

The crystal structure of jagoite

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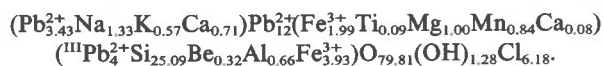
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Abstract

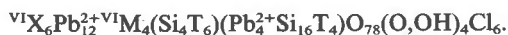
The crystal structure of jagoite ($a = 8.528(8)$, $c = 33.33(3)\text{\AA}$) was solved and refined in space group $P\bar{6}2c$ to $R_1 = 0.057$.

The structure is characterized by the presence of double and single tetrahedral layers connected by a sheet of iron and lead cations. Other lead cations as well as chloride anions are located inside the double layer. The single layer is characterized by an incomplete net of tetrahedra: the absent tetrahedron at the origin is replaced by the Fe(1) octahedron. The double layer is made up of two tetrahedral sheets, each of them built up of six membered rings of tetrahedra and PbO_3 ψ -tetrahedra.

The chemical data give rise to the following crystal chemical formula:



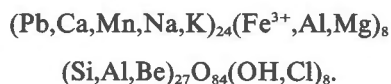
The corresponding idealized crystal chemical formula is



The chemical and structural data suggest ordering of silicon and iron in tetrahedral sites and of iron, magnesium, and manganese in octahedral sites. Possible ordering schemes, in space group $P31c$, are proposed.

Introduction

Jagoite is a rare lead and iron silicate, which was described from Långban, Sweden, by Blix *et al.* (1957). On the basis of its physical properties and chemical composition they suggested that jagoite is a sheet silicate with unit cell content



The absence of adequate data concerning its crystal chemistry and its classification among the silicate minerals led us to undertake a crystal structure analysis.

Experimental

The specimen of jagoite from Långban used in this study (NMNH #113302) was kindly given us by Dr. J. S. White of the Smithsonian Institution.

Whereas Blix *et al.* (1957) reported that jagoite is trigonal with Laue group $\bar{3}$, no systematic ex-

tinctions, and lattice parameters $a = 8.65(3)$ and $c = 33.5(1)\text{\AA}$, the many crystals we examined displayed the Laue symmetry $6/mmm$ and systematic extinctions in hhl for $l = 2n + 1$. This indicated $P6_3/mmc$, $P6_3mc$ and $P\bar{6}2c$ as possible space groups for jagoite. It is worthwhile to recall that Blix *et al.* (1957) reported that the "quality of the photographs was rather poor on account of the easiness with which the plates of jagoite are deformed." Actually, we too observed the easy deformability of jagoite crystals; notwithstanding, we obtained very fine diffraction patterns by carefully picking very tiny crystals.

From the many crystals we examined, a small platelet (nearly $0.17 \times 0.14 \times 0.03 \text{ mm}^3$) was chosen for intensity data collection. The lattice parameters, refined by least squares fitting of 18 medium range θ values, were $a = 8.528(8)$, $c = 33.33(3)\text{\AA}$, measured by a Philips PW1100 single crystal diffractometer, using graphite monochromatized $\text{MoK}\alpha$ radiation ($\lambda = 0.7107\text{\AA}$). A total of 3376 reflections were collected by the same diffractometer and the same radiation

using: ω scan from 2 to 26° θ , a scan width of 1° and a scan speed of 0.03° sec⁻¹. No crystal or counter instability was revealed by monitoring three reflections every three hours. Intensity data were corrected for Lorentz and polarization factors. An absorption correction was applied by the Ψ scan method developed by North *et al.* (1968) using two reflections.

The counter data confirmed the presence of the *c* glide plane and the hexagonal holohedral diffraction symmetry: the agreement index $R_{eq} = [\sum_{all} (n \sum_i w_i (F_i - F_i^2)) / \sum_{all} ((n-1) \sum_i w_i F_i^2)]^{1/2}$, calculated among equivalent reflections, was 0.046 assuming 6/*mmm* Laue symmetry (four equivalent sets) and 0.044 assuming $\bar{3}m$ symmetry (two equivalent sets). Therefore, the data were averaged to produce a unique set of 860 independent reflections, 92 of which were classified as unobserved having $|F_{hkl}| < 2\sigma(F_{hkl})$. The estimated standard deviations of observed structure factors were derived from the counting statistics. The statistical distribution and the average values of E_{hkb} calculated using the full set of independent diffractions, strongly indicated a non-centrosymmetric distribution of atoms in the structure, thus excluding *P6₃/mmc* as a possible space group. Moreover, the linear and planar concentrations of Patterson vectors seemed to indicate $\bar{P}6_2c$ as the correct space group (Buerger, 1950).

The structure determination was therefore undertaken in space group $\bar{P}6_2c$, by comparison of the *E* map analysis produced with the MULTAN program (Main *et al.*, 1971) and the distribution of the largest peaks in the Patterson synthesis. After a number of trials, differing mainly in the atomic scattering factors associated with the cationic positions, an optimal distribution of lead, iron and silicon cations produced a residual R_1 of 0.15, where $R_1 = \sum |F_o| - |F_c| / \sum |F_o|$. Subsequent localization of oxygen atoms through Fourier maps, full matrix least-squares refinement with weights assigned as the reciprocal variances of F_o , and anomalous dispersion corrections, led to $R_1 = 0.057$ for the observed reflections only. For all reflections R_1 was 0.069 and $R_2 = \sum w |F_o| - |F_c| / \sum w |F_o|^2$ was 0.049.

Different trials of anisotropic temperature factor refinement were unsuccessful, as they produced β_{ij} values leading to negative determinants. All scattering factors for neutral atoms and the anomalous dispersion correction factors were taken from the *International Tables for X-Ray Crystallography*, vol. IV, or calculated from them when a weighted average curve was used. Final atomic positional and thermal para-

Table 1. Final atomic positional and thermal parameters with esd's in parentheses

	x	y	z	B
Pb (1)	1/3	2/3	0.3305 (1)	0.69 (4)
Pb (2)	0.3679 (2)	0.4114 (2)	0.4243 (1)	0.82 (2)
Pb (3)	-0.1111 (3)	0.2772 (3)	1/4	1.89 (5)
Fe (1)	0	0	0.4302 (2)	0.24 (10)
SiFe (1)	0.2750 (10)	0	0	0.97 (14)
SiFe (2)	0	0	0.3031 (4)	1.22 (20)
Si (3)	2/3	1/3	0.4966 (5)	0.8 (3)
Si (4)	2/3	1/3	0.3387 (5)	0.5 (2)
	[2/3]	[1/3]	[0.3397]	
Si (5)	0.2903 (11)	0.0240 (13)	0.3626 (3)	0.6 (2)
O (1)	0.225 (3)	0.112 (4)	0.394 (1)	1.0 (4)
O (2)	0.103 (3)	0.222 (3)	0.463 (1)	0.4 (4)
O (3)	2/3	1/3	0.543 (1)	0.3 (6)
O (4)	0.169 (4)	0.477 (4)	0.520 (1)	2.0 (5)
O (5)	0.176 (3)	0.434 (3)	0.375 (1)	0.3 (4)
O (6)	0.989 (4)	0.187 (3)	0.319 (1)	1.7 (5)
O (7)	2/3	1/3	0.296 (1)	2.0 (9)
	[2/3]	[1/3]	[0.291]	
O (8)	0.860 (4)	0.370 (3)	0.358 (1)	2.2 (6)
O (9)	0	0	1/4	6 (2)
Cl	0.337 (2)	0.420 (2)	1/4	2.1 (3)

The bracketed positional parameters for Si(4) and O(7) atoms were obtained from ΔF syntheses.

rameters are reported in Table 1. Observed and calculated structure factors are reported in Table 2¹.

Structure description and discussion

The results of our study confirm the hypothesis made by Blix *et al.* (1957) about the classification of jagoite among the sheet silicates. In fact, its crystal structure is characterized by the presence of double and single tetrahedral layers such that alternating double and single layers are connected by a sheet of iron octahedra and lead polyhedra. Other lead cations as well as chloride anions are located inside the double layer. Figure 1 represents the crystal structure of jagoite in a slab parallel to (210), nearly *a*/2 thick, as seen along [100].

The single layer shown in Figure 2 is characterized by an incomplete net of tetrahedra: the absent tetrahedron at the origin is replaced by the Fe(1) octahedron. The Si(3) site is occupied by silicon cations, whereas the SiFe(1) site is nearly equally occupied by Si⁴⁺ and Fe³⁺ cations. It is interesting to note that this layer is similar to the [Zn₃Si₂O₄]¹⁴⁻ sheet, indicated by Moore and Araki (1978) as a pos-

¹ To receive a copy of Table 2, order document AM-81-165 from the Business Office, Mineralogical Society of America, 2000 Florida Avenue, N.W., Washington, D.C. 20009. Please remit \$1.00 in advance for the microfiche.

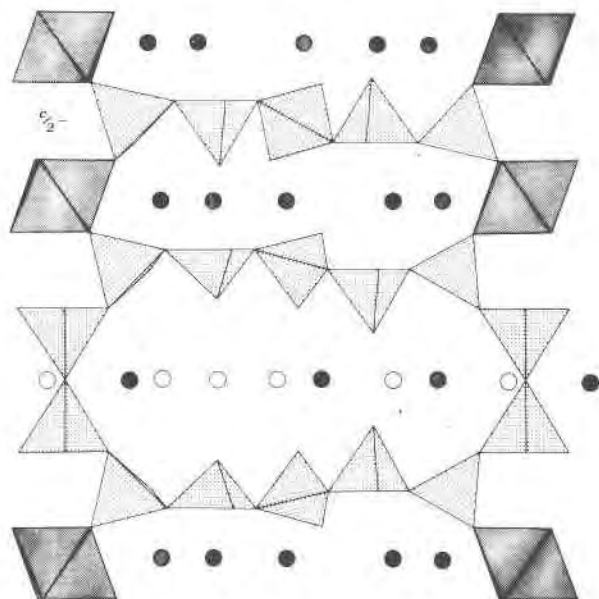


Fig. 1. Crystal structure of jagoite as seen along [100]. White circles represent chlorine atoms, shaded circles lead atoms.

sible structural component of kraisslite and mcgovernite. The double layer is composed of two linked tetrahedral sheets like that represented in Figure 3: each sheet is composed of six-membered rings of tetrahedra and ψ -tetrahedra, the latter being PbO_3 trigonal pyramids with an electron lone pair in the fourth ligand position. Whereas Si(4) and Si(5) are fully occupied by silicon cations, SiFe(2) is equally occupied

by Si^{4+} and Fe^{3+} cations. The atom O(9), which is the apical oxygen atom of the SiFe(2) tetrahedron, is located on the symmetry plane which repeats the tetrahedral sheet to produce the double layer. Pb(3) and Cl are located on this plane. The atom O(7), which is the apical oxygen atom of the Si(4) tetrahedron, and its mirror related equivalent make up the common edge of three symmetry-related, face-sharing Pb(3) octahedra (Fig. 3). The single and double layers are connected by a sheet composed of Fe(1) octahedra and Pb(2) polyhedra.

Bond lengths

The bond lengths in the various coordination polyhedra are given in Table 3, together with their standard deviations. Silicon cations are present in five crystallographically independent sites: three of them, Si(3), Si(4) and Si(5) have average Si–O distances of 1.60, 1.60 and 1.61 Å respectively. The corresponding average bond distances of the other two sites, SiFe(1) and SiFe(2), are 1.72 and 1.74 Å respectively, which indicate a nearly equal occupancy by Si^{4+} and Fe^{3+} cations, with possible minor substitution by beryllium and aluminum atoms. There is some ambiguity associated with the Si(4) tetrahedral site. Specifically, the least-squares refinement led to an improbable value for one Si(4)–O bond distance, namely a very short Si(4)–O(7) bond length of 1.41 Å, while the three crystallographically equivalent Si(4)–O(8) dis-

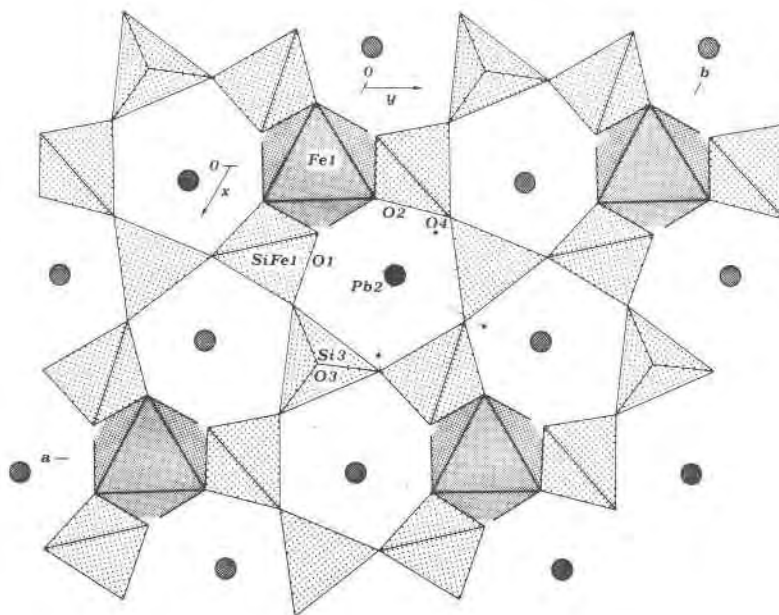


Fig. 2. Tetrahedral single layer of jagoite as seen along [001].

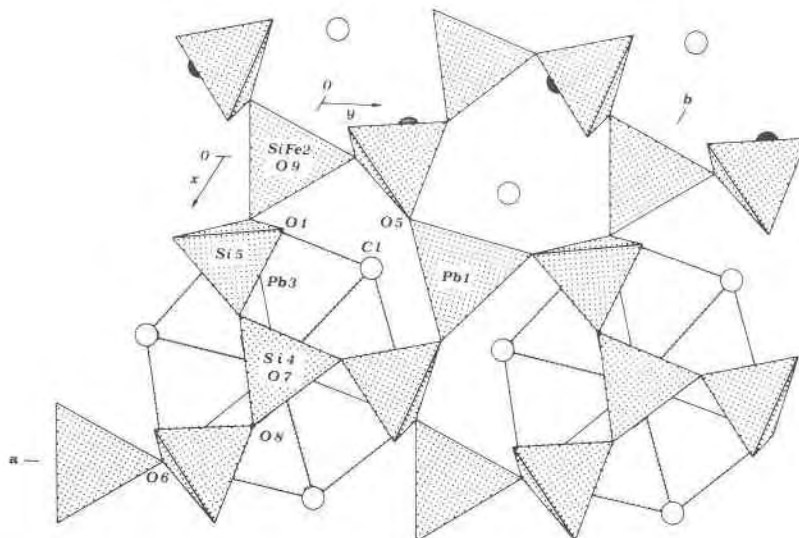


Fig. 3. One of the two sheets making up the double layer of jagoite as seen along [001].

tances are 1.66\AA long. Inspection of the bond angles $\text{O}(8)\text{-Si}(4)\text{-O}(8) = 104.8^\circ$ and $\text{O}(7)\text{-Si}(4)\text{-O}(8) = 113.8^\circ$ seemed to indicate that Si(4) was somewhat misplaced and that a regular tetrahedral coordination with reasonable bond distances could be obtained by shifting Si(4) along the threefold axis away from O(7). However, various refinement attempts resulted in a shift of the Si(4) atom from the "correct" starting position to the "wrong" one. On the other hand, a ΔF synthesis calculated with all the atoms, apart from Si(4) and O(7), gave two prominent peaks, corresponding to Si(4) and O(7) atoms, which together with the refined O(8) position defined a nearly regular tetrahedral coordination with Si(4)–O(7) and Si(4)–O(8) bond distances of 1.62 and 1.61\AA respectively. Therefore, we have reported in Table 1 the positional parameters for Si(4) obtained by least squares refinement, as well as, in brackets, those obtained from the ΔF synthesis. Likewise, Table 3 gives the Si(4)–O bond distances corresponding to the results of the least-squares refinement and, in brackets, those corresponding to the results of the ΔF synthesis. We suspect that the improbable results yielded by the least-squares refinement may be related to the proximity to Si(4) of three very heavy atoms, namely the Pb(3) atoms related by the threefold axis.

The Fe(1)–O mean bond length is 2.01\AA , in good agreement with the value 2.005\AA which is the sum of the effective ionic radii of $^{VI}\text{Fe}^{3+}$ and $^{III}\text{O}^{2-}$ (Shannon and Prewitt, 1969).

Lead cations are present in the crystal structure of jagoite in three crystallographically independent

sites. Pb(1) is bonded to three symmetry-related oxygen atoms, with Pb–O distances of 2.29\AA . The coordination is trigonal pyramidal with the lead atom at the vertex of the pyramid. This kind of coordination is conveniently called ψ -tetrahedral, assuming that an electron lone pair on the lead atom occupies the fourth ligand position. A similar coordination was found in alamosite (Boucher and Peacor, 1968) with Pb–O bond distances of 2.29 , 2.28 and 2.60\AA ; in linarite (Bachmann and Zemann, 1961) with bond distances of 2.38 and $2 \times 2.44\text{\AA}$; and in pyrobelonite (Donaldson and Barnes, 1955) with bond distances of 2.3 and $2 \times 2.5\text{\AA}$. In all these structures the mean bond length is larger than the value found in jagoite. Similar values were also found in larsenite (Prewitt *et al.*, 1967), with Pb(1)–O bond lengths of 2.26 , 2.31 and 2.46\AA and three longer distances of 2.88 , 3.15 and 3.18\AA . In trigonite (Pertlik, 1978) there are Pb(2)–O distances of 2.23 , 2.26 and 2.38\AA , and two longer distances of 2.80 and 2.89\AA ; the Pb(3)–O bond lengths are 2.26 , 2.27 and 2.34\AA with two longer distances of 2.67 and 3.14\AA . It is interesting to note that in jagoite Pb(1) is also weakly coordinated by three symmetry-related chlorine anions, with Pb(1)–Cl distance of 3.42\AA . The overall coordination polyhedron is a distorted trigonal antiprism.

Pb(2) is coordinated by eight oxygen atoms, with four short bond distances ranging from 2.39 to 2.58\AA and four long distances ranging from 2.39 to 3.30\AA . This kind of coordination is very common in lead compounds and like that of Pb(1) is a "one-sided" coordination, namely with short bonds to oxygen atoms disposed on one side and long bonds to addi-

Table 3. Bond lengths (Å) in the various coordination polyhedra with esd's in parentheses

Pb(1)-O(5) ^{VII}	2.29(2)	SiFe(1)-O(2) ^{XIII}	1.70(2)
-O(5) ^{VI}	2.29(2)	-O(2) ^{XII}	1.70(2)
-O(5) ^{VI}	2.29(2)	-O(4) ^{XIII}	1.74(2)
		-O(4) ^{XII}	1.74(2)
Pb(2)-O(2)	2.39(2)	average value	1.72
-O(5)	2.40(2)	SiFe(2)-O(6) ^{IV}	1.73(3)
-O(1) ^{IX}	2.41(3)	-O(6) ^{III}	1.73(3)
-O(3) ^{VII}	2.58(2)	-O(6) ^{VII}	1.73(3)
-O(5) ^{VI}	2.96(2)	-O(9)	1.77(2)
-O(8) ^V	2.97(3)	average value	1.74
-O(4) ^{XI}	3.06(2)	Si(3)-O(3) ^{IX}	1.55(4)
-O(4) ^X	3.30(2)	-O(4) ^{IX}	1.62(3)
average value	2.78	-O(4) ^X	1.62(3)
Pb(3)-O(7) ^{IV}	2.66(3)	-O(4) ^{XI}	1.62(3)
-O(7) ^{XIV}	2.66(3)	average value	1.60
-O(6) ^{IV}	2.71(3)	Si(4)-O(7)	1.41(6) [1.62]
-O(6) ^{XIV}	2.71(3)	-O(8) ^V	1.66(2) [1.61]
-Cl ^{VI}	2.85(1)	-O(8) ^V	1.66(2) [1.61]
-Cl ^I	2.88(1)	-O(8) ^{VII}	1.66(2) [1.61]
-O(9)	2.95(1)	-O(8)	1.66(2)
average value	2.77	average value	1.60
Fe(1)-O(2) ^I	1.98(2)	Si(5)-O(1) ^{VII}	1.54(3)
-O(2) ^{II}	1.98(2)	-O(6) ^{VIII}	1.61(3)
-O(2) ^{II}	1.98(2)	-O(8) ^{VIII}	1.64(1)
-O(1) ^I	2.05(2)	-O(5) ^{II}	1.64(2)
-O(1) ^{II}	2.05(2)	average value	1.61
-O(2) ^{II}	2.05(2)		
average value	2.01		

Symmetry code:

I	atom at	-y	x-y	z
II	" "	-x+y	-x	z
III	" "	-y	x-y	z
IV	" "	-1+x	y	z
V	" "	1-y	x-y	z
VI	" "	-x+y	1-x	z
VII	" "	1-y	1+x-y	z
VIII	" "	1-x+y	1-x	z
IX	" "	y	x	1-z
X	" "	1-x	-x+y	1-z
XI	" "	1+x-y	1-y	1-z
XII	" "	y	x	-1/2+z
XIII	" "	-x+y	-x	1/2-z
XIV	" "	-1+x	y	1/2-z

Bracketed values were obtained from ΔF syntheses.

tional oxygen atoms on the opposite side. The coordination polyhedron approaches a square antiprism.

By contrast, Pb(3) has "all-sided" coordination. Its coordination polyhedron is represented in Figure 3 as a distorted octahedron defined by four oxygen atoms (with bond distance 2×2.66 and 2×2.71 Å) and by two chlorine atoms, with bond distances 2.85 and 2.88 Å. A more distant, highly screened oxygen atom O(9) lies 2.95 Å from Pb(3) and was not taken into account in Figure 2.

Crystal chemistry

From the results of the crystal structure analysis and the preceding discussion, the following idealized crystal chemical formula may be derived for jagoite:



where T sites are occupied by silicon and trivalent iron, with minor amounts of beryllium and aluminum. The parentheses enclose the tetrahedral and ψ -tetrahedral cations in the single and in the double layers, respectively.

Table 4 reports the chemical analysis of Blix *et al.* (1957) together with the unit cell contents calculated on the basis of 56 total cations. On the basis of the preceding formula and the results given in Table 4, the actual crystal chemical formula of jagoite can be easily assessed.

(1) The chemical data indicate a deficiency of lead cations relative to the ideal number with the deficit being made up for by sodium, calcium, and potassium cations. Pb(1) and Pb(2) can be easily excluded as possible sites for such substitutions because of the short distances and the "one-sided" coordinations. On the other hand, the "all-sided" coordination, the consistently long bond distances and the relatively high thermal parameter suggest that the Pb(3) site actually receives the substituent cations.

(2) As discussed in the preceding section, silicon in the SiFe(1) and SiFe(2) sites, which are the T sites of the general ideal formula, can be substituted for by

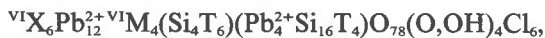
Table 4. Chemical analysis of jagoite (Blix *et al.*, 1957)

	weight percent	atoms per cell
SiO ₂	22.35	25.09
BeO	0.12	0.32
Al ₂ O ₃	0.50	0.66
Fe ₂ O ₃	7.00	5.92
TiO ₂	0.10	0.09
MgO	0.60	1.00
FeO	-	-
MnO	0.88	0.84
CaO	0.65	0.79
PbO	64.26	19.43
Na ₂ O	0.61	1.33
K ₂ O	0.37	0.53
Cl	3.25	6.18
H ₂ O ⁺	0.17	0.64
H ₂ O ⁻	0.19	
	101.05	
-O=Cl	0.73	
	100.32	

trivalent iron and minor amounts of beryllium and aluminum. Taking into account the amount of silicon, beryllium, and aluminum present, nearly four Fe^{3+} cations per unit cell may be placed in T sites, leaving about two Fe^{3+} for octahedral coordination in the Fe(1) site: its occupancy is completed by bivalent magnesium and manganese cations.

(3) The chemical analysis shows the presence of a definite, although small, water content. As the crystal structure does not present any void suitable for accommodating water molecules, the analytical water content probably corresponds to hydroxyl anions, which substitute for some oxygen anions. The O(7) site appears the most probable location for such a substitution, in view of the low bond strength sum to this atom (Table 5). The O-OH substitution in the O(7) site is probably linked to the substitution of bivalent by monovalent cations in the Pb(3) site.

To conclude we can write the following idealized crystal chemical formula for jagoite



where X corresponds to bivalent and monovalent cations in the Pb(3) site and M corresponds to trivalent and bivalent cations in Fe(1) site. The actual crystal chemical formula, on the basis of 56 total cations in the unit cell and collecting all tetrahedrally coordinated atoms, is $(\text{Pb}_{3.43}^{2+}\text{Na}_{1.33}\text{K}_{0.53}\text{Ca}_{0.71})_{\Sigma=6.00}\text{Pb}_{12}^{2+}(\text{Fe}_{1.99}^{3+}\text{Ti}_{0.09}\text{Mg}_{1.00}\text{Mn}_{0.84}\text{Ca}_{0.08})_{\Sigma=4.00}({}^{\text{III}}\text{Pb}_4^{2+}\text{Si}_{25.09}$

$\text{Be}_{0.32}\text{Al}_{0.66}\text{Fe}_{3.93}^{3+})_{\Sigma=34.00}\text{O}_{79.81}(\text{OH})_{1.28}\text{Cl}_{6.18}$ with only a small deficiency in the anionic content relative to the ideal one. We might also note here that the ratio of trivalent to bivalent M cations and the ratio of tetravalent to trivalent T cations are both close to 1:1.

Whereas the general topological features, the coordination geometry in the various structural sites, and the overall crystal chemistry of jagoite appear well established by the present structural study, some problems remain with regard to the real distribution of cations in the Fe(1), SiFe(1), and SiFe(2) sites. In this context we should recall the failure of our attempts to satisfactorily refine the structure with anisotropic temperature factors. As this circumstance is often indicative of a wrong choice of space group, we shall give further consideration to this problem.

The accurate interpretation of a number of diffraction patterns obtained from various crystals of jagoite led us to exclude $\bar{3}$ as the correct Laue group for those crystals and indicated $6/mmm$ to be the correct diffraction symmetry. Moreover the systematic absences indicated the presence of a c glide plane, which was also confirmed by the intensity measurements with the single crystal diffractometer. The choice of space group was thus restricted among $P6_3/mmc$, $P6_3mc$ or $P\bar{6}2c$. The structure analysis and solution was carried out in the latter space group. The two others can now be excluded because they would require a completely different topology for the crystal

Table 5. Electrostatic bond strength calculations (in v.u.)

	Pb (1)	Pb (2)	Pb (3)	SiFe (1)	SiFe (2)	Si (3)	Si (4)	Si (5)	Fe (1)	Σa_v
O (1)		0.404						1.249	0.447	2.100
O (2)		0.423		1.003					0.545	1.971
O (3)		0.278x3				1.215				2.049
O (4)		0.109		0.895		1.005				2.009
O (5)	0.535	0.414+0.130						0.954		2.033
O (6)			0.212		0.921			1.032		2.165
O (7)			0.235x3				1.005			1.710
O (8)		0.128					1.032	0.954		2.114
O (9)			0.133x3		0.823x2					2.045
Cl	0.119x2		0.378+0.353							0.969

Σa_v = sum of bond strengths reaching the anion.

Cation-chlorine strengths were calculated subtracting 0.41 Å from the corresponding distance. The parameters given by Brown and Wu (1976) were used.

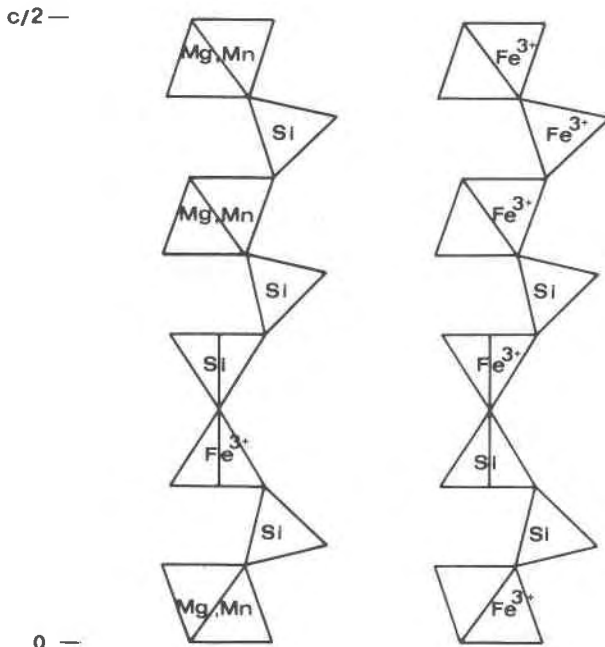


Fig. 4. Possible domains in the crystal structure of jagoite.

structure. It is, however, possible that ordering of cations gives rise to domains with space symmetry lower than $P\bar{6}2c$, the latter being only the average symmetry. One possible ordered distribution involves the corner sharing SiFe(2) tetrahedral pair, which has O(9) as the common corner. When one site is occupied by silicon, the other one could be occupied by trivalent iron or aluminum. The second ordered distribution involves the SiFe(1) tetrahedral site and the two adjacent Fe(1) octahedral sites. When SiFe(1) is occupied by silicon, Fe(1) could be occupied by a bivalent cation, Mg or Mn, whereas when SiFe(1) is occupied by Fe^{3+} or Al^{3+} , Fe(1) could be occupied by Fe^{3+} .

The chemical data, as we have stressed in the last paragraph of the preceding section, and the high thermal parameter of the oxygen anion O(9) support such ordered distributions. Figure 4 shows two ordering schemes having space group symmetry $P31c$, which is the highest symmetry subgroup of $P\bar{6}2c$ still preserving the c glide plane. The domains corresponding to these distributions and the two additional domains, which can be obtained by inter-

changing the corner sharing Si^{4+} and Fe^{3+} tetrahedra in the schemes of Figure 4, can occur simultaneously in the real structure of jagoite. It should be noted that the domains described in Figure 4, as well as the complementary pair, are quite different in chemistry. A transmission electron microscopy study would seem to be necessary to completely unravel the fine scale features of the crystal structure of jagoite.

Acknowledgment

Prof. G. Rossi and his colleagues of Istituto di Mineralogia dell'Università di Pavia are thanked for their assistance in intensity data collection.

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