American Mineralogist, Volume 58, pages 1080–1081, 1973

Unit Cell and X-Ray Powder Data for Metasideronatrite

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Abstract

The indexed powder pattern of metasideronatrite, $Na_4Fe_2(SO_4)_4(OH)_2 \cdot 3H_2O$, agrees well with the refined unit cell dimensions $a = 7.357$, $b = 16.002$, and $c = 7.102$ Å and space group *Pbnm or Pbn*2_1. A comparison of powder data for natural metasideronatrite and that produced from sideronatrite by dehydration over sulphuric acid by Cesbron (1964) shows some differences, possibly due to a difference in water content. Powder data for metasideronatrite and sideronatrite, $Na_4Fe_2(SO_4)_4(OH)_2 \cdot 6H_2O$ are distinctly different.

Metasideronatrite, $Na_4Fe_2(SO_4)_4(OH)_2 \cdot 3H_2O$, was first described by Bandy (1938). The mineral from Chuquicamata, Chile, was described as having a golden to straw yellow color and a fibrous habit. An analysis by E. P. Henderson provided the above formula, which is similar to that of sideronatrite, $Na_4Fe_2(SO_4)_4(OH)_2 \cdot 6H_2O$. According to Bandy (1938), metasideronatrite can be produced by dehydration of sideronatrite over sulfuric acid. However, Bandy stated that it was uncertain whether the natural metasideronatrite had ever undergone dehydration. Cesbron (1964) published unit cell and powder data for sideronatrite and powder data for metasideronatrite. For his work, Cesbron produced the metasideronatrite by the method discussed by Bandy.

The type collection at Colorado School of Mines contains an excellent specimen of metasideronatrite, T.M. 68·90, from Chuquicamata. The habit and color are the same as described by Bandy, and $\gamma = 1.634$ measured on fragments of the material agrees closely with the value 1.635 obtained by Bandy. The refractive index γ was chosen for measurement because it significantly exceeds any index for sideronatrite and thus aids in identification.

Single crystal Weissenberg and precession photographs of our sample showed the metasideronatrite to be orthorhombic with $a = 7.32$, $b = 15.95$ and $c = 7.09$ Å. The space group is either *Pbnm* or *Pbn*2_1 based on systematic absences, $0kl$: $k = 2n + 1$; $h0l$: $h + l = 2n + 1$, the orientation concurring with that given by Cesbron (1964) for the unit cell of sideronatrite which, incidentally, belongs to the same space group. Powder data obtained from Fe($K\alpha$) films were refined and indexed by the program of Evans, Appleman, and Handwerker (1963). The refined unit cell is $a = 7.357(3)$, $b = 16.002(4)$, and $c = 7.102(8)$.

TABLE 1. X-ray Powder Data for Metasideronatrite and Sideronatrite

Metasideronatrite						Sideronatrite			
	This paper			Cesbron (1964)			Cesbron (1964)		
h k l	d_{calc}	d_{obs}	I/I_o	d_{obs}	I/I_o	*h k l*	d_{obs}	I/I_o
0 2 0	8.001	8.051	90	7.93	60	0 2 0	10.2	100
1 1 0	6.684	6.682	70	6.63	40	1 1 0	6.78	40
1 2 0	5.415	5.412	20					
0 2 1	5.311	5.310	10	5.28	30	0 2 1	5.86	30
1 0 1	5.109	5.118	10	5.10	30	1 0 1	5.00	20
1 1 1	4.867	4.865	20	4.84	40			
1 2 1	4.306	4.303	15	4.29	30			
0 4 0	4.000	3.994	30	3.98	10			
2 0 0	3.678	3.680	100	3.66	100	2 1 0	3.58	40
0 0 2	3.551	--	--	3.54	5	0 0 2		
0 4 1	3.485	3.485	40	3.47	30			
						0 2 2	3.38	60
						1 5 1		
1 4 1	3.150	3.151	25	3.18	40	1 1 2	3.18	20
1 1 2 (?)	3.136	--	--	3.10	60	1 6 0	3.12	20
2 3 0	3.028	3.027	10	3.01	10	1 2 2	3.05	5
2 2 1	3.024					2 4 0	3.01	80
1 5 0	2.935	2.936	15	2.92	5			
						1 6 1	2.86	5
2 3 1	2.785	2.784	10	2.78	5			
1 3 2	2.743	2.749	50	2.73	80			
1 5 1	2.712	2.711	5			1 7 0	2.68	60
0 6 0	2.667	2.665	50	2.65	20	1 7 1		
2 1 2 (?)	2.523	--	--			2 5 1	2.54	10
1 6 0 (?)	2.507	--	--	2.51	10			
1 4 2	2.498	2.499	20	2.48	10	2 6 0	2.49	10
3 1 0	2.424	2.423	20	2.41	20	3 1 0	2.44	10
						2 3 2	2.38	20
3 0 1	2.318	2.313	5					
2 5 1	2.286	2.287	10					
3 3 0	2.228	2.227	20			1 1 3	2.25	10
3 2 1	2.226							
1 7 0	2.183	2.183	10					
2 6 0	2.159	2.161	5					

Intensities are relative.

The density measured by Bandy was 2.46 on natural material; however a measurement of the density of a 12.5 mg fragment of the T.M. 68·90 material produced a value of 2.68 by careful soaking of the fragment in toluene after weighing in air. From this measurement the unit cell contents are determined to be $Na_8Fe_4(SO_4)_8(OH)_4 \cdot 6H_2O$. Using this formula and the refined unit cell, density is calculated as 2.68 also.

The powder data for our metasideronatrite, that synthetic material of Cesbron, and his sideronatrite are compared in Table 1. There are some slight differences in line position for the two metasideronatrite patterns, possibly indicating a difference in water content between the synthetic and natural materials. There is, however, no other evidence to substantiate any difference in hydration state.

References

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Manuscript received, June 15, 1973; accepted for publication, July 24, 1973.