

Wang, S. (1983) Some problems concerning geochemistry of the Dading tin-iron ore deposits. *Bull. Inst. Min. Deposits, Chinese Acad. Geol. Sci.* **9**, 72.

Zhao, Y. (1984) The characteristics of volatile components and alkaline metasomatism in main skarn-type iron deposits in China and their role in ore formation. *Geochem.* **3**, 14-23.

Zhiji, R. (1984) Geochemical characteristics of tin-bearing magnetite-skarns. *Ibid.* **3**, 115-27.

[Manuscript received 30 November 1987; revised 1 February 1988]

© Copyright the Mineralogical Society

KEYWORDS: szaibelyite, fluorborite, borate, skarn, Tasmania, Australia.

Department of Geology, La Trobe University, Bundoora, Victoria 3083, Australia

T. A. P. KWAK
M. NICHOLSON

MINERALOGICAL MAGAZINE, DECEMBER 1988, VOL. 52, PP. 716-17

The crystallography of munitrite, $\text{NaVO}_3 \cdot (2-x)\text{H}_2\text{O}$

RECENTLY in these pages a new vanadium mineral from Pakistan was described by Butt and Mahmood (1983), which they referred to as 'partially dehydrated' $\text{NaVO}_3 \cdot 2\text{H}_2\text{O}$, and which they named 'munitrite' (name was approved by the International Commission on New Minerals and Mineral Names). The key defining data offered was a set of X-ray powder data, which they could not identify with any known phase. Butt and Mahmood found that their data fit those of Lukács and Strusievici (1962), given unindexed for synthetic $\text{NaVO}_3 \cdot 1.9\text{H}_2\text{O}$. In fact, the X-ray data of Butt and Mahmood match closely those for synthetic $\text{NaVO}_3 \cdot 1.89\text{H}_2\text{O}$, for which the crystal structure has been refined with high precision by Björnberg and Hedman (1977). The latter authors found a monoclinic unit cell in space group $P2_1/a$, with $a = 16.756(2)$, $b = 3.6391(3)$, $c = 8.023(a)\text{Å}$, and $\beta = 111.18(1)^\circ$, as measured from Guinier-Hägg powder data (unpublished). The orthorhombic unit cell found by Butt and Mahmood using Ito's method for indexing unknown powder patterns has 2.7 times the volume of the true cell, and there is no apparent relationship between the two cells. A least-squares refinement using the d spacings of Butt and Mahmood leads to $a = 16.72(2)$, $b = 3.636(3)$, $c = 8.015(6)\text{Å}$, and $\beta = 111.0(1)^\circ$, in good agreement with Björnberg and Hedman. The $\sigma(2\theta)$ value for 22 reflections is 0.072° for this calculation.

Butt and Mahmood report a chemical analysis in which the Na/V ratio is close to unity, but the water content corresponds to about $0.8\text{H}_2\text{O}$ instead of $2\text{H}_2\text{O}$ or $1.9\text{H}_2\text{O}$. Yet the unit cell

volume for their X-ray data is $455.0(6)\text{Å}^3$, only slightly smaller than $456.17(8)\text{Å}^3$ found by Björnberg and Hedman. As this difference corresponds to about $0.05\text{H}_2\text{O}$, it is apparent that the sample analysed by Butt and Mahmood was not pure. None of the prominent reflections for $\alpha\text{-NaVO}_3$ or $\beta\text{-NaVO}_3$ (Morris *et al.*, 1981) correspond to those given for munitrite.

A set of powder data attributed to Björnberg are recorded on Card No. 32-1201 of the JCPDS Powder Data Files, which, together with powder data calculated from the crystal structure, establishes the identity of the compound studied by Björnberg and Hedman (1977) and munitrite. In this laboratory, powder data for synthetic $\text{NaVO}_3 \cdot 1.9\text{H}_2\text{O}$ have been obtained by the Guinier-Hägg method. These data are listed in Table 1, along with those of Butt and Mahmood (1983), Lukács and Strusievici (1962), and the JCPDS data for comparison. Least-squares refinement of the unit cell parameters based on the data obtained in this laboratory (Table 1) led to values in close agreement with those of Björnberg and Hedman. Some recrystallized preparations have been found to give X-ray patterns of inferior quality with some lines broadened or missing, presumably because of partial loss of water from the structure. It is not known how much water can be lost while the structure is retained. It is best to define the composition of munitrite as $\text{NaVO}_3 \cdot (2-x)\text{H}_2\text{O}$, where x may vary from 0 to about 0.2.

The structure consists of a monoclinic arrangement of metavanadate $(\text{VO}_3)_n$ chains whose ele-

Table 1. X-ray powder data for munitrite, $\text{NaVO}_3 \cdot (2-x)\text{H}_2\text{O}$

(1)		(2)		(3)		(4)		(5)		(6)		(7)						
h k l	d(obs)	d(obs)	d(obs)	d(obs)	d(calc)	I(rel)	2 θ (obs)	h k l	h k l	d(obs)	d(obs)	d(obs)	d(obs)	d(calc)	I(rel)	2 θ (obs)	h k l	
2 0 0	7.851	7.86	7.82	7.831	7.818	100	11.29	2 0 0	4 0 3			1.8261	1.8251		3	49.90	4 0 3	
0 0 1		7.53	7.48	7.478	7.482	12	11.82	0 0 1	0 2 0	1.8195	1.83	1.820	1.8194	1.8198	26	50.09	0 2 0	
$\bar{2}$ 0 1	6.744	6.81	6.77	6.778	6.758	30	13.05	$\bar{2}$ 0 1	2 2 0	1.7710	1.78	1.772	1.7727	1.7724	10	51.51	2 2 0	
$\bar{4}$ 0 1	4.1344	4.16	4.13	4.136	4.129	33	21.47	$\bar{4}$ 0 1	$\bar{2}$ 2 1			1.7565	1.7572		5	52.02	$\bar{2}$ 2 1	
4 0 0	3.9178	3.93		3.913	3.909	5	22.71	4 0 0	8 0 1			1.7429	1.7434			52.46	8 0 1	
0 0 2	3.7300	3.76	3.74	3.743	3.741	11	23.75	0 0 2	$\bar{4}$ 2 1	1.6639	1.67	1.664	1.6646	1.6653		55.13	$\bar{4}$ 2 1	
$\bar{4}$ 0 2	3.3694	3.40	3.38	3.382	3.379	13	26.33	$\bar{4}$ 0 2	0 1 4			1.6636					0 1 4	
2 1 0		3.2972	3.32	3.30	3.301	3.300	42	26.99	6 1 2			1.6479	1.6480		4	55.73	6 1 2	
0 1 1				3.27	3.272	3.273	36	27.33	$\bar{10}$ 0 3			1.6118	1.6120		4	57.09	$\bar{10}$ 0 3	
$\bar{2}$ 1 1				3.204	3.210		2	27.76	$\bar{4}$ 2 2			1.6030	1.6022		3	57.44	$\bar{4}$ 2 2	
4 0 1			3.04	3.043				4 0 1	$\bar{6}$ 0 5			1.5639	1.5639		3	59.01	$\bar{6}$ 0 5	
2 0 2	2.9843	3.00	2.98	2.983	2.982	24	29.93	2 0 2	2 2 2			1.552	1.5530	1.5533	5	59.47	2 2 2	
2 1 1	2.8506	2.88	2.86	2.864	2.862	16	31.20	2 1 1	$\bar{10}$ 1 1			1.503	1.5043	1.5063		7	61.60	$\bar{10}$ 1 1
$\bar{6}$ 0 1	2.7877	2.81		2.794	2.794	5	32.00	$\bar{6}$ 0 1	$\bar{2}$ 2 3			1.5040					$\bar{2}$ 2 3	
$\bar{4}$ 1 1	2.7207	2.73	2.73	2.732	2.730	11	32.75	$\bar{4}$ 1 1	$\bar{4}$ 1 5	1.4679	1.47	1.468	1.4676	1.4677	7	63.32	$\bar{4}$ 1 5	
$\bar{2}$ 1 2		2.6847	2.70	2.69	2.686	2.686	39	33.33	$\bar{6}$ 1 5			1.437	1.4363	1.4369	3	64.86	$\bar{6}$ 1 5	
$\bar{2}$ 0 3			2.69	2.67	2.673	2.671	34	33.50	4 2 2			1.4301	1.4312	1.4306		4	65.18	4 2 2
4 1 0		2.64		2.663	2.664	13	33.62	4 1 0	10 0 1			1.3425	1.3425	1.3428		9	70.02	$\bar{4}$ 2 4
$\bar{6}$ 0 2			2.63	2.630	2.629	5	34.06	$\bar{6}$ 0 2	$\bar{2}$ 2 4			1.3425					$\bar{2}$ 2 4	
6 0 0		2.6127	2.62	2.61	2.604	2.606	7	34.40	$\bar{6}$ 2 5			1.1867	1.1851		2	81.03	$\bar{6}$ 2 5	
4 0 2	2.3207	2.33		2.3166	2.3172	2	38.84	4 0 2										
$\bar{2}$ 1 3			2.15	2.1533	2.1535	1	41.92	$\bar{2}$ 1 3										
$\bar{6}$ 1 2	2.1301	2.14	2.13	2.1310	2.1301	5	42.40	$\bar{6}$ 1 2										
$\bar{4}$ 1 3		2.0879		2.0956	2.0956	3	43.13	$\bar{4}$ 1 3										
8 0 1				2.0826	2.0836	5	43.41	8 0 1										
0 1 3				2.0563	2.0573	4	44.00	0 1 3										
$\bar{4}$ 0 4		1.9872	1.99	1.991	1.9886	1.9886	21	45.58	$\bar{4}$ 0 4									
$\bar{2}$ 0 4				1.9886				$\bar{2}$ 0 4										
4 1 2				1.9553	1.9547	4	46.40	4 1 2										
$\bar{6}$ 1 3			1.916	1.9155				$\bar{6}$ 1 3										
6 1 1	1.8934	1.90	1.897	1.8978	1.8979	14	47.89	6 1 1										
0 0 4				1.8702	1.8705	7	48.64	0 0 4										

Col. 1: Data of Butt and Mahmood (1983). The implied accuracy is evidently grossly exaggerated.

Col. 2: Data of Lukács and Strusievici (1962).

Col. 3: Data of Björnberg, from JCPDS Powder Data File Card No. 32-1200.

Col. 4: This work: Guinier-Högg method, $\text{CuK}\alpha_1$ radiation ($\lambda=1.54056 \text{ \AA}$), Si internal standard NBS SRM 640 ($a=5.4308 \text{ \AA}$).

Col. 5: Spacings calculated by least-squares analysis of data of col. 7; $\sigma(2\theta)=0.018^\circ$.

Col. 6: Intensities measured with Nonius Microdensitometer Model II from pattern of col. 4. Intensities for cols. 1, 2, 3 are comparable.

Col. 7: Data measured from pattern of col. 4.

ments are square pyramids linked in a zig-zag manner by sharing edges. The chain structure is consistent with the soft, fibrous character of the synthetic compound (crystallized from water at room temperature) and the radiating, fibrous habit as described for munitrite by Butt and Mahmood (1983).

References

Björnberg, A. and Hedman, B. (1977) *Acta Chem. Scand.* **A31**, 579-84.

KEYWORDS: munitrite, vanadate, crystallography.

Butt, K. A. and Mahmood, K. (1983) *Min. Mag.* **47**, 391-2.

Lukács, I. and Strusievici, C. (1962) *Z. anorg. allgem. Chem.* **315**, 323-6.

Morris, M. C., McMurdie, H. F., Evans, E. H., Paretzkin, B., Parker, H. S., and Panagiotopoulos, N. C. (1981) Standard X-ray diffraction powder patterns. *National Bureau of Standards Monograph* **25**, no. 18, pp. 67, 68.

[Manuscript received 11 January 1988; revised 18 February 1988]

© Copyright the Mineralogical Society