

The crystal structure of lawsonbauerite, $(\text{Mn},\text{Mg})_9\text{Zn}_4(\text{SO}_4)_2(\text{OH})_{22} \cdot 8\text{H}_2\text{O}$, and its relation to mooreite¹

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Abstract

Lawsonbauerite, $(\text{Mn},\text{Mg})_9\text{Zn}_4(\text{SO}_4)_2(\text{OH})_{22} \cdot 8\text{H}_2\text{O}$, is monoclinic, space group $P2_1/c$ with $a = 10.50(5)\text{\AA}$, $b = 9.64(5)\text{\AA}$, $c = 16.41(8)\text{\AA}$, $\beta = 95.21(10)^\circ$, and $Z = 2$. Like the closely related mineral mooreite, it contains brucite-like sheets of octahedrally coordinated Mg and Mn atoms; in lawsonbauerite, the sheets are parallel to (100). Two ninths of the sites are vacant, and oxygen atoms of the vacant sites are coordinated to tetrahedrally bonded zinc atoms above and below the sheet. Zinc atoms on adjacent sheets are bonded in a "cis" arrangement to an interlayer $[(\text{Mn},\text{Mg})(\text{OH})_2(\text{H}_2\text{O})_4]^{2-}$ octahedron, which provides the only linkage between successive sheets. Sulphate groups present in the inter-sheet region are loosely held by hydrogen bonds. Apart from its chemistry lawsonbauerite differs from mooreite by having more vacancies in the octahedral layer, and therefore a different arrangement of vacancies, zinc tetrahedra, and interlayer cations. The revision of the lawsonbauerite formula required by this structure analysis should also be applied to the isostructural mineral torreyite, which has $\text{Mg} > \text{Mn}$.

Introduction

Lawsonbauerite, previously defined as $(\text{Mn},\text{Mg})_5\text{Zn}_2(\text{SO}_4)(\text{OH})_{12} \cdot 4\text{H}_2\text{O}$, is a rare mineral found in only a few specimens from the Sterling Hill Mine, Ogdensburg, Sussex Co., New Jersey (Dunn *et al.*, 1979). Its formula implies close similarity to mooreite, $\text{Mg}_{9.1}\text{Mn}_{1.9}\text{Zn}_{4.0}(\text{SO}_4)_2(\text{OH})_{26} \cdot 8\text{H}_2\text{O}$, a rare mineral also found only at Sterling Hill (Bauer and Berman, 1929; Hill, 1980). The mooreite structure is based on brucite-like layers of octahedrally coordinated Mg and Mn cations with some vacant sites. Zinc atoms on both sides of the layer are bonded to hydroxyls around the vacant octahedral sites. The tetrahedral zinc atoms of adjacent layers are bonded through interlayer $\text{Mn}(\text{OH})_2(\text{H}_2\text{O})_4^{2-}$ and SO_4^{2-} groups (Hill, 1980). In order to determine the specific relations between lawsonbauerite and mooreite, a structure solution was attempted using a specimen of type lawsonbauerite, kindly provided by Mr. P. Dunn.

Experimental

Lawsonbauerite is monoclinic with space group $P2_1/c$. Lattice parameters are $a = 10.50(5)\text{\AA}$, $b =$

$9.64(5)\text{\AA}$, $c = 16.41(8)\text{\AA}$, $\beta = 95.21(10)^\circ$, $Z = 2$, as determined using Weissenberg and precession methods (Dunn *et al.*, 1979).

Intensity data were obtained from a fragment of a platy crystal, measuring $0.21 \times 0.19 \times 0.06$ mm, mounted for rotation about the b axis. Intensities were measured with a Supper-Pace diffractometer, which utilizes Weissenberg equinclination geometry, by scanning across a diffraction and measuring backgrounds on either side. $\text{MoK}\alpha$ radiation was used, and was monochromated with a flat graphite crystal, and detected with a scintillation counter. Intensities of 3045 symmetry-independent reflections ranging from $k = 0$ to $k = 9$ and with $\sin \theta < 0.46$ were measured, although mechanical limitations imposed more severe constraints on the higher levels. Of the reflections, 809 had intensities below observable limits. Data were corrected for Lorentz, polarization, and absorption effects ($\mu = 58.1 \text{ cm}^{-1}$) with a modified version of the program ABSRP written by Dr. C. W. Burnham. No extinction corrections were applied.

The first attempt to solve the structure was through a three-dimensional Patterson function, whose features confirmed the presence of a brucite-like sheet. Further study of the Patterson function was inconclusive, and the structure was therefore

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solved by direct methods using the computer program MULTAN (Main *et al.*, 1971). Two possible solutions were generated, one of which was clearly compatible with the presence of a brucite-like sheet having octahedral vacancies. With this solution, and reasonable crystal-chemical constraints, all atoms except those in the sulfate group were immediately located. At this point in the solution, it became apparent that the published chemical formula for lawsonbauerite was in error, and that the unit cell contains 18 (Mn,Mg) cations rather than 20 as previously reported (Dunn *et al.*, 1979). Refinement proceeded normally using the computer program RFIN2 (Finger and Prince, 1975) with neutral atom scattering factors of Doyle and Turner (1968) and the weighting scheme of Cruickshank (1965, p. 114). Atoms of the sulfate tetrahedron were located with a difference electron density function. In the final stages of refinement, atom site occupancies for octahedral cations were refined to determine occupancy of Mn and Mg. The overall M-cation occupancy refined to 69% Mn and 31% Mg, close to the 63% Mn found by electron microprobe chemical analysis (Dunn *et al.*, 1979). The final cycles of refinement involved determination of anisotropic temperature factors for oxygens of the sulfate group, as they were the only atoms expected to show significant anisotropy by analogy with the structure of mooreite (Hill, 1980). Hydrogen atoms were not directly located and therefore were not included in the refinement.

The final residuals were $R = 11.7\%$ ($R_w = 20.1\%$) for all reflections, and $R = 7.5\%$ ($R_w = 10.6\%$) for unrejected reflections. Rejected reflections included 809 for which F was less than the minimum observable, and 122 for which the individual R values were greater than 0.5. Of the latter reflections, all were less intense than 4 times the minimum observable limit, and 100 had intensities less than twice the minimum observable limit.

The final values of structure factors are listed in Table 1.² Atomic coordinates, isotropic temperature factors, and Mn occupancies are listed in Table 2. Anisotropic temperature factors for O(16)–O(19) are listed in Table 3.² Bond distances and angles were computed using the program ORFFE (Busing *et al.*, 1964) and selected values appear in Table 4.

Table 2. Final atom positions, isotropic temperature factors, and Mn occupancies

Atom	x	y	z	$B(\text{\AA}^2)$	% Mn Occupancy
M(1)	0	0	0	1.34(5)	71(1)
M(2)	.1551(2)	.3340(2)	.9999(1)	1.43(4)	62(1)
M(3)	.0123(2)	.1676(2)	.1688(1)	1.40(4)	68(1)
M(4)	.0025(2)	.4998(2)	.1672(1)	1.35(4)	70(1)
M(5)	.5021(2)	.4582(2)	.3006(1)	1.36(4)	74(1)
Zn(1)	.1828(2)	.3355(1)	.3466(1)	1.39(3)	
Zn(2)	.8372(1)	.3329(1)	.3237(1)	1.46(3)	
O(1)	.1060(8)	.1602(9)	.0611(5)	1.88(12)	
O(2)	.1029(8)	.5077(9)	.0613(5)	2.11(14)	
O(3)	.1182(7)	.0037(9)	.2303(5)	1.71(12)	
O(4)	.1270(8)	.3351(9)	.2290(5)	1.90(13)	
O(5)	.1164(7)	.5067(9)	.3951(5)	1.79(13)	
O(6)	.1290(7)	.1594(9)	.3965(5)	1.51(12)	
O(7)	.9136(7)	.3314(8)	.1080(5)	1.60(12)	
O(8)	.8964(8)	.1646(9)	.2690(5)	1.86(13)	
O(9)	.8943(7)	.3321(8)	.4404(5)	1.68(12)	
O(10)	.3714(8)	.3269(9)	.3536(5)	1.90(13)	
O(11)	.6481(7)	.3083(9)	.3070(5)	1.63(12)	
O(12)	.3895(8)	.3966(10)	.1733(5)	2.54(15)	
O(13)	.6250(8)	.1284(11)	.1939(6)	2.83(16)	
O(14)	.3950(8)	.0419(10)	.0825(5)	2.46(15)	
O(15)	.3850(8)	.0723(9)	.2870(5)	2.16(14)	
S	.5973(2)	.3148(3)	.0138(2)	1.58(5)	
O(16)	.6250(8)	.1260(10)	.4350(5)	2.41(15) ¹	
O(17)	.6656(8)	.1804(9)	.0240(5)	2.15(14) ¹	
O(18)	.6453(8)	.4074(10)	.0183(6)	2.62(15) ¹	
O(19)	.4586(8)	.2888(10)	.0164(5)	2.24(14) ¹	

¹ Equivalent isotropic temperature factor.

Because hydrogen atoms could not be located on difference electron density or electron density functions, their locations were inferred from crystal chemical constraints. The oxygen atoms associated with the brucite-like layer and the zinc tetrahedra, O(1)–O(11), are deduced to be hydroxyls from consideration of local charge balance as shown in Table 5 based on the method of Donnay and Allmann (1970), and analogy with the structures of brucite and mooreite (Hill, 1980). The oxygen atoms coordinated to the sulfur, O(16)–O(19), are assumed to form a SO_4 group, and thus have no associated hydrogen atoms. The remaining four oxygens, O(12)–O(15), are loosely coordinated around the interlayer M(5) cation, and are inferred to be H_2O molecules from their weak bonds, charge balance considerations, and from analogy with mooreite wherein the proton positions were determined directly, and refined (Hill, 1980). The system of hydrogen bonding is discussed below.

Description of structure

Octahedral layer

The basic structural units of lawsonbauerite are brucite-like sheets of Mn and Mg cations in octahedral coordination with hydroxyl ions. Two out of nine possible octahedral sites are vacant, in the pattern shown in Figure 1, resulting in bands of brucite-like structure oriented parallel to [010] and

²To receive a copy of Table 1 and Table 3, order document AM-82-209 from the Business Office, Mineralogical Society of America, 2000 Florida Ave. NW, Washington, D.C. 20009. Please remit \$1.00 in advance for microfiche.

Table 4. Selected interatomic distances and angles

M(1) Octahedron		M(5) Octahedron							
M(1) - 0(1)x2	2.106(8)	0(1) - 0(9)x2	2.853(12)	84.2(3)	M(5) - 0(11)	2.104(8)	0(11) - 0(10)	3.087(11)	94.0(3)
0(9)x2	2.149(8)	0(9)x2	3.157(11)	95.8(3)	0(10)	2.116(8)	0(15)	2.978(12)	86.5(3)
0(5)x2	2.209(8)	0(5)x2	3.182(11)	85.0(3)	0(13)	2.123(10)	0(14)	2.953(12)	84.8(3)
		0(5)x2	2.916(11)	95.0(3)	0(15)	2.240(8)	0(12)	3.451(12)	100.2(3)
average=2.155		0(9) - 0(5)x2	3.134(11)	91.9(3)	0(14)	2.271(9)	0(10) - 0(13)	3.006(13)	90.3(4)
		0(5)x2	3.029(11)	88.1(3)	0(12)	2.389(9)	0(14)	3.313(12)	98.0(3)
					average=2.215		0(13) - 0(15)	3.123(13)	91.4(3)
							0(14)	3.021(13)	86.8(4)
							0(12)	3.183(14)	87.9(4)
							0(15) - 0(14)	3.394(12)	97.6(3)
							0(12)	2.942(12)	78.9(3)
M(2) Octahedron		Zn(1) Tetrahedron							
M(2) - 0(2)	2.121(9)	0(2) - 0(1)	3.343(13)	103.6(3)	Zn(1) - 0(4)	1.973(8)	0(4) - 0(10)	3.146(11)	105.4(3)
0(1)	2.133(8)	0(2)	2.830(17)	82.8(4)	0(10)	1.982(8)	0(5)	3.208(11)	108.2(3)
0(2)	2.160(9)	0(7)	2.780(12)	80.9(3)	0(5)	1.986(8)	0(6)	3.235(11)	109.5(3)
0(7)	2.163(8)	0(6)	3.189(11)	96.0(3)	0(6)	1.989(8)	0(10) - 0(5)	3.319(11)	113.5(3)
0(6)	2.169(8)	0(1) - 0(7)	2.776(11)	80.5(3)			0(6)	3.154(11)	105.2(3)
0(9)	2.218(8)	0(6)	3.248(11)	98.0(3)	average=1.982		0(5) - 0(6)	3.344(12)	114.5(3)
average=2.161		0(9)	2.853(12)	81.9(3)					
		0(2) - 0(7)	3.181(11)	94.8(3)					
		0(6)	2.983(11)	87.1(3)					
		0(9)	3.121(12)	90.9(3)					
		0(7) - 0(9)	3.170(11)	92.7(3)					
		0(6) - 0(9)	3.119(11)	90.6(3)					
M(3) Octahedron		Zn(2) Tetrahedron							
M(3) - 0(7)	2.093(8)	0(7) - 0(1)	2.776(11)	82.7(3)	Zn(2) - 0(3)	1.946(8)	0(3) - 0(9)	3.254(10)	112.7(3)
0(1)	2.109(8)	0(8)	3.120(11)	94.9(3)	0(9)	1.962(8)	0(8)	3.266(12)	112.5(3)
0(3)	2.134(8)	0(4)	2.867(12)	83.8(3)	0(8)	1.982(8)	0(11)	3.202(10)	108.4(3)
0(8)	2.142(8)	0(5)	3.140(12)	92.4(3)	0(11)	2.001(8)	0(9) - 0(8)	3.253(11)	111.2(3)
0(4)	2.196(8)	0(1) - 0(3)	3.162(11)	96.3(3)	average=1.973		0(11)	3.252(11)	110.3(3)
0(5)	2.256(8)	0(4)	3.229(11)	97.2(3)			0(8) - 0(11)	3.075(11)	101.1(3)
average=2.155		0(5)	2.916(11)	83.8(3)					
		0(3) - 0(8)	2.922(12)	86.2(3)					
		0(4)	3.190(12)	94.9(3)					
		0(5)	3.076(12)	88.9(3)					
		0(8) - 0(4)	3.053(11)	89.5(3)					
		0(5)	3.095(11)	89.4(3)					
M(4) Octahedron		S Tetrahedron							
M(4) - 0(7)	2.070(8)	0(7) - 0(2)	2.780(12)	83.1(3)	S - 0(16)	1.472(9)	0(16) - 0(18)	2.422(12)	110.4(6)
0(2)	2.123(8)	0(3)	3.181(11)	96.1(3)	0(18)	1.477(9)	0(17)	2.385(13)	107.7(5)
0(8)	2.133(9)	0(4)	2.867(12)	83.2(3)	0(17)	1.482(9)	0(19)	2.444(12)	111.4(5)
0(3)	2.206(8)	0(6)	3.187(11)	94.6(3)	0(19)	1.487(9)	0(18) - 0(17)	2.396(12)	108.1(5)
0(4)	2.242(9)	0(2) - 0(8)	3.178(11)	96.6(3)			0(19)	2.436(13)	110.5(5)
0(6)	2.262(8)	0(4)	3.215(11)	94.8(3)	average=1.480		0(17) - 0(19)	2.411(12)	108.6(5)
average=2.173		0(6)	2.983(11)	85.7(3)					
		0(8) - 0(3)	2.922(11)	84.6(3)					
		0(4)	3.180(12)	93.2(3)					
		0(6)	3.081(12)	98.0(3)					
		0(3) - 0(4)	3.190(11)	91.0(3)					
		0(6)	3.115(11)	88.4(3)					

separated by bands of vacant sites. The octahedral layer is 2.24 Å thick away from the vacancies and 2.69 Å thick across the vacant site, giving the octahedral layer a periodic thickening and thinning along [001]. The M(1) and M(2) octahedra are quite regular, with M–O bond lengths ranging from 2.10 to 2.22 Å, and the M(3) and M(4) octahedra are more distorted, with bond lengths ranging from 2.07 to 2.26 Å. The longest bonds are to oxygen atoms adjacent to the vacant octahedral site.

Cations present in the octahedral layer are manganese and magnesium in a ratio of about 7:3. There is limited partitioning among the sites according to site size, or proximity to octahedral vacancies. The M(1) and M(4) sites, which are adjacent to two

vacant sites, have the greatest Mn occupancies, approximately 70%, and the M(2) and M(3) sites, which share one edge with a vacant site, have 62% and 58% Mn, respectively.

Vacant octahedral sites in the brucite-like layer share their upper and lower faces with $\text{Zn}(\text{OH})_4^{2-}$ tetrahedra. Zinc–oxygen bonds range from 1.946 to 2.001 Å, and O–Zn–O angles vary from 105.2 to 113.5°; both ranges are typical for $\text{Zn}(\text{OH})_4^{2-}$ tetrahedra.

Interlayer units

Between the brucite-like sheets is an interlayer slab (Fig. 2) which consists of the sulfate groups, and a (Mn,Mg) cation octahedrally coordinated to

Table 5. Balance of estimated bond valences for oxygen atoms

	M(1)	M(2)	M(3)	M(4)	M(5)	Zn(1)	Zn(2)	s	c ^v
O(1)	0.38	0.36	0.37						1.11 OH
O(2)		0.38		0.37					1.08 OH
		0.34							
O(3)			0.36	0.31			0.51		1.18 OH
O(4)			0.32	0.29		0.50			1.11 OH
O(5)	0.31		0.28			0.49			1.08 OH
O(6)		0.33		0.28		0.49			1.10 OH
O(7)		0.34	0.39	0.40					1.13 OH
O(8)			0.35	0.36			0.50		1.21 OH
O(9)	0.35	0.30					0.52		1.17 OH
O(10)				0.37	0.50				0.87 OH
O(11)				0.38		0.48			0.86 OH
O(12)				0.20					0.20 H ₂ O
O(13)				0.37					0.37 H ₂ O
O(14)				0.27					0.27 H ₂ O
O(15)				0.29					0.29 H ₂ O
O(16)								1.54	1.54 O ⁻
O(17)								1.51	1.51 O
O(18)								1.49	1.49 O
O(19)								1.47	1.47 O
A ^v	2.08	2.05	2.07	2.01	1.88	1.98	2.01	6.01	

two hydroxyls (in "cis" arrangement) and four water molecules. The (Mn,Mg)(OH)₂(H₂O)₄ octahedron is oriented with two faces essentially parallel to the brucite-like sheets. The two hydroxyl ions are shared with Zn tetrahedra on adjacent brucite-

like layers, thus linking the layers together. The octahedron is rather distorted, as the water molecules are only weakly bonded.

Sulfate groups are present in pairs between the rows of interlayer octahedra as shown in Figure 2.

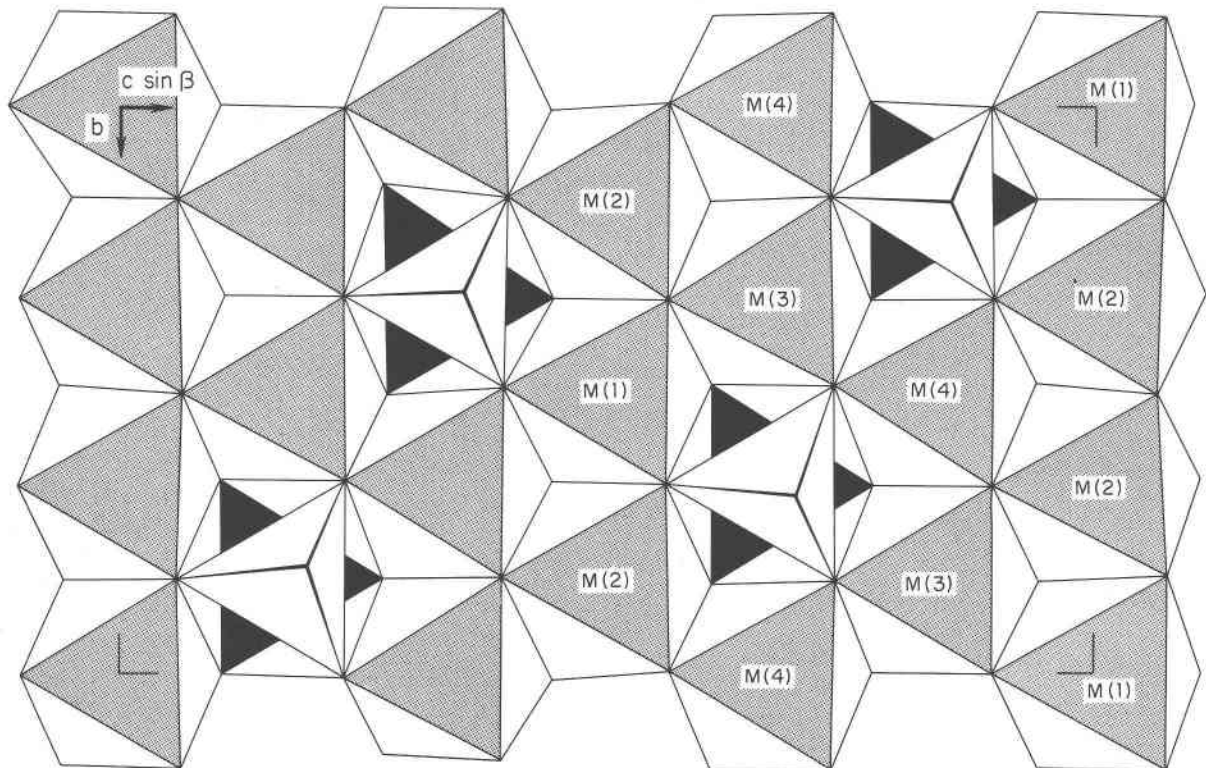


Fig. 1. Projection parallel to *a* of the octahedral brucite-like layer near *x* = 0. Above and below the octahedral sheet are ZnO₄ tetrahedra coordinated to vacant octahedral sites.

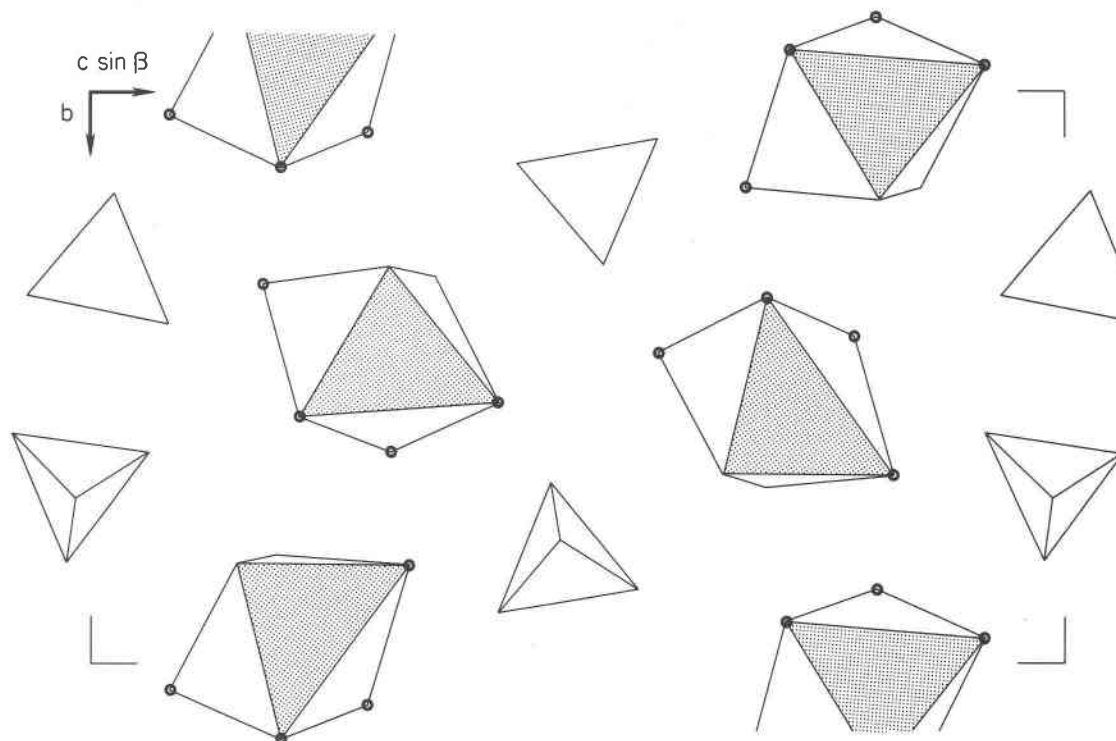


Fig. 2. Projection parallel to a of the interlayer region near $x = 0.5$. The M(5) octahedra share hydroxyls (shown as points) with ZnO_4 tetrahedra coordinated to the brucite-like layer. Sulfate groups (tetrahedra) have hydrogen bonds to water molecules (shown as circles) around the M(5) cations.

The sulfate groups are related through an inversion center, but oxygens on one sulfate group are not within hydrogen bonding distance of oxygens on the other. Temperature factors for oxygen in the sulfate group are not unusually large, unlike mooreite in which the sulfate oxygens have much larger temperature factors than other oxygens.

Hydrogen bonding

Locations and strengths of hydrogen bonds were computed using the method of Donnay and Allmann (1970), as shown in Table 5. None of the hydroxyls in the brucite-like layer receive a bond strength sum significantly different from 1.0, and the brucite-like sheet is inferred to have no strong hydrogen bonds. The hydroxyls and waters associated with the interlayer M(5) cation all receive bond strengths significantly different from their ideal values, and we infer that all are involved in hydrogen bonding. The strongest hydrogen bonds (shortest bond lengths) are between the bridging hydroxyls bonded to an M(5) cation, O(10) and O(11), and two water molecules coordinated to the adjacent M(5) cation [O(11)–O(13), 2.54Å; O(10)–O(15), 2.69Å]. The hydroxyls O(10) and O(11) are underbonded (Table 5)

and are receptors in the hydrogen bonds. The sulfate group oxygens are close enough to many of the interlayer water molecules, all overbonded, so that hydrogen bonding is likely. The pattern of bonding is complex, and is analogous to that in mooreite (Hill, 1980). Two sulfate group oxygens are close enough to hydroxyls of the brucite-like sheet [O(17)–O(9), 2.89Å; O(18)–O(7), 2.92Å] that hydrogen bonding is a possibility, but neither hydroxyl is overbonded significantly.

Torreyite chemistry

As noted by Dunn *et al.*, (1979), lawsonbauerite is the manganese analogue of torreyite (Bauer and Berman, 1929; Prewitt-Hopkins, 1949), a rare mineral also found only at Sterling Hill, New Jersey. This study therefore requires modification of the formula for torreyite, as given by Dunn *et al.* (1979), to $(Mg, Mn)_9Zn_4(SO)_2(OH)_{22} \cdot 8H_2O$.

Crystal chemistry

The structures of lawsonbauerite and mooreite (Hill, 1980) are quite similar. Both minerals have brucite-like layers with vacant octahedral sites. Zinc hydroxide tetrahedra share hydroxyls with the

vacant octahedral sites and with an interlayer (Mn, Mg)(OH)₂(H₂O)₄ polyhedron. Adjacent brucite-like sheets are linked together through the zinc tetrahedra and "cis" hydroxyls on the interlayer Mn octahedron. Sulfate groups in the interlayer region are held only by hydrogen bonds. Manganese is partitioned into the interlayer site, and into the larger octahedral sites adjacent to octahedral vacancies in the brucite-like layer.

The greatest difference between the two structures is in the pattern, or tessellation, of octahedral vacancies in the brucite-like layers: two of nine sites are vacant in lawsonbauerite, and two of eleven in moorite. Unlike the phyllosilicates, where large octahedral cations produce dilation of the brucite-like layer resulting in an incompatibility in the dimensions of the octahedral and tetrahedral layers, the tetrahedral zinc distribution is discontinuous and therefore does not constrain the dimensions of the octahedral layer. Therefore, one may expect to find many different tessellation patterns of octahedral vacancies in brucite-like sheets, independent of the interlayer cations or anions (see Hill, 1981, for references), and widely varying octahedral cation ratios in such structures depending on the chemical conditions during formation. Thus, the Mn equivalent of mooreite ought to be stable, and might be found in association with lawsonbauerite. Similarly, the ferrous iron equivalents of both lawsonbauerite and mooreite may be stable, perhaps in alterations of iron-zinc sulfide ores.

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