

Lileyite, $\text{Ba}_2(\text{Na,Fe,Ca})_3\text{MgTi}_2(\text{Si}_2\text{O}_7)_2\text{O}_2\text{F}_2$, a new lamprophyllite-group mineral from the Eifel volcanic area, Germany

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Abstract: The new Mg- and F-dominant lamprophyllite-group mineral lileyite (IMA 2011-021) was found at the Löhley quarry, Üdersdorf, near Daun, Eifel Mountains, Rhineland-Palatinate (Rheinland-Pfalz), Germany, and named for the old name of the type locality, Liley. Associated minerals are nepheline, leucite, augite, magnetite, fluorapatite, perovskite, götzenite. Lileyite is brown, translucent; streak is white. It forms platy crystals up to $0.1 \times 0.3 \times 0.5$ mm in size and their clusters up to 1 mm across on the walls of cavities in an alkaline basalt. Lileyite is brittle, with Mohs hardness of 3–4 and perfect cleavage on (001). D_{calc} is 3.776 g/cm^3 . The new mineral is biaxial (+), $\alpha = 1.718(5)$, $\beta = 1.735(5)$, $\gamma = 1.755(5)$, $2V$ (meas.) = $75(15)^\circ$, $2V$ (calc.) = 86° . The IR spectrum is given. The chemical composition is (EDS-mode electron microprobe, mean of 5 analyses, wt%): SiO_2 28.05, BaO 26.39, TiO_2 18.53, Na_2O 6.75, MgO 4.58, FeO 4.48, CaO 2.30, SrO 2.23, MnO 1.44, K_2O 1.41, Nb_2O_5 0.95, F 3.88, $-\text{O}=\text{F}_2$ -1.63; total 99.36. The empirical formula based on 18 anions is: $\text{Ba}_{1.50}\text{Sr}_{0.19}\text{K}_{0.26}\text{Na}_{1.89}\text{Ca}_{0.36}\text{Mn}_{0.18}\text{Mg}_{0.99}\text{Fe}_{0.54}\text{Ti}_{2.01}\text{Nb}_{0.06}\text{Si}_{4.06}\text{O}_{16.23}\text{F}_{1.77}$. The simplified formula is: $\text{Ba}_2(\text{Na,Fe,Ca})_3\text{MgTi}_2(\text{Si}_2\text{O}_7)_2\text{O}_2\text{F}_2$. The crystal structure was solved using single-crystal X-ray diffraction data ($R = 0.024$). Lileyite is monoclinic, space group $C2/m$, $a = 19.905(1)$, $b = 7.098(1)$, $c = 5.405(1)$ Å, $\beta = 96.349(5)^\circ$, $V = 758.93(6)$ Å³, $Z = 2$. The strongest lines of the powder diffraction pattern [d , Å (I , %) (hkl)] are: 3.749 (45) (31–1), 3.464 (76) (510, 311, 401), 3.045 (37) (51–1), 2.792 (100) (221, 511), 2.672 (54) (002, 601, 20–2), 2.624 (43) (710, 42–1). Type material is deposited in the collections of the Fersman Mineralogical Museum of the Russian Academy of Sciences, Moscow, Russia, registration number 4106/1.

Key-words: lileyite, new mineral, lamprophyllite group, heterophyllosilicates, crystal structure, Eifel, Germany.

1. Introduction

Lamprophyllite-group minerals (Back & Mandarino, 2008) belong to the large family of heterophyllosilicates, *i.e.* minerals whose crystal structures are based on the *HOH* layers consisting of one inner octahedral (*O*) and two outer heteropolyhedral (*H*) sheets. The stoichiometry of heterophyllosilicates can be described by the following general formula (after Ferraris & Gula, 2005; some designations are changed): $A_2\{M_4[L_2X_{2+p}(\text{Si}_2\text{O}_7)_2]Y_2\}W$, where *A* are low-field-strength interlayer cations (typically, alkaline and alkaline-earth), *M* are octahedral cations of the *O* sheet, *L* are cations with 5- or 6-fold coordination

belonging to the *H* sheet, *X* and *Y* are O, F and OH; *W* are H_2O molecules and complex anions; $p = 0-2$.

Distinctive features of lamprophyllite-group minerals are: (a) the absence of *W*-components; (b) 5-fold coordination of *L* cations, and consequently zero *p* value. The general crystal chemical formula of lamprophyllite, barytolamprophyllite, ericssonite and ferroericssonite (Kampf *et al.*, 2011) is $^{[10-11]}A_2 [^{[6]}M1 \ ^{[6]}M2_2 \ ^{[6]}M3 \ X_2] [^{[5]}L_2 (\text{Si}_2\text{O}_7)_2 \text{O}_2]$ where *A* = **Ba**, **Sr**, **K**, **Na**, **Ca**, \square ; *M1* = **Na**, **Mn**²⁺; *M2* = **Na**, **Mn**²⁺, **Fe**²⁺, **Ca**; *M3* = **Ti**, **Mn**²⁺, **Mg**, **Fe**³⁺, **Fe**²⁺; *L* = **Ti**, **Fe**³⁺; *X* = **OH**, **O**, **F** (species-defining components of valid mineral species are given in bold type). In these minerals (Si_2O_7) groups link to the *trans*

edges of the same octahedron of the *O* sheet, unlike the related triclinic (space group *P1*) mineral schüllerite (Chukanov *et al.*, 2011) that has a different topology of the *HOH* layer corresponding to “linkage 3” (Sokolova, 2006) where two (Si_2O_7) groups link to two octahedra adjacent approximately along the diagonal *yz*. In schüllerite and nabalamprophyllite (space group *P2/m*; Chukanov *et al.*, 2004) *A*-, *M*-, *L*- and *X*-sites are transformed in pairs of non-equivalent sites. For lamprophyllite, barytolamprophyllite and ericssonite two polytypes are known: *2M* (space group *C2/m*) and *2O* (space group *Pnmm*): Peng & Chang, 1965; Moore, 1971; Krivovichev *et al.*, 2003; Sokolova & Hawthorne, 2008. In the latter paper, the orthorhombic polytype of barytolamprophyllite is erroneously named “orthorhombic polytype of nabalamprophyllite”. Nabalamprophyllite and barytolamprophyllite have different crystal-chemical formulae. Barytolamprophyllite, including the sample described by Sokolova & Hawthorne (2008), has one interlayer cation site that is Ba-dominant. Unlike barytolamprophyllite, nabalamprophyllite contains two interlayer cation sites, occupied predominantly with Na and Ba (Chukanov *et al.*, 2004).

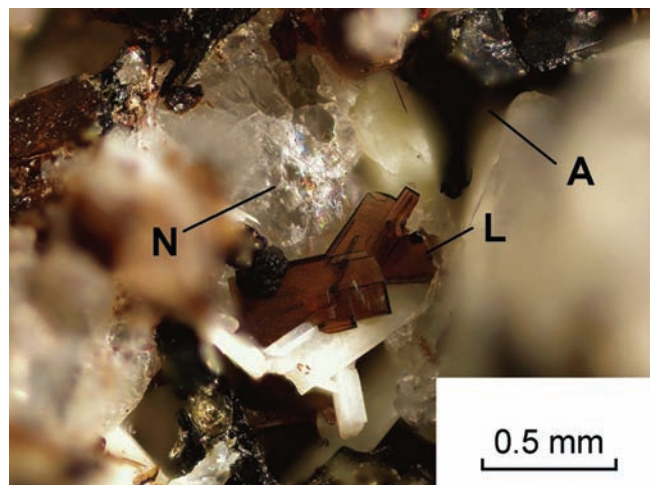
The present paper is a description of a new mineral species, lileyite (Cyrillic: лилейит), and its crystal structure. Lileyite is a member of the lamprophyllite group, an analogue of barytolamprophyllite-*2M* with Mg predominant in *M3* site and F predominant in *X* site and “linkage 1” according to Sokolova (2006). It is named for the old name of the type locality, Liley (Dechen, 1861). The mineral and its name have been approved by the IMA Commission on New Minerals, Nomenclature and Classification (IMA no. 2011-021).

The type material is deposited in the collection of the Fersman Mineralogical Museum of the Russian Academy of Sciences, Moscow, Russia, registration number 4106/1.

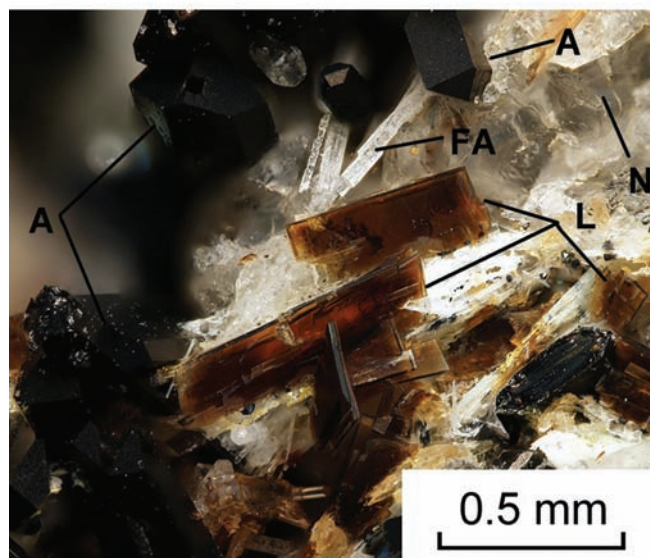
2. Occurrence, general appearance and physical properties

Specimens with lileyite were collected in the Löhley quarry, Üdersdorf, near Daun, Eifel Mountains, Rhineland-Palatinate (Rheinland-Pfalz), Germany. Associated minerals are nepheline, leucite, augite, magnetite, fluorapatite, perovskite and götzenite. Götzenite is partly substituted with an X-ray amorphous silicate of Ca and Ti with variable stoichiometry (white in Fig. 1a). Earlier, in the same assemblage at Löhley, another lamprophyllite-group mineral, schüllerite, $\text{Ba}_2\text{Na}(\text{Mn,Ca})(\text{Fe}^{3+}, \text{Mg}, \text{Fe}^{5+})_2\text{Ti}_2(\text{Si}_2\text{O}_7)_2(\text{O,F})_4$, visually indistinguishable from lileyite, was discovered (Chukanov *et al.*, 2011). All these minerals occur in miarolitic cavities of alkaline basalt.

Lileyite is brown, translucent; streak is white. It forms platy crystals up to $0.1 \times 0.3 \times 0.5$ mm in size and their clusters up to 1 mm across on the walls of cavities in an alkaline basalt (Fig. 1). The main crystal form is $\{100\}$.



a



b

Fig. 1. Platy crystals of lileyite (L) with nepheline (N), augite (A) and fluorapatite (FA). Photo: F. Kruijen.

The new mineral is brittle, with Mohs hardness of 3–4 and perfect cleavage on (001). D_{calc} is 3.776 g/cm^3 . Lileyite is optically biaxial (+), $\alpha = 1.718(5)$, $\beta = 1.735(5)$, $\gamma = 1.755(5)$, $2V$ (meas.) = $75(15)^\circ$, $2V$ (calc.) = 86° . Dispersion is medium, $r > v$. Orientation: $X = a$; Y coincides with the elongation direction of crystals. Pleochroism is medium, Z (greyish-brown) $> Y$ (light brown) $> X$ (colourless).

The IR spectrum of lileyite (Fig. 2a) is different from those of other members of the lamprophyllite group (Fig. 2b–d). Absorption bands in the IR spectrum of lileyite and their assignments are (cm^{-1} ; s – strong band): 1032 s, 957 s, 901 s, 854 s (Si–O stretching vibrations), 680 (O–Si–O bending vibrations of Si_2O_7 groups), 578, 529 (Ti–O stretching vibrations of the TiO_5 polyhedra), 458 s,

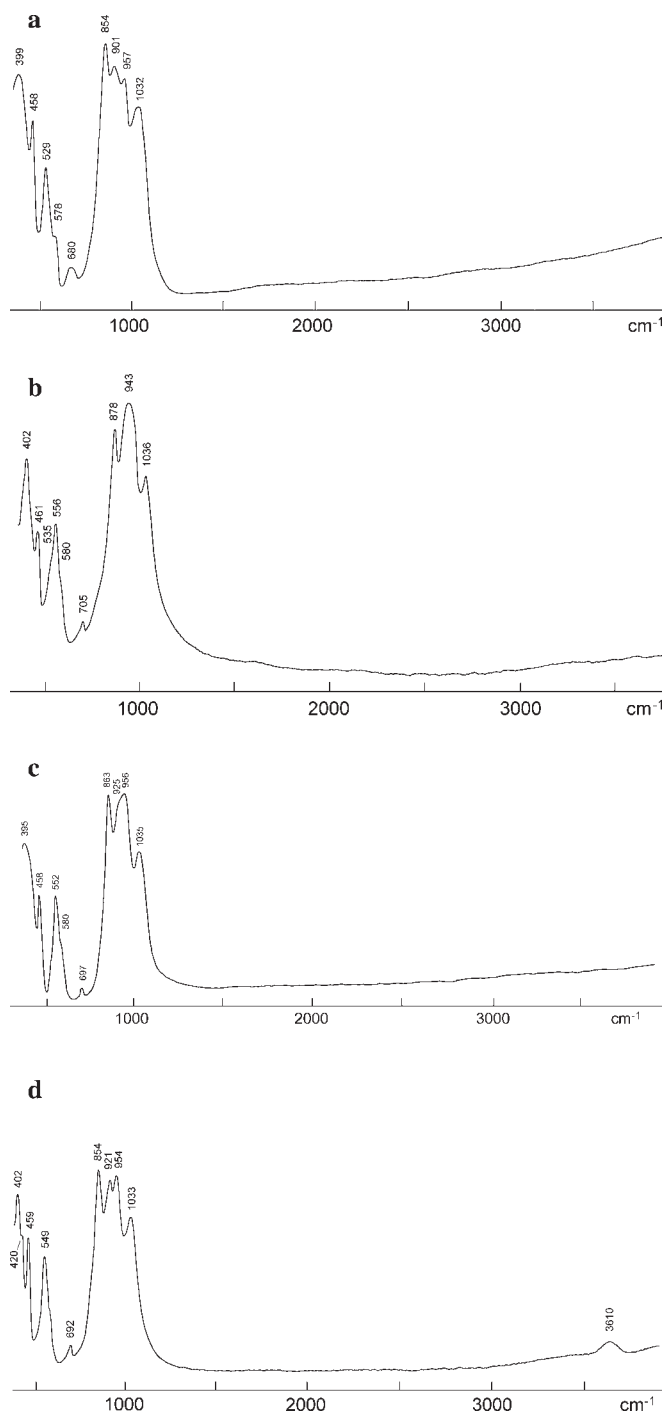


Fig. 2. IR spectra of titanium lamprophyllite-group minerals: lileyite (a); lamprophyllite from Mt. Flora, Lovozero massif, Kola peninsula, Russia (b); barytolamprophyllite from Mt. Kukisvumchorr, Khibiny massif, Kola peninsula, Russia (c); and nabalamprophyllite from the Inaglik alkaline-ultrabasic massif, South Yakutia, Russia (d).

399 cm^{-1} (combination of Si-O-Si bending vibrations and stretching vibrations of the MO_6 octahedra where $M = \text{Mg, Fe, Mn, Ca}$). Bands with frequencies above 1100 cm^{-1} (that could correspond to stretching

Table 1. Chemical composition of lileyite.

Constituent	wt%	Range	SD	Probe standard
SiO_2	28.05	27.90–28.23	0.1	SiO_2
BaO	26.39	25.48–27.19	0.6	BaSO_4
TiO_2	18.53	18.34–18.75	0.15	MnTiO_3
Na_2O	6.75	6.24–7.33	0.3	Albite
MgO	4.58	4.32–4.77	0.1	Diopside
FeO	4.48	4.29–4.61	0.1	Fe_2O_3
CaO	2.30	2.11–2.60	0.2	Wollastonite
SrO	2.23	1.83–2.78	0.25	SrF_2
MnO	1.44	1.31–1.64	0.1	MnTiO_3
K_2O	1.41	1.20–1.59	0.1	Microcline
Nb_2O_5	0.95	0.72–1.27	0.15	Nb
F	3.88	3.67–4.19	0.2	CaF_2
O = F	–1.63			
Total	99.36			

vibrations of H-, B- or C-bearing groups) are absent in the IR spectrum.

3. Chemical data

Five electron-microprobe analyses were carried out using VEGA TS 5130MM SEM equipped with EDX analyser (INCA Si(Li) detector), at an operating voltage of 15.7 kV and a beam current of 0.5 nA. The program INCA Energy 200 was used for the analytical data calculation.

H_2O and CO_2 were not analysed because of the absence of bands corresponding to vibrations of O-H and C-O bonds in the IR spectrum. The contents of P, S, Al, V, Cr, Ni, Zn, Y, Zr, Ln, Th and U were found to be below detection limits. Analytical results are given in Table 1. The empirical formula of lileyite (based on 18 anions O+F *pfu*) is: $\text{Ba}_{1.50}\text{Sr}_{0.19}\text{K}_{0.26}\text{Na}_{1.89}\text{Ca}_{0.36}\text{Mn}_{0.18}\text{Mg}_{0.99}\text{Fe}_{0.54}\text{Ti}_{2.01}\text{Nb}_{0.06}\text{Si}_{4.06}\text{O}_{16.23}\text{F}_{1.77}$.

The simplified formula is $\text{Ba}_2(\text{Na,Fe,Ca})_3\text{MgTi}_2(\text{Si}_2\text{O}_7)_2\text{O}_2\text{F}_2$, taking into account the structural data (see below).

4. Crystal structure and X-ray powder diffraction data

Single-crystal X-ray studies of lileyite were carried out using an Xcalibur S CCD diffractometer; 3022 independent reflections ($|I| > 3\sigma$) were used for the structure determination. The crystal structure has been solved and refined using AREN and Jana programs (Andrianov, 1987; Petricek *et al.*, 2006). Mixed scattering curves were used for the composite cation sites. The details of data collection and structure refinement are given in Table 2. The results of the crystal structure refinement are given in Fig. 3 and 4 and Tables 3–6.

Table 2. Crystal parameters, data collection and single-crystal structure refinement details for lileyite.

a (Å)	19.905 (1)
b (Å)	7.098 (1)
c (Å)	5.405 (1)
β (°)	96.349 (5)
V (Å ³)	758.93 (6)
Space group	$C2/m$
Z	2
Absorption coefficient (mm ⁻¹)	7.033
$F(000)$	812
D_x (g/cm ³)	3.804
Crystal size (mm)	0.24 × 0.21 × 0.18
Radiation/filter	MoK α /graphite
θ_{\max} – for structure refinement (°)	55.17
$R(\text{int})$ (%)	5.03
Reflection collected	24082
Independent reflections	3436
$ F > 3\sigma_F$	3191
Refinement method	Full-matrix least squares on F^2 with fixed weight scheme $1/(\sigma^2 F +0.0009F^2)$
Number of refined parameters	80
Final $R(\text{obs})$ (%) [$ F > 3\sigma_F$]	3.05
wR_2	4.46
S	1.17

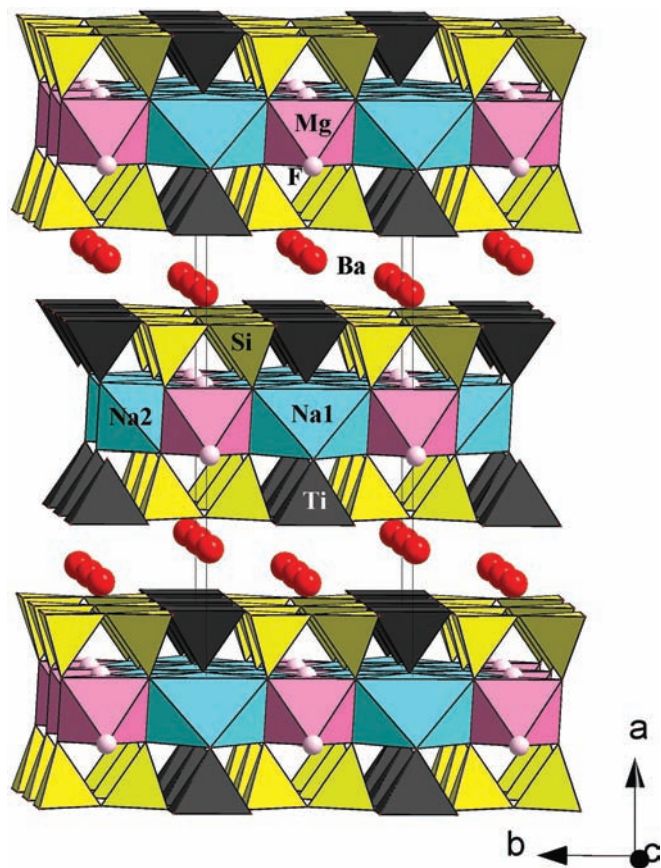


Fig. 3. The crystal structure of lileyite (general view).

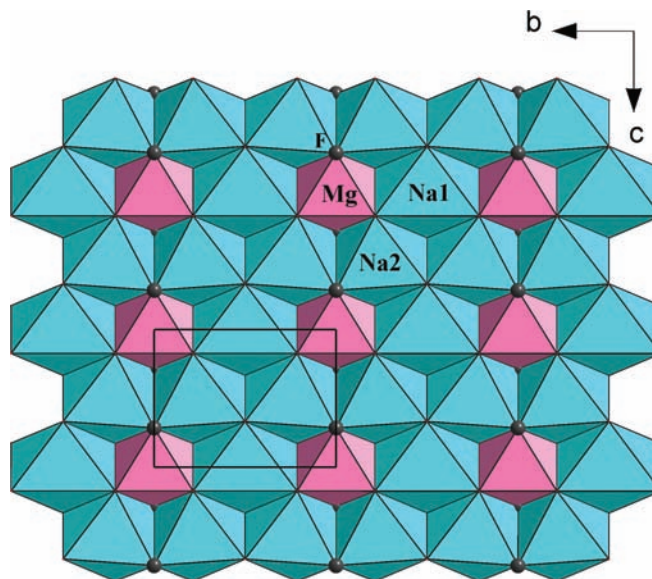


Fig. 4. The octahedral sheet in lileyite.

Lileyite is isostructural with $2M$ polytypes of lamprophyllite, barytolamprophyllite, ericssonite and ferroericssonite and is structurally related to nabalamprophyllite and schüllerite (Table 7).

A characteristic feature of the Na-dominant Na2 site is its ability to incorporate the bivalent cations Ca^{2+} , Fe^{2+} and Mn^{2+} (Peng *et al.*, 1984; Rastsvetaeva *et al.*, 1990, 1995). Large cations (Ba^{2+} , Sr^{2+} , K^+) are situated in the interlayer space. Fluorine is concentrated in the F site, as seen from bond valence calculations (Table 5). High valence sums for the Mg and Na2 sites with mixed occupancy (2.36 and 1.66, respectively) are consistent with the mean charge of cations in these sites (2.30 and 1.55, respectively).

The refined crystal-chemical formula of lileyite is $[\text{Ba}_{0.75}\text{K}_{0.15}\text{Sr}_{0.1}]_2[\text{Na}(\text{Na}_{0.45}\text{Ca}_{0.20}\text{Fe}^{2+}_{0.25}\text{Mn}_{0.10})_2(\text{Mg}_{0.80}\text{Fe}^{3+}_{0.10}\text{Ti}_{0.10})(\text{F}_{0.80}\text{O}_{0.20})_2][(\text{Ti}_{0.95}\text{Nb}_{0.05})_2(\text{Si}_2\text{O}_7)_2\text{O}_2]$, where interlayer contents, O sheet and H sheet are given in square brackets.

The X-ray powder diffraction data for lileyite (Table 8) were collected with a STOE IPDS II single-crystal diffractometer equipped with an image plate detector (MoK α radiation; the distance between sample and detector was 200 mm) using the Gandolfi method. They are well indexed in the monoclinic unit cell found by single-crystal studies; the unit-cell parameters refined from the powder data are: $a = 19.94(2)$, $b = 7.094(7)$, $c = 5.404(6)$ Å, $\beta = 96.23(8)^\circ$, $V = 760(2)$ Å³.

5. Discussion

Members of the lamprophyllite-barytolamprophyllite isomorphous series are typical accessory minerals of peralkaline (agpaitic) rocks and pegmatites. The content of MgO

Table 3. Fractional atomic coordinates, site multiplicities (W), refined number of electrons (e_{ref}), equivalent atom displacement parameters (B_{eq}) and site population for lileyite.

Site	x	y	z	W	e_{ref}	$B_{\text{eq}}, \text{\AA}^2$	Site population
Ba	0.2827 (1)	0	0.2623 (1)	4i	49	0.77 (1)	Ba _{0.75} K _{0.15} Sr _{0.1}
Ti	0.1458 (1)	0	0.7068 (1)	4i	23.4	0.59 (1)	Ti _{0.95} Nb _{0.05}
Mg	0	0.5	0	2b	14.4	0.86 (2)	Mg _{0.8} Fe ³⁺ _{0.1} Ti _{0.1}
Na1	0	0	0	2a	11.0	0.77 (5)	Na
Na2	0	0.2594 (1)	0.5	4h	17.9	0.98 (1)	Na _{0.45} Ca _{0.2} Fe ²⁺ _{0.25} Mn _{0.1}
Si	0.1386 (1)	0.2819 (1)	0.2041 (1)	8j	14.0	0.51 (2)	Si
O1	0.1713 (1)	0.1889 (1)	0.4657 (1)	8j		0.88 (2)	O
O2	0.1715 (1)	0.1876 (1)	0.9714 (1)	8j		0.86 (2)	O
O3	0.1696 (1)	0.5	0.2164 (2)	4i		0.78 (2)	O
O4	0.0579 (1)	0.2867 (1)	0.1735 (2)	8j		1.18 (5)	O
O5	0.0604 (1)	0	0.6671 (3)	4i		1.63 (7)	O
F	0.4443 (1)	0	0.2848 (4)	4i		1.67 (8)	F _{0.8} O _{0.2}

Table 4. Anisotropic displacement parameters (U) for lileyite.

Site	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ba	0.01464 (8)	0.00940 (8)	0.00941 (7)	0	0.00095 (5)	0
Ti	0.00979 (13)	0.00761 (13)	0.00630 (12)	0	0.00066 (10)	0
Mg	0.0113 (3)	0.0016 (3)	0.0151 (4)	0	-0.0110 (3)	0
Na1	0.0113 (6)	0.0092 (6)	0.0080 (5)	0	0.0048 (4)	0
Na2	0.0192 (3)	0.0174 (3)	0.0144 (2)	0	0.0049 (2)	0
Si	0.00874 (16)	0.00533 (16)	0.00624 (15)	0.00007 (12)	0.00052 (13)	-0.00028 (12)
O1	0.0164 (5)	0.0082 (4)	0.0074 (4)	-0.0005 (4)	0.0008 (4)	0.0019 (3)
O2	0.0168 (5)	0.0078 (4)	0.0084 (4)	-0.0001 (4)	0.0023 (4)	-0.0025 (3)
O3	0.0137 (7)	0.0049 (6)	0.0107 (6)	0	0.0006 (5)	0
O4	0.0085 (4)	0.0152 (6)	0.0196 (6)	0.0002 (4)	-0.0004 (4)	-0.0016 (5)
O5	0.0118 (7)	0.0343 (14)	0.0134 (8)	0	0.0004 (6)	0
F	0.0221 (10)	0.0321 (13)	0.0241 (10)	0	0.0054 (8)	0

Table 5. Bond valence calculations for lileyite^a.

Site	Ba	Ti	Mg	Na1	Na2	Si	V_i
O1	(0.28+ 0.19) ^{(×2)↓}	0.65 ^{(×2)↓}				0.99 ^{↓→}	2.11
O2	(0.28+ 0.19) [→]	0.65 [→]				1.00	2.11
O3	(0.28+ 0.19) ^{(×2)↓}	0.64 ^{(×2)↓}				0.90 ^{(×2)→}	2.27
O4	(0.27+ 0.20) ^{↓→}		0.37 ^{(×4)↓}	0.16 ^{(×4)↓}	0.32 ^{(×2)↓}	1.08 ^{↓→}	1.93
O5		1.41 ^{↓→}	0.37 [→]	0.16 [→]	0.32 [→]		2.17
F			0.28 ^{(×2)↓}	0.28 ^{(×2)↓}	0.24 ^{(×2)↓→}		0.98
V_i	2.35	3.99	0.44 ^{(×2)↓} 0.44 [→]	1.20	0.27 ^{(×2)↓→}	3.97	

Note: ^aCalculated with parameters taken from Brown (1981).

Table 6. Bond lengths [Å] in coordination polyhedra of lileyite.

Ba-O1	2.7550(14) 2×	Na1-O4	2.4655(16) 4×
Ba-O1'	2.9066(15) 2×	Na1-O5	2.260(3) 2×
Ba-O2	2.7553(14) 2×	<i>Mean</i>	2.3970
Ba-O2'	2.8959(14) 2×		
Ba-O3	2.852(2)	Na2-F	2.2854(18) 2×
Ba-O3'	2.8736(19)	Na2-O4	2.2206(17) 2×
<i>Mean</i>	2.8351	Na2-O5	2.3269(15) 2×
		<i>Mean</i>	2.2776
Ti-O1	1.9777(14) 2×	Si-O1	1.6264(14)
Ti-O2	1.9772(14) 2×	Si-O2	1.6257(15)
Ti-O5	1.695(2)	Si-O3	1.6642(9)
<i>Mean</i>	1.9210	Si-O4	1.6019(15)
		<i>Mean</i>	1.6296
Mg-F	1.989(3) 2×		
Mg-O4	2.0642(16) 4×		
<i>Mean</i>	2.0391		

in these minerals does not exceed 1.5 wt% (Zaitsev & Kogarko, 2002; Azarova, 2004).

Alkaline basalts of the Eifel volcanic area contain basaltic (magnesian) clinopyroxene and, routinely, olivine as main rock-forming components (Wörner & Wright, 1984). These rocks are much more enriched in Mg than the majority of agpaitic rocks that typically host titanium lamprophyllite-group minerals. This seems to be the main cause of magnesium enrichment of lileyite. The incorporation of bivalent cations in the Ti-dominant *M3* site of lamprophyllite and barytolamprophyllite from peralkaline rocks is hindered also by charge-balance conditions because of high contents of univalent alkali metals in these minerals.

Lileyite and all associated primary minerals practically do not contain hydrogen. This is an indication that a high-

Table 7. Comparative data for monoclinic titanium lamprophyllite-group minerals.

Mineral	Lileyite	Barytolamprophyllite	Lamprophyllite	Nabalamprophyllite	Schüllerite
Simplified formula	Ba ₂ (Na,Fe,Ca) ₃	Ba ₂ (Na,Fe,Mn) ₃ Ti ₃	Sr ₂ (Na,Fe,Mn) ₃ Ti ₃	Ba(Na,Ba)Na ₃	Ba ₂ Na(Mn,Ca)(Fe ³⁺ ,Mg,Fe ²⁺) ₂
	MgTi ₂ (Si ₂ O ₇) ₂ O ₂ F ₂	(Si ₂ O ₇) ₂ O ₂ (O,OH,F) ₂	(Si ₂ O ₇) ₂ O ₂ (O,OH,F) ₂	Ti ₃ (Si ₂ O ₇) ₂ O ₂ (OH) ₂	Ti ₂ (Si ₂ O ₇) ₂ (O,F) ₄
Space group	<i>C2/m</i>	<i>C2/m</i>	<i>C2/m</i>	<i>P2/m</i>	<i>P1</i>
<i>a</i> , Å	19.905	19.833	19.431	19.741	5.4027
<i>b</i> , Å	7.0976	7.089	7.086	7.105	7.0656
<i>c</i> , Å	5.4051	5.393	5.392	5.408	10.2178
α , °	96.349	96.66	96.75	96.67	99.816
β , °	2	2	2	2	99.624
γ , °					90.084
<i>Z</i>					1
Strong lines of the X-ray powder-diffraction pattern: <i>d</i> , Å (<i>I</i> , %)	3.749 (45) 3.464 (76) 3.045 (37) 2.884 (36) 2.792 (100) 2.672 (54) 2.624 (43) 2.140 (52)	3.447 (70) 3.294 (50) 2.801 (100) 2.153 (90) 1.790 (70) 1.601 (80) 1.482 (90)	3.73 (40) 3.43 (55) 3.27 (40) 2.874 (40) 2.773 (100) 2.130 (45) 1.477 (45)	9.87 (96) 3.75 (65) 3.45 (90) 3.275 (78) 3.040 (41) 2.797 (100) 2.610 (43)	9.96 (29) 3.308 (45) 2.791 (100) 2.664 (46) 2.609 (36) 2.144 (52) 2.110 (31)
Optical data:					
α	1.718	1.735–1.743	1.733–1.751	1.750	1.756
β	1.735	1.741–1.754	1.740–1.760	1.755	1.773
γ	1.755	1.767–1.778	1.769–1.781	1.799	1.780
Optical sign, 2V	+86	+30–+45	+21 – +43	+40	–40° (meas.), –68° (calc.)
Density, g/cm ³	3.776	3.62–3.66	3.44–3.53	3.65	3.974 (calc.)
IR absorption bands, cm ⁻¹	1032 957 901 854 680 578 529 458 399	1035 956 925 863 697 580 552 458 395	3610 1036 943 878 705 580 556 535 461 402	1033 954 921 854 692 580 549 459 420 402	1013 892 849 526 454 389
Source	This work	Peng & Chang (1965); Peng <i>et al.</i> (1984); Rastsvetaeva <i>et al.</i> , (1995); Feklichev (1989); this work	Vlasov <i>et al.</i> (1966); Saf'yanov <i>et al.</i> , (1983); Rastsvetaeva <i>et al.</i> , (1990); Feklichev (1989); this work	Chukanov <i>et al.</i> (2004); this work	Chukanov <i>et al.</i> (2011)

Table 8. X-ray powder diffraction data for lileyite.

I_{obs}	d_{obs}	I_{calc}	d_{calc}^a	hkl
31	9.96	44	9.891	200
5	4.520	1	4.516	201
6	4.283	3	4.265	11-1
21	4.121	22	4.112	111
45	3.749	49	3.746	31-1
76	3.464	33, 55, 14	3.456, 3.456, 3.453	510, 311, 401
34	3.324	28, 29	3.340, 3.297	220, 600
37	3.045	47	3.043	51-1
13	2.961	19	2.960	60-1
36	2.884	26, 15	2.885, 2.883	22-1, 420
100	2.792	100, 27	2.790, 2.787	221, 511
54	2.672	16, 11, 37	2.686, 2.681, 2.668	002, 601, 20-2
43	2.624	39, 28	2.626, 2.612	710, 42-1
10	2.469	4, 1, 4, 3	2.478, 2.475, 2.461, 2.461	40-2, 421, 71-1, 112
7	2.426	3, 6	2.433, 2.416	31-2, 620
5	2.348	7	2.347	80-1
7	2.271	9	2.271	312
14	2.220	9, 6, 7	2.228, 2.227, 2.205	51-2, 330, 60-2
52	2.140	8, 31, 17, 18	2.142, 2.142, 2.139, 2.132	131, 022, 621, 22-2
31	2.031	9, 20, 4, 3, 13	2.032, 2.031, 2.031, 2.030, 2.028	42-2, 530, 331, 91-1, 512
12	1.980	17, 4, 7	1.982, 1.978, 1.958	71-2, 602, 82-1
5	1.935	7, 4	1.936, 1.927	53-1, 10.0.-1
2	1.895	6	1.889	911
4	1.865	8	1.865	531
7	1.813	14	1.814	730
19	1.774	27	1.774	040
5	1.714	5, 7	1.714, 1.713	113, 11.1.-1
2	1.684	5	1.684	10.0.-2
6	1.653	9, 2, 1	1.657, 1.652, 1.652	51-3, 60-3, 241
5	1.640	6	1.636	313
23	1.602	10, 20, 14	1.603, 1.601, 1.599	22-3, 10.2.1, 023
5	1.556	2, 8	1.556, 1.555	71-3, 73-2
2	1.524	4	1.522	64-1
25	1.478	7, 2, 3, 23, 3, 16, 2	1.481, 1.480, 1.480, 1.479, 1.479, 1.477, 1.476	042, 12.0.-2, 641, 12.2.-1, 423, 24-2, 13.1-1
5	1.457	11	1.456	732
4	1.433	9, 3	1.433, 1.433	93-2, 13-3
4	1.414	2, 1, 1, 7	1.415, 1.415, 1.415, 1.413	84-1, 133, 11.3.-1, 14.0.0
1	1.375	3, 2, 2	1.382, 1.371, 1.370	53-3, 333, 841
10	1.343	6, 10	1.343, 1.341	004, 12.0.2
6	1.309	2, 5	1.308, 1.308	10.2.-3, 55-1
2	1.288	3, 2	1.286, 1.285	823, 551
2	1.265	2, 1	1.268, 1.263	750, 22-4
3	1.248	2, 1, 1	1.249, 1.249, 1.248	71-4, 42-4, 152
3	1.214	1, 1, 3	1.216, 1.215, 1.213	62-4, 55-2, 514
3	1.191	3, 3	1.192, 1.190	950, 91-4
2	1.184	3, 2	1.187, 1.183	10.2.3, 060

Note: ^aCalculated with single-crystal unit-cell parameters. For calculated X-ray data, only reflections with intensities ≥ 1 are given.

temperature, pneumatolytic origin of lileyite is more probable than a hydrothermal one.

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References

- Andrianov, V.I. (1987): Development of the system of crystallographic programs RENTGEN for the computers NORD, CM-4 and EC. *Kristallografiya*, **32**, 228–231 (in Russian).
- Azarova, Y.V. (2004): Genesis and typomorphism of lamprophyllite – barytolamprophyllite series minerals from lujavrite-malignite complex of Khibiny massif. *New Data Mineral.*, **39**, 65–70.
- Back, M.E. & Mandarino, J.A. (2008): Fleischer's glossary of mineral species. 10th Edition, The Mineralogical Record Inc., Tucson, 345 p.
- Brown, I.D. (1981): The bond-valence method: an empirical approach to crystal structure and bonding. in "Structure and Bonding in Crystals II", M. O'Keeffe & A. Navrotsky, eds., Academic Press, New York, 1–30.
- Chukanov, N.V., Moiseev, M.M., Pekov, I.V., Lazebnik, K.A., Rastsvetaeva, R.K., Zayakina, N.V., Ferraris, G., Ivaldi, G. (2004): Nabalamprophyllite $\text{Ba}(\text{Na},\text{Ba})\{\text{Na}_3\text{Ti}[\text{Ti}_2\text{O}_2\text{Si}_4\text{O}_{14}](\text{OH},\text{F})_2\}$, a new layered lamprophyllite-group mineral from the alkaline-ultrabasic massifs Inagli and Kovdor, Russia. *Zapiski Vserossiiskogo Mineralogicheskogo Obshchestva*, **133**, 1, 59–72 (in Russian).
- Chukanov, N.V., Rastsvetaeva, R.K., Britvin, S.N., Virus, A.A., Belakovskiy, D.I., Pekov, I.V., Aksenov, S.M., Ternes, B. (2011): Schüllerite, $\text{Ba}_2\text{Na}(\text{Mn},\text{Ca})(\text{Fe}^{3+},\text{Mg},\text{Fe}^{2+})_2\text{Ti}_2(\text{Si}_2\text{O}_7)_2\text{O},\text{F})_4$, a new mineral from the Eifel volcanic region, Germany. *Zap. Vserossiiskogo Mineralogicheskogo Obshchestva*, **140**, 1, 67–75 (in Russian).
- Dechen, H.V. (1861): Geognostischer Führer zu der Vulkanreihe der Vorder-Eifel. Verlag Henry and Cohen, Bonn, 190 p. (in German).
- Feklichev, V.G. (1989): Diagnostic constants of minerals. Nedra, Moscow, 479 p (in Russian).
- Ferraris, G. & Gula, A. (2005): Polysomatic aspects of microporous minerals – heterophyllosilicates, palysepioles and rhodesite-related structures. In Micro- and Mesoporous Mineral Phases. *Rev. Mineral. Geochem.*, **57**, 69–104.
- Kampf, A.R., Roberts, A.C., Venance, K.E., Dunning, G.E., Walstrom, R.E. (2011): Ferrocicssonite, the Fe^{2+} analogue of ericssonite, from Eastern Fresno County, California, U.S.A. *Can. Mineral.*, **49**, 587–594.
- Krivovichev, S.V., Armbruster, T., Yakovenchuk, V.N., Pakhomovsky, Y.A., Men'shikov, A., Yu., P. (2003): Crystal structures of lamprophyllite-2M and lamprophyllite-2O from the Lovozero alkaline massif, Kola peninsula, Russia. *Eur. J. Mineral.*, **15**, 711–718.

- Moore, P.B. (1971): Ericssonite and orthoericssonite. Two new members of the lamprophyllite group from Långban, Sweden. *Lithos*, **4**, 137–145.
- Peng, T.C. & Chang, C.H. (1965): New varieties of lamprophyllite–barytolamprophyllite and orthorhombic lamprophyllite. *Sci. Sin.*, **14**, 1827–1840.
- Peng, Z., Zhang, J., Shu, J. (1984): The crystal structure of barytolamprophyllite. *Kexue Tongbao*, **29**, 237–241.
- Petricek, V., Dusek, M., Palatinus, L. (2006): Jana 2006. Structure determination software programs. Institute of Physics, Praha Czech Republic.
- Rastsvetaeva, R.K., Evsyunin, V.G., Konev, A.A. (1995): Crystal structure of K-barytolamprophyllite. *Crystallogr. Rep.*, **40**, 472–474.
- Rastsvetaeva, R.K., Sokolova, M.N., Gusev, A.I. (1990): Refined crystal structure of lamprophyllite. *Mineralogicheskii Zhurnal*, **5**, 25–28 (in Russian)
- Saf'yanov, Y.N., Vasil'eva, N.O., Golovachev, V.P., Kuz'min, E.A., Belov, N.V. (1983): The crystal structure of lamprophyllite. *Dokl. Akad. Nauk SSSR*, **269**, 117–120 (in Russian).
- Sokolova, E. (2006): From structure topology to chemical composition. I. Structural hierarchy and stereochemistry in titanium disilicate minerals. *Can. Mineral.*, **44**, 1273–1330.
- Sokolova, E. & Hawthorne, F.C. (2008): From structure topology to chemical composition. IV. Titanium silicates: the orthorhombic polytype of nabalamprophyllite from the Lovozero massif, Kola Peninsula, Russia. *Can. Mineral.*, **46**, 1323–1331.
- Vlasov, K.A., Kuz'menko, M.V., Es'kova, E.M. (1966): The Lovozero Alkaline Massif. Publishing House of the Academy of Sciences of the USSR, Moscow, 627 p. (in Russian).
- Wörner, G. & Wright, T.L. (1984): Evidence for magma mixing within the Laacher See magma chamber (East Eifel, Germany). *J. Volcanol. Geotherm. Res.*, **22**, 301–327.
- Zaitsev, V.A. & Kogarko, L.N. (2002): Compositions of minerals of the lamprophyllite group from alkaline massifs worldwide. *Geochem. Int.*, **40**, 313–322.

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