BRIEF COMMUNICATIONS

CRYSTAL STRUCTURE OF $ZnWO_4$

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I. S. Potkin (Institute of Synthesis of Mineral Raw Materials) has produced semitransparent dark-red prismatic crystals of $ZnWO_4$ by hydrothermal synthesis. Euhedral specimens were measured with a GD-1 optical goniometer; Table 1 gives the results from measurements on 20 crystals, which show that the external form is pseudoorthorhombic. The true symmetry was established only by x-ray examination.

The crystal (Fig. 1) consists of a combination of the {100} and {010} pinakoids with the {120}, {110}, {210}, {310}, {102}, {011}, {111}, {$\bar{1}$11}, {121}, {$\bar{1}$21} (pseudo)-orthorhombic prisms.

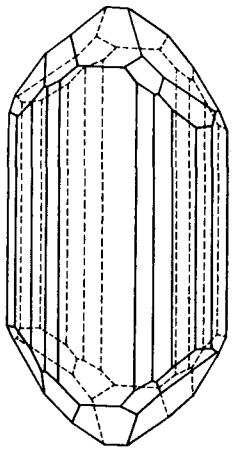

Fig. 1. Isometric projection of $ZnWO_4$ crystal.

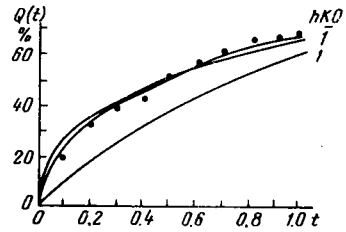

Fig. 2. Statistical demonstration that $ZnWO_4$ is centrosynometric.

$ZnWO_4$ powder was used on Cu radiation with a Ni filter (URS-50I). Table 2 gives the interplanar distances and the indices assigned to some of the reflections by reference to the isostructural $MgWO_4$ [1].

The full study was based on crystals of cross-section 0.2 × 0.3 mm elongated on c. The monoclinic cell of $ZnWO_4$ was determined with a DRON-1 diffractometer and has parameters $a = 4.72 \pm 0.01$, $b = 5.70 \pm 0.005$, $c = 4.95 \pm 0.005$ Å, and $\beta = 90°05' \pm 2'$, which agree with previous data [2]. The specific gravity of 7.8 means that the cell contains two $ZnWO_4$ molecules. The hk0, hk1, 0kl, h0l reflections were recorded with KFOR and Weissenberg cameras on Mo radiation ($\max \sin\vartheta/\lambda = 1.27$ Å^{-1}). The intensities were estimated visually on a $\sqrt[4]{2}$ scale.

The diffraction group 2/mP – / c corresponds to the space groups Pc and P2/c. Tests for the piezoelectric effect (at the Department of Crystal Physics, Moscow University) gave a negative result; goniometry and a statistical test (Fig. 2) by

TABLE 1. Goniometer Results

Symbol	ρ_c	φ_c	ρ_{in}	φ_{in}	Symbol	ρ_c	φ_c	ρ_{in}	φ_{in}
120	90°	31°06′	90°	31°04′	011	41°04′	0	41°05′	0°03′
110	90°	50 22′	90°	50°25′	102	27°44′	90°	27°50′	89°58′
210	90°	67°30′	90°	67°29′	121	63°50′	31°06′	63°50′	31°08′
310	90°	74°33′	90°	74°16′	121	116°10′	31°06′	116°10′	31°06′
100	90°	90°	90°	90°	111	53°50′	50°22′	53°43′	50°20′
010	90°	0	90°	0	111	126°10′	50°22′	126°17′	50°20′

TABLE 2

d, Å	I/I_1	hkl	d, Å	I/I_1	hkl	d, Å	I/I_1	hkl	d, Å	I/I_1	hkl
6.1085	2		1.8234	13		1.3037	2		1.0606	4	
5.7313	22	010	1.7693	46		1.2920	1		1.0584	3	
4.7051	26	100	1.7680	30		1.2663	3		1.0546	5	
3.7385	34	011	1.6980	28	221.202	1.2099	10		1.0293	5	
3.6391	38	110	1.6865	6		1.2051	5		1.0288	13	
2.9308	100	111	1.6639	6		1.2025	4		1.0100	9	
2.9159	98	111	1.5796	1	013	1.1943	4		0.9966	2	
2.8488	77	020	1.5621	2	300	1.1863	18		0.9891	3	
2.4947	40	002.021	1.5024	15	113	1.1853	20		0.9827	3	
2.4422	11	120	1.4963	14	113	1.1748	10		0.9783	5	
2.3476	16	200	1.4839	10		1.1481	3		0.9537	6	
2.2032	25	102	1.4663	9		1.1314	2		0.9519	5	
2.0570	4	112	1.4333	42		1.1110	17		0.9502	5	
2.0316	5	112	1.3896	39		1.1048	5		0.9493	4	
1.9811	6	211	1.3291	15		1.0854	15		0.9481	4	
1.9080	10		1.3184	14		1.0840	14		0.9369	6	
1.8675	10	022	1.3169	13		1.0795	10		0.9351	8	

TABLE 3. Atomic Coordinates in Zn Tungstate

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
W	0.000	0.179	0.250	O_1	0.220	0.110	0.950
Zn	0.500	0.674	0.250	O_2	0.260	0.380	0.390

TABLE 4. Interatomic Distances in $ZnWO_4$

Zn polyhedron			W polyhedron		
Distance, Å			Distance, Å		
Zn—O	2.14 (2)	O—O 2.88 (1)	W—O	1.83 (2)	O—O 2.86 (1)
	2.10 (2)	3.16 (2)		1.84 (2)	2.70 (2)
	2.06 (2)	2.84 (2)		2.18 (2)	2.78 (2)
O—O	2.82 (2)	2.86 (1)	O—O	2.48 (2)	2.87 (1)
	2.82 (2)	2.82 (2)		2.86 (2)	2.82 (2)

the method of [3] make group P2/c (C_{2h}^4) more probable.

Projections were used. The Patterson projections (simple and weighted) confirmed that the structure is of wolframite type [2, 4], with Zn and W on two-fold axes. The structure was refined via a series of electron-density projections. The O atoms were located from difference series. The xy and xz projections were used to refine the coordinates by least squares ($R_{hk0} = 9.4\%$, $R_{h0l} = 10.8\%$).

Table 3 gives the mean coordinates, while Table 4 gives the interatomic distances calculated from these.

Figure 3 shows the characteristic zigzag of Zn octahedra in projection along the b axis.

The Zn octahedra in $ZnWO_4$ are more nearly isometric than the analogous Ni and Cd ones in $NiWO_4$ [5] and $CdWO_4$ [6]. The W octahedra (as in other representatives of the wolframite type) have four short distances and two longer ones.

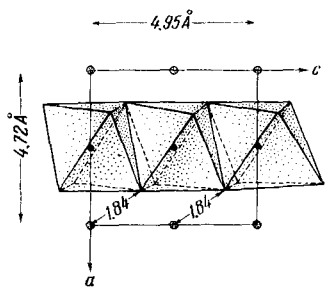

Fig. 3. Zigzag of Zn octahedra in $ZnWO_4$.

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