y), 1245  
Xieite, 1246  
Ximengite polymorph, 448, 449  
Xocolatlite, 1246  
Xocomecatlite, 1246  
Xonotlite, 1246
- Y**  
Yafsoanite, 695  
Yangzhumingite, 295  
Yarrowite, 1247  
Yavapaiite, 478  
Yecoraite, 1247

- Ye'elimit, 1247  
Yimengite, 1247  
Yingjiangite, 1247  
Yoshimuraite, 337  
Yttriaite-(Y), 1248  
Yttrium barium borate  $\text{YBa}_3\text{B}_9\text{O}_{18}$ , 70  
Yttrium hydroxychloride hydrate, 543  
Yttrium iron antimony(V) oxide pyrochlore-type, 172  
Yttrium metaphosphate, 428  
Yttrium oxide, 172  
Yttrium tungstate, 717  
Yttrium vanadyl oxyseLENITE, 660  
Yttrium vanadyl oxytellurite, 694  
Yukonite, 1248  
Yuksporite, 1248  
Yurmarinite, 1248  
Yushkinite, 1249  
Yvonite, 1249
- Z**
- Žabińskiite, 1249  
Zadovite, 1249  
Zaherite, 518  
Zálesíte, 1250  
Zanazziite, 1250  
Zaratite, 1250  
Zdeněkite, 1250  
Zellerite, 1251  
Zemannite, 698, 1251  
Zemkorite, 1251  
Zhangpeishanite, 1251  
Zhemchuzhnikovite, 109  
Ziesite, 1252  
Ziesite and blossite polymorph, 582  
Ziminaite, 588
- Ziminaite monoclinic polymorph, 583  
Zinc basic pyrovanadate hydrate, 577  
Zinc hydroxychloride, 544  
Zinc hydroxyfluoride, 234  
Zinc iron(III) orthovanadate, 576  
Zincite, 206, 1252  
Zinc molybdate, 676  
Zincoberaunite, 350  
Zincobotryogen, 528  
Zincochromite, 1252  
Zincocopiapite, 1252  
Zinc orthoborate hydroxide, 38  
Zinc orthoborate orthophosphate, 39  
Zinc orthovanadate, 576  
Zincospiroffite, 1253  
Zincovelesite- $6N6S$ , 220  
Zincovoltaite, 531  
Zinc stannate, 174  
Zinc telluromolybdate, 676  
Zinc vanadyl oxide  $\text{Zn}(\text{VO}_2)_2\text{O}_2$ , 578  
Zinc vanadyl phosphate, 429  
Zinkenite, 1253  
Zippeite, 1253  
Zircon, 1253  
Zirconium acid arsenate monohydrate, 616  
Zirconium acid phosphate monohydrate, 429, 430  
Zirconium basic oxalate, 103  
Zirconium molybdenum oxide (monoclinic), 677  
Zirconium molybdenum oxide (trigonal), 678  
Zirconolite- $2M$ , 218  
Zoisite, 1254  
Zorite, 1254  
Zuktamurrite, 1254  
Zunyite, 1254  
Zýkaite, 1255