Name and formula

Reference code:	96-101-1157
Mineral name:	Wakefieldite (Y)
Compound name:	Wakefieldite (Y)
Common name:	Wakefieldite (Y)
Chemical formula:	$Y_{4.00}V_{4.00}O_{16.00}$

Crystallographic parameters

Crystal system:	Tetragonal
Space group:	I 41/a m d
Space group number:	141
a (Å):	7.1260
b (Å):	7.1260
c (Å):	6.1790
Alpha (°):	90.0000
Beta (°):	90.0000
Gamma (°):	90.0000
Calculated density (g/cm^3):	4.31
Volume of cell (10^6 pm^3):	313.77
RIR:	5.99

Subfiles and quality

Subfiles:	User Inorganic, User Mineral
Quality:	User From Structure (=)

Comments

Creation Date:	2/8/2021 1:59:10 PM
Modification Date:	2/8/2021 1:59:10 PM
Cross-References:	COD:96-101-1157
Structure TIDY:	Transformed from space group: "I41/AMD1" to space group: "I 41/a m dZ".

Structure TIDY: Applied Origin shift (x, y, z): -0.25, -0.25, -0.25

Structure TIDY: Applied Transformation matrix:
Structure TIDY: 1, 0, 0
Structure TIDY: 0, 1, 0
Structure TIDY: 0, 0, 1
Structure TIDY: TRANS Origin 0 0 1/2
Publication title: Die Kristallstruktur von Yttriumvanadat
COD database code: 1011156

References

Structure: Broch, E, *Zeitschrift fuer Physikalische Chemie, Abteilung B: Chemie der Elementarprozesse, Aufbau der Materie*, **20**, 345 - 350, (1933)

Peak list

No.	h	k	l	d [Å]	2θ [°]	I [%]
1	1	0	1	4.66839	18.995	5.2
2	2	0	0	3.56300	24.971	100.0
3	2	1	1	2.83233	31.563	1.3
4	1	1	2	2.63384	34.011	69.6
5	2	2	0	2.51942	35.606	14.3
6	2	0	2	2.33419	38.538	8.1
7	3	0	1	2.21715	40.660	8.6
8	1	0	3	1.97867	45.822	4.1
9	3	2	1	1.88245	48.309	7.6
10	3	1	2	1.82061	50.061	49.8
11	4	0	0	1.78150	51.238	16.3
12	2	1	3	1.72983	52.885	2.0
13	4	1	1	1.66443	55.136	0.7
14	4	2	0	1.59342	57.819	11.0
15	3	0	3	1.55613	59.341	0.2
16	0	0	4	1.54475	59.822	1.4
17	4	0	2	1.54331	59.884	0.4
18	3	3	2	1.47564	62.934	12.9
19	3	2	3	1.42605	65.389	0.0
20	2	0	4	1.41728	65.845	8.6
21	4	2	2	1.41616	65.904	0.4
22	4	3	1	1.38874	67.377	2.7
23	4	1	3	1.32395	71.157	1.2
24	2	2	4	1.31692	71.595	10.8
25	5	2	1	1.29393	73.071	0.0
26	3	1	4	1.27412	74.396	0.2
27	5	1	2	1.27331	74.452	11.2
28	4	4	0	1.25971	75.394	3.2
29	1	0	5	1.21763	78.488	0.2
30	6	0	0	1.18767	80.870	4.0
31	5	0	3	1.17198	82.183	0.9
32	4	0	4	1.16710	82.602	3.3
33	2	1	5	1.15220	83.910	1.1
34	6	1	1	1.15100	84.017	0.3
35	5	3	2	1.13642	85.349	8.5
36	6	2	0	1.12672	86.261	4.1
37	5	2	3	1.11330	87.562	0.9
38	4	2	4	1.10911	87.978	9.6

39	6	0	2	1.10858	88.031	0.0
40	3	0	5	1.09630	89.277	0.0
41	5	4	1	1.09527	89.384	0.1

Structure

No.	Name	Element	X	Y	Z	Biso	sof	Wyck.
1	Y1	Y	0.00000	0.75000	0.12500	0.5000	1.0000	4a
2	V1	V	0.00000	0.25000	0.37500	0.5000	1.0000	4b
3	O1	O	0.00000	0.06000	0.23000	0.5000	1.0000	16h

Stick Pattern