

PETARASITE, $\text{Na}_5\text{Zr}_2\text{Si}_6\text{O}_{18}(\text{Cl},\text{OH}) \cdot 2\text{H}_2\text{O}$,
A ZEOLITE-TYPE ZIRCONOSILICATE

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ABSTRACT

Petarasite, $\text{Na}_5\text{Zr}_2\text{Si}_6\text{O}_{18}(\text{Cl},\text{OH}) \cdot 2\text{H}_2\text{O}$, from Mont St-Hilaire, Quebec, is monoclinic, space group $P2_1/m$, with cell dimensions a 10.7956(8), b 14.4928(16), c 6.6229(6) Å, β 113.214(5)°; $Z = 2$. The crystal structure has been determined by direct methods and refined by least squares to a R factor of 0.051, based on 2947 observed reflections. The crystal structure of petarasite is an open three-dimensional framework, with the composition $\text{Zr}_2\text{Si}_6\text{O}_{18}$, consisting of corner-sharing, six-membered silicate rings and ZrO_6 octahedra. Elliptical channels (3.5 x 5.5 Å), defined by mixed six-membered rings, consisting of pairs of SiO_4 tetrahedra linked by Zr octahedra, run parallel to the b and c axes. Other channels limited by silicate rings run parallel to c . Two sodium atoms and the water molecules are located in channels parallel to b , whereas the third sodium atom and the Cl and (OH) ions are located in channels parallel to c . The average Si-O and Zr-O bond distances are 1.615 and 2.091 Å, respectively. All three sodium atoms are seven coordinated. The Cl and (OH) ions are solely bonded to the sodium atoms and are partially disordered. Structurally, petarasite is related to other zircono- (or titano-) silicates such as lovozerite, $\text{Na}_2[\text{ZrSi}_6\text{O}_{12}(\text{OH})_6]$, and kazakovite, $\text{Na}_6\text{Mn}[\text{TiSi}_6\text{O}_{18}]$.

Keywords: petarasite, zirconosilicate, six-membered rings, framework structure.

SOMMAIRE

La pétarasite, $\text{Na}_5\text{Zr}_2\text{Si}_6\text{O}_{18}(\text{Cl},\text{OH}) \cdot 2\text{H}_2\text{O}$, du mont St-Hilaire, Québec, cristallise dans le groupe $P2_1/m$, avec la maille: a 10.7956(8), b 14.4928 (16), c 6.6229(6) Å, β 113.214(5)°, et $Z = 2$. Sa structure, déterminée par méthodes directes, a été affinée par moindres carrés, jusqu'au résidu $R = 0.051$, sur 2947 réflexions observées. Elle consiste en une charpente tridimensionnelle, ouverte, de composition $\text{Zr}_2\text{Si}_6\text{O}_{18}$, formée d'anneaux à six tétraèdres SiO_4 et d'octaèdres ZrO_6 à sommets communs. Des tunnels de section elliptique (3.5 x 5.5 Å), parallèles aux axes b et c , sont ménagés

par des anneaux mixtes à six maillons qui consistent en paires de tétraèdres SiO_4 reliées par les octaèdres. Les anneaux silicatés définissent aussi des tunnels parallèles à c . Les tunnels suivant b contiennent 2 atomes de sodium, ainsi que les molécules d'eau; les tunnels parallèles à c renferment un troisième sodium et les ions chlore et hydroxyle. La moyenne des liaisons Si-O est 1.615; celle des distances Zr-O, 2.091 Å. Les atomes de sodium sont tous trois heptacoordonnés. Les ions Cl et OH, partiellement désordonnés, ne sont liés qu'aux atomes de sodium. Structuellement, la pétarasite se rattache aux zircono- (et titano-) silicates, tels la lovozerite $\text{Na}_2[\text{ZrSi}_6\text{O}_{12}(\text{OH})_6]$ et la kazakovite $\text{Na}_6\text{Mn}[\text{TiSi}_6\text{O}_{18}]$.

(Traduit par la Rédaction)

Mots-clés: pétarasite, zirconosilicate, anneaux à six côtés, charpente (structure en -).

INTRODUCTION

Petarasite is a new sodium zirconosilicate mineral from Mont St-Hilaire, Quebec, with the empirical chemical composition $(\text{Na}_{4.89}\text{Ca}_{0.13}\text{K}_{0.08})(\text{Zr}_{2.01}\text{Ti}_{0.01})\text{Si}_6\text{O}_{18}[(\text{OH})_{0.80}\text{Cl}_{0.48}] \cdot 3.01\text{H}_2\text{O}$ (Chao *et al.* 1980). It occurs as irregular grains up to 10 mm across in a xenolith in nepheline syenite, in association with catapleite, apatite and zircon. Chao *et al.* have determined the chemical composition and crystallographic and optical properties of petarasite. They found it to be monoclinic, space group $P2_1/m$ or $P2_1$, with unit-cell dimensions a 10.791(4), b 14.505 (5), c 5.626(2) Å, β 113.21(3)°; $Z = 2$.

CRYSTAL DATA

A small cleavage fragment of petarasite was ground to a sphere with a diameter of 0.25 mm (Bond 1951), which was mounted on the computer-controlled single crystal X-ray diffractometer (Syntex P1). The unit-cell dimensions were redetermined by least-squares refine-

TABLE 1. CRYSTAL DATA FOR PETARASITE

Petasarite, $\text{Na}_3\text{Zr}_2\text{Si}_6\text{O}_{18}(\text{Cl},\text{OH})\cdot 2\text{H}_2\text{O}$	
Light greenish yellow transparent grains from Mont St. Hilaire, Quebec, Canada	
Monoclinic, $2/m$	Space group: $P 2_1/m$
a : 10.7956(8) Å	Cell content: $2[\text{Na}_3\text{Zr}_2\text{Si}_6\text{O}_{18}(\text{Cl},\text{OH})\cdot 2\text{H}_2\text{O}]$
b : 14.4928(16) Å	D_m : 2.88 g cm ⁻³
c : 6.6229(6) Å	D_o : 2.86 g cm ⁻³
β : 113.214(5)°	$\lambda(\text{MoK}\alpha)$: 0.71069 Å
V : 952.32 Å ³	$\mu(\text{MoK}\alpha)$: 17.38 cm ⁻¹

ment of the 2θ values (between 22 and 38°) measured for 15 reflections and their symmetry equivalents, using Mo $K\alpha$ radiation (Table 1). These cell dimensions are in good agreement with those determined by Chao *et al.* (1980).

COLLECTION OF THE INTENSITY DATA

The X-ray intensity data were collected from the single crystal sphere by the θ - 2θ method, using graphite-monochromatized Mo $K\alpha$ radiation and a scintillation counter. The variable scan method was used, with the minimum scan-rate being 1°/min. (50 kV, 12.5 mA). All reflections within the 2θ limit of 65° were collected in a quadrant, *i.e.*, a total of 3734 reflections, out of which 787 were below $3\sigma(I)$, where $\sigma(I)$ is the standard deviation of the intensity I , as determined from the counting statistics. The measured intensities were corrected for Lorentz, polarization and absorption factors.

DETERMINATION AND REFINEMENT OF THE STRUCTURE

An $N(Z)$ test of the measured X-ray intensities indicated that the centric space group $P2_1/m$ is most likely to be correct. The crystal structure has been determined by symbolic addition (Karle & Karle 1966), using the computer program MULTAN (Germain *et al.* 1971). In addition to the three origin-determining reflections, signs of four reflections were determined through the Σ_1 relationship, and five reflections were assigned symbols. The first E map indicated the positions of zirconium, two silicon and three oxygen atoms. Cycles of least-squares refinement, followed by difference-Fourier syntheses, brought out the missing silicon, oxygen and sodium atoms, the water molecules and the Cl and (OH) ions. Least-squares refinement at this stage indicated a negative temperature-factor for Na(3); subsequently, 0.20 Ca and 0.80 Na were assigned to this site,

which made the temperature factor positive. The R factor at this stage was 0.080. Subsequently, the occupancy and positional parameters of Cl and the (OH) ions were refined, resulting in a lowering of the R factor to 0.069. Final refinement was carried out using anisotropic temperature factors and the block-diagonal least-squares-refinement program CRYLSQ (Stewart *et al.* 1972), with one block assigned to each atom. The atomic scattering factors for Na, Ca, Zr, Si, O and Cl were taken from Cromer & Mann (1968), corrected for anomalous dispersion (Cromer & Liberman 1970). The observed structure factors were weighted by the formula $1/\sigma^2(F_o)$, where $\sigma(F_o)$ is the standard deviation of the measurement of the structure factor F_o . The final R factor, based on all observed reflections, is 0.051. The final refinement resulted after seven cycles; even though very close to convergence, the refinement still showed oscillations in both positional and thermal parameters for Na(3), which is highly anisotropic, and, surprisingly, for Zr. Attempts to refine the structure in the space group $P2_1$ were unsuccessful. The final positional and thermal parameters are listed in Table 2. Observed and calculated structure factors (Table 3) have been deposited and may be obtained at nominal charge from the Depository of Unpublished Data, CISTI, National Research Council of Canada, Ottawa, Ontario K1A 0S2. Bond lengths and angles are presented in Table 4. The average standard deviations in Na-O, Zr-O and Si-O bond lengths are 0.005, 0.003 and 0.005 Å, respectively; in the O-Zr-O and O-Si-O angles, they are 0.1 and 0.2°, respectively. Because of low partial occupancy, the positional coordinates of the (OH) ions are not very reliable. Hence they have been omitted from a discussion of the crystal structure. The third water molecule shown in the empirical formula was not found; thus the ideal structural formula for petasarite is $\text{Na}_3\text{Zr}_2\text{Si}_6\text{O}_{18}(\text{Cl},\text{OH})\cdot 2\text{H}_2\text{O}$.

DESCRIPTION OF THE STRUCTURE

The three-dimensional framework

The crystal structure of petasarite is an open three-dimensional framework with the composition $[\text{Zr}_2\text{Si}_6\text{O}_{18}]$, consisting of corner-sharing, six-membered silicate rings and ZrO_6 octahedra. Elliptical channels (3.5 x 5.5 Å) defined by mixed six-membered rings, consisting of pairs of $[\text{SiO}_4]$ tetrahedra linked by Zr octahedra, run parallel to the b and c axes (Figs. 1, 2).

TABLE 2. PETARASITE: POSITIONAL AND THERMAL PARAMETERS

	x^*	y	z	u_{11}^+	u_{22}	u_{33}	u_{12}	u_{13}	u_{23}
Na (1)	53703(26)	11999(18)	94377(40)	409(14)	269(16)	315(12)	119(13)	189(11)	99(11)
Na (2)	96816(26)	11801(17)	4734(36)	400(14)	213(14)	224(11)	-90(11)	102(10)	-35(10)
Na (3)	75350(52)	25000	53730(128)	238(22)	70(22)	1619(66)	-	229(33)	-
Zr	75341(4)	1483(3)	50974(6)	62(1)	15(1)	39(1)	-2(2)	35(1)	-3(2)
Si (1)	4177(11)	14185(9)	59651(18)	71(5)	18(5)	52(5)	5(4)	31(4)	1(4)
Si (2)	25281(13)	5076(8)	99330(18)	79(4)	50(5)	36(4)	4(5)	23(4)	-2(4)
Si (3)	46055(11)	14000(8)	39881(18)	61(5)	22(5)	71(5)	-7(4)	35(4)	-5(4)
O(1)	5903(47)	25000	54621(72)	152(22)	43(22)	161(21)	-	98(18)	-
O(2)	89046(32)	12341(23)	57443(54)	105(14)	73(17)	229(16)	-20(13)	93(13)	-31(13)
O(3)	9220(30)	7970(22)	44176(46)	121(14)	57(15)	74(13)	47(12)	51(11)	17(11)
O(4)	13872(35)	12679(26)	85457(48)	271(19)	165(19)	72(14)	143(16)	45(13)	9(13)
O(5)	80161(31)	514(24)	84919(46)	156(15)	128(18)	60(12)	-58(14)	54(11)	-14(11)
O(6)	70604(32)	1230(25)	17083(45)	168(15)	113(17)	66(12)	44(15)	69(11)	0(12)
O(7)	38504(34)	11045(25)	14028(48)	213(17)	159(19)	80(14)	-103(15)	57(13)	-27(13)
O(8)	61709(30)	12247(23)	46523(52)	82(14)	61(17)	225(16)	26(13)	73(12)	6(13)
O(9)	43210(47)	25000	41461(78)	122(22)	58(23)	228(24)	-	68(19)	-
O(10)	39821(31)	8351(23)	54458(48)	130(15)	70(16)	107(14)	-58(13)	70(12)	-16(12)
w(1)(H ₂ O)	10237(77)	25000	16018(107)	575(46)	261(39)	394(36)	-	308(34)	-
w(2)(H ₂ O)	39241(63)	25000	82389(92)	399(34)	145(30)	283(29)	-	211(26)	-
Cl	75124(32)	25000	521(48)	352(14)	177(12)	435(16)	-	164(12)	-
(OH) (1)	86880(360)	25000	-2220(564)	625(99)	-	-	-	-	-
(OH) (2)	70151(644)	25000	11946(972)	528(157)	-	-	-	-	-

+ Anisotropic temperature factor expression ($\times 10^3$), $\exp[-2\pi^2(\frac{1}{2}u_{11}^2 a^{*2} + u_{22}^2 b^{*2} + u_{33}^2 c^{*2} + 2u_{12}^* hka^* b^* \cos \gamma^* + 2u_{13}^* hka^* c^* \cos \beta^* + 2u_{23}^* klb^* c^* \cos \alpha^*)]$; isotropic temperature factors, $u(\times 10^2)$
 Occupancies: Na(3): Na 0.80; Ca 0.20; Cl: 0.75; (OH)(1): 0.25; (OH)(2): 0.12.
 Standard deviations in parentheses. Positional coordinates $\times 10^5$.

Other channels limited by silicate rings run parallel to *c*. The sodium atoms, Na(1) and Na(2), and the water molecules w(1) and w(2) are located in channels parallel to *b*, whereas Na(3) and the Cl atoms and (OH) ions are located in channels parallel to *c*.

Conformation of the six-membered silicate ring

The [Si₆O₁₈] ring, of point-group symmetry *m*, deviates considerably from hexagonal symmetry. It can be considered as formed by two [Si₂O₇] groups, one pointing up and the other pointing down, bridged by two separate [SiO₄] groups (Fig. 3). This situation is similar to that found in lovozerite, Na₂ZrSi₆O₁₂(OH)₆ (Ilyukhin & Belov 1960); however, in lovozerite, the ring has a *chair* configuration, whereas in petarasite it is nearly planar. The Si-O-Si angles within the [Si₂O₇] groups [Si(1)-O(1)-Si(1)′ 148.6°; Si(3)-O(9)-Si(3)′ 154.5°] are much larger than the other two between the [Si₂O₇] groups and the isolated [SiO₄] tetrahedra [Si(1)-O(5)-Si(2) 135.1°; Si(2)-O(7)-Si(3) 136.4°]. The maximum deviation of the silicon atoms from the least-square plane passed through the bridging oxygen atoms [O(1), O(4), O(7) and O(9)] is 0.06 Å (Table 5).

The average Si-O bond length within the

three crystallographically independent silicate tetrahedra is 1.615 Å. Each silicate tetrahedron shares two corners with adjacent silicate tetrahedra, and each of the other two corners are shared with Zr octahedra and Na polyhedra. The average Si-O bond involved in bridging two Si atoms is significantly larger (1.632 Å) than the average nonbridging ones (1.604 Å).

The Zr octahedron

The Zr octahedron is nearly regular; the Zr-O distances vary from 2.082 to 2.103 Å, and the O-Zr-O angles from 82.4 to 95.9°. The average Zr-O distance, 2.091 Å, is significantly larger than that (2.074 Å) found in zektzerite, NaLiZrSi₆O₁₅, where Zr octahedra share edges with LiO₄ tetrahedra (Ghose & Wan 1978).

The sodium polyhedra

All three sodium atoms are seven-coordinated. The Na(1)O₅(H₂O)Cl and Na(2)O₅(H₂O)Cl polyhedra are distorted monocapped octahedra, whereas the Na(3)O₆Cl polyhedron is a distorted hexagonal pyramid (Fig. 4). For a proper shielding of the charge of the Na(3) ion, a second Cl atom may be considered part of the Na(3) coordinations [Na(3)-Cl 3.520 Å];

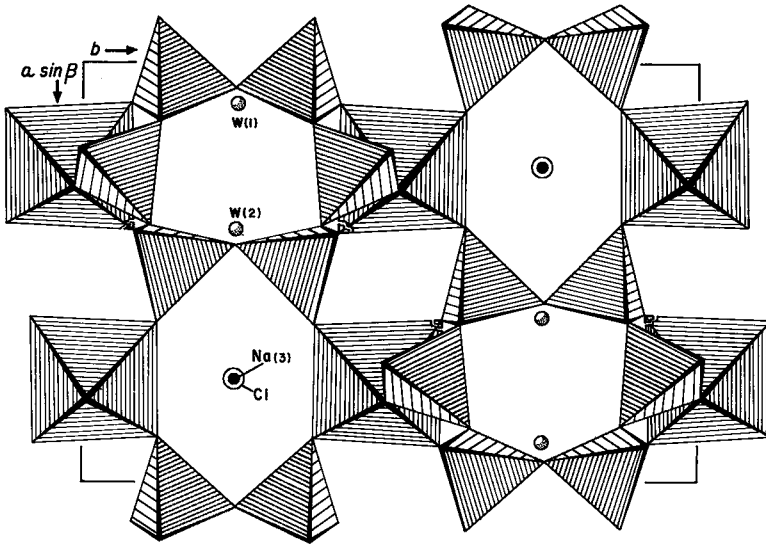


FIG. 1. Petarasite, $\text{Na}_5\text{Zr}_2\text{Si}_6\text{O}_{18}(\text{Cl},\text{OH})\cdot 2\text{H}_2\text{O}$: partial projection of the structure down the c axis, showing the corner-sharing, six-membered silicate rings and ZrO_6 octahedra. Note the elliptical channels parallel to the c axis, which accommodate $\text{Na}(3)$ and Cl atoms.

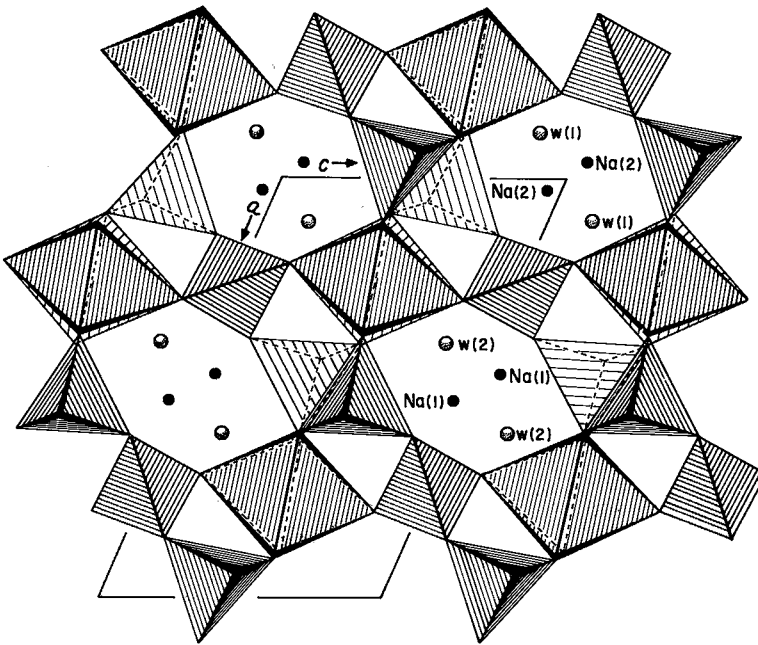


FIG. 2. Petarasite: partial projection of the structure down the b axis showing elliptical channels parallel to b , which house the sodium atoms $\text{Na}(1)$ and $\text{Na}(2)$ and the water molecules. The six-membered silicate rings and the rest of the structure can be reconstructed by passing mirror planes through vertices of silicate tetrahedra pointing up (or down).

TABLE 4. PETARASITE: BOND LENGTHS (Å) AND ANGLES (°)

The Na(1) Polyhedron		The Na(2) Polyhedron	
Na(1) - O(6)	2.421(4)	Na(2) - O(2)	2.907(4)
Na(1) - O(6)'	3.093(4)	Na(2) - O(3)	2.484(4)
Na(1) - O(7)	2.468(5)	Na(2) - O(4)	2.625(5)
Na(1) - O(8)	3.213(5)	Na(2) - O(5)	2.402(4)
Na(1) - O(10)	2.528(4)	Na(2) - O(5)	2.914(4)
Na(1) - W(2)	2.375(5)	Na(2) - W(1)	2.337(5)
Na(1) - Cl	2.885(4)	Na(2) - Cl	2.951(4)
Mean of 6 Na - O distances	2.683	Mean of 6 Na - O distances	2.612
The Na(3) Polyhedron		The Zr Octahedron	
Na(3) - O(2)	2.308(5)	Zr - O(2)	2.086(3)
Na(3) - O(2)'	2.308(5)	Zr - O(3)	2.082(3)
Na(3) - O(8)	2.293(5)	Zr - O(5)	2.103(3)
Na(3) - O(8)''	2.293(5)	Zr - O(6)	2.097(3)
Na(3) - O(1)	3.276(4)	Zr - O(8)	2.084(3)
Na(3) - O(9)	3.237(4)	Zr - O(10)	2.092(3)
Na(3) - Cl	3.109(3)	Mean 2.091	
Na(3) - Cl'	3.520(4)	O(2) - O(3)	2.954(5)
Mean of 6 Na - O distances	2.619	O(2) - O(5)	2.923(5)
		O(2) - O(6)	3.083(4)
		O(3) - O(5)	2.748(5)
		O(3) - O(6)	2.878(5)
		O(3) - O(10)	2.950(4)
		O(3) - O(8)	3.099(5)
		O(5) - O(8)	3.055(4)
		O(5) - O(10)	2.985(4)
		O(6) - O(8)	2.958(5)
		O(6) - O(10)	2.902(5)
		O(8) - O(10)	2.989(5)
		O(1) - Si(1) - O(2)	109.7(2)
		O(1) - Si(1) - O(3)	108.3(2)
		O(1) - Si(1) - O(4)	105.4(2)
		O(2) - Si(1) - O(3)	115.8(2)
		O(2) - Si(1) - O(4)	106.5(2)
		O(3) - Si(1) - O(4)	110.7(2)
		Mean 109.4	
		O(4) - Si(2) - O(5)	108.5(2)
		O(4) - Si(2) - O(6)	110.5(2)
		O(4) - Si(2) - O(7)	105.5(2)
		O(5) - Si(2) - O(6)	114.9(2)
		O(5) - Si(2) - O(7)	109.9(2)
		O(6) - Si(2) - O(7)	107.2(2)
		Mean 109.4	
		O(7) - Si(3) - O(8)	106.5(2)
		O(7) - Si(3) - O(9)	107.1(2)
		O(7) - Si(3) - O(10)	110.0(2)
		O(8) - Si(3) - O(9)	110.1(2)
		O(8) - Si(3) - O(10)	113.9(2)
		O(9) - Si(3) - O(10)	109.0(3)
		Mean 109.4	
		Si(1) - O(1) - Si(1)'	148.6(4)
		Si(2) - O(7) - Si(2)	136.0(3)
		Si(3) - O(9) - Si(3)'	154.5(4)
The Si(1) Tetrahedron		Hydrogen Bonds	
Si(1) - O(1)	1.628(2)	W(1) - O(1)	2.775(10)
Si(1) - O(2)	1.604(4)	W(1) - O(4)	2.840(8)
Si(1) - O(3)	1.612(4)	W(1) - O(4)'	2.840(8)
Si(1) - O(4)	1.619(3)	W(2) - O(9)	2.906(9)
Mean 1.618		W(2) - O(7)	2.936(6)
		W(2) - O(7)'	2.936(6)
O(1) - O(2)	2.642(5)		
O(1) - O(5)	2.626(4)		
O(1) - O(4)	2.591(4)		
O(2) - O(3)	2.725(6)		
O(2) - O(4)	2.590(5)		
O(3) - O(4)	2.867(5)		
Mean 2.640			
The Si(2) Tetrahedron			
Si(2) - O(4)	1.638(4)		
Si(2) - O(5)	1.604(4)		
Si(2) - O(6)	1.611(4)		
Si(2) - O(7)	1.626(4)		
Mean 1.619			
O(4) - O(5)	2.631(5)		
O(4) - O(6)	2.569(5)		
O(4) - O(7)	2.596(5)		
O(5) - O(6)	2.710(5)		
O(5) - O(7)	2.642(5)		
O(6) - O(7)	2.604(5)		
Mean 2.642			
The Si(3) Tetrahedron			
Si(3) - O(7)	1.637(3)		
Si(3) - O(8)	1.590(3)		
Si(3) - O(9)	1.635(2)		
Si(3) - O(10)	1.602(4)		
Mean 1.616			
O(7) - O(8)	2.586(4)		
O(7) - O(9)	2.631(5)		
O(7) - O(10)	2.654(5)		
O(8) - O(9)	2.644(5)		
O(8) - O(10)	2.675(5)		
O(9) - O(10)	2.635(4)		
Mean 2.638			
Si - Si Distances		Si - O - Si Angles	
Si(1) - Si(1)'	3.135(2)	Si(1) - O(1) - Si(1)'	148.6(4)
Si(1) - Si(2)	3.020(2)	Si(2) - O(7) - Si(2)	136.0(3)
Si(2) - Si(3)	3.028(2)	Si(3) - O(9) - Si(3)'	154.5(4)
Si(3) - Si(3)'	3.188(2)		

(with standard deviations in parentheses)

the Na(3) polyhedron is a distorted hexagonal bipyramid. Other than this long distance, the other Na-Cl distances average 2.982 Å, which is considerably larger than the Na-Cl distance in sodium chloride (2.820 Å). Interestingly, the Cl atom is bonded to six sodium atoms in a distorted octahedral coordination, as in NaCl. The average Na-(H₂O) distance, 2.356 Å, is considerably shorter than the average Na-O distance, 2.673 Å.

The water molecules and the proposed hydrogen bonding

The water molecules w(1) and w(2) are located on mirror planes within channels parallel to *b*. The hydrogen atoms associated with the water molecules can occur either on the mirror plane or across it, the former possibility being more likely on account of the near neighbor environments. The oxygen atom O(1) located on the mirror plane is the acceptor of one H bond from w(1) [O(1)-w(1) 2.775 Å]. The other H bond appears to be bifurcated, with the two O(4) oxygen atoms across the mirror plane being the acceptors [O(1)-O(4) 2.840 Å]. The water molecule w(3) has a similar arrangement; O(9) on the mirror plane is one acceptor [O(9)-w(3) 2.906 Å] and the two O(7) atoms across the mirror plane are acceptors of the other bifurcated H bond [O(7)-w(2) 2.936 Å].

RELATED STRUCTURES

Although the presence of six-membered silicate rings is well known from minerals such as beryl, cordierite and diopside, petarasite belongs structurally to the group of sodium zircono- (or titano-) silicates such as lovozerite Na₂ZrSi₆O₁₂(OH)₈ (Ilyukhin & Belov 1960) and kazakovite Na₃Mn{Ti[Si₆O₁₈]} (Vorontsov *et al.* 1979) [*cf.*, the synthetic phase, Na₃Cd₃[Si₆O₁₈] (Simonov *et al.* 1967)]. All these phases are characterized by an open corner-sharing zircono- (or titano-) silicate framework with open channels that house the sodium atoms and, as in petarasite, water molecules and chlorine atoms as well. In all cases, the diameter of the open channel is defined by mixed six-membered rings of alternating [Si₂O₇] groups and Zr (or Ti) octahedra. Another zeolite-type zirconosilicate from Mont St-Hilaire is lemoynite, (Na,K)₂CaZr₂Si₁₀O₃₈·5-6H₂O, with large channels parallel to [100], [101] and [001], where the Na, K and Ca atoms and the water molecules are located (LePage & Perrault 1976).

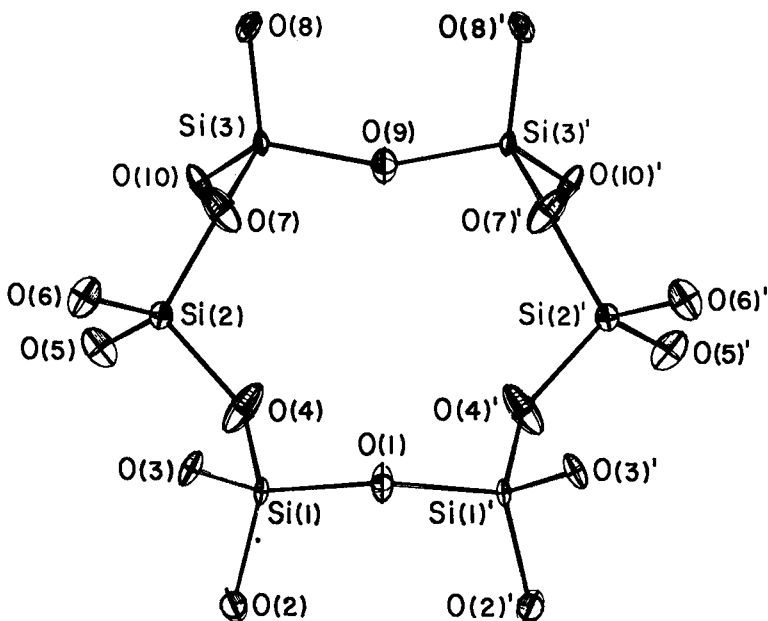


FIG. 3. Petarasite: configuration of the silicate ring $[\text{Si}_6\text{O}_{18}]$, showing the thermal vibration ellipsoids.

TABLE 5. RING ANGLES, PLANE AND DEVIATION OF RING PLANE FOR THE SIX-MEMBERED SILICATE RING IN PETARASITE

Ring atoms	Si-O-Si angles ($^\circ$)				
O(1)-Si(1)-O(4)-Si(2)-O(7)-Si(3)-	Si(1)-O(1)-Si(1)	148.6(4)			
O(9)-Si(3)-O(7)-Si(2)-O(4)-Si(1)-	Si(1)-O(4)-Si(2)	135.1(3)			
	Si(2)-O(7)-Si(3)	136.4(3)			
	Si(3)-O(9)-Si(3)	154.5(4)			
Parameters of plane* defined by ring oxygens					
A	B	C	D		
9.6341	0	-5.0762	-2.5637		
Deviations (\AA) from ring-planes defined by six oxygens					
Si(1)	-0.062	O(2)	-1.407	O(6)	1.187
Si(2)	-0.043	O(3)	1.210	O(8)	1.071
Si(3)	-0.010	O(5)	-1.367	O(10)	-1.440

*The equation of the plane in direct space are of the form $Ax + By + Cz = D$, where x, y, z are the atomic coordinates in $\frac{a}{2}$ units and D is the distance of the plane from the origin in \AA units.

The $[\text{ZrSi}_5\text{O}_{13}]$ framework in lemoynite contains silicate layers that consist of six-membered silicate rings.

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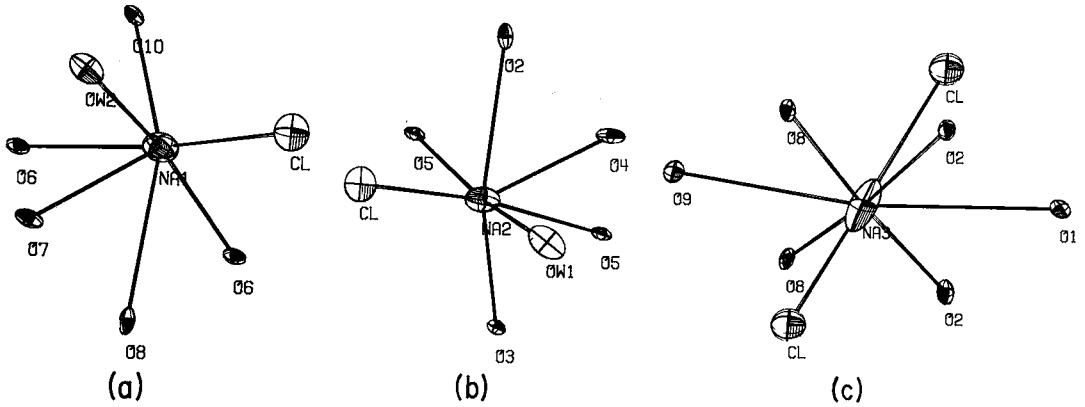


FIG. 4. Petarasite: coordination of the sodium atoms showing thermal vibration ellipsoids. The unusually anisotropic "thermal" vibration of Na(3), which is partly replaced by Ca, might be due to positional disorder.

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