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MINERALOGICAL NOTES

The Unit Cell of Volborthite

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Abstract

Indexed powder diagrams of volborthite, $Cu_3(VO_4)_2 \cdot 3H_2O$, from Monument Valley, Arizona, disclose it to be monoclinic (space group *C*2, *Cm*, or *C*2/*m*), the unit cell [$a = 10.604(2)$, $b = 5.879(1)$, $c = 7.202(2)$ Å, $\beta = 94.81(2)°$][1] containing two formula units. Calculated density, 3.52 g/cm³, compares with 3.42 g/cm³, the value measured by Guillemin (1956).

Introduction

In the Mineralogical Museum, Copenhagen, Guinier-Hägg powder diffraction exposures have formed part of the routine examination of newly acquired mineral specimens since 1971. Such an examination of volborthite from Monument No. 1 Mine, Monument Valley, Navajo County, Arizona, permitted indexing of the pattern and thus, for the first time, determination of its unit cell. The specimen (M.M. No. 1972.307), according to Witkind (1961), originates from the outermost zone of oxidized minerals of the ore body, the mineral assemblage of which includes carnotite, hewettite, metatyuyamunite, rauvite, tyuyamunite, and volborthite. The specimen consists of a light gray siltstone matrix profusely covered on one side with olive green to citron yellowish-green microcrystalline globules of volborthite, some of which are themselves partly covered with numerous small crystals.

X-Ray Diffraction Data

Guillemin (1956) published an unindexed powder pattern of volborthite, which is reproduced by Joint Committee of Powder Diffraction Standards, card no. 12–523. No other diffraction data were found.

Our pattern is in excellent agreement with this standard, except for some splitting up of the lines due to the Guinier-technique. The pattern was readily indexed by the method of Ito (1950). Least squares refinement gave the following unit cell dimensions: $a_0 = 10.604 \pm 0.002$ Å, $b_0 = 5.879 \pm 0.001$ Å, $c_0 = 7.202 \pm 0.002$ Å, and $\beta = 94.81 \pm 0.02°$.

TABLE 1. X-Ray Diffraction Data for Volborthite

JCPDS, card no. 12-523		Present investigation[xx]				
Int.	d (Å)	Int.	$d_{obs.}$ Å	$10^4\ Q_{obs.}$ (Å^{-2})	$10^4\ Q_{calc.}$ (Å^{-2})	hkl
100	7.26	10	7.16	195.0	194.2	001
20	5.21	3	5.291	357.2	358.2	200
		4	5.136	379.1	378.9	110
		1	4.426	510.3	508.1	$20\bar{1}$
10	4.19[x]				550.9	$11\bar{1}$
10	4.03	5	4.103	594.1	595.2	111
					596.6	201
10	3.56	1	3.583	779.0	776.6	002
30	3.08	5	3.090	1047.1	1046.3	$20\bar{2}$
		4	3.022	1094.9	1095.4	310
40	2.98	5	2.998	1112.4	1111.2	$11\bar{2}$
		1	2.940	1157.3	1157.3	020
80	2.87	5	2.887	1199.8	1199.8	112
		5	2.859	1223.5	1223.1	$31\bar{1}$
					1223.4	202
20	2.71	5	2.722	1349.7	1351.4	021
					1355.9	311
20	2.64	7	2.643	1432.1	1432.9	400
80	2.56	7	2.571	1513.3	1515.5	220
		5	2.551	1537.2	1538.6	$40\bar{1}$
					1665.4	$22\bar{1}$
					1715.6	401
					1739.2	$31\bar{2}$
					1747.4	003
80	2.38	7	2.389	1752.2	1753.9	221
					1933.9	022
					1972.9	$20\bar{3}$
					2004.7	312
30	2.21	1	2.216	2036.3	2032.5	$40\bar{2}$
					2059.9	$11\bar{3}$
					2192.7	113
10	2.12[x]				2203.6	$22\bar{2}$
					2238.4	203
30	2.04	4	2.049	2381.9	2380.7	222
					2386.6	402
					2528.3	510
					2590.2	420
					2611.8	$51\bar{1}$
					2643.6	$31\bar{3}$
					2693.4	130
		1	1.9247	2699.3	2695.9	$42\bar{1}$
					2833.1	511
		1	1.8688	2863.3	2865.5	$13\bar{1}$
					2872.9	421
					2904.7	023
					2909.7	131
10	1.85	1	1.8521	2915.1	2914.8	$40\bar{3}$
					3041.9	313
		1	1.8021	3079.2	3083.6	$51\bar{2}$
30	1.78	2	1.7946	3105.0	3106.5	004
		3	1.7876	3129.2	3130.2	$22\bar{3}$
			1.7703	3191.0	3189.8	$42\bar{2}$
					3224.1	600
					3285.5	$60\bar{1}$
					3287.7	$20\bar{4}$
		3	1.7170	3392.2	3395.7	223
					3396.9	$11\bar{4}$
30	1.71				3409.9	330
		2	1.7081	3427.7	3425.8	$13\bar{2}$
					3445.9	403
					3514.3	132
30	1.67		1.6838	3527.1	3526.2	512
					3537.7	$33\bar{1}$
					3543.9	422

[x] *Lines in position of strong quartz lines.*

[xx] *Pattern obtained with Guinier Hägg focusing camera, radius 40.3 mm. CuKα_1 ($\lambda = 1.54051$ Å) radiation, Ni-filter, and curved crystal monochromator. Internal standard quartz. Intensities visually estimated. All possible Q-values below $Q_{calc} = 3550.0$ have been calculated.*

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[1] Numbers in parentheses represent estimated standard deviation in respect to the last decimal cited. (See *Am. Mineral.* **59,** 223.

The systematic reflection condition led to the space-groups *C*2, *Cm*, or *C*2/*m*. Multiple indexed lines were omitted from the least squares refinement. The formula $Cu_3(VO_4)_2 \cdot 3H_2O$, unit cell volume = 447.42 Å^3, and $Z = 2$, gives the calculated density $D_x = 3.52$ g/cm^3. Guillemin (1956) has measured the density as 3.42 g/cm^3.

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