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/cm³): 4.31 Volume of cell (10⁶ pm³): 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

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User: User Date: 5/22/2023 Time: 3:37:50 PM

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)

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Peak list

No.	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	1715 40.660		
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	

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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

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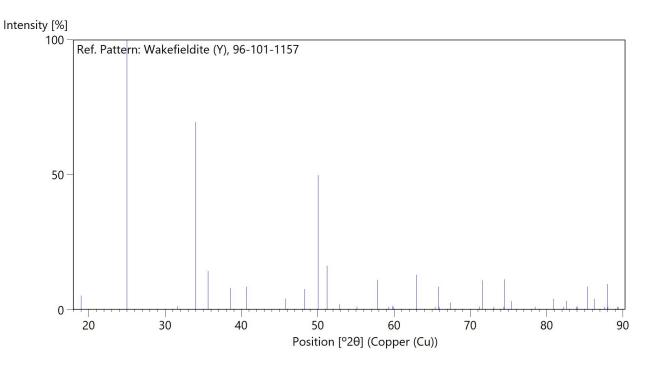
User: User

Structure

No.	Name	Element	Х	Υ	Z	Biso	sof	Wyck.
1	Y1	Υ	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	01	0	0.00000	0.06000	0.23000	0.5000	1.0000	16h

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Stick Pattern



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