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The crystal structure of orthoericssonite

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Abstract

Orthoericssonite from the Hijikuzu mine, Iwate Prefecture, Japan, $(Ba_{0.7}Sr_{0.3})(Mn^{2+}{}_{1.4}Fe^{2+}{}_{0.6})(Fe^{3+}{}_{0.9}Ti_{0.1})Si_2O_7(O,OH)_2$, is orthorhombic, space group *Pnmn*, with unit cell parameters $a=20.230(5)$, $b=6.979(2)$, $c=5.392(2)$ Å and $Z=4$. The crystal structure has been determined based on three-dimensional Patterson and Fourier syntheses and refined to $R=0.054$ for 1626 independent reflections.

The structure contains composite sheets each built up of a pair of quasi-silicate sheets consisting of Si_2O_7 groups and square pyramids formed by oxygen atoms about Fe^{3+}, intercalating between the pair a sheet of octahedra formed by oxygen atoms about Mn^{2+}. The composite sheets are separated by (Ba, Sr) atoms. The orthoericssonite structure can be derived from a monoclinic subcell, which has dimensions $a'=10.19$, $b'=6.979$, $c'=5.392$Å, β 96°45′ and $P2/m$, after polysynthetically twinning them on {100}, with a glide reflection having the glide component of $^b/_2$ as twin operation. If the subcells are juxtaposed on {100}, with a glide of $^b/_2$, stepwise in one direction, the ericssonite cell is obtained. The relationship between orthoericssonite and ericssonite thus offers an example of cell twinning.

The minerals containing quasi-silicate sheets can be structurally classified in terms of different combinations of the stackings of various types of quasi-silicate sheets and intersheet cations or groups.

Introduction

Orthoericssonite, $BaMn_2^{2+}Fe^{3+}[O|OH|Si_2O_7]$, is the orthorhombic dimorph of ericssonite, and both were firstly described by Moore (1971) from Långban, Sweden. Matsubara and Nagashima (1975) have reported the second occurrence of orthoericssonite from the thermally metamorphosed manganese deposit of the Hijikuzu mine, Iwate Prefecture, Japan. A chemical analysis gave the empirical formula $(Ba_{0.688}Sr_{0.256}K_{0.024}Na_{0.013}Li_{0.003})_{\Sigma 0.984}(Mn^{2+}{}_{1.435}Fe^{2+}{}_{0.546}Mg_{0.086})_{\Sigma 2.067}(Fe^{3+}{}_{0.931}Ti_{0.093}Al_{0.034})_{\Sigma 1.058}Si_{2.062}O_{7.000}(O_{1.389}(OH)_{0.611})_{\Sigma 2.000}$ on the basis of O=9, specifying the mineral to be a strontian and ferroan variety.

The structure model of ericssonite has been already proposed with reference to that of lamprophyllite by Moore (1971), who also discussed geometrical similarities between ericssonite and orthoericssonite and that between lamprophyllite* (monoclinic) and orthorhombic lamprophyllite. However, the material studied by Moore (1971) was not a single but an intergrown body composed of ericssonite and orthoericssonite, impeding his structural description of them.

Here the structure of orthoericssonite from the Hijikuzu mine is described together with the discussion on the structural relationship between orthoericssonite and ericssonite. Also a structural classification of minerals involving quasi-silicate sheets is proposed.

Experimental

A single crystal was isolated from the analysed specimen (NSM M-20799) deposited in Department of Geology, National Science Museum, Tokyo, Japan. The size of the crystal was approximately 0.15×0.12×0.08 mm.

The four-circle diffractometer study suggested the space group to be *Pnmn* or *Pn2n*, revising the previous result by Matsubara and Nagashima (1975). The centric space group was preferred from the expected analogy with orthorhombic lamprophyllite discussed by Peng and Chang (1965) and Moore (1971).

The unit cell parameters a=20.230(5), b=6.979(2), c=5.392(2)Å were obtained from diffractometry using graphite monochromatized MoKα radiation (λ= 0.71069Å). The ω-2θ scan technique was used to measure intensities of reflections in the limit of $2\theta=90°$. A total of 2409 independent reflections were measured, of which 1626 had intensities larger than $3\sigma(I)$ and were used for the structure refinement. The intensities were corrected for Lorentz and polarization effects and reduced to structure factors.

Refinement of the structure

To determine the heavy metal positions, a three-dimensional Patterson synthesis was carried out. The atomic scattering factor for each ion was taken from International Tables for X-ray Crystallography (1968). Based on the chemical composition, the barium, manganese and iron metal sites were respectively assigned to be composed of 70% Ba and 30% Sr, 70% Mn^{2+} and 30% Fe^{2+}, and 90% Fe^{3+} and 10% Ti.

From the Patterson map, the three kinds of heavy metal positions were directly determined, showing that their arrangements were very similar to

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* The name lamprophyllite was originally used to indicate the orthorhombic lamprophyllite (Gossner and Drechsler, 1935). Woodrow (1964), however, used the name lamprophyllite for monoclinic barium-dominant "lamprophyllite". Peng and Chang (1965) referred to the minerals of lamprophyllite group, using the name lamprophyllite and barytolamprophyllite for monoclinic lamprophyllite and its barium-dominant one, respectively.

those of lamprophyllite. The structure of lamprophyllite (Woodrow, 1964) then served for allocating initial positions of silicon and oxygen atoms in the orthoericssonite structure.

The structure thus derived was refined with the least-squares program LINUS (Coppens and Hamilton, 1970); the isotropic refinement converged to give the value of $R=0.063$. Four more cycles of least-squares calculations using anisotropic temperature factors for all atoms reduced the R value to 0.054 for 1626 reflections. After absorption correction ($\mu=115.5\,\mathrm{cm}^{-1}$), however, the similar calculations gave 0.064, giving no significant change in atomic parameters. Although three-dimensional difference Fourier synthesis was carried out, it was impossible to locate hydrogen positions.

The final atomic coordinates and thermal parameters are given in Table 1, interatomic distances and angles in Table 2, and the observed and calculated structure factors in another table*, respectively.

TABLE 1. Atomic coordinates and thermal parameters.

Atom	x	y	z	$B_{eq.}$	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Ba	0.22483(3)	0	0.1644(1)	0.76	5.3	35.7	61.8	0	0.0	0
Mn 1	0	0.2596(2)	0	0.73	6.4	33.1	43.1	0	4.5	0
Mn 2	0	0	0.5	0.85	5.6	43.1	67.4	0	1.1	0
Mn 3	0	0.5	0.5	0.53	3.7	33.8	27.2	0	3.2	0
Fe	0.14291(6)	0.5	0.1663(3)	0.41	2.4	29.7	23.3	0	0.8	0
Si	0.13640(8)	0.2262(2)	0.6644(4)	0.42	2.8	19.4	37.1	0.7	0.8	−2.4
O 1	0.0507(4)	0	0.1657(20)	1.22	7.1	71.0	95.2	0	−0.2	0
O 2	0.1582(4)	0	0.6624(24)	1.36	6.5	15.9	232	0	0.5	0
O 3	0.0567(2)	0.2465(7)	0.6617(12)	0.81	3.4	52.7	72.6	2.8	3.4	5.0
O 4	0.1708(3)	0.3087(10)	0.9137(10)	1.04	4.9	85.4	55.9	1.9	−1.4	−16.7
O 5	0.1722(3)	0.3086(9)	0.4180(10)	0.98	5.1	71.6	60.8	0.1	3.4	21.0
O 6	0.0523(3)	0.5	0.1730(16)	0.59	2.7	36.5	52.4	0	1.1	0

The anisotropical thermal parameters ($\times 10^4$) are of the form: $\exp[-(h^2\beta_{11}+k^2\beta_{22}+l^2\beta_{33}+2hk\beta_{12}+2hl\beta_{13}+2kl\beta_{23})]$. Standard deviations are in parentheses.

Description of the structure

The structure of orthoericssonite contains Si_2O_7 groups, which are joined together with square pyramids formed by oxygen atoms about Fe^{3+} to form a sheet parallel to {100}. This is the type of the sheets which were found in astrophyllite, lamprophyllite and others, and designated by Takéuchi and Joswig (1967) as quasi-silicate sheets because they simulate the tetrahedral sheets in

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* The copy of this table is available from the author.

TABLE 2. Interatomic distances(Å) and angles(°).

	Distances(Å)	Angles(°)		Distances(Å)	Angles(°)
Mn 1 octahedron			*Mn 2 octahedron*		
2×Mn 1-O 1	2.266(8)		2×Mn 2-O 1	2.074(10)	
2×Mn 1-O 3	2.156(8)		4×Mn 2-O 3	2.244(5)	
2×Mn 1-O 6	2.192(7)		mean	2.187(7)	
mean	2.205(8)				
O 1-O 1	2.721(13)	73.8(4)	4×O 1-O 3	3.182(11)	94.9(2)
2×O 1-O 3	3.219(11)	93.4(3)	4×O 1-O 3	2.923(8)	85.1(2)
2×O 1-O 3	2.923(8)	82.7(4)	2×O 3-O 3	2.880(7)	79.9(2)
2×O 1-O 6	3.4899(2)	103.1(3)	2×O 3-O 3	3.441(7)	100.2(2)
2×O 3-O 6	3.277(9)	97.8(3)			
2×O 3-O 6	2.963(7)	85.9(3)			
O 6-O 6	2.820(10)	80.1(3)			
Mn 3 octahedron			*Fe square pyramid*		
4×Mn 3-O 3	2.281(5)		2×Fe-O 4	1.989(6)	
2×Mn 3-O 6	2.056(8)		2×Fe-O 5	1.995(6)	
mean	2.206(6)		Fe-O 6	1.834(6)	
			mean	1.960(6)	
2×O 3-O 3	2.880(7)	78.3(2)	O 4-O 4	2.670(9)	84.3(2)
2×O 3-O 3	3.538(7)	101.7(2)	2×O 4-O 5	2.720(8)	86.1(3)
4×O 3-O 6	3.175(9)	94.0(2)	2×O 4-O 6	3.080(9)	107.3(3)
4×O 3-O 6	2.963(7)	86.0(2)	O 5-O 5	2.672(9)	84.1(2)
			2×O 5-O 6	3.069(8)	106.5(3)
Si tetrahedron			*Ba polyhedron*		
Si-O 2	1.639(2)		Ba-O 2	3.005(12)	
Si-O 3	1.620(5)		Ba-O 2	3.024(12)	
Si-O 4	1.619(6)		2×Ba-O 4	2.769(6)	
Si-O 5	1.619(6)		2×Ba-O 4	2.837(6)	
mean	1.624(4)		2×Ba-O 5	2.764(6)	
			2×Ba-O 5	2.809(6)	
O 2-O 3	2.679(8)	110.6(3)	mean	2.839(7)	
O 2-O 4	2.558(9)	103.5(5)			
O 2-O 5	2.540(9)	102.5(5)	2×O 2-O 4	3.944(10)	84.9(2)
O 3-O 4	2.714(7)	113.9(3)	2×O 2-O 5	2.540(9)	52.1(2)
O 3-O 5	2.716(8)	114.0(4)	2×O 2-O 4	2.558(9)	52.2(1)
O 4-O 5	2.673(8)	111.3(3)	2×O 2-O 5	3.932(10)	84.7(2)
			2×O 4-O 5	2.720(8)	58.9(2)
Si-O 2-Si		148.8(3)	2×O 4-O 5	3.280(8)	72.0(2)
			O 4-O 4	2.670(9)	56.1(2)
			2×O 4-O 5	3.280(8)	71.7(2)
			2×O 4-O 5	2.673(8)	56.5(2)
			2×O 4-O 5	3.779(9)	84.0(2)
			O 5-O 5	2.672(9)	56.8(2)

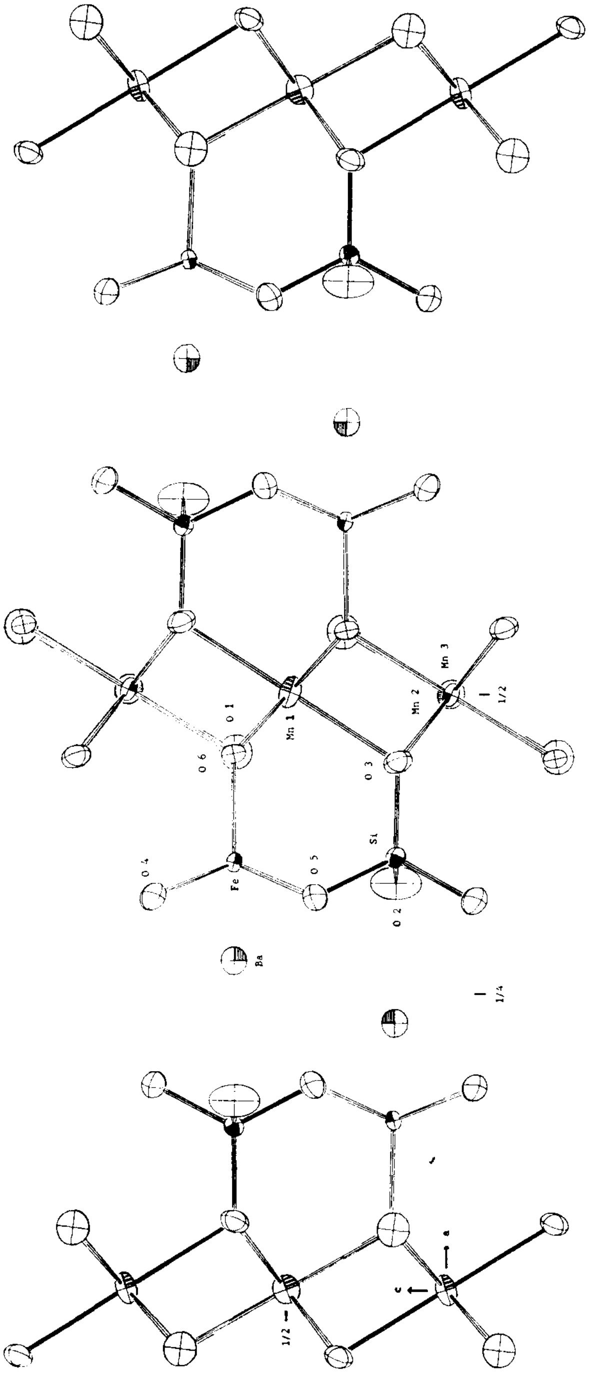

FIG. 1. Projection of the structure along the *b*-axis.

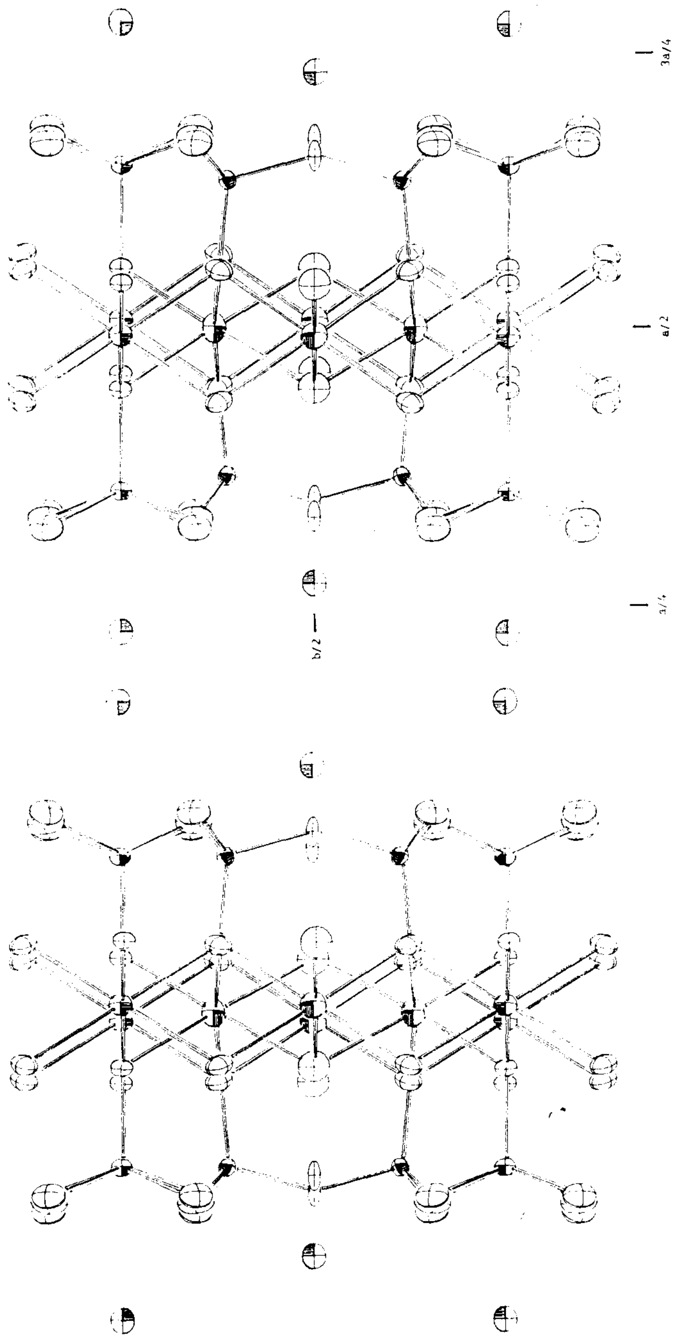

FIG. 2. Stereographic projection of the structure along the *c*-axis.

common sheet silicates like micas. A pair of these sheets in orthoericssonite form between them a sheet of octahedra formed by oxygen atoms about Mn. The large cations Ba(Sr) occur between these composite sheets, thus constructing the bulk of the orthoericssonite. This structural feature accounts for the perfect cleavage of this mineral parallel to {100}.

Quasi-silicate sheet: The sheet is formed by sharing the corner oxygen atoms, O(4) and O(5), of Si_2O_7 sorosilicate groups and $Fe^{3+}O_5$ square pyramids (Fig. 1). Each sorosilicate group and square pyramid also share apical oxygen atoms, O(3) and O(6), with $Mn^{2+}O_6$ octahedra, respectively (Fig. 1). The bridge bonds of the silicate group have a length of 1.639(2)Å and they are significantly longer than non-bridge bonds (Table 2). The distances between Fe^{3+} and oxygens bonded to Si are similar to each other [Fe-O(4) 1.989(6)Å; Fe-O(5) 1.995(6)Å] and are much longer than the apical bond, Fe-O(6) 1.834(6)Å, the oxygen atom of which is bonded to Mn. The mean Fe^{3+}-O distance of 1.960(6)Å is considerably shorter than those of $Fe^{3+}O_6$ octahedra in other silicates. Note that this is the first example of the square pyramidal coordination of oxygen atom about Fe^{3+} in the mineral structures so far reported, though

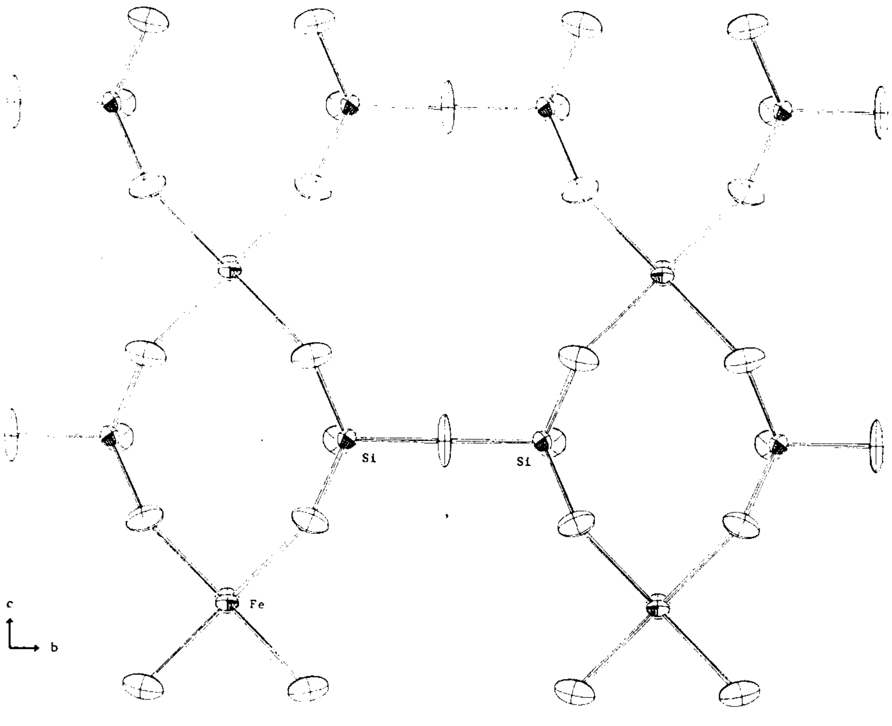

FIG. 3. A projection of Si_2O_7-$Fe^{3+}O_5$ sheet.

such a coordination is rather common for the cations like Ti and V as has been found in lamprophyllite (Woodrow, 1964), yoshimuraite (Takéuchi and Haga; 1971, 1978) and haradaite (Takéuchi and Joswig, 1967).

Octahedral sheet: Three non-equivalent manganese atoms are situated on the {100} plane and are densely packed between a pair of quasi-silicate sheets. The octahedral sheet is constituted by sharing the apical oxygens, O(1), O(3) and O(6), of three kinds of MnO_6 octahedra. Among the apical oxygens, O(3) and O(6) are also shared with two opposite quasi-silicate sheets. The chemical formula requires the presence of OH ion. A part of O(1) is most likely to be hydroxyl radical than the other oxygen atoms (Fig. 1). The Mn(1)-O distances range from 2.156(8)Å to 2.266(8)Å with a mean value 2.205(8)Å. The Mn(2)-O and Mn(3)-O octahedra have two short Mn-O bonds of equal distance, 2.074(10)Å and 2.056(8)Å, and four long bonds of equal distance, 2.244(5)Å and 2.281(5)Å with a mean value of 2.187(7)Å and 2.206(6)Å, respectively.

Ba polyhedra: The barium atoms are situated nearly on the *n*-glide planes parallel to {100} and in between the quasi-silicate sheets. The atom is ten-coordinated, the Ba-O distances ranging from 2.764(6)Å to 3.024(12)Å with a mean value of 2.839(7)Å. The BaO_{10} polyhedron can be regarded as a hetero-polar prism whose bottom is a distorted hexagon and top is a square. If two oxygen atoms located farther than 3.0Å from barium atom are not considered, eight oxygen atoms form a truncated square pyramids.

Discussion

The crystal structure of orthoericssonite is very similar to that of lamprophyllite, $(Sr, Ba, K)(Na, Ti)_2(TiO)[Si_2O_7](OH)$, determined with the projection along the *z*-axis by Woodrow (1964). Moore (1971) has already discussed the structural relationship between orthoericssonite and ericssonite to be very close to that between orthorhombic lamprophyllite and lamprophyllite, and also suggested that ericssonite was isotypic with lamprophyllite. In the structure of orthoericssonite can be taken a monoclinic subcell having $P2/m$ and parameters of $a'=10.19$, $b'=6.979$, $c'=5.392$Å, $\beta=96°45'$, which are geometrically related to the orthoericssonite cell parameters (given by subscript or): $a'\cdot\sin\beta={}^1/_2 a_{or}$, $b'=b_{or}$, $c'=c_{or}$. This subcell is dimensionally close to the unit cell of bafertisite (Peng and Sheng, 1963). The true cell of orthoericssonite can be derived by twinning the monoclinic subcells (Fig. 4) on {100}, with a glide reflection having the glide component of ${}^b/_2$ as a twin operation. If the monoclinic subcells are juxtaposed on {100} with a glide of ${}^b/_2$ stepwise only in one direction, we obtain a unit cell having $a_e=20.37$, $b_e=6.979$, $c_e=5.392$Å, $\beta=96°45'$ and space

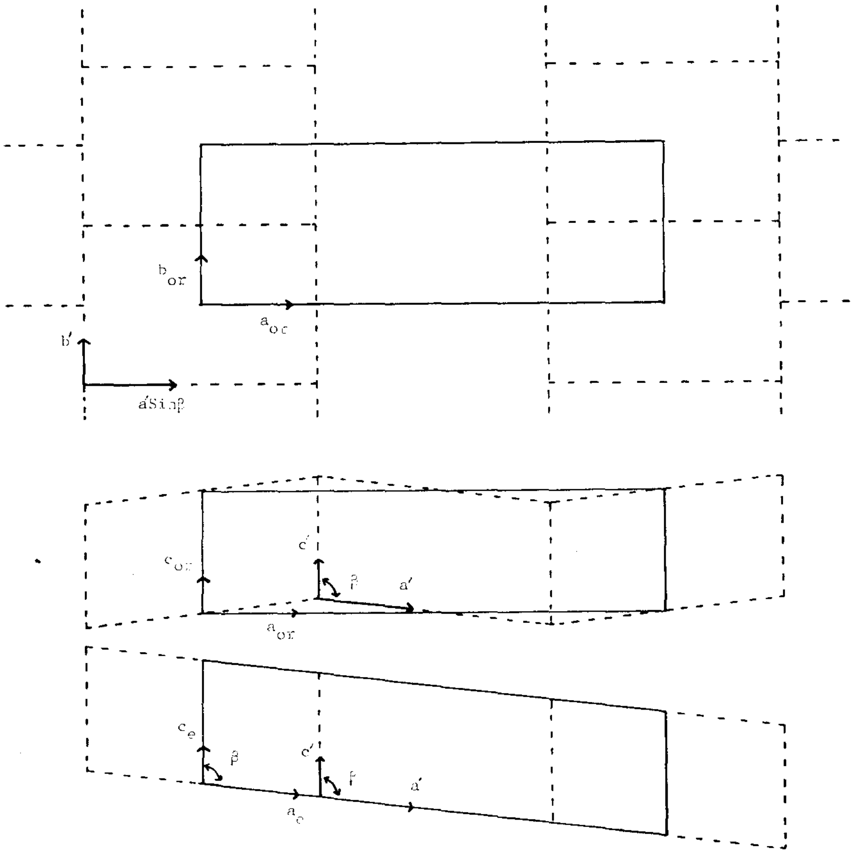

FIG. 4. The geometrical relationships of ericssonite and orthoericssonite cells.

group $C2/m$ (Fig. 4), the cell corresponding to the true cell of ericssonite. These values are very similar to that of real ericssonite obtained by Moore (1971). Thus, the structural relationship between orthoericssonite and ericssonite can be explained by twinning on {100} of the monoclinic subcell, and offers a new example of cell twinning originally advocated by Ito (1950). Such a relationship may account for the nature of intergrowth of ericssonite and orthoericssonite observed in the Långban material (Moore, 1971).

As already pointed out by Moore (1971), the structural relationship between orthorhombic lamprophyllite and lamprophyllite is quite similar to that between orthoericssonite and ericssonite.

Therefore, the structure of orthorhombic lamprophyllite and lamprophyllite are very probably isotypic with orthoericssonite and ericssonite, respectively, in principal cation substitutions being $\mathrm{Ba} \rightleftarrows \mathrm{Sr}$, $\mathrm{Mn} \rightleftarrows (\mathrm{Na, Ti})$, and $\mathrm{Fe} \rightleftarrows \mathrm{Ti}$.

The structural relationship and the problem of polysynthetic twinning on {100} between monoclinic and triclinic members in allied silicate minerals as yoshimuraite, lomonossovite and astrophyllite may be clear through the consideration on the twinning of {100} of subcells and the ordering of octahedral cations.

Table 3. Unit cell parameters, chemical formulae and cations in each sheet of

			A	B	C
I	a :	Lamprophyllite	Sr_2	Na_3Ti or $(Na,Ti)_4$	$Ti_2[Si_2O_7]_2$
		Barytolamprophyllite	$(Ba,Ca,Sr)_2$	Na_3Ti or $(Na,Ti)_4$	$(Ti,Fe''')_2[Si_2O_7]_2$
		Orthorhombic lamprophyllite	Sr_2	Na_3Ti or $(Na,Ti)_4$	$Ti_2[Si_2O_7]_2$
		Ericssonite	Ba_2	Mn_4	$Fe_2'''[Si_2O_7]_2$
		Orthoericssonite	$(Ba,Sr)_2$	$(Mn,Fe'')_4$	$(Fe''',Ti)_2[Si_2O_7]_2$
		Bafertisite	Ba_2	Fe''_4	$Ti_2[Si_2O_7]_2$
		Manganese analogue of bafertisite	Ba_2	$(Mn,Fe'',Fe''')_4$	$Ti_2[Si_2O_7]_2$
	b :	Yoshimuraite	$(Ba,Sr)_4[(P,S)O_4]_2$	$(Mn,Fe'',Mg)_4$	$(Ti,Fe''')_2[Si_2O_7]_2$
		Innelite	$Ba_4[(S,Si)O_4]_2$	$(Na,K,Mn,Ti)_4$	$Ti_2[Si_2O_7]_2$
		Murmanite	$(H_2O)_{8-6}$	$Na_2(Mn,Fe'',Mg)Ti$	$Ti_2[Si_2O_7]_2$
		Epistolite	$(H_2O)_{4-2}$	$(Na,Ca)_2Ti_2$	$(Nb,Ti)_2[Si_2O_7]_2$
	c :	Lomonossovite	$Na_4[PO_4]_2$	$Na_2(Mn,Fe'',Ca,Mg)Ti$	$Na_2Ti_2[Si_2O_7]_2$
		β-lomonossovite	$Na_3H_3[PO_4]_2$	Na_2Ti_2	$Na_2Ti_2[Si_2O_7]_2$
	d :	Astrophyllite	$(K,Na)_3$	$(Fe'',Mn)_7$	$Ti_2[Si_4O_{12}]_2$
		Magnesium astrophyllite	K_2Na_2	$(Fe'',Mn)_5Mg_2$	$Ti_2[Si_4O_{12}]_2$
		Hydroastrophyllite	$(H_3O,K,Ca)_3$	$(Fe'',Mn)_{5-6}$	$(Ti,Nb)_2[(Si,Al)_4O_{12}]_2$
		Kupletskite	$(K,Na)_3$	$(Mn,Fe'')_7$	$(Ti,Nb)_2[Si_4O_{12}]_2$
		Cesium kupletskite	$(Cs,K,Na)_3$	$(Mn,Fe'')_7$	$(Ti,Nb)_2[Si_4O_{12}]_2$
		Niobophyllite	$(K,Na)_3$	$(Fe'',Mn)_{6-7}$	$(Nb,Ti)_2[Si_4O_{12}]_2$
		Zircophyllite	$(K,Na,Ca)_3$	$(Mn,Fe'')_7$	$(Zr,Nb)_2[Si_4O_{12}]_2$
II		Rosenbuschite		$(Ca,Na)_3(Ti,Mn)$	$Ca_2NaZr[Si_2O_7]_2$
		Seidozerite		Na_2MnTi	$(Na,Ca)_2(Zr,Ti)_2[Si_2O_7]_2$
III		Haradaite	$(Sr,Ba)_2$	-	$V_2[Si_2O_7]_2$
		Suzukiite	$(Ba,Sr)_2$		$V_2[Si_2O_7]_2$

1. Peng & Chang (1965), 2. Moore (1971), 3. This paper, 4. Peng & Shen (1963), 8. Khalilov & Makarov (1966), 9. Rastsvetaeva *et al.* (1974), 10 X-ray Laboratory, Nickel *et al.* (1964), 14. Kapustin (1972), 15. Shibaeva *et al.* (1963), 16. Skszat

The letters in parentheses in the column for cell parameters indicate the figures

The structures of minerals here discussed (Table 3) consists basically of sheets composed of Si_2O_7 with their bases all in nearly one plane and five- (or six-) fold and six- (or eight-) fold polyhedra which are lodged by such cations as Ti, Fe, Zr, Nb, Ca, Na, V and Mn. These quasi-silicate sheets may be classified into the following three types in terms of the cation polyhedra which

quasi-silicates sheet minerals.

Anions and Groups	Cell parameters a	b	c	α	β	γ	Reference
$(O,OH,F)_4$	9.72×2	7.05	5.43	—	96°30′	—	1
$(O,OH,F)_4$	9.98×2	7.07	5.43	—	96°30′	—	1
$(O,OH,F)_4$	9.66×2	7.05	5.43	—	—	—	1
$O_2(OH)_2$	10.23×2	7.03	5.34	—	95°30′	—	2
$(O,OH)_4$	10.12×2	6.98	5.39	—	—	—	3
$O_2(OH)_2$	10.98	6.8	5.36	—	94°	—	4
$(O,OH,F)_4$							5
$O_2(OH)_2$	14.71(b)	7.00(a)	5.39	90°12′(β)	93°30′(α)	95°18′	6
$(O,OH,F)_4$	14.76	7.14	5.38	90°	95°	99°	7
O_2	11.94(c)	7.00	5.45(a)	88°55′(γ)	100°26′	96°(α)	8
$(O,OH)_4$	12.07(c)	7.08	5.41(a)	88°36′(γ)	96°06′	103°03′(α)	8
O_2	14.65(c)	7.03	5.40(a)	89°(γ)	96°	100°(α)	8
O_4	14.23(c)	7.13×2	5.34(a)	89°06′(γ)	105°52′	102°33′(α)	9
$(O,OH,F)_7$	11.77	11.86	5.42	101°53′	94°25′	113°21′	10
$(O,OH,F)_7$	10.56	6.57×3.5	5.35	—	102°	—	10
$(O,OH,F)_7$	11.86	11.98	5.42	103°25′	95°09′	112°12′	10
$(O,OH,F)_7$							11
$(O,OH,F)_7$	10.58×2(c)	11.74	5.41(a)	102°23′(γ)	90°	89°(α)	12
$(O,OH)_{7-8}$	11.66(c)	11.88	5.391(a)	103°06′(γ)	94°30′	113°06′(α)	13
$(O,OH,F)_7$							14
$(F,O)_4$	10.12	7.27(c)	5.70×2(b)	91°20′	111°50′(γ)	99°40′(β)	15
$O_2(F,OH)_2$	9.15×2(c)	7.10	5.54(a)	—	102°43′	—	16
	14.64(b)	7.06(a)	5.33	—	—	—	17
	15.26(b)	7.09(a)	5.36	—	—	—	18

5. Ganzeev *et al.* (1971), 6. Watanabe *et al.* (1961), 7. Kravchenko *et al.* (1961), Hubei Geologic College (1974), 11. Semenov (1956), 12. Efimov *et al.* (1971), 13. & Simonov (1965), 17. Takéuchi & Joswig (1967), 18. Watanabe *et al.* (priv. comm.)

after the original axial settings.

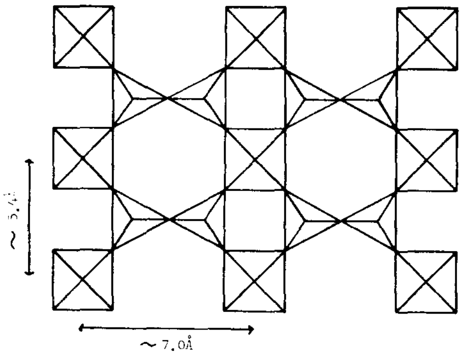

FIG. 5. A schematic representation of the type 1 sheet.

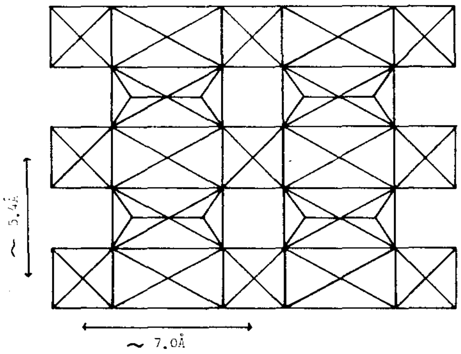

FIG. 6. A schematic representation of the type 2 sheet.

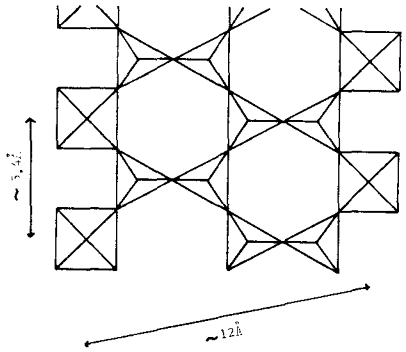

FIG. 7. A schematic represention of the type 3 sheet.

link together the Si_2O_7 groups. Type 1 sheet is formed by Si_2O_7 group and five- or six-fold coordinated polyhedron, sharing four corners with neighbours (Fig. 5). The repeat distances of this sheet are characterized by approximately 5.4 and 7.0(=3×2.33)Å. Type 2 sheet is achieved when the hexagonal open space of type 1 sheet is occupied by Na and Ca octahedron (or hexagonal pyramid) (Fig. 6). The repeat distances of this sheet are characterized by the lengths approximately 5.4 (or 2×5.4 if cations in octahedral site are ordered) and 7.0 (=3×2.33)Å. Type 3 sheet is formed by $(Si_2O_7)_2$ group and Ti and Nb octahedron (Fig. 7). The repeat distances of this sheet are approximately 5.4 and 11.7(=5×2.33) or 23.3(=10×2.33)Å.

These quasi-silicate sheets sandwich the dense-packed octahedral sheets which are morphologically very similar to trioctahedral ones of layer silicates. The cations in the octahedral sheet are mainly occupied by Ti, Fe, Mn, Na, Ca, Mg and Nb. Almost all of the minerals here referred to have such larger cations as Ba, Sr, K and Na, and groups as (PO_4) and H_2O disjoining the composite sheets consisting of two quasi-silicate sheets and one octahedral sheet. In case of absence of interlayer cations as seen in rosenbuschite and seidozerite, their composite sheets are directly joined by sharing the edges of octahedra in quasi-silicate sheets. The arrangement of the octahedra in these minerals is of three-dimensional linkage type. Therefore, Takéuchi and Joswig (1967) excluded them from quasi-silicate sheet mineral.

The mineral containing quasi-silicate sheets are built up of different combinations of the stacking of various types of the sheets. If $A(A_1$ and $A_2)$, B and $C(C_1$, C_2 and $C_3)$ represent the interlayer (cations and groups), the octahedral sheet and the quasi-silicate sheet (Type 1, 2 and 3), respectively, the following groups can be derived. In only haradaite, a pair of the quasi-silicate sheets are directly joined by sharing the apical oxygen atoms of SiO_4 tetrahedra and as a result Si_4O_{12} chains are formed (Takéuchi and Joswig, 1967). Yet, the structure still retains the nature of a layer silicate.

I. CBCACBC group

a. Lamprophyllite subgroup ($C_1BC_1A_1C_1BC_1$)

The repeat distances of the stacks ("basal spacings") is characterized by the length of about $n\times10$Å where $n=1$ or 2. This subgroup includes barytolamprophyllite, orthorhombic lamprophyllite, ericssonite, orthoericssonite, bafertisite and manganese analogue of bafertisite (Ganzeev *et al.*, 1971).

b. Yoshimuraite subgroup ($C_1BC_1A_2C_1BC_1$)

The repeat distance on the stack is characterized by the length of about

14Å. This subgroup includes innelite, murmanite and epistolite.

c. Lomonossovite subgroup ($C_2BC_2A_2C_2BC_2$)

The repeat distance on the stack is characterized by the length of 12–14Å. This subgroup includes beta-lomonossovite.

d. Astrophyllite subgroup ($C_3BC_3A_1C_3BC_3$)

The repeat distance on the stack is characterized by the length of about 10Å or 2×10Å. This subgroup includes magnesium astrophyllite, hydroastrophyllite, kupletskite, cesium kupletskite, niobophyllite and zircophyllite.

II. Rosenbuschite group ($C_2BC_2C_2BC_2$)

The repeat distance on the stack is characterized by the length of about 10Å or 2×10Å. This group includes seidozerite.

III. Haradaite group ($C_1C_1A_1C_1C_1$)

The repeat distance on the stack is characterized by the length of about 7Å. This group includes Ba analogue of haradaite, which is newly found and described under the name suzukiite (Watanabe *et al.*, priv. comm.).

The unit cell parameters, chemical formulae and cations in each sheet of them are summarized in Table 3. Some of unit cell parameters are given in terms of the manner that {100} is parallel to the layers.

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