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Citation: *The Journal of Chemical Physics* **75**, 5456 (1981); doi: 10.1063/1.441947

View online: <http://dx.doi.org/10.1063/1.441947>

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Piezoelectric $K_3Ta_3B_2O_{12}$: Crystal structure at room temperature and crystal growth

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(Received 1 June 1981; accepted 14 August 1981)

$K_3Ta_3B_2O_{12}$ is a new piezoelectric material that crystallizes in the hexagonal system with space group $P\bar{6}2m$ and one formula unit in the unit cell. The lattice constants are $a = 8.781\,58 \pm 0.000\,04$ and $c = 3.899\,02 \pm 0.000\,02$ Å at 298 K ($\lambda_{CuK\alpha} = 1.540\,598$ Å). The integrated intensities of a full sphere of reciprocal space, with radius $(\sin \theta)/\lambda \leq 1.15$ Å⁻¹, were measured with a CAD-4 diffractometer and resulted in 1050 independent reliable structure factors. The crystal structure was solved by means of Patterson and Fourier series and was refined by the method of least squares, with final agreement factor $R = 0.0133$. Corner-sharing triads of TaO_6 octahedra are stacked along the c axis and are connected by planar BO_3 groups. The resulting large trigonally girdled pentagonal prismatic interstices are occupied by the K^+ ions. The average Ta–O distance is 1.973 Å in a strongly distorted octahedron. The B–O distance is 1.364 ± 0.004 Å and the average K–O distance is 2.992 Å. The absolute sense of each polar axis has been determined and the piezoelectric d_{22} coefficient measured as 1.6 ± 0.1 pC N⁻¹. Piezoelectricity has not been detected in the related material $K_3Nb_3B_2O_{12}$, neither has evidence been found for a quadrupling in the a axis of $K_3Ta_3B_2O_{12}$ such as is readily observed in $K_3Nb_3B_2O_{12}$.

INTRODUCTION

Colorless and transparent single crystals of high refractive index with formula initially taken to be $KTaBO_{4.5}$ or $KNbBO_{4.5}$ were prepared by high temperature solution of Ta_2O_5 or Nb_2O_5 in potassium metaborate. An excess of B_2O_3 in the melt was required to reduce the high vapor pressure of KBO_2 at the solution temperature. Crystals were extracted from the solidified melts by boiling the mass in water: the resulting phases were identified by x-ray powder photography. The tantalum-containing crystals gave a strong response in our modified Giebe–Sheibe apparatus,¹ while the niobium-containing crystals did not produce a detectable signal. The results of the present structural study on the new piezoelectric “ $KTaBO_{4.5}$ ” show that the correct formula is $K_3Ta_3B_2O_{12}$. The atomic arrangement² in the related material $K_3Nb_3B_2O_{12}$ has an a axis repeat quadruple that of the present material.

EXPERIMENTAL

A sphere of $K_3Ta_3B_2O_{12}$, with radius 0.0886(28) mm,³ was ground and mounted with random orientation on a Pyrex capillary. A full sphere of reciprocal space, with radius $(\sin \theta)/\lambda = 1.15$ Å⁻¹, was measured using an Enraf-Nonius CAD-4 diffractometer controlled by a PDP 11/40-8e minicomputer operating under Enraf-Nonius software.⁴ $MoK\alpha$ radiation reflected from a graphite monochromator was used in an $\omega - 2\theta$ scanning mode of angular range $1.10^\circ + 0.35^\circ \tan \theta$. The maximum counting time was 600 s, resulting in a precision, as given by the counting statistics, not less than 1.5%. The algorithm for measuring the integrated intensities has previously been described.⁵ Five standard reflections were measured hourly, of which four varied less than 1% and the weak fifth less than 2.2% over the length of the experiment, on average. No correction was made

for these small variations, but corrections were made for the effects of Lorentz, polarization and absorption. The transmission factors ranged from 0.023 to 0.075.

A total of 11 541 structure factors were measured with 1946 remaining after symmetry related values were averaged. Standard deviations were derived from the expression $\sigma^2 F^2_{meas} = V_1 + V_2(F_{meas})^4$ + larger of $[V_3(F_{meas})^4 \text{ or } V_4]$, where V_1 is the variance due to counting statistics, $V_2 = 0.0038$, $V_3 = 0.0115$, and V_4 is the variance derived from differences among equivalent members of a form.⁶ Terms for which $|F_{meas}|^2 < 3\sigma|F_{meas}|^2$ were eliminated as unobserved and hence unreliable, resulting in a total of 1050 F_{meas} that were included in the following analysis. An isotropic extinction correction⁷ was applied in the course of least-squares refinement, with coefficient $g = 9.66(26) \times 10^2$ and a maximum correction of 57.0% in $F(00.1)$. The magnitudes of the symmetry-independent but Bijvoet-pair related F_{meas} and σF_{meas} are given in Ref. 8, on the final least-squares derived absolute scale.

CRYSTAL GROWTH

Colorless hexagonal prisms of $K_3Ta_3B_2O_{12}$ or $K_3Nb_3B_2O_{12}$ were obtained by dissolving Ta_2O_5 or Nb_2O_5 in molten KBO_2 with an excess of B_2O_3 . Crystals of $K_3Ta_3B_2O_{12}$ having dimensions about $2 \times 2 \times 5$ mm resulted from a charge of 23.26 g K_2CO_3 , 17.68 g Ta_2O_5 , and 10.46 g B_2O_3 in a 100 ml platinum crucible. The covered crucible was horizontally loaded into a resistively heated furnace at about 1075 K. The temperature was raised at furnace rate to 1475 K, held for 4 h to allow reaction and solution of the constituents, and then lowered at the controlled rate of 3 K h⁻¹ to about 775 K, whereupon the furnace power was shut off and the system allowed to cool to room temperature. The flux is soluble in hot water; addition of HCl hastens dissolution without visibly etching the crystals.

A number of chemical analyses led to an initial formu-

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lation of $KTaBO_{4.5}$ for the Ta-containing crystals. The subsequent x-ray diffraction analysis showed that errors in the wet-chemical analyses substantially exceeded those given by the reproducibility.

Crystals of $K_3Nb_3B_2O_{12}$ were grown by a similar method. A charge of 22.10 g K_2CO_3 , 10.64 g Nb_2O_5 , and 14.00 g B_2O_3 heated from 1075 K as before, brought to 1400 K, held for 5 h, and cooled as for the Ta-containing material resulted in crystals with dimensions about $0.5 \times 0.5 \times 2.0$ mm.

CRYSTAL DATA

$K_3Ta_3B_2O_{12}$ has formula weight (fw) of 873.765 and is hexagonal with lattice constants of $a = 8.78158(4)$ and $c = 3.89902(2)$ Å at 298 K, as measured on two different crystal specimens with $CuK\alpha_1$ radiation ($\lambda = 1.540598$ Å) and a modified⁹ version of Bond's precision lattice constant diffractometer.¹⁰ Values of $a = 8.7836(17)$ and $c = 3.9023(6)$ Å were obtained on the CAD-4 diffractometer with $MoK\alpha$ radiation using 21 well-centered reflections with $25^\circ < 2\theta < 68^\circ$: values of $a = 8.780(1)$ and $c = 3.899(1)$ Å resulted from a Debye-Scherrer camera of diameter 114.6 mm with $CrK\alpha$ radiation. Neither set differs significantly from the more accurate lattice constants. The volume of the unit cell is 260.394 Å³. $D_m = 5.61(19)$ based on the mass of a sphere with diameter $1.427(17)$ mm and $D_x = 5.572$ g cm⁻³ for one fw per unit cell.

The absorption coefficient¹¹ for $MoK\alpha$ radiation is 34.7 mm⁻¹ and for the sphere used $\mu R = 3.07$. The average refractive index for this uniaxial crystal is 2.01, with birefringence of 0.13 at 298 K. The crystal habit is columnar, elongated along $[00.1]$ with $\{10.0\}$ prominent and $\{11.0\}$ occasionally developed. Observation of a single independent piezoelectric coefficient $d_{22} = 1.6(1)$ pC N⁻¹ at 298 K, together with the intensity distribution in reciprocal space, reduced the choice of space group to $P31m$ or $P\bar{6}2m$. Determination that the diffraction symmetry is $6/mmm$ with no systematically absent reflections, together with the results of structural refinement, eliminated the trigonal possibility and confirmed the space group as $P\bar{6}2m$.

SOLUTION AND REFINEMENT OF THE $K_3Ta_3B_2O_{12}$ STRUCTURE

The predominant Ta-Ta vectors were readily recognizable in the three-dimensional Patterson function. Least-squares refinement of the atomic parameters for the single Ta atom in space group $P31m$ gave $R = 0.108$ for 1928 F_{meas} , and a difference Fourier series yielded the location of the K and three independent O atoms. These calculations were made on the PDP 11/40 mini-computer using Enraf-Nonius programs.¹² Least-squares refinement reduced R to 0.041 and the resulting difference Fourier series revealed the location of one B atom. Refinement of the 37 variable parameters in $P31m$ gave $R = 0.016$ and $wR = 0.022$ (see Ref. 6 for definitions) but produced no evidence for the second independent B atom expected for the formula $KTaBO_{4.5}$. Subsequently, new chemical analyses confirmed the structural formula $K_3Ta_3B_2O_{12}$.

TABLE I. Structural refinement indicators for $K_3Ta_3B_2O_{12}$ at 298 K.^a

Parameters varied	Number of parameters	R	wR	S
xyz, B	14	0.0294	0.0386	1.020
$\bar{x}\bar{y}\bar{z}, B$	14	0.0422	0.0686	1.519
xyz, β_{ij}	26	0.0133	0.0167	0.445
$\bar{x}\bar{y}\bar{z}, \beta_{ij}$	26	0.0319	0.0460	1.223

^aThe total number of F_{meas} used in least-squares refinement is 1050. See Ref. 6 for definitions of R , wR , and S . All refinements included the single scale factor and an isotropic extinction factor as variables.

All z coordinates in $P31m$ were found to be close to 0 or $\frac{1}{2}$ at this refinement stage, and values of $F(hk \cdot l)$ and $F(hk \cdot \bar{l})$ were noted to be closely comparable. These two classes of reflection were thereupon averaged to give the 1050 F_{meas} in Ref. 8, satisfying the requirements of $P\bar{6}2m$ symmetry and the observed relations among the piezoelectric moduli. Refinement in $P\bar{6}2m$ gave $R = 0.0149$ and $wR = 0.0184$ after all parameter shifts had become very small. Further refinement was continued on the Honeywell 6080 computer under ORFLS-3,¹³ since it had previously been found¹⁴ that one or more algorithms used in the least-squares program of Ref. 12 were in error. Agreement factors for the final models investigated are presented in Table I. In each case, the largest parameter shift had a magnitude less than 1% of the error in that parameter.

The agreement between each pair of F_{meas} and F_{calc} was examined in a δR normal probability plot,¹⁵ which was found to depart only slightly from linearity except for a few points in the extrema. The two largest departures were $F(00.1)$ and $F(00.2)$, which are the two reflections most strongly affected by extinction. On excluding these two terms, refinement resulted in $R = 0.0130$, $wR = 0.0163$, and $S = 0.438$ with no parameter changing more than 0.3σ between the two sets except for $Ta \beta_{11}$, $Ta \beta_{22}$, and $Ta \beta_{33}$. Elimination of $F(00.1)$ and $F(00.2)$ was thus not considered to be justified; hence, the position coordinates of Table II and the anisotropic temperature coefficients of Table III are based on the full set of 1050 structure factors. The slope of the δR plot is 0.429, indicating that σF_{meas} has been overestimated on average by a factor of 2.3, probably a consequence of overestimating V_3 .

The largest integrated feature in the final difference Fourier series, based on the data in Ref. 8, corresponds to less than $1e$ at the origin: this feature could be interpreted as a fragment less than 20% of a boron atom or, more likely, as a residual error in the difference series since the next highest remaining features are only slightly smaller and are located at about 0.15 Å on either side of Ta. Attempts at refining both occupancy and isotropic temperature factors for this feature at the origin, assuming it to be a boron atom, did not lead to convergence and gave negative values for the temperature factor. All other features correspond to less than $0.2e$.

TABLE II. Atomic coordinates in $K_3Ta_3B_2O_{12}$ at 298 K.^a

Atom	x	y	z
K	0	0.404 30(11)	0.500 00
Ta	0	0.753 63(1)	0
B	0.333 33	0.666 67	0
O(1)	0	0.737 2(3)	0.500 00
O(2)	0	0.181 5(3)	0
O(3)	0.316 3(3)	0.503 5(3)	0

^aValues without errors (see Ref. 3) are determined by symmetry and are not varied in the refinement process.

ABSOLUTE SENSE OF THE POLAR AXES

The absolute sense of each polar diad axis, normal to the crystal a_1 , a_2 , or a_3 axes and to the c axis, may be determined by means of the anomalous scattering of MoK α radiation by the K, Ta, B, and O atoms that cause $SF(hkl) \neq S(\bar{h}\bar{k}\bar{l})$. Hamilton's method¹⁶ allows the F hypothesis that the model with $\bar{x}\bar{y}\bar{z}$ coordinates fits the F_{meas} in Ref. 8 better than that with xyz coordinates to be tested. The theoretical value of $wR(\bar{x}\bar{y}\bar{z})/wR(xyz)$ at the half-percent significance level, for 1050 independent F_{meas} and 26 variables, is $R_{1,1024,0.005} = 1.0040$. The experimental value from Table I is 2.755; hence, the hypothesis can be rejected with confidence. The hypothesis is also rejected on the basis of the indicators in Table I for the isotropic model ($R_{exp} = 1.777$ versus $R_{1,1036,0.005} = 1.004$). The atomic coordinates in Table I hence represent the absolute polarity of $K_3Ta_3B_2O_{12}$ at 298 K in terms of the Miller indices and F_{meas} listed in Ref. 8.

Experimental determination of the absolute sense of $[11.0]$ in a crystal of $K_3Ta_3B_2O_{12}$ may be made by consultation with Table IV. In particular, it is to be noted that $F^2(hh \cdot 0)/F^2(\bar{h}\bar{h} \cdot 0)$ is 1.07 for $h = 2$, 1.18 for $h = 5$, and 0.92 for $h = 6$, a characteristic grouping of intensity ratios that is readily recognizable experimentally.

AMPLITUDES OF VARIATION

The hypothesis that the atomic vibrations in $K_3Ta_3B_2O_{12}$ at 298 K are isotropic rather than anisotropic may also be tested by means of Hamilton's method.¹⁶ The experimental ratio $wR(\text{isotropic})/wR(\text{anisotropic}) = 2.311$ from Table I whereas $R_{12,1024,0.005} = 1.014$; hence, the hypoth-

TABLE IV. Absolute sense of polar $[11.0]$.^a

$hh \cdot 0$	$F_{meas}(+)$	$F_{calc}(+)$	$F_{meas}(-)$	$F_{calc}(-)$
11.0	135.4(3.1)	134.1	136.8(3.2)	136.3
22.0	90.3(2.4)	88.1	87.5(1.8)	85.8
33.0	131.3(2.9)	132.9	128.8(2.9)	131.4
44.0	113.2(2.7)	115.9	115.9(2.7)	118.6
55.0	66.6(2.0)	66.3	61.2(2.0)	61.7
66.0	27.3(1.3)	26.6	28.5(1.3)	28.4
77.0	65.7(2.0)	65.6	66.0(1.8)	67.6
88.0	59.6(1.9)	60.1	57.2(1.9)	58.2
99.0	38.9(1.6)	38.9	37.8(1.5)	38.8

^aBased on MoK α anomalous scattering differences between $F(hh \cdot 0)$ and $F(\bar{h}\bar{h} \cdot 0)$ and the atomic coordinates of Tables II and III and values in Ref. 8, with $hh \cdot 0$ denoted by (+) and $\bar{h}\bar{h} \cdot 0$ by (-). Estimated standard deviations in F_{meas} are probably overestimated by the factor of 2.3; see the text.

esis may be rejected at the half-percent significance level. The anisotropy in the amplitudes of thermal vibration is indicated directly by the ratios of maximum to minimum root-mean-square amplitudes given in Table V: the ratios range from a factor of about 1.3 for Ta and B to greater than a factor of 2 for O(3). All amplitudes in Table V are quite small, corresponding to a characteristic temperature Θ that is expected to be larger than 325 K. The root-mean-square radial thermal amplitudes are 0.119(2) Å for K, 0.064(1) Å for Ta, 0.088(5) Å for B, and range from 0.092(6) to 0.119(2) Å for O.

ATOMIC ARRANGEMENT AND INTERATOMIC DISTANCES

The $K_3Ta_3B_2O_{12}$ crystal contains stacked triads of TaO_6 octahedra, each of which shares two O(2) corners in the equatorial or basal plane and two O(1) apical corners, as illustrated in Fig. 1. These stacks are joined by planar BO_3 groups, with K^+ ions occupying the resulting interstitial pentagonal prisms. All interatomic distances less than 3.2 Å, except for O-O contacts, are given in Table VI as calculated from the position coordinates of Table II and the best lattice constants given under Crystal Data. Estimated standard deviations were computed from the variance-covariance matrix derived from the final cycle of least-square refinement by the ORFFE program.¹³

The average Ta-O distance of 1.973 Å in Table VI is very close to the average distance of 1.981 Å found in

TABLE III. Anisotropic temperature coefficients in $K_3Ta_3B_2O_{12}$.^a

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
K	609(12)	268(13)	1714(36)	134	0	0
Ta	123(1)	111(2)	706(5)	55	0	0
B	215(21)	215	1380(143)	107	0	0
O(1)	621(44)	339(53)	765(77)	170	0	0
O(2)	184(23)	137(36)	2004(126)	68	0	0
O(3)	390(20)	201(17)	2859(109)	168(15)	0	0

^aBased on the exponential expression— $(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)$. The coefficients are $\times 10^5$. See also footnote a to Table II.

TABLE V. Root-mean-square amplitudes of thermal vibration along the principal ellipsoid axes in $K_3Ta_3B_2O_{12}$ at 298 K.

Atom	1 (Å)	2 (Å)	3 (Å)
K	0.089(2)	0.115(1)	0.146(2)
Ta	0.057(1)	0.061(1)	0.074(1)
B	0.079(5)	0.079(5)	0.103(5)
O(1)	0.077(4)	0.100(8)	0.145(6)
O(2)	0.063(8)	0.077(6)	0.124(4)
O(3)	0.070(6)	0.108(3)	0.148(3)

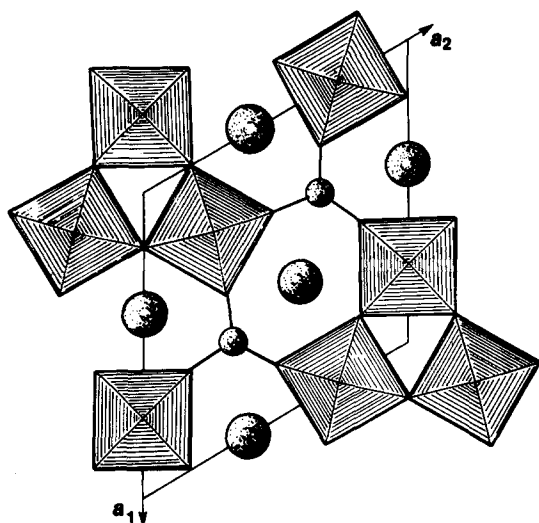


FIG. 1. View of the $K_3Ta_3B_2O_{12}$ structure along the hexagonal axis. The triads of TaO_6 octahedra are shown with triangular octahedral faces shaded. The K^+ ion is the larger circle. The BO_3 groups connecting the octahedra are shown with the B-O bonds in heavy outline.

$LiTaO_3$,¹⁷ although the spread of individual distances in piezoelectric $K_3Ta_3B_2O_{12}$ is significantly less than that in ferroelectric $LiTaO_3$. The Ta-O octahedron in $K_3Ta_3B_2O_{12}$ is strongly distorted, with the O(1)-Ta-O(1) angle = $171.6(2)^\circ$; the remaining axial octahedral angles are both $179.5(2)^\circ$, as illustrated in Fig. 2(a). The deformability of TaO_6 and similar octahedra permits polarization reorientation and is essential for the reversal of the spontaneous polarization observed in many such octahedral ferroelectrics.

The coordination of the K^+ ion may be regarded as 13-fold, if all K-O contacts less than 3.2 Å are included, as illustrated in Fig. 2(b). In this case, the coordination polyhedron is a pentagonal prism with an equatorial trigonal girdle of oxygen atoms, having an average K-O distance of 2.993 Å. The coordination number of oxygen in this polyhedron is three; hence, the K-O distance predicted with Shannon's radii¹⁸ is 3.00 Å, in good agreement with experiment. If contacts longer than 3.00 Å are neglected, the coordination number of potassium becomes seven and the resulting polyhedron forms a capped trigonal prism with average K-O distance of 2.872 Å; the corresponding predicted¹⁸ value is 2.87 Å.

The BO_3 group, which joins the stacks of TaO_6 triads, is geometrically planar and regular with O-B-O angle of 120° and B-O distance of 1.364 Å. The B-O distance given¹⁹ by Zachariasen for the BO_3 group is 1.365 Å, in excellent agreement with the present value.

COMPARISON OF $K_3Ta_3B_2O_{12}$ WITH $K_3Nb_3B_2O_{12}$ AND RELATED SILICON OXIDES

$K_3Ta_3B_2O_{12}$ is structurally the simplest known member of a family of related materials, all of which are reported to crystallize with trigonal or hexagonal symmetry and have either the c axis doubled or the a axis quadrupled in length (see Table VII). The subcell of

TABLE VI. Metal- and boron-oxygen distances in $K_3Ta_3B_2O_{12}$ at 298 K.^a

Ta-O(2)	1.942(3) Å ($\times 2$)	K-O(3)	2.762(3) Å ($\times 2$)
-O(1)	1.955(3) Å ($\times 2$)	-O(3)	2.914(4) Å ($\times 4$)
-O(3)	2.022(4) Å ($\times 2$)	-O(1)	2.924(3) Å
B-O(4)	1.364(4) Å ($\times 3$)	-O(1)	3.121(3) Å ($\times 2$)
		-O(3)	3.139(4) Å ($\times 4$)

^aThe digit following the multiplication sign denotes the number of equivalent distances formed by symmetry about the central atom.

$K_3Nb_3B_2O_{12}$ is closely comparable to the unit cell of $K_3Ta_3B_2O_{12}$, but rotation photographs about the a axis of $K_3Nb_3B_2O_{12}$ clearly reveal intermediate layers corresponding to the $4a$ spacing, whereas no evidence for such quadrupling is seen on very heavily exposed rotation photographs of $K_3Ta_3B_2O_{12}$. It is also noteworthy that, whereas crystals of $K_3Ta_3B_2O_{12}$ produce very strong resonance signals on a Giebe-Sheibe piezoelectric detector,¹ those of $K_3Nb_3B_2O_{12}$ give no signal. Direct

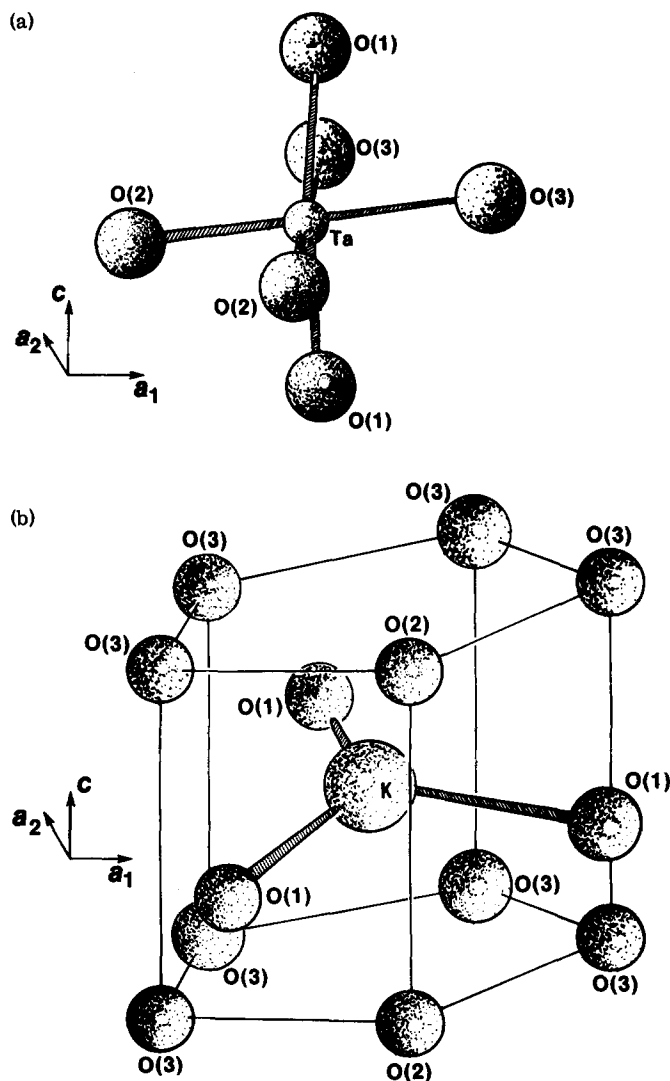


FIG. 2. (a) Perspective view of the TaO_6 octahedron. (b) Perspective view of 13-coordinated oxygen atoms about the K^+ ion.

TABLE VII. Crystallographic data for compounds of the $K_3Ta_3B_2O_{12}$ family.^a

Compound	S. G.	<i>a</i> (Å)	<i>c</i> (Å)	<i>Z</i>	Reference
$K_3Ta_3B_2O_{12}$	$P\bar{6}2m$	8.78158(4)	3.89902(2)	1	Present work
$K_3Nb_3B_2O_{12}$	$P31m(?)$	$4 \times 8.753(5)$	3.966(1)	16	2
$K_3Ta_3B_2O_{12}$...	8.775(5)	3.897(1)	1	2
$Ba_3Ta_6Si_4O_{23}$	$P\bar{6}2m$	8.997(3)	7.745(5)	1	20
$Ba_3Ta_6Si_4O_{26}$	$P\bar{6}2m$	8.99(1)	7.79(1)	1	20
$Ba_3Nb_6Si_4O_{26}$	$P\bar{6}2m$	9.00(1)	7.89(1)	1	21
$Sr_3Ta_6Si_4O_{26}$	$P\bar{6}2m$	8.913(5)	7.633(5)	1	22
$K_6Ta_6Si_4O_{26}$	$P\bar{6}2m$	9.066(5)	7.873(5)	1	22
$K_6Nb_6Si_4O_{26}$	$P\bar{6}2m$	9.032(5)	8.041(5)	1	22

^aS. G. is the space group, and *Z* the number of formula units per unit cell.

attempts at detecting the only independent piezoelectric modulus were unsuccessful: the upper limit on d_{22} was placed at about 4×10^{-2} pC N⁻¹.

Atomic coordinates reported² for the substructure of $K_3Nb_3B_2O_{12}$ differ by less than one estimated standard deviation from those given in Table II. The 16 subunits arrayed within the true unit cell are nearly identical. The lack of piezoelectric response and the minor violations noted² in the intensity relationships required for the assumed space group $P31m$ suggest that this assumption may be in error: additional study is needed before the arrangement of the 16 subunits of $K_3Nb_3B_2O_{12}$ in the true unit cell is regarded as confirmed.

Six related alkali or alkaline-earth tantalum or niobium silicon oxides have now been reported²⁰⁻²² with unit cells that are multiples of that of $K_3Ta_3B_2O_{12}$, (see Table VII) and with similar atomic arrangement. The common motif is the triad of corner-sharing TaO_6 and NbO_6 octahedra joined by planar BO_3 groups as in $K_3Ta_3B_2O_{12}$, or by ditetrahedral Si_2O_7 groups as in $Ba_3Ta_6Si_4O_{26}$. The large resulting interstices, sometimes described as "pentagonal tunnels," are similar to the polyhedron shown in Fig. 2(b) and are occupied either by K, Sr, or Ba.

All NbO_6 or TaO_6 octahedra reported in these compounds are distorted with Nb-O distances ranging from 1.918 to 2.056 Å²¹ and 1.84 to 2.14 Å,² and Ta-O from 1.94 to 2.06 Å²⁰ and 1.918 to 2.056 Å.²¹

PIEZOELECTRIC d_{22} COEFFICIENT

The point group of $K_3Ta_3B_2O_{12}$ permits only one independent piezoelectric coefficient $d_{21} = -d_{22} = 2d_{16}$, which was measured by a static method.²³ Pairs of (11.0) faces were ground on a large prism and coated with Engelhard's flexible silver coating. Tensile stress in the range 5 to 10 N mm⁻² applied to these faces gave a very reproducible polarization that was measured with a Keithley 610C electrometer. The resulting value for d_{22} was 1.6(1) pC N⁻¹.

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