

The crystal structure of curetonite, a complex heteropolyhedral sheet mineral

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ABSTRACT

The crystal structure of curetonite, $\text{Ba}[(\text{Al,Ti})(\text{PO}_4)(\text{OH},\text{O})\text{F}]$, monoclinic, $a = 6.977(2)$, $b = 12.564(4)$, $c = 5.223(1)$ Å, $\beta = 102.15(2)^\circ$, $V = 447.6(6)$ Å³, $P2_1/n$, has been solved by direct methods and refined to an R index of 3.7% using $\text{MoK}\alpha$ X-ray data. There is one unique P position tetrahedrally coordinated by four O atoms, and there are two unique Al positions octahedrally coordinated by $4\text{O} + 2\text{OH}$ and $4\text{O} + 2\text{F}$, respectively. These octahedra and tetrahedra link by sharing corners to form a sheet of general stoichiometry $\text{M}(\text{TO}_4)_\phi_2$ that constitutes the structural unit of the mineral. The sheets are linked by tenfold-coordinated interstitial Ba atoms. The $\text{M}(\text{TO}_4)_\phi_2$ sheet is topologically identical to the structural unit in laueite (Moore, 1965, 1975), but the intersheet linkage by Ba atoms is very different from that in laueite, which occurs through $\text{Mn}^{2+}(\text{H}_2\text{O})_4(\text{O})_2$ octahedra. Nevertheless, the valence-matching principle (Brown, 1981) is maintained in both structures, as the Lewis acidities of the interstitial cations Ba ($= 0.20$ vu) and $\text{Mn}^{2+}(\text{H}_2\text{O})_4(\text{O})_2$ ($= 0.20$ vu) match the Lewis basicity ($= 0.18$ vu) of the constituent structural unit.

INTRODUCTION

Curetonite is a barium aluminum hydroxy-phosphate from Golconda, Nevada, that was originally described by Williams (1979). It occurs as bright yellow-green or nickel green crystals in veins of coarse-grained barite and euhedral adularia that cut massive barite in a series of sericitic, phosphatic, and black organic cherts and shales. The formula of curetonite was given as $\text{Ba}_4\text{Al}_3\text{Ti}(\text{PO}_4)_4(\text{O},\text{OH})_6$, which may be generalized to $\text{R}_4[\text{M}_4(\text{PO}_4)_4\phi_6]$, where R is a large low-valence cation, M is a medium-sized divalent to tetravalent cation (0.5–0.8 Å), and ϕ is an unspecified anion. An interest in the structural topology of $\text{M}(\text{TO}_4)_\phi_n$ minerals (Hawthorne, 1990) and the acquisition of a suitable crystal of curetonite prompted the current study.

EXPERIMENTAL METHODS

The crystal used in this work was mounted on a Nicolet R3m automated four-circle diffractometer equipped with a Mo X-ray tube. Twenty-five reflections were measured on a random-orientation photograph and aligned automatically on the diffractometer. From the resulting setting angles, least-squares refinement gave the cell dimensions listed in Table 1, together with the orientation matrix. Intensity data were collected according to the procedure of Hawthorne and Groat (1985). A total of 2668 reflections was measured to a maximum 2θ angle of 60° . Ten strong reflections uniformly distributed with regard to 2θ were measured at 10° intervals of ψ (the azimuthal angle corresponding to the rotation of the crystal about its diffraction vector). These data were used to calculate an absorption correction, modeling the crystal as an ellipsoid and reducing the azimuthal R index from 11.3 to 3.3%; this correction was then applied to the nor-

mal intensity data. Data were corrected for Lorentz and polarization effects, averaged, and reduced to structure factors; the R index for the averaging procedure was 4.4%. A reflection was considered as observed if its magnitude exceeded that of 5 sd on the basis of counting statistics. Miscellaneous information pertaining to data collection and structure refinement is given in Table 1.

Subsequent to the data collection, the crystal was analyzed by electron microprobe according to the procedure of Hawthorne et al. (1993); results (average of ten spot analyses) are given in Table 2. The formula unit was calculated on the basis of six anions, assuming stoichiometric (H_2O) , and is also given in Table 2.

STRUCTURE SOLUTION AND REFINEMENT

Scattering curves for neutral atoms, together with coefficients of anomalous dispersion, were taken from the *International Tables for X-ray Crystallography*, vol. 4 (Ibers and Hamilton, 1974). R and R_w indices are of the conventional form and are given as percentages.

The structure was solved by direct methods. The E statistics indicated that the structure was centrosymmetric. The situation with regard to systematic absences was somewhat ambiguous. The presence of both an n glide ($h0l$, $h + l = 2n$) and a 2_1 axis ($0k0$, $k = 2n$) was suggested, but there were a number of weak violations to both those conditions. We suspected that the violations were due to double diffraction, but ψ scanning showed that at least some of them [e.g., 050 , $I = 1133(118)$] were observed. However, we decided to adopt the higher symmetry initially, and we looked for a solution in the space group $P2_1/n$. The solution with the highest combined figure of merit refined to an R index of 3.7% for a model with anisotropic displacements and variable scattering

TABLE 1. Miscellaneous information for curetonite

<i>a</i> (Å)	6.977(2)	crystal size (mm)	0.16 × 0.21 × 0.04
<i>b</i> (Å)	12.564(4)	radiation/mono	MoK α /Gr
<i>c</i> (Å)	5.223(1)	no. of intensities	2688
β (°)	102.15(2)	no. of $ F_o > 5\sigma$	1248
<i>V</i> (Å ³)	447.7(2)	$R_{\text{azimuthal}}$ (%)	11.3 → 3.3
Space group	$P2_1/n$	R_{obs} (%)	3.7
		$R_{\text{w,obs}}$ (%)	3.6
Cell content:	4[Ba(Al,Ti)(PO ₄)(OH)F]		

powers at the Al1 and Al2 sites. During the refinement, one of the (monovalent) anion positions had an anomalously small equivalent isotropic displacement parameter (0.004) and an anomalously short Al- ϕ distance. This suggested the presence of F at this position; replacement of the O scattering curve by the F scattering curve removed the anomaly in the equivalent isotropic displacement parameter and accounts for the short Al- ϕ distance. Attempts to refine the structure in lower symmetry ($P2_1$, Pn , or $P\bar{1}$) were unsuccessful, presumably because of the very few (perhaps a dozen) weak reflections violating $P2_1/n$ symmetry.

Final atomic positions and displacement parameters are given in Table 3, selected interatomic distances are given in Table 4, observed and calculated structure factors are listed in Table 5,¹ and empirical bond-valence values are shown in Table 6.

DISCUSSION

Local coordination

Details of the cation-coordination polyhedra are shown in Figure 1 and Table 4. There is one Ba position surrounded by ten anions between 2.6 and 3.2 Å, and the bond valence sums of Table 6 suggest that all must be considered to be bonded to the central cation. There is one P position surrounded by four O²⁻ anions in a moderately distorted tetrahedral arrangement, and the observed P-O distances are in the range typically found in oxide and oxysalt structures.

There are two Al positions, both on special positions with $\bar{1}$ symmetry. Al1 is surrounded by a distorted octahedral arrangement of O²⁻ and OH⁻ anions, the two OH⁻ anions occurring in a trans arrangement, as dictated by the inversion symmetry of the coordination polyhedron. Site-scattering refinement showed Al1 to contain the transition metal in curetonite (Al1 = 0.66Al + 0.34 Ti), which accounts for the longer $\langle\text{Al1}-\phi\rangle$ distance of 1.933 Å (Table 4) and the bond valence sum of 3.31 vu (Table 6) at the Al1 site. Al2 is surrounded by a distorted octahedral arrangement of O²⁻ and F⁻ anions, again with the monovalent F⁻ anions in a trans arrangement. The $\langle\text{Al2}-\phi\rangle$ distance of 1.865 Å is quite short for an ⁶Al ϕ_6 polyhedron but agrees reasonably well with the distance

TABLE 2. Electron microprobe analysis* and formula unit** for curetonite

P ₂ O ₅	22.83	P	0.985
Al ₂ O ₃	13.20		
TiO ₂	4.08	Al	0.792
V ₂ O ₅	0.65	Ti	0.156
MgO	0.27	V	0.027
BaO	51.30	Mg	0.021
SrO	0.10	Total	0.996
H ₂ O	(2.50)		
F	6.46	Ba	1.024
Total	101.39	Sr	0.003
O \equiv F	-2.72	Total	1.027
Total	98.67	F	1.041
		OH	0.850
		Total	1.891

* Weight percent.

** Calculated on the basis of six anions.

of 1.875 Å calculated for an AlO₄F₂ octahedron from the sum of the appropriate ionic radii (Shannon, 1976).

The chemical formula of curetonite

The chemical formula of curetonite was originally given by Williams (1979) as Ba₄Al₃Ti(PO₄)₄(O,OH)₆, as compared with the formula 4[Ba(Al_{0.83}Ti_{0.17})(PO₄)(OH,-O)F], derived from the structure solution, and the formula 4{Ba(Al_{0.79}Mg_{0.02}Ti_{0.16}V_{0.03})(PO₄)[F_{1.04}(OH)_{0.85}O_{0.11}]}, derived from the electron microprobe analysis. Ti is not an essential chemical constituent of the formula, and the ideal end-member composition is BaAl(PO₄)(OH)F. Site-scattering refinement shows Ti to order at the Al1 site; the bond valence sum at Al1 (Table 6) is 3.31 vu, in good agreement with the mean aggregate cation valence of 3.34 vu at Al1 indicated by the site-scattering refinement. Ti enters the ideal curetonite formula by means of the substitution Ti⁴⁺ + O²⁻ → Al³⁺ + OH⁻, and the bond valence table (Table 6) shows that O²⁻ must be incorporated at the O4 position. This substitution suggests an aggregate anion charge of 1.34 vu at O4, in good agreement with the incident bond valence sum of 1.43 vu.

If there is no Ti in the structure, then the O4 anion position must be completely occupied by OH. This, in turn, means that the sum at the O4 site must be much less than that observed in Ti-bearing curetonite (i.e., 1.43 vu: Table 6), which would require a strong decrease in the Ba-O4 interaction (as well as the Al1-O4 interaction). It is not clear whether this decrease is possible. Thus the curetonite structure may require significant Ti content for its stability.

Structure topology

The basic structural unit of curetonite is shown in Figure 2, a corner-sharing octahedral-tetrahedral sheet of general stoichiometry M(T ϕ_4) ϕ_2 , where M is a sixfold-coordinated cation, T is a fourfold-coordinated cation, and ϕ represents unspecified simple anions. The sheet shows two very common structural motifs. Of prime importance are the butlerite-type M(TO₃) ϕ chains (Fanfani et al., 1971) parallel to the *a* axis and involving both Al1

¹ A copy of Table 5 may be ordered as Document AM-94-555 from the Business Office, Mineralogical Society of America, 1130 Seventeenth Street NW, Suite 330, Washington, DC 20036, U.S.A. Please remit \$5.00 in advance for the microfiche.

TABLE 3. Final atomic parameters for curetonite

Site	x	y	z	U_{eq}	U_{11}^*	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ba	0.31601(4)	0.32090(3)	0.45914(7)	171(1)	135(2)	123(2)	219(2)	53(1)	-44(1)	-17(1)
P	0.3036(2)	0.1135(1)	-0.0694(2)	85(3)	93(4)	73(5)	87(5)	-8(5)	16(4)	-4(4)
Al1	0	1/2	0	120(5)	211(9)	78(9)	81(8)	-16(7)	48(6)	-52(6)
Al2	1/2	1/2	0	95(5)	92(8)	94(10)	100(9)	16(9)	23(7)	12(7)
O1	0.2105(5)	0.2235(3)	-0.0701(8)	143(10)	161(15)	109(18)	167(18)	7(16)	56(13)	21(13)
O2	0.4330(5)	0.0927(3)	0.2030(7)	133(10)	172(15)	106(17)	105(16)	12(15)	-10(13)	11(13)
O3	-0.0584(5)	0.3858(3)	0.2290(7)	110(9)	105(13)	113(16)	121(15)	7(14)	44(12)	5(12)
O4	0.2636(5)	0.4474(3)	0.0679(7)	108(9)	85(13)	131(17)	123(16)	52(14)	54(12)	34(12)
O5	0.6445(5)	0.4724(3)	0.3497(7)	129(10)	132(14)	155(19)	99(16)	37(15)	23(12)	59(13)
F	0.0521(4)	0.1306(2)	0.3945(6)	143(9)	130(12)	113(15)	176(15)	10(13)	15(10)	-16(11)

* $U_i \times 10^4$.

and Al2 octahedra, as well as the PO₄ tetrahedra. These are M ϕ_5 chains of trans corner-sharing octahedra that are linked lengthwise by sharing corners with TO₄ tetrahedra (Fig. 3a). Adjacent chains link by sharing corners between tetrahedra and octahedra to form a sheet (Fig. 2). This polyhedral condensation is interesting, as it gives rise to another common chain motif. There are kröhnkite-type M(TO₄)₂ ϕ_2 chains (Hawthorne and Ferguson, 1975) parallel to the c axis (Fig. 3b), involving the Al1 octahedra (cross-shaded in Fig. 2) and the PO₄ tetrahedra; it is these chains that give rise to the ~5.2-Å c repeat and cross-link through the Al2 octahedra to form the complete sheet.

In two papers of seminal importance in structural crystallography, Moore (1970, 1975) examined geometrical and topological stereoisomerism among chain and sheet structures involving M ϕ_5 chains. He identified seven topologically distinct M ϕ_5 chains involving intrachain linkage by TO₄ groups (Moore, 1970), and showed that ligand stereoisomerism results in 21 distinct arrangements. The structural unit of curetonite is one of these arrangements. The M ϕ_5 chain in curetonite (Fig. 3a) is the type I chain typified by laucite (Moore, 1965). There are three distinct types of trans ligand isomerism in this type I chain (Fig. 4): (H₂O)(H₂O), O₂O_i, or (H₂O)_iO_i (Moore, 1975). The situation is slightly different here, as the intersheet linkage involves Ba rather than M²⁺ ϕ_6 octahedra, and the non-

O_i linkages are not H₂O but F; however, in terms of the sheet topology this is not significant. In curetonite the Al1 ϕ_6 octahedron is of type Ib, and the Al2 ϕ_6 octahedron is of type Ia (substituting F for H₂O), identical to the situation in laucite. The structural units in curetonite (Fig. 2) and laucite (Moore, 1965, 1975) are thus topologically identical.

Interstitial linkage of structural units

As discussed by Moore (1970, 1975) and Fanfani et al. (1978), there are several structure types based on these M(TO₄) ϕ_2 sheets that involve M ϕ_5 octahedral corner-sharing chains (Baur, 1969; Baur and Rama Rao, 1967; Moore and Araki, 1974a, 1974b). Curetonite is unusual among this group in that the sheets are cross linked by Ba rather than (M²⁺ ϕ_6)²⁺ octahedra (Fig. 5). Hawthorne (1985, 1992a) has shown how to examine interstitial linkage between structural units; the structural unit is treated as a complex oxyanion, and the interstitial species is treated as a complex cation. This produces a binary representation of even the most complicated structure, and we can examine the interaction between the two components using the valence-matching principle of Brown (1981). According to the valence-matching principle, the Lewis basicities of these units should match the Lewis acidities of the interstitial species to which they are bonded. Brown (1981) listed Lewis acidities for simple cations of relevance here.

The ideal structural unit in curetonite is [Al₂(PO₄)₂(OH)₂F₂]⁴⁻. Following Hawthorne (1992a), we

TABLE 4. Selected interatomic distances (Å) in curetonite

Ba-O1	2.885(4)	Al1-O2a,d	×2	1.917(4)
Ba-O1a	2.889(4)	Al1-O3,e	×2	1.965(4)
Ba-O1b	2.808(4)	Al1-O4,e	×2	1.916(3)
Ba-O2	3.145(4)	⟨Al1-O⟩		1.933
Ba-O3	2.834(3)			
Ba-O3b	2.803(4)			
Ba-O4	2.700(4)	Al2-O4,i	×2	1.879(4)
Ba-O5j	2.987(4)	Al2-O5,i	×2	1.923(3)
Ba-F	2.816(3)	Al2-Fc,h	×2	1.793(3)
Ba-Fg	2.646(3)	⟨Al2-O⟩		1.865
⟨Ba-O⟩	2.889			
P-O1	1.527(4)			
P-O2	1.538(3)			
P-O3f	1.569(4)			
P-O5d	1.542(4)			
⟨P-O⟩	1.544			

Note: equivalent positions: a = x, y, z + 1; b = x + 1/2, \bar{y} + 1/2, z + 1/2; c = \bar{x} + 1/2, y + 1/2, z + 1/2; d = x - 1/2, \bar{y} + 1/2, z - 1/2; e = \bar{x} , y + 1, z; f = x + 1/2, \bar{y} + 1/2, z - 1/2; g = x, \bar{y} + 1/2, z + 1/2; h = x, \bar{y} + 1/2, z - 1/2; i = \bar{x} + 1, y + 1, z; j = \bar{x} + 1, y + 1, z + 1.

TABLE 6. Bond valence* arrangement in curetonite

	Ba	Al1	Al2	P	Total
O1	0.203 0.201 0.245			1.296	1.944
O2	0.111	0.572 ^{×2} ↓		1.256	1.939
O3	0.230	0.509 ^{×2} ↓		1.153	2.140
	0.248				
O4	0.323	0.573 ^{×2} ↓	0.532 ^{×2} ↓		1.428
O5	0.159		0.482 ^{×2} ↓	1.242	1.883
F	0.173		0.509 ^{×2} ↓		0.910
	0.229				
Total	2.122	3.308	3.046	4.947	

* Calculated from the curves of Brown (1981).

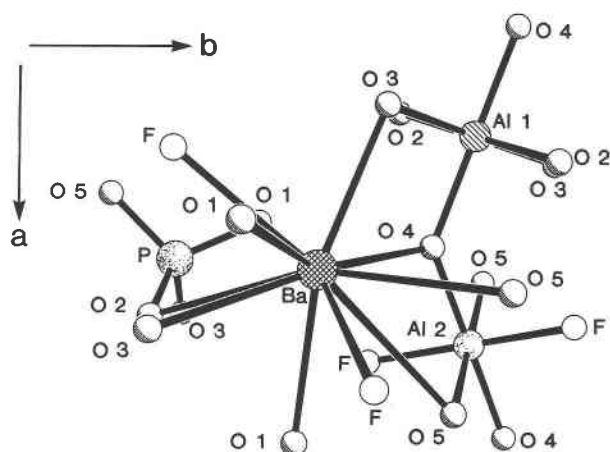


Fig. 1. Details of the coordination polyhedra in curetonite; Ba is crosshatched, Al1 is line-shaded, P and Al2 are dot-shaded, and anions are open circles.

assume a mean divalent-anion coordination number of 4 and a mean monovalent-anion coordination number of 3. This requires $4 \times 4 \times 2 + 2 \times 3 \times 2 = 44$ bonds per $[\text{Al}_2(\text{PO}_4)_2(\text{OH})_2\text{F}_2]^{4-}$ fragment in the structural unit. There are $6 \times 2 + 4 \times 2 + 1 \times 2 = 22$ bonds within each $[\text{Al}_2(\text{PO}_4)_2(\text{OH})_2\text{F}_2]$ fragment of the structural unit, and hence each of these fragments requires $44 - 22 = 22$ bonds from the interstitial cations that hold the structural units together. The charge on the structural unit is 4^- , and therefore the Lewis basicity of the structural unit is $\frac{1}{2} = 0.18$ vu. The valence-matching principle indicates that the interstitial cation species in curetonite should have a Lewis acidity of 0.18 vu. Inspection of the table

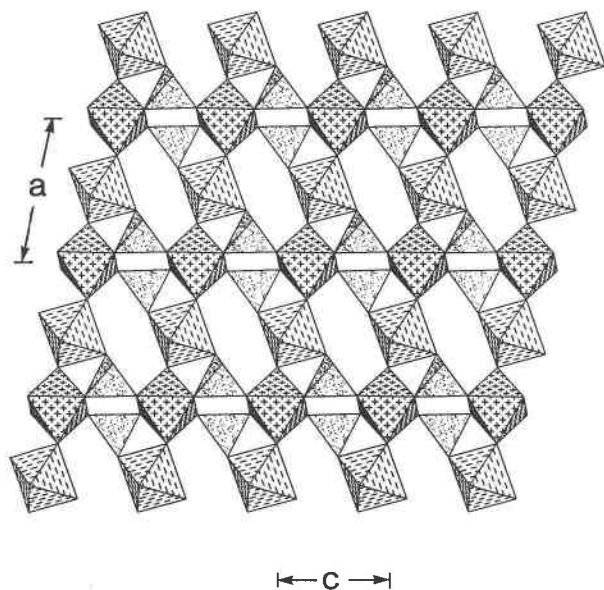


Fig. 2. The $\text{M}(\text{TO}_4)_2$ sheet in curetonite, projected down $[010]$; Al1 ϕ_i are shaded with crosses, Al2 ϕ_i are dash-shaded, and PO_4 are dot-shaded.

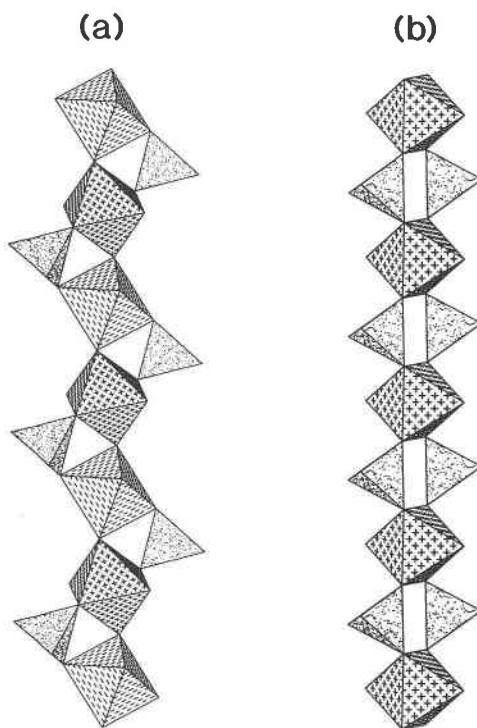


Fig. 3. The prominent chain motifs within the $\text{M}(\text{TO}_4)_2$ sheet of curetonite: (a) the $\text{M}(\text{TO}_4)_2$ laueite-type chain, (b) the $\text{M}(\text{TO}_4)_2$ kröhnkite-like chain.

of Lewis acidities of common cations (Brown, 1981; Hawthorne, 1992a) shows that Ba at 0.20 vu is close to the ideal value of 0.18 vu and hence can be the interstitial cation in curetonite.

Is the valence-matching principle observed in laueite, in which the interstitial cation is Mn^{2+} ? The Lewis basicity of the laueite sheet is 0.20 vu, very similar to that of the curetonite sheet. However, the Lewis acidity of Mn^{2+} is 0.36 vu (Brown, 1981); how is the Mn^{2+} able to function as the interstitial cation in laueite? In laueite, the interstitial Mn^{2+} does not bond directly to the structural units at all of its ligands. The coordination of the interstitial Mn^{2+} is actually $\text{Mn}^{2+}(\text{H}_2\text{O})_4(\text{O}_i)_2$, where O_i represents an O atom linked to the tetrahedrally coordinated cation. Thus we must consider the $\text{Mn}^{2+}(\text{H}_2\text{O})_4(\text{O}_i)_2$ group as a complex cation and take into account the

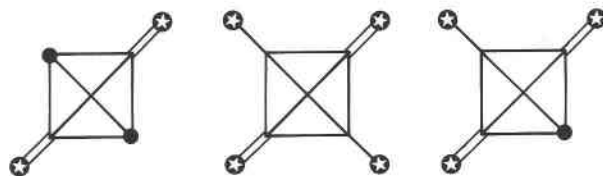


Fig. 4. The distinct ligand arrangements on a type I $\text{M}\phi_i$ chain viewed along the chain direction; tetrahedrally coordinated cations are shown as starred circles, and H_2O groups are shown as solid circles; after Moore (1975).

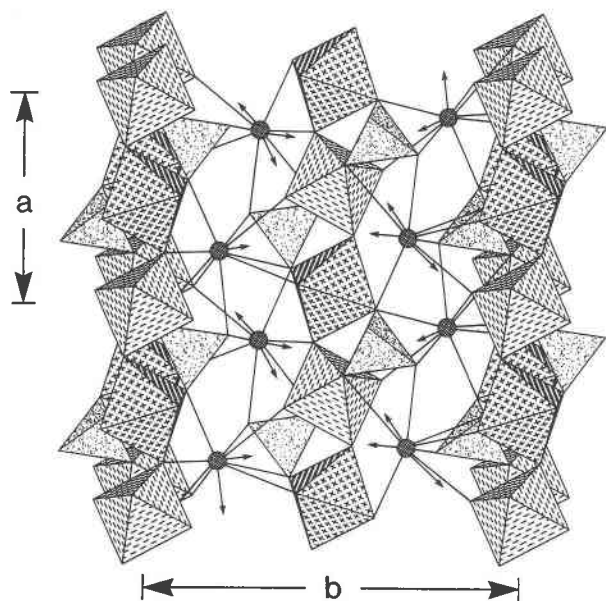


Fig. 5. The structure of curetonite projected onto (001), showing the intersheet linkage by interstitial Ba atoms.

transformer effect of H_2O (Hawthorne, 1992b). In this case, the effective Lewis acidity of the complex $Mn^{2+}(H_2O)_4(O)_2$ cation is $2/(4 \times 2 + 2) = 0.20$ vu, and therefore it can function as the interstitial (complex) cation for the structural unit of laueite.

Do we expect to find Ca as an interstitial cation in these types of structure? The Lewis acidity of Ca is 0.28 vu, and thus it does not match the Lewis basicity of 0.18 vu for this type of heteropolyhedral sheet. However, the Lewis acidity of Ca can be moderated by its bonding to H_2O to form a complex cation. Thus Ca could form a complex cation of the form $Ca(H_2O)_4(O)_3$, with an effective Lewis acidity of $2/(4 \times 2 + 3) = 0.18$ vu, and function as an interstitial cation in these types of structure.

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