

THE CRYSTAL STRUCTURE OF FENCOOPERITE: UNIQUE $[\text{Fe}^{3+}_3\text{O}_{13}]$ PINWHEELS CROSS-CONNECTED BY $[\text{Si}_8\text{O}_{22}]$ ISLANDS

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ABSTRACT

The crystal structure of fencooperite, ideally $\text{Ba}_6\text{Fe}^{3+}_3\text{Si}_8\text{O}_{23}(\text{CO}_3)_2\text{Cl}_3\cdot\text{H}_2\text{O}$, has been solved in the trigonal space-group $P3m1$, with a 10.7409(5), c 7.0955(4) Å, V 708.9(1) Å³ and $Z = 1$. The final residual index for observed reflections is 0.038. The uniqueness of the fencooperite structure is a result of two previously unknown fundamental building blocks (*FBB*). The islands of silica tetrahedra form $[\text{Si}_8\text{O}_{22}]$ units described as double open-branched triple tetrahedra sharing vertices along [001]. The other unique *FBB* consists of three (Fe^{3+}O_5) tetragonal pyramids having one of the O atoms common to all three polyhedra, forming a pinwheel trimer $[\text{Fe}_3\text{O}_{13}]$. The pronounced optical absorption is attributed to this coordination complex of iron. This trimer cross-links the $[\text{Si}_8\text{O}_{22}]$ islands to form a framework structure. The framework supports intersecting tunnels in all three crystallographic directions that are filled by Ba and Cl atoms and by H_2O and CO_3 groups. The structure of fencooperite is compared to that of gillespite, pellyite, titantaramellite and orthoericssonite. In gillespite and pellyite, individual polyhedra of Fe^{2+} in four-fold coordination with oxygen cross-link sheets and chains of silica tetrahedra, whereas the chains of Fe^{3+} in (titan)taramellite having six-fold coordination with oxygen cross-links island rings of silica tetrahedra. In orthoericssonite, which has the same five-fold coordination of Fe^{3+} as fencooperite, the Fe^{3+} polyhedra cross-link $[\text{Si}_2\text{O}_7]$ groups into sheets.

Keywords: fencooperite, unique crystal structure, hydrated barium–iron silicate–carbonate–chloride, ferric iron, five-fold coordination, pinwheel.

SOMMAIRE

La structure cristalline de la fencooperite, dont la formule idéale serait $\text{Ba}_6\text{Fe}^{3+}_3\text{Si}_8\text{O}_{23}(\text{CO}_3)_2\text{Cl}_3\cdot\text{H}_2\text{O}$, a été résolue en termes du groupe spatial trigonal $P3m1$, avec a 10.7409(5), c 7.0955(4) Å, V 708.9(1) Å³ et $Z = 1$. Le résidu final pour toutes les réflexions observées est égal à 0.038. La particularité de la structure de la fencooperite vient de la présence de deux modules structuraux non connus antérieurement. Des îlots de tétraèdres de silice forment des modules de stoechiométrie $[\text{Si}_8\text{O}_{22}]$, que l'on peut décrire comme tétraèdres triples doublement et ouvertement branchés partageant un coin le long de [001]. L'autre module structural contient trois pyramides (Fe^{3+}O_5) ayant une des atomes d'oxygène en commun aux trois polyèdres, pour former un trimère en "moulinet à vent" de composition $[\text{Fe}_3\text{O}_{13}]$. L'absorption optique prononcée serait due à cette coordinence du fer. Ce trimère rattache les îlots $[\text{Si}_8\text{O}_{22}]$ pour former la trame de la structure. Cette trame contient des canaux dans les trois directions cristallographiques, remplis par des atomes de Ba et de Cl et par des groupes de H_2O et de CO_3 . La structure de la fencooperite montre des points communs avec celles de la gillespite, la pellyite, la titantaramellite et l'orthoericssonite. Dans la gillespite et la pellyite, des polyèdres individuels contenant le Fe^{2+} tétra-coordonné par l'oxygène rattachent les feuillets et les chaînes de tétraèdres de silice, tandis que dans la titantaramellite, les chaînes contenant le Fe^{3+} hexa-coordonné par l'oxygène rattachent les anneaux d'îlots de tétraèdres de silice. Dans l'orthoericssonite, qui partage avec la fencooperite le Fe^{3+} en coordinence cinq, les polyèdres rattachent les groupes $[\text{Si}_2\text{O}_7]$ en feuillets.

(Traduit par la Rédaction)

Mots-clés: fencooperite, structure cristalline unique, silicate–carbonate–chlorure hydraté de barium et de fer, fer ferrique, coordinence cinq, "moulinet à vent".

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INTRODUCTION

Fencooperite, ideally $\text{Ba}_6\text{Fe}^{3+}_3\text{Si}_8\text{O}_{23}(\text{CO}_3)_2\text{Cl}_3 \cdot \text{H}_2\text{O}$, is a recently described mineral species (Roberts *et al.* 2001) from Trumbull Peak, Mariposa County, California. The crystal-structure analysis was essential to the description of this new species, as insufficient material was available to determine the valence of iron, and the content of H_2O and CO_2 . These three chemical parameters were readily determined with a solution of the crystal structure.

Dunning & Cooper (1999) described the mineralogy of the barium silicates found at Trumbull Peak. In their description, fencooperite is referred to as mineral UKTP-1, a Ba-Fe silicate. Further to this label, Dunning (pers. commun. 2001) states that: "Fencooperite occurs exclusively in one lens associated with gillespite, sanbornite, titantaramellite, Fe-Cl analogues of ericssonite and orthoericssonite, pyrrhotite, bigcreekite, alforsite, barite, macdonaldite, a Ba-Fe-Mn-Ca silicate-phosphate (Mineral 27 in Dunning & Cooper 1999) and with erite in a quartz matrix. In a second lens about 20 meters to the south, the only minerals identified in this quartz-rich lens are walstromite, pellyite, fresnoite, bigcreekite, benitoite, titantaramellite, a hydrous silicate (mineral 21 in Dunning & Cooper 1999), barite and some sanbornite." In the paragenetic sequence given by Roberts *et al.* (2001), the crystallization of fencooperite follows barite, is contemporaneous with celsian, alforsite and likely titantaramellite, and precedes gillespite and sanbornite.

X-RAY CRYSTALLOGRAPHY
AND CRYSTAL-STRUCTURE DETERMINATION

Precession single-crystal photographs initially showed fencooperite to be hexagonal with diffraction symmetry $6/mmm$ (Roberts *et al.* 2001). It was not until the crystal-structure analysis was completed that it became evident that fencooperite is trigonal (pseudo-hexagonal). Two sets of intensity data were collected on different crystals in an attempt to improve the refinement. In fact, there was remarkably little difference between the two refinements, but the marginally better experiment is described in full here. Comparing the two refinements, there are exact parallels, problematic anisotropic-displacement parameters, disparate bond-lengths in SiO_4 tetrahedra and poor bond-valence sums. These problems are without doubt a signature of the poor crystallinity or granular nature of fencooperite.

In the final data-collection, a fragment of fencooperite measuring $50 \times 40 \times 20 \mu\text{m}$ was mounted on a CCD-equipped Bruker *P4* fully automated four-circle diffractometer operated at 50 kV and 40 mA. With the CCD detector, almost a full sphere of intensity data were collected out to $2\theta = 60^\circ$ using a 120 s frame time and a crystal-to-detector distance of 40 mm. With these operating conditions, no decrepitation was evident in the final analysis of the intensity standards. Information

relevant to the data collection and structure determination is given in Table 1. The three-dimensional data were reduced for Lorentz, polarization, and background effects and multiply-measured reflections were averaged using the Bruker program SAINT. An empirical plate-absorption correction was done on the basis of 3998 reflections and reduced the merging *R* of this data set from 5.35% before the absorption correction to 4.79% after it.

All calculations were done with the Siemens SHELXTL Version 5.03 system of programs, which incorporates scattering factors of neutral atoms taken from the International Tables for Crystallography, Vol. C (1992). During the initial examination of the reduced dataset to determine a starting space-group, sixteen possible space-groups were considered (eight trigonal and eight hexagonal). Phasing of a set of normalized structure-factors gave a mean value $|E^2 - 1|$ of 0.800. This *E* statistic is indicative of a non-centrosymmetric crystal structure, which proved to be the correct interpretation. A calculated sharpened Patterson function for space group *P3* (the lowest symmetry possible among the sixteen space-groups) located the two *Ba* sites and ten other lighter-element sites. This model refined to *R* = 0.174 for observed data with $F_o > 4\sigma(F_o)$. Additional *O* and *C* sites were added following a series of ΔF synthesis maps, which, in turn, reduced the *R* index to 0.080 (observed data). In the final least-squares refinement, all atomic positions were refined with anisotropic-displacement factors to a residual of *R* = 0.048 (observed data in space group *P3*). The program MISSYM (Le Page 1987) suggested the possible presence of a mirror plane, and space group *P3m1* proved to be the correct choice of symmetry; the final refinement reduced *R* to 0.038 (observed data). MISSYM (Le Page 1987) also indicated that most of the structure is consistent with space group *P6m2*, thus it is not surprising that the diffraction symmetry is consistent with $6/mmm$. The addition of an isotropic-extinction factor did not improve the results, nor was there any evidence of merohedral twinning. The maximum and minimum electron-densities in the final cycle of refinement were +2.76 and -1.83 $e^-/\text{\AA}^3$. Table 2 contains the final positional coordinates, anisotropic-displacement factors, equivalent isotropic-displacement parameters and bond-valence sums, and Table 3 con-

TABLE 1. FENCOOPERITE: DATA COLLECTION AND STRUCTURE-REFINEMENT INFORMATION

Simplified formula: $\text{Ba}_6\text{Fe}^{3+}_3\text{Si}_8\text{O}_{23}(\text{CO}_3)_2\text{Cl}_3 \cdot \text{H}_2\text{O}$	
Space Group: <i>P3m1</i> (No. 156)	μ 10.4 mm^{-1}
Radiation: $\text{MoK}\alpha$	Reflections collected 6694
<i>a</i> 10.7409(5) \AA	Unique reflections 1560
<i>c</i> 7.0955(4) \AA	Observed reflections ($> 4\sigma F_o$) 1335
<i>V</i> 708.9(1) \AA^3	<i>R</i> (int) = 0.0611
<i>Z</i> = 1	Goof = 1.215 (all data)
$R = \Sigma(F_o - F_c) / \Sigma F_o =$	$wR^2 = [\Sigma w(F_o - F_c)^2 / \Sigma w(F_o)^2] = 0.091$
0.038 (for F_o), 0.051 (for all <i>F</i>) and	for $w = 0.0387$
0.044 (for all <i>F</i> merged)	

TABLE 2. FENCOOPERITE: ATOMIC COORDINATES, ANISOTROPIC DISPLACEMENT PARAMETERS (\AA^2) AND BOND VALENCE SUMS

Site	Wy*	x	y	z	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{eq}	BVS**
Ba1	3d	0.82749(5)	0.17251(5)	0	0.0101(3)	0.0101(3)	0.0447(6)	0.0003(2)	-0.0003(2)	0.0053(4)	0.0216(2)	1.84
Ba2	3d	0.51607(5)	0.48393(5)	0.5006(2)	0.0132(3)	0.0132(3)	0.0091(3)	-0.0001(2)	0.0001(2)	0.0032(4)	0.0134(2)	2.45
Fe	3d	0.4373(1)	0.5627(1)	0.0010(3)	0.0075(7)	0.0075(7)	0.0115(9)	0.0002(3)	-0.0002(3)	0.0015(7)	0.0098(5)	2.58
Si1	1a	0	0	0.7218(8)	0.005(2)	0.005(2)	0.010(3)	0	0	0.0027(9)	0.007(1)	4.09
Si2	3d	0.1678(2)	0.3356(5)	0.7284(5)	0.015(1)	0.007(2)	0.002(2)	0.002(1)	0.0008(6)	0.0036(8)	0.0092(7)	4.05
Si3	1a	0	0	0.2789(8)	0.010(2)	0.010(2)	0.004(2)	0	0	0.0053(9)	0.008(1)	4.19
Si4	1d	0.1669(2)	0.8331(2)	0.2704(6)	0.020(1)	0.020(1)	0.006(2)	-0.0011(5)	0.0011(5)	0.019(1)	0.0118(7)	3.94
C1	1c	2/3	1/3	0.181(5)							0.049(9)	3.91
C2	1c	2/3	1/3	0.716(5)							0.039(8)	3.82
O1	1a	0	0	0.498(3)	0.065(13)	0.065(13)	0.009(9)	0	0	0.032(6)	0.047(8)	2.32
O2	3d	0.0822(5)	0.1644(10)	0.797(1)	0.030(4)	0.014(5)	0.008(4)	0.005(3)	0.002(2)	0.007(2)	0.019(2)	2.08
O3	6e	0.3316(8)	-0.0777(8)	0.804(1)	0.014(4)	0.036(4)	0.025(3)	0.017(3)	0.011(3)	0.014(3)	0.024(1)	1.93
O4	3d	0.167(1)	0.334(2)	0.505(2)	0.119(9)	0.019(6)	0.007(5)	-0.004(4)	-0.002(2)	0.010(3)	0.060(5)	2.01
O5	3d	0.0819(5)	0.1638(9)	0.199(1)	0.015(3)	0.011(4)	0.009(4)	-0.002(4)	-0.001(1)	0.006(2)	0.012(2)	2.09
O6	6e	0.5933(7)	-0.0769(8)	0.196(1)	0.011(3)	0.025(4)	0.023(3)	-0.011(3)	0.000(3)	0.010(3)	0.019(2)	1.94
O7	1b	1/3	2/3	-0.006(3)	0.007(5)	0.007(5)	0.041(11)	0	0	0.003(2)	0.018(4)	1.86
O8	3d	0.5972(5)	0.4028(5)	0.176(3)	0.041(6)	0.041(6)	0.100(12)	-0.008(4)	0.008(4)	0.018(7)	0.062(3)	1.94
O9	3d	0.7366(4)	0.2634(4)	0.711(2)	0.027(5)	0.027(5)	0.055(8)	-0.004(3)	0.004(3)	0.014(5)	0.036(3)	2.02
OW10	1b	1/3	2/3	0.504(4)	0.052(9)	0.052(9)	0.041(12)	0	0	0.026(5)	0.048(6)	0.14
Cl***	3d	0.8361(4)	0.1639(4)	0.501(1)	0.031(2)	0.031(2)	0.032(3)	0.000(1)	-0.000(1)	0.008(3)	0.034(1)	0.87

* Wyckoff notation

** bond valence sums (valence units) calculated using the parameters of Brese & O'Keeffe (1991)

*** assuming 0.54 Cl + 0.46 OH atoms from the chemical analysis (Roberts *et al.* 2001)

tains selected interatomic distances and angles. Observed and calculated structure-factors have been submitted to the Depository of Unpublished Data, CISTI, National Research Council of Canada, Ottawa, Ontario K1A 0S2, Canada.

DESCRIPTION AND DISCUSSION OF THE STRUCTURE

There are nine cation sites in fenicooperite: two cation sites contain Ba, one Fe, four Si and two C. The *Ba1* site is at the center of an irregular polyhedron approximating an incomplete, doubly terminated hexagonal prism (Fig. 1a). This polyhedron best describes the 13-fold coordination of the *Ba1* site. Eleven of the coordinating anions are O atoms ranging in distance from 2.660 to 3.130 Å (mean 2.978 Å) to the Ba atom. The other two anions are the Cl apices of the dipyrmaid at distances of approximately 3.55 Å. In contrast to this Ba site is the *Ba2* site at the center of a polyhedron simply described as singly terminated hexagonal prism (Fig. 1b). In this Ba-centered polyhedron with 12-fold coordination, the apex is an H₂O group (denoted OW10). The 10 O anions (including OW10) have bond lengths ranging from 2.751 to 3.399 Å (mean 2.943 Å). The remainder of the polyhedron comprises two Cl anions at 2.992 Å. The bond-valence sums of the two Ba sites differ considerably, and neither is ideal. Refinement of the site occupancy of both sites reveals no replacement by cations or vacancy. The *Fe* site is bonded to five oxygen atoms; four of these define a near-perfect square at a bond distance average of 2.024 Å, the fifth oxygen atom completes a square or tetragonal pyramidal polyhedron with a considerably shorter bond-length, 1.934 Å. Using the bond-valence parameters of Brese & O'Keeffe (1991), the bond strength of the iron

is 2.58 valence units, *i.e.*, it is underbonded. The next-nearest oxygen atom (O8) is at 3.22 Å, which does not increase the bond strength to any appreciable extent. The reason for the poor agreement between the calculated and the theoretical value of 3 is not clearly understood,

TABLE 3. FENCOOPERITE: SELECTED BOND LENGTHS(Å) AND ANGLES(°)

Ba polyhedra			
Ba1-O9	2.660(12)	Ba2-O8	2.751(16)
-O8 x 2	2.884(8)	-O3 x 2	2.760(7)
-O6 x 2	2.947(7)	-O6 x 2	2.778(6)
-O3 x 2	2.965(8)	-O9 x 2	2.849(7)
-O5 x 2	3.120(4)	-Cl x 2	2.992(4)
-O2 x 2	3.130(4)	-O4 x 2	3.255(6)
-Cl	3.543(8)	-OW10	3.399(9)
-Cl'	3.559(8)		
Fe ³⁺ tetragonal pyramid			
Fe-O7	1.934(2)	O7-Fe-O6 x 2	103.8(6)
-O3 x 2	2.021(7)	O7-Fe-O3 x 2	101.7(6)
-O6 x 2	2.028(7)	O6-Fe-O6	88.5(4)
		O6-Fe-O3 x 2	86.6(3)
		O3-Fe-O3'	87.0(4)
Silicate tetrahedra			
Si1-O1	1.59(3)	O1-Si1-O2 x 3	109.3(4)
-O2 x 3	1.62(1)	O2-Si1-O2' x 3	109.6(4)
Si2-O4	1.59(2)	O3-Si2-O4 x 2	109.5(4)
-O3 x 2	1.617(8)	O2-Si2-O4	106.7(6)
-O2	1.67(1)	O3'-Si2-O3	114.9(5)
		O2-Si2-O3 x 2	107.9(4)
Si3-O1	1.55(3)	O1-Si3-O5 x 3	110.3(4)
-O5 x 3	1.624(9)	O5-Si3-O5' x 3	108.6(4)
Si4-O6 x 2	1.608(8)	O6-Si4-O6'	115.3(5)
-O5	1.66(1)	O5-Si4-O5 x 2	107.5(3)
-O4	1.66(2)	O4-Si4-O6 x 2	109.2(4)
		O4-Si4-O5	107.9(6)
Carbonate groups			
C1-O8 x 3	1.293(9)	O8-C1-O8	119.9(2)
C2-O9 x 3	1.302(8)	O9-C2-O9	119.9(2)

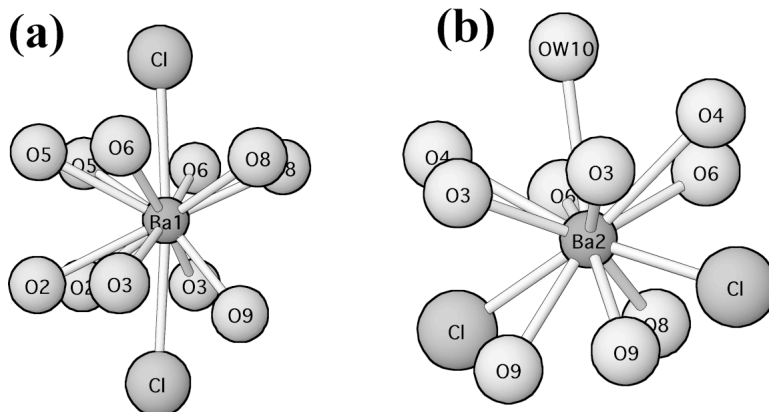


FIG. 1. The Ba site coordinations in fencooperite. An oblique projection approximately along [110] with [001] vertical: (a) the *Ba1* site, and (b) the *Ba2* site.

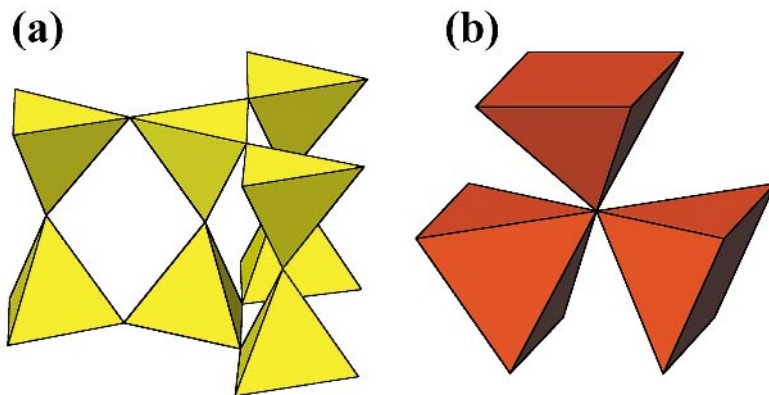


FIG. 2. The fundamental building blocks (FBB) in fencooperite. (a) The $[\text{Si}_8\text{O}_{22}]$ island unit in oblique projection approximately along [110], with [001] vertical. (b) The $[\text{Fe}^{3+}_3\text{O}_{13}]$ pinwheel trimer in oblique projection approximately along [001], with [010] horizontal.

but there may be factors such as covalent bonding and the uniqueness of the trimer complex described below that are not considered in the calculation. The only other mineral known to contain this rather unique coordination for Fe^{3+} is orthoericssonite (Matsubara 1980). In that structure, the mean $\text{Fe}^{3+}\text{-O}$ distance is 1.960 Å, which is somewhat shorter than the 2.006 Å of fencooperite, but 10% of the site is occupied by Ti^{4+} , which would shorten the bond lengths. If in fact the square pyramidal site contains both Fe^{3+} and Fe^{2+} , the residual positive charge could be attained by additional H^+ cations. The infrared-absorption spectrum (Roberts *et al.* 2001) and the bond-valence calculations do not

indicate any contribution from a $(\text{HCO}_3)^-$ ion, so one might assume that the proton is associated with O7. Here again, in the IR spectrum, there is only a broad shallow band in the O-H stretching region, which does not support a model for more OH^- anions. The four SiO_4 tetrahedra are somewhat irregular, with Si-O bond lengths varying from 1.55 to 1.67 Å (1.619 Å is the overall average for silicate tetrahedra), and O-Si-O bond angles varying from 106.7 to 115.3° (the ideal is 109.47°). The two carbonate groups are regular, trigonal planar.

The uniqueness of the fencooperite structure is a result of two previously undiscovered fundamental building blocks (FBB). The islands of silica tetrahedra form

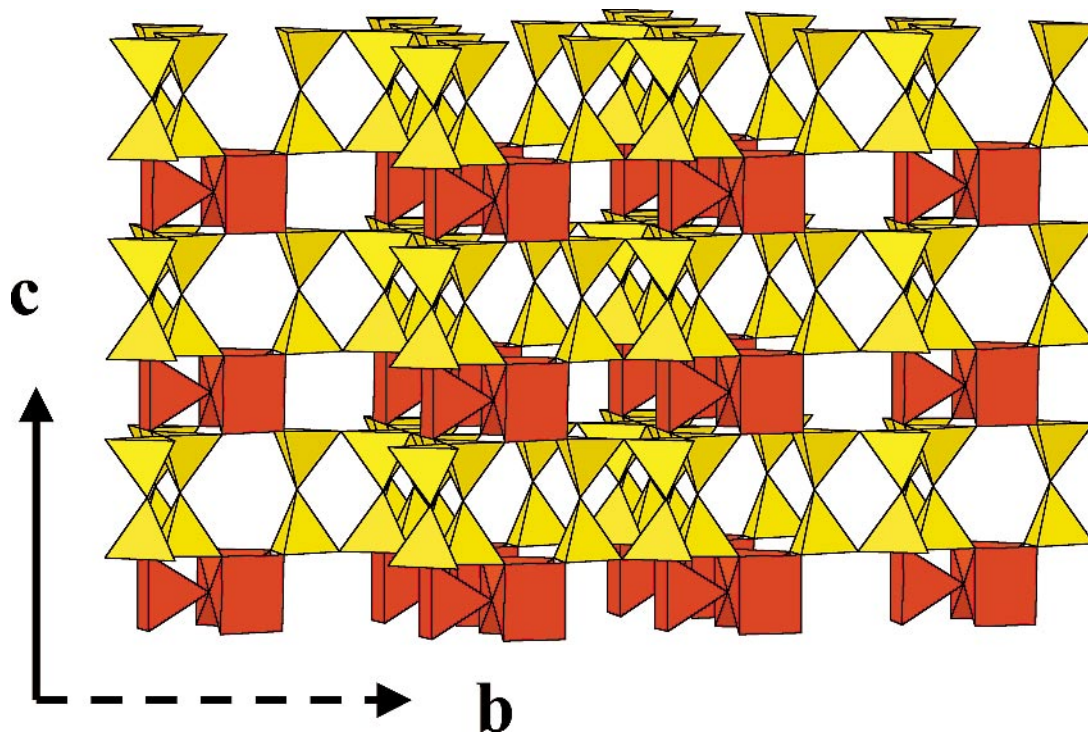


FIG. 3. The fencooperite framework in oblique projection approximately along $[110]$, with $[001]$ vertical, displaying the fundamental building blocks $[\text{Si}_8\text{O}_{22}]$ in yellow and $[\text{Fe}^{3+}_3\text{O}_{13}]$ in red.

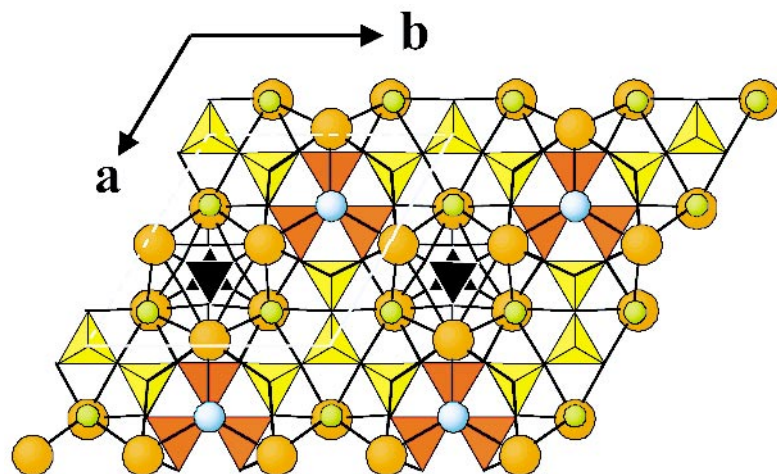


FIG. 4. The fencooperite structure projected along $[001]$. The Ba atoms are shown in orange, the (SiO_4) tetrahedra, in yellow, and the $(\text{Fe}^{3+}\text{O}_5)$ tetragonal pyramids, in red; the (CO_3) polyhedra are black triangles, the Cl atoms are shown in green, and the (H_2O) groups, in blue. The unit cell is outlined.

[Si₈O₂₂] units described as double open-branched triple tetrahedra sharing vertices along [001] (Fig. 2a). The only FBB that vaguely resembles this is found in the crystal structure of synthetic NaBa₃Nd₃[Si₂O₇][Si₄O₁₃] (Malinovskii *et al.* 1983). In that structure, the [Si₄O₁₃] group would be equivalent to one-half of the doubled FBB in fencooperite *i.e.*, a single-layer open-branched triple tetrahedra. The other unique FBB consists of three [Fe³⁺O₅] tetragonal pyramids with one of the O atoms common to all three polyhedra, [Fe₃O₁₃] (Fig. 2b). This pinwheel trimer cross-links the [Si₄O₁₃] islands forming a framework structure (Fig. 3). The framework supports intersecting tunnels in all three crystallographic directions, which are filled by Ba and Cl atoms and by H₂O and CO₃ groups (Fig. 4). The H₂O group (OW10) has site symmetry *3m*, which contradicts the point-group symmetry *2mm* for a H₂O group, necessitating disorder of the H atoms. This disorder is manifested in the apparent lack of hydrogen bonds. There are three O4 atoms at a distance of 3.09 Å, which is too long for any appreciable hydrogen-bonding effects. Inspection of Figure 4, in conjunction with Table 2, shows the close proximity of symmetry in this structure to space-group symmetry *P6m2* (origin at $\frac{2}{3}, \frac{1}{3}, 0$), a supergroup of *P3m1*. This similarity explains the diffraction symmetry *6/mmm* noted earlier in this paper. The two CO₃ groups are what lowers the rotation symmetry from a 6-fold axis to a 3-fold axis, and the displacement of these two groups to unequal distances above and below *z* = 0 destroys the inversion point, resulting in the space group *P3m1*. Space group *P31m* requires reorientation to a non-standard, larger unit-cell.

McDonald *et al.* (2000) discussed the unusual occurrence of five-coordinate Ti⁴⁺ with a distorted square pyramidal geometry in yoshimuraite. In fencooperite, the same unusual polyhedron is observed with Fe³⁺. The electronic configuration *d⁵* for Fe³⁺ has five 3*d* electrons. In this distorted polyhedron, the electrons will most likely be high spin, with three unpaired electrons (Cotton & Wilkinson 1980). There is little doubt that this electronic configuration in the [Fe³⁺O₅] tetragonal pyramids gives rise to the striking optical properties of fencooperite. Fencooperite, like Fe-rich tourmaline, is strongly dichroic, with $\omega \gg \epsilon$ in plane-polarized light. A much rarer optical property is its dichroism in unpolarized light, like that of Fe-bearing cordierite and zoisite.

Although the fencooperite structure is unique, it is worth comparing structural features with those of some of its coexisting phases. Gillespite, BaFe²⁺[Si₄O₁₀], has corrugated sheets of (SiO₄) tetrahedra that are cross-linked by (Fe²⁺O₄) polyhedra with a square-planar geometry (Hazen & Finger 1983). Pellyite, Ba₂CaFe²⁺₂[Si₆O₁₇], has chains of six-membered rings of (SiO₄) tetrahedra cross-linked into sheets by (Fe²⁺O₄) tetrahedra (Meagher 1976). Titantaramellite, Ba₄(Ti,Fe³⁺)₄[B₂Si₈O₂₇]O₂Cl, has four-membered rings of (SiO₄) tetra-

hedra cross-linked into sheets by chains of edge-sharing [(Ti,Fe³⁺)O₆] octahedra (Mazzi & Rossi 1980). Orthoericssonite and ericssonite, BaMn²⁺₂Fe³⁺Si₂O₇(O,OH)₂, contain composite sheets of [Si₂O₇] groups cross-linked by (Fe³⁺O₅) square pyramids interlayered by sheets of (MnO₆) octahedra and Ba atoms. The distribution of silica tetrahedra and the five-fold coordination of iron in fencooperite seem to be a crystal-chemical hybrid of the structures found in these other phases. In gillespite and pellyite, individual polyhedra of Fe²⁺ in four-fold coordination with oxygen cross-link sheets and chains of silica tetrahedra, whereas in (titan)taramellite the chains of Fe³⁺ having six-fold coordination with oxygen cross-link isolated rings of silica tetrahedra. Perhaps the most closely related mineral to fencooperite from the point of view of crystal chemistry would be orthoericssonite, with Fe³⁺ in five-fold coordination and forming an integral part of the quasi-silicate sheet. It should be noted that the five-fold coordination noted in fencooperite is also observed for Fe²⁺ in graftonite (Kostiner & Rea 1974), but it seems that in the Trumbull Peak locality, the paragenesis is such that this coordination complex is primarily, and probably entirely, dominated by Fe³⁺.

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