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New data on lacroixite, $NaAlFPO_4$

Part I. Occurrence, physical properties and chemical composition

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Part II. Crystal structure

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Abstract

Museum specimens of lacroixite from the type locality (near Greifenstein, German Democratic Republic) were restudied. The mineral occurs in druses of a lithium-bearing granite in close association with viitaniemiite. Being similar in appearance it is difficult to distinguish between these two minerals, and therefore physical properties measured from viitaniemiite have been cited for lacroixite in the literature.

Lacroixite, NaAlFPO, is monoclinic, space group $C2/c$, $a = 6.414$, $b = 8.207$, $c = 6.885$Å, $\beta = 115.47°$ and $Z = 4$. The strongest peaks in the X-ray diffractogram are 3.155(100)(112), 2.895(98)(200), 2.476(57)(022,130), 4.73(51)(110), 2.166(43)(131), 4.627(32)(111). The specific gravity is 3.29 and hardness 4–5.

The mineral is colorless or gray, biaxial with $\alpha = 1.546$, $\beta = 1.563$, $\gamma = 1.580$, $-2V$ (meas.) = 89°, $-2V$ (calc.) = 89.1° and $r < v$. The characteristic bands in the IR spectrum are 3388, 2924, 2854, 1075, 567, 474, 396, 325 and 304 cm^{-1}.

The structure of lacroixite has been solved by Patterson and Fourier methods. After the least-square refinement the final R is 0.034 for 468 (2σ observed) reflections collected on a computer-controlled four-circle diffractometer. The structure contains chains of corner-sharing AlO_4F_2 octahedra cross-linked by PO_4 tetrahedra. The resulting large cavities in the framework are filled with Na atoms in 7-fold coordination. The octahedral chains, which are parallel to the c-axis, are kinked, the Al–F–Al angle being 142.7°. Bond distance averages are $^{[7]}$Na–(O,F) 2.356, $^{[6]}$Al–(O,F) 1.864, $^{[4]}$P–O 1.543Å.

Lacroixite is the phosphate analog of durangite, $NaAlFAsO_4$; both are isostructural with high temperature ($A2/a$) titanite, $CaTiOSiO_4$.

Part I. Occurrence, physical properties and chemical composition

Introduction

The rare phosphate mineral lacroixite was originally described by Slavik (1914, 1915) from druses of a lithium-bearing granite near Greifenstein, German Democratic Republic. Only three other localities have been reported since then by Mrose (1971). Because many of the properties were unknown or uncertain due to the paucity of the mineral, Mrose (1971) studied the type samples and redefined lacroixite. She has given the space group, unit cell data, the six main X-ray powder reflections, and proposed the formula $NaAlFPO_4$ for the mineral. The description is, however, a short abstract without any detailed information of the chemistry and optical properties of the mineral.

Because the chemical data given by Slavik (1914, 1915) are not in good agreement with the formula of Mrose (1971), and because the properties and structure of lacroixite are not fully known, the present authors restudied lacroixite samples from the type locality. Several small mineral fragments designated as lacroixite, and one piece of a druse wall were at the authors' disposal. These were from the Staatliches Museum für Mineralogie und Petrologie zu Dresden, the Mineralogical Museum of Harvard University and the U.S. National Museum of Natural History (Washington, D.C.).

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Occurrence

According to the original description of Slavik (1914) lacroixite occurs in druses of a lithium-bearing granite near Greifenstein, Saxony, German Democratic Republic. The associated minerals are quartz, potassium feldspar, tourmaline and dark Li-bearing mica. Smaller amounts of childrenite, ježekite, apatite, and roscherite were encountered as euhedral crystals in cavities. Lacroixite appears to have formed at an early to intermediate stage in the sequence of cavity mineralization. The mineral occurs as small crystal aggregates or rarely as subhedral crystals between the cavity minerals.

The studies carried out by the present authors confirmed Slavik's observations except that many of the specimens labelled lacroixite contain viitaniemiite in close association. A piece of rock from a cavity wall (specimen HMM 86746 from the Harvard Mineralogical Museum) exhibits subhedral to euhedral crystals of feldspar, quartz, and tourmaline. Two small gray grains containing both viitaniemiite and lacroixite were detected between the quartz and feldspar crystals. Thin section studies revealed that lacroixite occurs as small crystals between very thin (less than 0.02 mm), altered viitaniemiite crystal plates. A small prismatic crystal of dark green tourmaline was found as in inclusion in one sample. The Greifenstein viitaniemiite is in appearance very like that from Viitaniemi (see Lahti, 1981). Lacroixite and viitaniemiite are similar in color and difficult to recognize with the naked eye.

Physical properties

Lacroixite is gray or colorless and its luster vitreous. Some of the crystal fragments studied are transparent and exhibit a few faces. The refractive indices of the mineral are $\alpha = 1.546 \pm 0.001$, $\beta = 1.563 \pm 0.001$, $\gamma = 1.580 \pm 0.001$, $\gamma - \alpha = 0.034$. They were measured with the immersion method in Na light. The indices of refraction of the liquids were tested on an Abbe refractometer. The optic axial angle is $-2V$ (meas.) $= 89° \pm 1°$ and $r < v$. They were determined with a universal stage from a thin section containing small fragments of lacroixite. The measured optic axial angle agrees well with the calculated value, $-2V$ (calc.) $= 89.1°$.

Slavik (1914) did not determine all of the refractive indices; hence, he only reports a median value of 1.57 for his specimen. Larsen and Berman (1934) gave the refractive indices of lacroixite as follows: $\alpha = 1.545$, $\beta = 1.554$, $\gamma = 1.565$, $-2V$ near 90°; unfortunately they did not study their material in detail. Because these values differ slightly from those measured by us, we also determined the refractive indices of viitaniemiite associated with lacroixite. Fragments from the same specimen that Larsen and Berman (1934) used in their studies were at the authors' disposal (specimen HMM 87273, Harvard University, Mineralogical Museum). Our results are consistent with those reported by Larsen and Berman (1934) and indicate that their measurements were carried out on viitaniemiite.

The specific gravity of lacroixite was determined using methylene iodide–acetone solutions and a Westphal balance. The fragments showed some small differences in specific gravity probably due to cracks and inclusions. The specific gravity of the heaviest fragment, 3.29, is identical to the calculated density 3.29 g/cm^3. The much lower value of 3.126 given by Slavik (1914) is too low for lacroixite, but may represent the specific gravity of altered viitaniemiite.

Chemical composition

Lacroixite was analyzed at the Geological Survey of Finland using the electron microanalyser technique. The analyses given in Table 1 were obtained using a Jeol Superprobe at an operating voltage of 15 kV, a sample current of 20 nA and a beam diameter of 20 nm. The standards were albite for Na, spodumene for Al, apatite for P and synthetic MgF_2 (and CeF_2) for F. The chemical formula calculated on the basis of 10 (O + F) and with Z = 4 is $Na_{0.9}AlFPO_4$, which is very near to the ideal formula of lacroixite, $NaAlFPO_4$. The paucity of material precluded the analysis of water. The IR-spectrum and the structure determination indicates, however, that there are no water of crystallization or OH groups in the structure.

The original analytical data by Slavik showed (wt.%): Na_2O 14.92, CaO 19.46, MnO 8.43, Al_2O_3 18.87, P_2O_5 28.83, F 6.53, SiO_2 0.95, ign. loss 5.46, total 100.70. According to Slavik, the results are only preliminary, due to the paucity of the material. Electron microprobe analyses of the Greifenstein viitaniemiite performed during our studies gave the following results (wt.%): Na_2O 11.7, CaO 12.6, FeO 6.2, MnO 3.7, Al_2O_3 22.7, P_2O_5 27.7 and F 11.9. The composition varies, however, between different samples but it resembles closely the composition of Finnish viitaniemiite (Lahti, 1981).

The analytical data indicate that the sample analyzed by Slavik (1914) was probably a mixture of minerals consisting mainly of viitaniemiite. Slavik (1915) reported that a re-

Table 1. The chemical composition of lacroixite

	1	2		3
Al_2O_3	32.1	31.1	Al	1.0
Na_2O	16.4	18.9	Na	0.9
P_2O_5	44.7	43.3	P	1.0
F	12.3	11.6	F	1.0
	105.5		O	4.0
-O	5.17			
	100.3			

1. Lacroixite, Greifenstein. Microprobe analysis by Tuula Hautala.
2. Theoretical composition of $NaAlFPO_4$.
3. Atoms in the formula computed on the basis of 5 (O+F) from the chemical analysis.

analysis of lacroixite did not show any calcium. At this time his sample probably consisted largely of lacroixite (according to the definition of Mrose); unfortunately the results are only qualitative. In her short abstract Mrose (1971) does not give any chemical analyses, although she does present the correct chemical formula for lacroixite based on its crystallographic relation to durangite, $NaAlFAsO_4$.

Crystallography

Lacroixite was studied with X-ray diffractometer and single crystal methods. The **a**-, **b**- and **c**-axis, 0-, 1- and 2-level precession photographs were taken using Zr-filtered Mo radiation. The precession photographs exhibit monoclinic symmetry. The systematic absences ($h + k = 2n + 1$ in hkl and $l = 2n + 1$ in $h0l$ reflections) are consistent with the space group $C2/c$ (15) and Cc (9).

The X-ray powder diffraction data and cell dimensions obtained with the diffractometer method using Ni-filtered Cu radiation with a quartz standard are given in Table 2. The cell dimensions are consistent with those obtained with four-circle diffractometer during the crystal structure analysis (see Table 5) and with those given by Mrose (1971) although her determinations indicate a somewhat greater cell volume for the mineral.

Table 2. X-ray powder diffraction data on lacroixite, Greifenstein, Saxony. Diffractometer, Ni-filtered Cu radiation (Cu$K\alpha$ = 1.54178Å), quartz as an internal standard

hkl	d meas.	d calc.	I/I_o	hkl	d meas.	d calc.	I/I_o
110	4.73	4.73	51	202	1.772	1.772	5
*11$\bar{1}$	4.627	4.629	32	042	1.713	1.712	8
021	3.423	3.424	18	*20$\bar{4}$	1.709	1.709	15
111	3.254	3.254	23	33$\bar{1}$b	1.676	1.675	1
*11$\bar{2}$	3.155	3.156	100	*33$\bar{2}$	1.661	1.662	10
*002	3.107	3.108	17	11$\bar{4}$ } b	1.657	1.659 }	10
*200	2.895	2.895	98	24$\bar{2}$ }		1.656 }	
20$\bar{2}$	2.804	2.803	19	*222	1.627	1.627	12
22$\bar{1}$	2.525	2.526	18	330 }	1.578	1.579 }	27
022 }	2.476	2.477 }	57	22$\bar{4}$ }		1.578 }	
130 }		2.473 }		24$\bar{3}$ }	1.494	1.497 }	4
220	2.365	2.366	6	42$\bar{2}$ }		1.492 }	
11$\bar{3}$	2.202	2.204	9	15$\bar{2}$	1.481	1.480	2
*131	2.166	2.166	43	133	1.461	1.462	3
13$\bar{2}$	2.136	2.136	9	*043	1.458	1.458	3
040 }	2.054	2.052 }	8	$\bar{4}$00	1.448	1.448	4
31$\bar{1}$ }		2.052 }		13$\bar{4}$ }	1.440	1.440 }	9
*31$\bar{2}$	2.027	2.027	10	42$\bar{3}$ }		1.439 }	
221	1.990	1.991	4	331	1.415	1.415	2
041b	1.950	1.948	5	*40$\bar{4}$	1.402	1.402	5
*22$\bar{3}$	1.931	1.931	14	33$\bar{4}$ }	1.374	1.374 }	4
310	1.880	1.879	4	312 }		1.373 }	
132b	1.782	1.782	1				

b broad peak
* used in computing unit cell dimensions: a= 6.414 Å, b= 8.207 Å, c= 6.885 Å and β= 115.47°.

Before the redefinition of lacroixite (Mrose, 1971) the mineral described on JCPDS-card 13-587 (specimen from Greifenstein) was called lacroixite: afterwards the name was changed to "unknown mineral". The first of the present authors (S.L.) showed that the mineral described could be viitaniemiite and therefore the card was renamed viitaniemiite. During this study we confirmed that the X-ray powder diffraction pattern of the Greifenstein viitaniemiite is identical to that of Viitaniemi and Francon viitaniemiite (Lahti, 1981, and Ramik et al., 1983) and the unit cell data given for viitaniemiite by Mrose (1971) and Pajunen and Lahti (1984) are close to each other.

Infrared spectrum

The infrared spectrum was recorded with a Perkin-Elmer 983 spectrophotometer fitted with the Data Station 36 computer at the Technical Research Center of Finland. The spectrum was recorded with two methods: (1) The conventional pressed disc technique, in which 1 mg of the lacroixite powder was ground with 300 mg KBr. The spectra obtained are given in Figure 1(a). (2) The nujol technique, whereby the spectrum was recorded using nujol—mineral emulsion to prevent the bands caused by the humidity absorbed from the air during grinding of the sample. The spectrum is given in Figure 1(b). Even the nujol causes some additional bands, i.e., 3000–2800, 1460, 1380 and 720 cm^{-1}.

The following bands were recorded for lacroixite using the conventional pressed disc technique: 3434, 2924, 2854, 1630, 1075, 808, 567, 474, 396, 325, and 304 cm^{-1}. Because the spectrum shows bands characteristic of water and OH vibrations (3434, 1630 and 808 cm^{-1}), the nujol technique was also used. Strong OH stretching vibrations are assigned to the high frequency region between 3400 and 3550 cm^{-1} in many phosphates and silicates including titanite (Plyusina and Zajtseva, 1971), which is structurally similar to lacroixite.

Figure 1(b) shows that the two bands at 1630 and 808

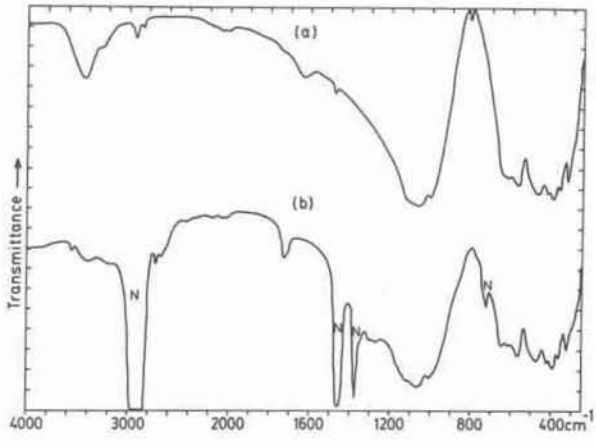

Fig. 1. The infrared spectrum of lacroixite recorded using a) conventional pressed KBr-disc technique b) nujol technique. The bands marked with N are derived from nujol.

cm^{-1} are lacking and that only a weak broad band at 3388 cm^{-1} is visible in the spectrum recorded using the nujol technique. This indicates that lacroixite has no water of crystallization, but that very limited substitution of F by OH may be possible. Bands 3434, 1630 and 808 cm^{-1} in the spectrum recorded using the conventional pressed disc technique are assigned to the vibrations of molecular water absorbed by the sample; these bands were present also in pure KBr discs.

Lacroixite has a broad absorption band at 1200–950 cm^{-1}. This may be attributed to the stretching vibrations of PO_4 tetrahedra or to 2νAl–F and 2νAl–O overtones as in durangite (Sumin de Portilla, 1974), which is an arsenate analog of lacroixite. The medium to low frequency region is also quite complex. P–O bending vibrations (Povarennyh, 1972, Fransolet and Tarte, 1977) and probably the stretching vibrations of Al–F and Al–O (Sumin de Portilla, 1974) may be the cause of bands below 650 cm^{-1}.

Part II. Crystal structure

Experimental

For the structure analysis a transparent crystal fragment of lacroixite measuring about 0.5 × 0.5 × 0.8 mm was separated from the type material.

The unit cell dimensions (298° K) given in Table 5 were obtained by least-squares refinement of angular settings of 15 reflections centered on a Nicolet P3 automatic four-circle diffractometer using graphite monochromated Mo$K\alpha$ radiation ($\lambda = 0.7107$Å). The intensity data were measured using the ω-scan method with variable scan speed. Two standard reflections measured for every 50 reflections showed no systematic variation. Of the 554 reflections with $3° < 2\theta < 60°$, 468 were regarded as observed ($I > 2\sigma(I)$). The intensities were corrected for Lorentz and polarization effects, but no corrections for absorption were applied ($\mu = 16.7\ cm^{-1}$).

Although lacroixite was suspected to be isostructural with durangite, the structure was determined independently using Patterson and Fourier methods. The structure was refined with the full-matrix, least-squares method using anisotropic temperature factors. The function minimized was $\Sigma w\|F_o| - |F_c\|^2$ with unit weights. The atomic scattering factors used were those of Cromer and Mann (1968). The refinement converged to an R factor of 0.034, $R_w = 0.042$ and $S = (\Sigma w \Delta F^2/(m - n))^{0.5} = 10.2$. On the difference map the electron density was largest 0.28 eÅ^3, in the vicinity of the phosphorus atom. The calculations were performed on a UNIVAC 1100 computer using programs of the XRAY76 system (Stewart, 1976). The final atomic parameters are listed in Table 3 and the interatomic distances and bond angles are given in Table 4. Observed and calculated structure factors[1] are on deposit.

Discussion of the structure

The structure of lacroixite contains chains of corner-sharing AlO_4F_2 octahedra cross-linked by PO_4 tetrahedra. The resulting large cavities in the framework are filled by Na atoms in seven-fold coordination. Figure 2 shows a stereoscopic view of the structure. The octahedral chains, which are parallel to the **c** axis of the mineral, are kinked, the Al–F–Al angle being 142.7(1)°.

The AlO_4F_2 octahedra are nearly ideal. The phosphate groups are slightly deformed tetrahedra with O–P–O angles in the range 105.8–110.4°. Na occupies an irregular seven-coordinated polyhedron between the chains.

Lacroixite ($NaAlFPO_4$, with $Z = 4$) is the phosphate analog of durangite ($NaAlFAsO_4$), which according to Kokkoros (1938), is isostructural with titanite ($CaTiOSiO_4$). Speer and Gibbs (1976) showed that there are two titanite polymorphs in nature, the one with space group $P2/a$ and the other with $A2/a$ (or $C2/c$ using our axes). Our structural analysis confirmed that the space group of lacroixite is $C2/c$ and, like durangite, the mineral is isostructural with the high temperature variety of titanite (space group $A2/a$).

Table 5 presents the unit cell data and the mean cation-

[1] To receive a copy of the structure factors, order Document AM-85-270 from the business Office, Mineralogical Society of America 2000 Florida Avenue, N.W., Washington, D.C. 20009. Please remite $5.00 in advance for the microfiche.

Table 3. Atomic coordinates and anisotropic thermal vibration parameters for lacroixite

Atom	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Al	0.0	0.0	0.0	0.0037(5)	0.0043(5)	0.0035(5)	0.0002(4)	0.0007(4)	-0.0004(4)
Na	0.0	0.6685(2)	0.25	0.0147(9)	0.0083(9)	0.0297(11)	0.0	0.0025(8)	0.0
P	0.0	0.3178(1)	0.25	0.0035(4)	0.0042(4)	0.0046(4)	0.0	0.0008(3)	0.0
O(1)	0.0939(4)	0.2095(3)	0.1218(3)	0.0060(9)	0.0055(9)	0.0072(9)	-0.0008(7)	0.0018(7)	-0.0007(7)
O(2)	0.1915(4)	0.4310(3)	0.4032(3)	0.0052(9)	0.0077(9)	0.0089(9)	-0.0006(7)	0.0017(7)	-0.0011(7)
F	0.0	-0.0708(3)	0.25	0.0099(11)	0.0055(10)	0.0049(10)	0.0	0.0032(8)	0.0

The values of x, y, z are given in fractional coordinates, the anisotropic temperature factor is of the form $\exp(-2\pi^2(U_{11}a^{*2}h^2 + U_{22}b^{*2}k^2 + U_{33}c^{*2}l^2 + 2U_{12}a^*b^*hk + 2U_{13}a^*c^*hl + 2U_{23}b^*c^*kl))$. Estimated standard deviations in parentheses refer to the last digits.

Table 4. Interatomic distances and angles for lacroixite

Al	-	O(1)	1.895(2)	O(1)	-	Al	-	$O(2)^{i}$	91.8(1)	O(1)	-	$O(2)^{i}$	2.712(3)
Al	-	$O(2)^{i}$	1.882(2)	O(1)	-	Al	-	F	90.0(1)	O(1)	-	F	2.626(3)
Al	-	F	1.816(1)	$O(2)^{i}$	-	Al	-	F	89.8(1)	$O(2)^{i}$	-	F	2.610(3)
Na	-	$O(1)^{ii}$	2.387(2)	$O(1)^{ii}$	-	Na	-	$O(1)^{iii}$	79.9(1)	$O(1)^{ii}$	-	$O(1)^{iii}$	3.185(4)
Na	-	$O(1)^{iii}$	2.567(2)	$O(1)^{ii}$	-	Na	-	$O(1)^{iv}$	93.7(1)	$O(1)^{ii}$	-	$O(1)^{iv}$	3.617(3)
Na	-	O(2)	2.304(3)	$O(1)^{ii}$	-	Na	-	O(2)	124.8(1)	$O(1)^{ii}$	-	O(2)	4.157(3)
Na	-	F^{vi}	2.141(3)	$O(1)^{ii}$	-	Na	-	$O(2)^{v}$	70.6(1)	$O(1)^{ii}$	-	$O(2)^{v}$	2.712(3)
				$O(1)^{ii}$	-	Na	-	F^{vi}	81.9(1)	$O(1)^{ii}$	-	F^{vi}	2.973(3)
				$O(1)^{iii}$	-	Na	-	F^{vi}	67.0(1)	$O(1)^{iii}$	-	F^{vi}	2.624(3)
				$O(1)^{iii}$	-	Na	-	O(2)	129.6(1)	$O(1)^{iii}$	-	O(2)	4.409(3)
				$O(1)^{iii}$	-	Na	-	$O(2)^{v}$	91.4(1)	$O(1)^{iii}$	-	$O(2)^{v}$	3.490(3)
				O(2)	-	Na	-	$O(2)^{v}$	64.4(1)	O(2)	-	$O(2)^{v}$	2.455(3)
P	-	O(1)	1.546(3)	O(1)	-	P	-	$O(1)^{v}$	109.7(2)	O(1)	-	$O(1)^{v}$	2.528(4)
P	-	O(2)	1.540(2)	O(1)	-	P	-	O(2)	110.3(1)	O(1)	-	O(2)	2.531(3)
				O(1)	-	P	-	$O(2)^{v}$	110.4(1)	O(1)	-	$O(2)^{v}$	2.533(3)
				O(2)	-	P	-	$O(2)^{v}$	105.8(2)	O(2)	-	$O(2)^{v}$	2.455(3)

Symmetry code (i) = 1/2 - x, -1/2 + y, 1/2 - z (ii) = -1/2 + x, 1/2 + y, z (iii) = -x, 1 - y, -z
(iv) = x, 1 - y, 1/2 + z (v) = -x, y, 1/2 - z (vi) = x, 1 + y, z

anion distances of lacroixite, durangite, titanite and three other structurally similar minerals. Detailed discussion of the titanite and other derivative structures have been presented by several authors e.g., Mongiorni and Sanseverino (1968), Taylor and Brown (1976), Speer and Gibbs (1976), and Higgins and Ribbe (1977). Table 5 shows that SiO_4 groups in the titanite structure may be replaced by AsO_4 and PO_4 groups. Lacroixite, isokite and panasqueiraite are the three known phosphates structurally similar to titanite, although detailed crystal structure analyses of the two last mentioned minerals are lacking (Isaacs and Peacor, 1981). In lacroixite and durangite the seven coordinated Ca atoms of titanite are replaced by Na atoms, and the octahedral Ti atoms by Al atoms. Fluorine occupies the same site in lacroixite and in other isostructural minerals as does the non-tetrahedral oxygen in titanite. The OH groups replace this site in panasqueiraite and may also partly replace it in titanite (Sahama 1946, Higgins and Ribbe, 1976).

The unit cell volume of lacroixite is much smaller than that of the other minerals isostructural with it due to the small size of the Al octahedra and P tetrahedra. The large octahedral Mg, Ti and Sn atoms cause lengthening of especially the **b**- and **c**-axes in the structure. The chemical analyses of the Greifenstein lacroixite do not show any marked replacement and the chemical and structural data are therefore consistent with each other.

Lacroixite occurs closely associated with viitaniemiite as a hydrothermal cavity mineral. The structure of each mineral exhibits kinked chains of Al octahedra with a period of 7Å linked by P tetrahedra (cf. Pajunen and Lahti 1984). This kind of chain structure is especially characteristic of many low-temperature phosphate minerals that occur, like lacroixite and viitaniemiite, in granitic pegmatites and their cavities (Moore, 1970).

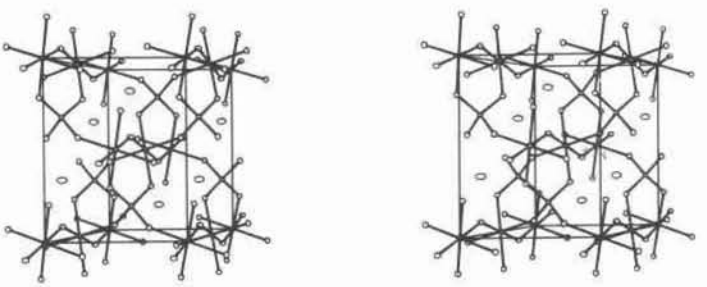

Fig. 2. Stereoscopic view of the lacroixite structure. The origin is at the lower left hand corner, **a** is horizontal, **b** is vertical and **c** towards viewer.

Table 5. Comparisons between the unit cell data and structure of lacroixite (the present study), isokite (Deans et al., 1955), panasqueiraite (Isaacs and Peacor, 1981), durangite (Kokkoros, 1938), tilasite (Bladh et al., 1972), titanite (Mongiorni and Sanseverino, 1968) and malayaite (Higgins and Ribbe, 1977).

	Lacroixite $NaAlFPO_4$	Isokite $CaMgFPO_4$	Panasqueiraite $CaMg(OH)PO_4$	Durangite $NaAlFAsO_4$	Tilasite $CaMgFAsO_4$	Titanite $CaTiOSiO_4$	Malayaite $CaSnOSiO_4$
a(Å)	6.411(2)	6.535	6.52	6.53	6.688	6.555	6.667
b(Å)	8.210(2)	8.753	8.75	8.46	8.944	8.718	8.906
c(Å)	6.883(2)	6.919	7.16	7.30	7.570	7.073	7.149
β(°)	115.45 (3)	112.33	109.5	119.37	121.17	113.97	113.3
V($Å^3$)	327.13	366.09	385.05	351.45	397.45	369.34	389.86
4 coord. cation	P	P	P	As	As	Si	Si
c-a distance(Å)*	1.543	-	-	1.68	1.684	1.663	1.641
6 coord. cation	Al	Mg	Mg	Al	Mg	Ti	Sn
c-a distance(Å)*	1.864	-	-	1.84	2.060	1.930	2.042
7 coord. cation	Na	Ca	Ca	Na	Ca	Ca	Ca
c-a distance(Å)*	2.356	-	-	2.44	2.466	2.436	2.483

* the mean distance between cation and anions.

\- not known

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