Crystal structures of lamprophyllite-2*M* and lamprophyllite-2*O* from the Lovozero alkaline massif, Kola peninsula, Russia

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Abstract: The crystals of lamprophyllite-2*M* and lamprophyllite-2*O* were found coexisting in an ussingite-microcline-sodalite veins in the Alluaiv Mt., Lovozero alkaline massif, in association with ussingite, aegirine, microcline, sodalite, albite, mangan-neptunite, vuonnemite, sphalerite, lomonosovite and betalomonosovite. The chemical composition of the polytypes corresponds to the formula $(Sr_{1.18}Na_{0.66}Ca_{0.12})_{\Sigma 1.96}Na(Na_{1.30}Mn_{0.36}Fe_{0.22}Mg_{0.12})_{\Sigma 2.00}Ti_3O_2(Si_2O_7)_2(OH)_2$. The structures of lamprophyllite-2*M* (*C*2/*m*, $a = 19.215(5)$, $b = 7.061(2)$, $c = 5.3719(15)$ Å, $\beta = 96.797(4)°$, V = 723.7(4) Å^3) and lamprophyllite-2*O* (*Pnmn*, $a = 19.128(4)$, $b = 7.0799(14)$, $c = 5.3824(11)$ Å, V = 728.9(3) Å^3) have been refined to $R = 0.040$ for 688 reflections ($|F_o| \geq 4\sigma_F$) and to $R = 0.084$ for 571 reflections ($|F_o| \geq 4\sigma_F$), respectively. The structures of both polytypes are based on the *HOH* layer consisting of a central *O* sheet of edge-sharing $Na(1)O_6$, $Na(2)O_6$ and $Ti(2)O_6$ octahedra sandwiched between two heterophyllosilicate *H* sheets. The *H* sheet is built by corner-sharing of $Ti(1)O_5$ square pyramids and Si_2O_7 groups and consists of two types of rings of polyhedra: (i) six-membered rings (6*R*) formed by two Si_2O_7 groups and two TiO_5 square pyramids and (ii) four-membered rings (4*R*) formed by two silicate tetrahedra and two TiO_5 square pyramids. The Sr atom is located in the interlayer and is coordinated by six anions from 6*R* of the upper *H* sheet and four anions from 4*R* of the lower *H* sheet. The difference between monoclinic and orthorhombic lamprophyllites can be described in terms of different orientations of *HOH* layers. Whereas in lamprophyllite-2*M*, all *HOH* layers are in the same orientation, in lamprophyllite-2*O*, two adjacent layers are in different orientations.

Key-words: lamprophyllite, polytypism, Lovozero alkaline massif.

Introduction

Lamprophyllite, $(Sr,Ba)_2Na_3Ti_3O_2(Si_2O_7)_2(OH)_2$, was first described in 1894 by W. Ramsay and V. Hackman from the nepheline-syenite of the Kola peninsula, Russia. Later, lamprophyllite from alkaline complexes of the Kola peninsula was re-investigated in a number of works (Fersman, 1926; Bonshtedt, 1930; Balashov & Turanskaya, 1960; Belyaevskaya & Borutsky, 1993; Yakovenchuk *et al.*, 1999, *etc.*) and the mineral was found in other alkaline massifs in the world: Tertiary Gardiner complex, east Greenland (Johnsen *et al.*, 1994), Inagli massif, southern Yakutia (Lazebnik *et al.*, 1998), Pegmatite Peak, Bearpaw Mts., Montana (Chakhmouradian & Mitchell, 1999), Oldoinyo Lengai, Tanzania (Dawson, 1998; Dawson & Hill, 1998), *etc*. A Ba-analogue of lamprophyllite, barytolamprophyllite, was described by Dudkin (1959) from the Khibiny massif, Kola peninsula, and from other mineral localities (Kapustin, 1973; Johnsen *et al.*, 1994).

The crystal structure of lamprophyllite was first studied by Gossner & Drexler (1935) who suggested that the mineral is orthorhombic. The structure was solved by Woodrow (1964) who reported lamprophyllite to be monoclinic, space group *C*2/*m*. Peng & Chang (1965) proposed that there are two varieties of lamprophyllite, of which the orthorhombic one was that studied by Gossner & Drexler (1935), whereas the monoclinic modification was investigated by Woodrow (1964). Moore (1971) presented further evidence for the existence of orthorhombic and monoclinic modifications of lamprophyllite. However, all further structural studies of lamprophyllite (Saf'yanov *et al.*, 1983; Rastsvetaeva *et al.*, 1990) and barytolamprophyllite (Peng *et al.*, 1984; Rastsvetaeva & Dorfman, 1995; Rastsvetaeva *et al.*, 1995) were performed in the monoclinic space group *C*2/*m*. On the basis of TEM and X-ray powder diffraction studies of lamprophyllites from the Tertiary Gardiner complex, east Greenland, Johnsen (1996) demonstrated the presence of both monoclinic and

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Table 1. Crystallographic data for lamprophyllite-2*O* and lamprophyllite-2*M*.

	lamprophyllite-2*O*	lamprophyllite-2*M*
a (Å)	19.128(4)	19.215(5)
b (Å)	7.0799(14)	7.061(2)
c (Å)	5.3824(11)	5.3719(15)
β (°)	-	96.797(4)
V (Å^3)	728.9(3)	723.7(4)
Space group	*Pnmn*	*C2/m*
F_{000}	737	737
μ (cm^{-1})	70.36	70.36
Crystal size (mm)	0.26 x 0.18 x 0.03	0.30 x 0.14 x 0.04
Radiation	Mo*K*α	Mo*K*α
Total Ref.	1800	1607
Unique $|F_o| \geq 4\sigma_F$	571	688
R_{int}	0.067	0.045
Θ range	3.07-26.35	3.08-27.60
*R*1	0.084	0.040
*wR*2	0.234	0.103
s	1.12	1.05
D_{calc} (g/cm^3)	3.49	3.49

Note: $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR2 = \{\Sigma[w(F_o{}^2 - F_c{}^2)^2]/\Sigma[w(F_o{}^2)^2]\}^{1/2}$;
$s = \{\Sigma[w(F_o{}^2 - F_c{}^2)]/(n - p)\}^{1/2}$ where *n* is the number of reflections and *p* is the number of refined parameters.

orthorhombic modifications. It is noteworthy that the orthorhombic modification constituted more than 50 % of the sample and that the chemical compositions of both modifications were identical. Partial Rietveld analysis of the sample provided unit-cell parameters *a* = 19.480(2), *b* = 7.1043(4), *c* = 5.4086(3) Å, β = 96.789(6)° for the monoclinic lamprophyllite (space group *C2/m*) and *a* = 19.356(2), *b* = 7.1040(4), *c* = 5.4083(3) Å for the orthorhombic lamprophyllite (space group *Pnmn*). A structural model was suggested for the orthorhombic structure and the following polytypes were identified: lamprophyllite-2*M*, lamprophyllite-2*O* and barytolamprophyllite-2*M*.

The relationships between the structure of lamprophyllite and the structures of other layered titano- and niobosilicates have long been recognized (Belov, 1965; Matsubara, 1980). The common feature of these minerals is the presence of so-called *HOH* layers (Ferraris *et al*., 1996; Ferraris, 1997) composed of an octahedral *O* sheet sandwiched between two heterophyllosilicate *H* sheets. In turn, the *H* sheet consists of silicate groups or chains interlinked by Ti octahedra or square pyramids. A comprehensive account of the crystal chemistry of this group of titanosilicates is given by Egorov-Tismenko & Sokolova (1990), Sokolova (1998), Ferraris (1997), and Christiansen *et al*. (1999); for more recent studies on this subject see McDonald *et al*. (2000), Ferraris *et al*. (2001a, b), Sokolova & Hawthorne (2001), and Piilonen *et al*. (2000, 2001). Because of the layered structure, polytypism is frequent in this group of minerals (Christiansen *et al*., 1999).

Among minerals, the most close analogues of lamprophyllite polytypes are ericssonite and orthoericssonite described by Moore (1971) from Långban, Sweden. These two minerals have the same formula $BaMn_2^{2+}Fe^{3+}(Si_2O_7)O$ (OH) and occur together in the same crystal (Moore, 1971).

However, in contrast to lamprophyllite, orthoericssonite (space group *Pnmn*) is the more abundant phase than ericssonite (space group *C2/m*). Matsubara (1980) solved the structure of orthoericssonite on a crystal from the Hijikuzu mine, Iwate Prefecture, Japan, and demonstrated that the structure is closely related to one of monoclinic lamprophyllite. The *HOH* layer in orthoericssonite has the composition $[Mn_2^{2+}Fe^{3+}(Si_2O_7)O(OH)]$, where Mn^{2+} is solely incorporated into the *O* sheet and the *H* sheet is built by corner sharing of $Fe^{3+}O_5$ tetragonal pyramids and Si_2O_7 groups. According to Matsubara (1980), the chemical relations between lamprophyllite and orthoericssonite can be described by the substitution schemes Ba $\leftrightarrow$ Sr, Mn $\leftrightarrow$ (Na,Ti) and Fe $\leftrightarrow$ Ti.

The aim of the present study is to report results of crystal-structure refinements of two co-existing lamprophyllite polytypes from the Lovozero massif, Kola peninsula, Russia.

Occurrence and chemical composition

The lamprophyllite crystals used in this study were found in an ussingite-microcline-sodalite vein in the Alluaiv Mt., Lovozero alkaline massif, in association with ussingite, aegirine, microcline, sodalite, albite, manganneptunite, vuonnemite, sphalerite, lomonosovite and betalomonosovite. X-ray powder diffraction studies of the lamprophyllite sample from the above mentioned association indicated presence of two different but closely related phases. Subsequent single-crystal Weissenberg photographs showed that the sample consists of orthorhombic and monoclinic modifications of lamprophyllite, crystals of which are almost indistinguishable without detailed examination.

Table 2a. Atomic coordinates and displacement parameters ($\times 10^4$ Å^2) for lamprophyllite-$2O$.

Atom	x	y	z	U_{iso}	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ti(1)	0.34914(12)	0	0.1442(4)	27(8)	10(13)	23(13)	48(14)	0	2(8)	0
Ti(2)	0	0	0	254(14)	240(30)	54(18)	470(30)	0	-280(20)	0
Si	0.14413(14)	0.2161(4)	0.1440(5)	41(8)	90(20)	50(20)	120(30)	0	-24(14)	0
Na(1)	½	0.2588(5)	0	85(14)	120(50)	80(50)	130(60)	0	-50(30)	0
Na(2)	½	0	½	110(30)	135(12)	97(12)	145(13)	0	-1(7)	0
Sr	0.21584(10)	0	0.6453(4)	126(8)	10(13)	23(13)	48(14)	0	2(8)	0
OH(1)	0.0570(6)	0	0.702(2)	190(30)						
O(2)	0.3239(4)	0.1864(10)	0.3952(13)	110(16)						
O(3)	0.3250(4)	0.1867(10)	0.8900(12)	97(16)						
O(4)	0.1777(5)	0	0.1448(16)	50(20)						
O(5)	0.0593(4)	0.2044(10)	0.1478(13)	102(17)						
O(6)	0.4376(7)	0	0.141(2)	190(30)						

Table 2b. Residual peaks in the difference-Fourier map of lamprophyllite-$2O$ related to lamprophyllite-$2M$.

Peak	x	y	z	Height (e)	Peak	x	y	z	Height (e)
Ti(1)'	0.350	0	0.559	3.39	*Na*(1)'	-0.003	0.233	-0.212	2.45
Ti(2)'	-0.001	0	0.699	2.92	*Na*(2)'	0.498	0	0.223	1.47
Si'	0.144	0.225	0.567	2.30	*Sr*'	0.216	0	0.053	3.27

The chemical analyses were performed using CAMECA MS-46 electron microprobe operating at 20 kV and 20-40 nA. The following standards were used: lorenzenite (Na and Ti), pyrope (Mg), diopside (Ca, Si), wadeite (K), $MnCO_3$ syn. (Mn), hematite (Fe), celestine (Sr), Nb metal. (Nb) and $BaSO_4$ syn. (Ba). The chemical analyses showed that both monoclinic and orthorhombic lamprophyllites have nearly the same chemical composition (average of analyses of three crystals, 6-8 points for each; wt. %): Na_2O 12.38, MgO 0.66, SiO_2 32.20, K_2O 0.45, CaO 0.84, TiO_2 30.30, MnO 3.49, FeO 2.08, SrO 16.43, Nb_2O_5 0.43, BaO 0.49, sum 99.75. The empirical chemical formula, calculated on the basis of Si = 4, is $(Na_{2.98}Sr_{1.18}Mn_{0.37}Fe_{0.22}Mg_{0.12}Ca_{0.11}K_{0.07}Ba_{0.02})_{\Sigma5.07}(Ti_{2.83}Nb_{0.02})_{\Sigma2.85}Si_4O_{17.28}$. This formula is in good agreement with the site-occupancy refinements for the cation positions (see below).

Experimental

Data collection

Single crystals of lamprophyllite-$2M$ and lamprophyllite-$2O$ selected for data collection were mounted on a Bruker PLATFORM goniometer equipped with a 1K SMART 1000 CCD (charge-coupled device) detector with a crystal-to-detector distance of 5.4 cm. The data were collected using monochromatic Mo$K\alpha$ X-radiation and frame widths of 0.3° in ω, with 30 s used to acquire each frame. More than a hemisphere of three-dimensional data were collected for each crystal. Miscellaneous information regarding data collection and structure refinement is given in Table 1. The data were reduced using the Bruker program SAINT. A semi-empirical absorption-correction based upon the intensities of equivalent reflections was applied, and the data were corrected for Lorentzation, and background effects.

Structure solution and refinement

Scattering curves for neutral atoms, together with anomalous dispersion corrections, were taken from *International Tables for X-Ray Crystallography, Vol. IV* (Ibers & Hamilton, 1974). The Bruker SHELXTL Version 5.1 system of programs was used for the refinement of the crystal structure.

The crystal structure of lamprophyllite-$2M$ was refined in space group $C2/m$ on the basis of atomic coordinates taken from Rastsvetaeva *et al.* (1995). The final refinement included atomic-positional and anisotropic displacement parameters of all atoms, and a refinable weighting scheme of the structure factors. The refinement resulted in a final agreement index ($R1$) of 4.0 %, calculated for 688 unique observed reflections ($|Fo| \geq 4\sigma F$) and a goodness-of-fit (S) of 1.05.

The crystal structure of lamprophyllite-$2O$ was solved by direct methods and the atoms were subsequently renumbered in one-to-one correspondence to the atom numbers in the structure lamprophyllite-$2M$. The non-standard setting $Pnmn$ was chosen for the orthorhombic structure in order to facilitate comparison of $2M$ and $2O$ polytypes. Attempts to refine all atoms anisotropically resulted in non-positive definite displacement parameters for Si and some O atoms and these were refined isotropically. The final refinement included positional and isotropic displacement parameters for all atoms, and anisotropic displacement parameters for Sr, Ti, and Na positions. $R1$ converged at 8.4 %, calculated for 571 unique observed reflections ($|Fo| \geq 4\sigma F$) yielding a goodness-of-fit (S) of 1.12. The high $R1$ index is probably due to stacking faults observed in the orthorhombic polytype (Johnsen 1996). Analysis of the six strongest residual peaks in difference Fourier maps demonstrated that they are located on the same levels along the a axis (direction of stacking of the HOH layers) as the Si, Ti, Na and Sr atoms (Table 2b). The residual electron density peaks

Table 3. Atomic coordinates and displacement parameters ($\times 10^4$ Å^2) for lamprophyllite-2M.

Atom	x	y	z	U_{iso}	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ti(1)	0.15057(6)	0	0.70775(19)	56(4)	214(6)	128(6)	116(5)	0	9(3)	0
Ti(2)	0	½	0	246(7)	146(11)	77(11)	85(9)	0	27(7)	0
Si	0.14390(6)	0.28459(18)	0.2049(2)	78(4)	74(7)	46(7)	45(6)	0	0(4)	0
Na(1)	0	0.2590(3)	½	102(6)	288(12)	50(11)	339(12)	0	-222(9)	0
Na(2)	0	0	0	174(9)	103(7)	51(7)	78(6)	4(4)	0(4)	10(5)
Sr	0.28418(5)	0	0.26213(16)	153(4)	190(20)	170(20)	172(19)	0	62(16)	0
OH(1)	0.4425(3)	0	0.2758(9)	169(11)	160(30)	140(30)	220(20)	0	50(20)	0
O(2)	0.17480(17)	0.1889(5)	0.4674(6)	155(8)	155(18)	158(19)	146(15)	61(14)	-5(13)	-28(14)
O(3)	0.17532(17)	0.1875(5)	0.9712(6)	143(8)	127(17)	138(19)	166(15)	-54(14)	28(13)	-21(13)
O(4)	0.1777(2)	0.5000	0.2200(8)	113(10)	130(20)	50(20)	150(20)	0	-13(18)	0
O(5)	0.05951(17)	0.2965(4)	0.1725(6)	127(8)	92(16)	87(18)	198(16)	-18(14)	-1(13)	5(14)
O(6)	0.0623(3)	0	0.6677(9)	200(12)	120(20)	350(30)	130(20)	0	2(19)	0

observed for the 2O polytype approximately correspond to the cation positions of the 2M polytype and are a direct result of the stacking faults common for the 2O polytype. The random stacking disorder usually results in broadening of non-family reflections known as the v uroviΔ effect (Nespolo & Ferraris, 2001). Ferraris *et al.* (2001c) demonstrated for mica polytypes where electron residues occur with shifts $\pm$ $b/3$ from the cation positions, that this stacking disorder can be modelled by applying separate scale factors to family and non-family reflections (in the case of mica polytypes, reflections with $k = 3n$ and $k \neq 3n$, respectively). However, in the case of lamprophyllite-2O, the shifts of the residual peaks along the c axis are different for the octahedral sheets, heterophyllosilicate sheets and sheets of the Sr atoms. As a consequence, family and non-family reflections cannot be defined and the disorder cannot be modelled by applying separate scale factors for different groups of reflections. From the height of the electron residues in the difference Fourier map, the amount of the 2M polytype domains within the crystal of the 2O polytype can be estimated as approximately 5 %.

The final atomic parameters for lamprophyllite-2O and lamprophyllite-2M are listed in Tables 2a and 3, respec-tively, selected interatomic distances are in Table 4. Observed and calculated structure-factors are available from the authors upon request or through the E.J.M. Editorial Office, Paris.

Structure description

Overview of the structures

The structures of both polytypes of lamprophyllite are shown in Fig. 1. They are based on the same *HOH* layer depicted in Fig. 2a. This layer consists of a central *O* sheet of edge-sharing Na(1)O$_6$, Na(2)O$_6$, and Ti(2)O$_6$ octahedra sandwiched between two heterophyllosilicate *H* sheets. In lamprophyllites, the *H* sheet (Fig. 2b) is built by corner-sharing of Ti(1)O$_5$ square pyramids and Si$_2$O$_7$ groups and consists of two types of rings of polyhedra: (i) six-membered rings (6R) formed by two Si$_2$O$_7$ groups and two TiO$_5$ square pyramids and (ii) four-membered rings (4R) formed by two silicate tetrahedra and two TiO$_5$ square pyramids. Sr is in the interlayer and is coordinated by six anions from the 6R of the upper *H* sheet and four anions from the 4R of the lower *H* sheet. The coordination of Sr is

Table 4. Selected bond lengths (Å) for lamprophyllite-2O and lamprophyllite-2M.

| Bond	2O	2M	Bond	2O	2M
Ti(1)-O(6)	1.69(1)	1.684(5)	Na(1)-O(5)	2.225(7) 2x	2.225(3) 2x
Ti(1)-O(2)	1.950(7) 2x	1.951(3) 2x	Na(1)-OH(1)	2.230(9) 2x	2.291(3) 2x
Ti(1)-O(3)	1.957(7) 2x	1.955(3) 2x	Na(1)-O(6)	2.314(8) 2x	2.310(3) 2x
<Ti(1)-O>	1.90	1.90	<Na(1)-ϕ*>	2.26	2.28
Ti(2)-OH(1)	1.94(1) 2x	1.950(5) 2x	Na(2)-O(6)	2.27(1) 2x	2.264(5) 2x
Ti(2)-O(5)	2.003(7) 4x	1.995(3) 4x	Na(2)-O(5)	2.510(7) 4x	2.509(3) 4x
<Ti(2)-ϕ*>	1.98	1.98	<Na(2)-O>	2.43	2.43
Si-O(3)	1.605(7)	1.609(4)	Sr-O(2)	2.705(7) 2x	2.699(4) 2x
Si-O(5)	1.625(8)	1.612(4)	Sr-O(3)	2.724(7) 2x	2.697(4) 2x
Si-O(2)	1.626(7)	1.612(3)	Sr-O(4)	2.786(9)	2.774(5)
Si-O(4)	1.659(5)	1.652(2)	Sr-O(4)	2.791(9)	2.792(5)
<Si-O>	1.63	1.62	Sr-O(2)	2.798(7) 2x	2.822(4) 2x
			Sr-O(3)	2.801(7) 2x	2.792(4) 2x
			<Sr-O>	2.76	2.76

* ϕ = O, OH
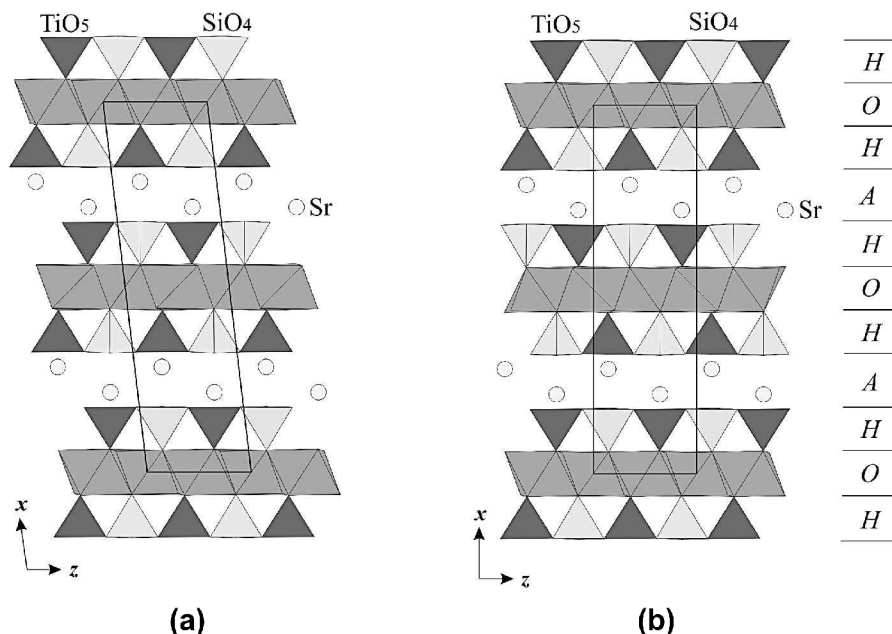
Fig. 1. The crystal structures of lamprophyllite-2*M* (a) and lamprophyllite-2*O* projected along the *b* axis.

preserved in both polytypes. The difference between mono-clinic and orthorhombic lamprophyllites can be viewed in the arrangements of adjacent octahedral sheets shown in Fig. 2c, d. Whereas in lamprophyllite-2*M*, all octahedral sheets in the *HOH* layers are in the same orientation, in lamprophyllite-2*O*, adjacent octahedral sheets have oppo-site orientations.

The symmetry of the *HOH* layers is the same in both structures and corresponds to the layer group *P*12/*m*1

considering only the symmetry elements present in the space group. Two adjacent *HOH* layers in lamprophyllite-2*M* are related by the *C*-translation (= $^1/_2$(a + b)) or the 2_1 screw axis perpendicular to the *b* axis (both these opera-tions do not change the layer orientation). In contrast, two adjacent *HOH* layers in lamprophyllite-2*O* are related by the 2_1 screw axis parallel to the *c* axis or by the *n* glide plane parallel to (100) (these operations change the layer orientation).
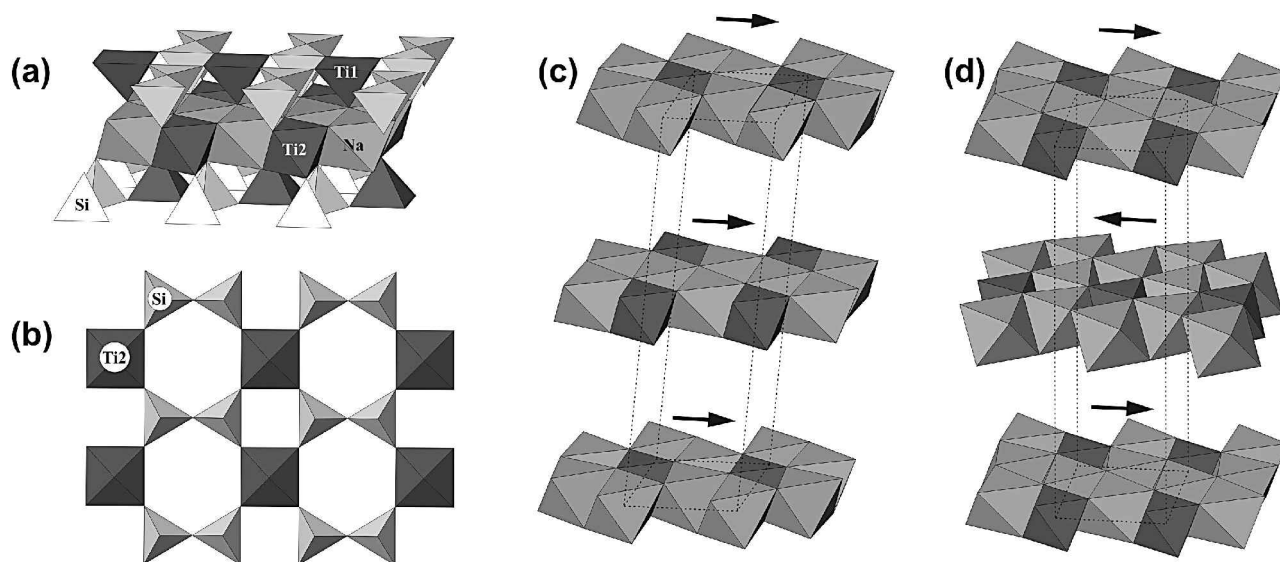

Fig. 2. The *HOH* layer in lamprophyllite-2*M* and lamprophyllite-2*O* (a), the *H* sheet (b), and arrangements of octahedral sheets in the struc-tures of lamprophyllite-2*M* (c) and lamprophyllite-2*O* (c). In (c) and (d), arrows are used to indicate orientations of the octahedral sheets.

Table 5. Numbers of electrons and occupancies for cation positions in lamprophyllite-$2O$ and lamprophyllite-$2M$.

Atom	Number of electrons		Occupancy*
	$2O$	$2M$	
Ti(1)	22.00	22.00	$Ti_{1.00}$
Ti(2)	22.00	22.00	$Ti_{1.00}$
Si	14.00	14.00	$Si_{1.00}$
Na(1)	15.29	15.51	$Na_{0.65}Mn_{0.18}Fe_{0.11}Mg_{0.06}$
Na(2)	9.90	11.00	$Na_{1.00}$
Sr	27.74	27.36	$Sr_{0.59}Na_{0.33}Ca_{0.06}$

* calculated on the basis of chemical analyses

Crystal-chemical formula: $(Sr_{1.18}Na_{0.66}Ca_{0.12})_{\Sigma1.96}Na(Na_{1.30}Mn_{0.36}Fe_{0.22}Mg_{0.12})_{\Sigma2.00}$
$Ti_3(Si_2O_7)_2(OH)_2O_2$

Cation positions, their occupancies and bond-valence sums

Number of electrons for the cation positions and their occupancies are given in Table 5. Table 6 provides bond-valence sums for all atoms in the structure calculated on the basis of bond-valence parameters given by Brese & O'Keeffe (1991). The full occupancy of the Ti(1) and Ti(2) positions by Ti is in good agreement with the bond-valence sums of ~ 4 valence units (v.u.). The occupancy of the Na(2) position in lamprophyllite-$2O$ is slightly lower than that in lamprophyllite-$2M$, however, the bond-valence sums are close to the expected values of 1.0 v.u. The refinement shows that the number of electrons for the Na(1) position in both polytypes is higher than 11.0 which would be expected for the pure Na position, whereas the bond-valence sums for this position is around 1.7 v.u. Analysis of bond lengths given in Table 4 shows that Na(1) site is in octahedral coordination to six anions with a relatively short average $<$Na(1)-$\phi>$ distance (ϕ = O, OH) of ~ 2.3 Å. This is a clear indication that this position is also occupied by divalent cations (Mn^{2+}, Fe^{2+}, Mg^{2+}), in good agreement with previous structural studies of lamprophyllite (*e.g.*, Rastsvetaeva *et al.*, 1995). The Sr positions in lamprophyllite-$2O$ and lamprophyllite-$2M$ have approximately the same site-scattering factors and cation occupancies (Table 5). The refined occupancies of cation positions are in good agreement with the results of chemical analyses confirming that, in our sample, lamprophyllite-$2O$ and lamprophyllite-$2M$ have nearly the same chemical composition $(Sr_{1.18}Na_{0.66}Ca_{0.12})_{\Sigma1.96}Na(Na_{1.30}Mn_{0.36}Fe_{0.22}Mg_{0.12})_{\Sigma2.00}$ $Ti_3(Si_2O_7)_2(OH)_2O_2$.

The bond-valence sums for the OH(1) positions in lamprophyllite-$2O$ and lamprophyllite-$2M$ are 1.33 and 1.23 v.u., respectively, which is in a good agreement with their assignment to hydroxyl groups.

Discussion

The structure refinement of lamprophyllite-$2O$ confirmed the suggestion of Matsubara (1980) that the 'orthorhombic lamprophyllite' is isotypic to orthoericssonite. A comparison of the unit-cell parameters of lamprophyllite polytypes, barytolamprophyllite, ericssonite and orthoericssonite is given in Table 7. As can be seen, the *b* and *c* parameters are almost identical, whereas the *a* parameter varies from structure to structure. In fact, the *b* and *c* parameters are within the *HOH* layer, whereas the *a* parameter depends upon the size of the cation located in the interlayer.

Matsubara (1980) explained relationships between ericssonite and orthoericssonite in terms of tropochemical cell-twinning (Takéuchi, 1997). For the orthorhombic and monoclinic structures, a monoclinic subcell can be defined that has symmetry $P2/m$ and unit-cell parameters *a'* ~ 9.5-10.2, *b'* ~ 7.0, *c'* ~ 5.4 Å. The structure of lamprophyllite-$2O$ and orthoericssonite can be obtained by twinning the subcell by the {100} plane. The structures of lamprophyllite-$2M$, barytolamprophyllite-$2M$ and ericssonite can be derived from the subcell by the {100} glide plane with the *b*/2 glide component.

According to Ferraris (1997) and Ferraris *et al.* (2001b), lamprophyllite-$2O$, lamprophyllite-$2M$ and barytolamprophyllite-$2M$ are members of the baferitisite polysomatic series which have the general formula

$$A_2\{Y_4[Z_2(O')_{2+p}Si_4O_{14}](O'')_2\}W,$$
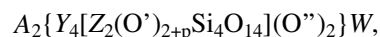
where $[Z_2(O')_{2+p}Si_4O_{14}]$ is the formula of the heterophyllosilicate *H* sheet (*Z* is a cation either in fivefold ($p = 0$) or sixfold ($p = 1$ or 2) coordination), $\{Y_4[Z_2(O')_{2+p}Si_4O_{14}](O'')_2\}$ is the formula of the *HOH* sheet (O' and O''' are

Table 6. Bond-valence sums (v.u.) for atoms in lamprophyllite-$2O$ and lamprophyllite-$2M$.

Atom	$2O$	$2M$	Atom	$2O$	$2M$
Ti(1)	4.15	4.18	OH(1)	1.33	1.23
Ti(2)	3.83	3.85	O(2)	2.05	2.08
Si	3.95	4.03	O(3)	2.08	2.09
Na(1)	1.76	1.67	O(4)	2.14	2.19
Na(2)	1.15	1.16	O(5)	2.07	2.11
Sr	1.76	1.79	O(6)	2.18	2.21

Table 7. Crystallographic information on minerals of the lamprophyllite group.

	Space-group type	a, Å	b, Å	c, Å	β, °	V, Å^3	Reference
lamprophyllite-2M	$C2/m$	19.215	7.061	5.372	96.797	723.7	This work
lamprophyllite-2O	$Pnmn$	19.128	7.080	5.382	-	728.9	This work
barytolamprophyllite-2M	$C2/m$	19.744	7.099	5.409	96.77	752.9	Rastsvetaeva & Dorfman (1995)
ericssonite	$C2/m$	20.42	7.03	5.34	95.5	763.0	Moore (1971)
orthoericssonite	$Pnmn$	20.230	6.979	5.392	-	761.3	Matsubara (1980)

anions that are not bonded to Si), A and W are species in the interlayer. Note that the bafertisite series is defined as having Si_2O_7 groups as necessary constituents of the H heterophyllosilicate sheet (Ferraris *et al.*, 2001b).

For lamprophyllite-2O, lamprophyllite-2M and barytolamprophyllite-2M, A = Sr or Ba, Y = Na, ^{VI}Ti, Z = ^{V}Ti, $p = 0$, O' = O^{2-}, O" = OH$^-$. For ericssonite and orthoericssonite, A = Ba, Y = Mn, Z = ^{V}Fe^{3+}, $p = 0$, O' = O^{2-}, O" = OH$^-$. These minerals are the only minerals of the bafertisite polysomatic series that have $p = 0$. If $p = 2$, the Z cation is in octahedral coordination with its apical vertex pointing into the interlayer space (bafertisite and delindeite are examples of this configuration). In the case of $p = 1$, this vertex is shared with the ZO_6 octahedron from the adjacent HOH layer (*e.g.*, in the structure of seidozerite). In the structures of betalomonosvite and lomonosovite ($p = 2$), the interlayer space contains W = Na$^+$ and PO$_4^{3-}$ ions.

It is interesting to note that, from the viewpoint of mutual orientations of adjacent octahedral O sheets, the structures of lamprophyllite-2O and lamprophyllite-2M are related to the structures of the $C2/m$ and $Pnmn$ amphiboles if the latter are considered as layered structures (Hawthorne, 1981). As in lamprophyllite-2O and lamprophyllite-2M, the adjacent octahedral sheets in the $Pnmn$ and $C2/m$ amphiboles are related by the 2_1 screw axis parallel to the c axis and by the C-translation, respectively. The symmetry operation, corresponding to the 2_1 screw axis parallel to the c axis, changes the orientation of the octahedral sheet, whereas the C-translation does not. This relationship between the adjacent layers has also recently been observed by Ferraris *et al.* (2001c) for phlogopite-2O and phlogopite-1M from the Khibiny alkaline massif, Kola peninsula, Russia.

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