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X-RAY CRYSTALLOGRAPHY AND CRYSTAL CHEMISTRY OF GOWERITE, $CaO \cdot 3B_2O_3 \cdot 5H_2O$*

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The new mineral gowerite, $CaO \cdot 3B_2O_3 \cdot 5H_2O$, was recently described by Erd, McAllister, and Almond (1959). The present note gives the results obtained from an *x*-ray study of single crystals of gowerite. The crystals were examined on a quartz-calibrated precession camera, using Cu/Ni radiation ($\lambda CuK\alpha = 1.5418$ Å); film measurements were corrected for both horizontal and vertical shrinkage. The following crystallographic data were obtained: monoclinic, $P2_1/n$-C_{2h}^5 (no. 14), $a = 11.03 \pm 0.04$, $b = 16.40 \pm 0.05$, $c = 6.57_7 \pm 0.02$ Å, $\beta = 90°56' \pm 05'$, $a:b:c = 0.673:1:0.401$; cell volume 1190 Å^3; calculated density 1.98_2 g. cm.$^{-3}$ for cell contents $4[CaO \cdot 3B_2O_3 \cdot 5H_2O]$, observed specific gravity 2.00 ± 0.01 (Erd *et al.*, 1959). An alternative description of the unit cell is $P2_1/a$, $a = 12.93$, $b = 16.40$, $c = 6.57_7$ Å, $\beta = 121°30'$, $a:b:c = 0.788:1:0.401$. The transformation from the $P2_1/a$ to the $P2_1/n$ setting is given by the matrix 101/010/001.

The morphology of gowerite crystals and a sketch of a typical crystal are given by Erd *et al.* (1959). The crystals used in the present study can be described, in accordance with either the $P2_1/a$ or $P2_1/n$ setting, as follows: prismatic needles, elongated [001], flattened on {010}, with small {100}, {110}, {140}, and terminating form, for $P2_1/n$, {111}, optical orientation $Y = b$, $Z \wedge c = 27°$. The present description is the same as that given by Erd *et al.* (1959), except that these authors called the terminating form {001?}.

An *x*-ray powder pattern of gowerite was taken with Cu/Ni radiation in a 114.59 mm. diameter camera and the measurements from the resulting film were corrected for shrinkage. Interplanar spacings were calculated from the single crystal data for $d \geq 2.250$ Å and indexed on the $P2_1/n$ orientation; the powder film results, and the diffractometer results of Erd *et al.* (1959) are compared in Table 1.

It has been pointed out (Christ, 1959) that crystals of formula $MO \cdot 3B_2O_3 \cdot xH_2O$ (where M represents a bivalent cation) may be explained by postulating either discrete polyions of composition $[B_3O_3(OH)_4]^{-1}$, or polymerization products resulting from these polyions by the splitting out of water. This structural unit, consisting of two boron-oxygen triangles and a boron-oxygen tetrahedron linked at corners

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TABLE 1. *X*-RAY POWDER DATA FOR GOWERITE, $CaO \cdot 3B_2O_3 \cdot 5H_2O$

Monoclinic $P2_1/n-C_{2h}^5$: $a=11.03\pm0.04$, $b=16.40\pm0.05$, $c=6.57_7\pm0.02$ Å; $\beta=90°56'\pm05'$

Measured				Calculated[1]	
Erd *et al.* (1959)[2]		Present Study[3]		d_{hkl}	hkl
I	d_{hkl}	I	d_{hkl}		
2	9.18	25	9.2_0	9.15	110
10	8.23	100	8.2_3	8.20	020
<1	6.61	5	6.5_7	6.58	120
		2	6.0_7	6.10	011
<1	5.64	2	5.64	5.689	$\bar{1}01$
				5.608	101
<1	5.52			5.513	200
1	5.40	5	5.37	5.374	$\bar{1}11$
				5.306	111
				5.225	210
1	5.15	5	5.13	5.130	021
1	4.91	5	4.89	4.898	130
				4.674	$\bar{1}21$
				4.629	121
				4.575	220
				4.204	031
				4.122	$\bar{2}11$
5	4.11	20	4.09_4	4.100	040
2	4.07			4.061	211
<1	3.95		3.94_5	3.942	$\bar{1}31$
1	3.92	10b		3.914	131
1	3.88		to	3.882	230
2	3.85		3.83_6	3.843	140
				3.779	$\bar{2}21$
<1	3.74	2	3.72_4	3.732	221
				3.586	310
				3.479	041
				3.360	$\bar{2}31$
1	3.36	10	3.34_5	3.354	320
<1	3.32			3.326	231, $\bar{1}41$
				3.310	141
				3.290	240
				3.288	002
1	3.23	2	3.22_8	3.230	$\bar{3}01$
				3.224	012

[1] All calculated interplanar spacings listed for $d_{khl} \geq 2.250$ Å.

[2] *X*-ray diffractometer data, unfiltered Fe radiation, only lines due to FeKα, $\lambda=1.9373$ Å, are given.

[3] Corrected for shrinkage; b=broad. Radiation: Cu/Ni, λCuK$\alpha=1.5418$ Å. Lower limit of 2θ measurable, approximately 7° (13 Å). Film no. 13540. Camera diameter, 114.59 mm.

TABLE 1 (*continued*)

Measured				Calculated[1]	
Erd *et al.* (1959)[2]		Present Study[3]		d_{hkl}	hkl
I	d_{hkl}	I	d_{hkl}		
6	3.19	45	3.18_6	3.186	301
				3.170	$\bar{3}11$
2	3.15	2	3.13_9	3.144	150
				3.128	311
				3.108	$\bar{1}12$
				3.081	112
1	3.06	5	3.04_9	3.052	022
				3.050	330
<1	3.01			3.006	$\bar{3}21$
1	2.97			2.970	321
<1	2.96	10	2.960	2.954	$\bar{2}41$
				2.953	$\bar{1}22$
				2.935	051
1	2.93			2.931	241
				2.930	122
				2.844	$\bar{2}02$
				2.841	$\bar{1}51$
				2.831	151
1	2.82	10	2.816	2.819	250
				2.818	032
				2.804	202
				2.802	$\bar{2}12$
				2.781	$\bar{3}31$
1	2.77	10	2.768	2.764	212
				2.756	400
				2.753	331
				2.739	$\bar{1}32$
				2.737	340
4	2.73	25	2.728	2.733	060
				2.721	132
				2.718	410
				2.687	$\bar{2}22$
2	2.65	10	2.648	2.653	160, 222
				2.613	420
				2.599	$\bar{2}51$
				2.583	251
				2.565	042
1	2.54	5	2.531	2.537	$\bar{3}41$
				2.526	$\bar{4}11$
				2.524	061
				2.523	$\bar{2}32$
				2.516	341
				2.505	$\bar{1}42$
<1	2.50			2.498	411
				2.495	232
				2.491	142

TABLE 1 (*continued*)

Measured				Calculated[1]	
Erd *et al.* (1959)[2]		Present Study[3]		d_{hkl}	*hkl*
I	d_{hkl}	I	d_{hkl}		
				2.464	$\bar{1}61$
<1	2.46	2	2.458	2.461	430
				2.457	161
				2.449	260
				2.447	350
				2.443	$\bar{3}12$
				2.441	$\bar{4}21$
				2.415	421
				2.405	312
				2.365	$\bar{3}22$
		2	2.334	2.337	$\bar{2}42$
				2.331	322
				2.322	052
				2.316	$\bar{4}31$
				2.314	242
				2.302	$\bar{3}51$
				2.300	$\bar{2}61$
1	2.29	10	2.294	2.294	431
				2.292	170
				2.289	261
				2.287	440
				2.285	351
				2.278	$\bar{1}52$
				2.267	152
				2.251	$\bar{3}32$
1	2.17	5	2.165		
1	2.13	5	2.128		
<1	2.11	5	2.109		
<1	2.08	2	2.079		
1	2.06	5	2.060		
<1	2.05				
<1	2.00	5	2.015		
<1	1.995	5	1.998		
		2	1.966		
<1	1.946	2	1.942		
<1	1.924				
<1	1.896	5b	1.895		
<1	1.868				
<1	1.865	2b	1.861		
1	1.797	5b	1.795		
<1	1.755	2	1.756		
1	1.730	5b	1.726		
1	1.590	plus additional lines, all with I≤2			
plus additional lines all with I<1					

to form a ring, would be analogous to the one triangle-two tetrahedra ring found, e.g., in meyerhofferite, $CaB_3O_3(OH)_5 \cdot H_2O$, (Christ and Clark 1956) and the two triangles-two tetrahedra ring found in borax, $Na_2B_4O_5(OH)_4 \cdot 8H_2O$, (Morimoto, 1956). It has, in fact, been postulated that discrete $[B_3O_3(OH)_4]^{-1}$ polyions exist in aqueous solutions (Ingri, Lagerström, Frydman, and Sillén, 1957), and that monoclinic metaboric acid, HBO_2, contains infinite chains of composition $[B_3O_4(OH)_2]_n^{-n}$ (Zachariasen, 1952).

For gowerite, the space group $P2_1/a$ (or $P2_1/n$) and the unit-cell contents $4[CaO \cdot 3B_2O_3 \cdot 5H_2O]$ are consistent with the presence of insular polyions, $[B_3O_3(OH)_4]^{-1}$, dimers, $[B_6O_7(OH)_6]^{-2}$, or infinite chains, $[B_3O_4(OH)_2]_n^{-n}$. The structural formulas corresponding to these three possibilities would be for gowerite, $Ca[B_3O_3(OH)_4]_2 \cdot H_2O$, $CaB_6O_7(OH)_6 \cdot 2H_2O$, and $Ca[B_3O_4(OH)_2]_2 \cdot 3H_2O$, respectively. The determination of the crystal structure of gowerite is currently in progress by the present authors.

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