Mineralogical Magazine, February 2017, Vol. 81(1), pp. 175–181

Lobanovite, $K_2Na(Fe^{2+}_4Mg_2Na)Ti_2(Si_4O_{12})_2O_2(OH)_4$, a new mineral of the astrophyllite supergroup and its relation to magnesioastrophyllite

Elena Sokolova[1,*], Fernando Cámara[2], Frank C. Hawthorne[1], Evgeny I. Semenov[3] and Marco E. Ciriotti[4]

[1] Department of Geological Sciences, University of Manitoba, Winnipeg, Manitoba R3T 2N2, Canada
[2] Dipartimento di Scienze della Terra, Università degli Studi di Torino, via Valperga Caluso 35, I-10125 Torino, Italy
[3] Fersman Mineralogical Museum, Russian Academy of Sciences, Leninskii Prospekt, 18-2, 119071 Moscow, Russia
[4] AMI – Associazione Micromineralogica Italiana, via San Pietro 55, I-10073 Devesi-Ciriè, Italy

[*Received 9 November 2015; Accepted 31 January 2016; Associate Editor: Sergey Krivovichev*]

ABSTRACT

Lobanovite, $K_2Na(Fe^{2+}_4Mg_2Na)Ti_2(Si_4O_{12})_2O_2(OH)_4$, is a new mineral of the astrophyllite supergroup from Mt. Yukspor, the Khibiny alkaline massif, Kola Peninsula Russia. It has been known previously under the following names: monoclinic astrophyllite, magnesium astrophyllite, magnesiumastrophyllite and magnesioastrophyllite but has never been formally proposed and approved as a valid mineral species by the Commission on new Minerals, Nomenclature and Classification of the International Mineralogical Association. It has now been revalidated and named lobanovite after Dr. Konstantin V. Lobanov, a prominent Russian ore geologist who worked in the Kola Peninsula for more than forty years (Nomenclature voting proposal 15-B). Lobanovite has been described from pegmatitic cavities on Mt. Yukspor where it occurs as elongated bladed crystals, up to 0.04 mm wide and 0.2 mm long, with a straw yellow to orange colour. Associated minerals are shcherbakovite, lamprophyllite, delindeite, wadeite, umbite and kostylevite. Lobanovite is biaxial (–) with refractive indices ($\lambda = 589$ nm) $\alpha = 1.658$, $\beta_{calc.} = 1.687$, $\gamma = 1.710$; $2V_{meas.} = 81.5–83°$. Lobanovite is monoclinic, space group *C*2/*m*, $a = 5.3327(2)$, $b = 23.1535(9)$, $c = 10.3775(4)$ Å, $\beta = 99.615(1)°$, $V = 1263.3(1)$ Å^3, $Z = 2$. The six strongest reflections in the powder X-ray diffraction data [*d* (Å), I, (*hkl*)] are: 3.38, 100, (003); 2.548, 90, (063); 10.1, 80, (001); 3.80, 60, (042,131); 3.079, 50, (132,062); 2.763, 90, ($\bar{1}71$). The chemical composition of lobanovite was determined by electron-microprobe analysis and the empirical formula $(K_{1.97}Ba_{0.01})_{\Sigma1.98}(Na_{0.65}Ca_{0.14})_{\Sigma0.79}$ $(Fe^{2+}_{3.18}Mg_{2.02}Na_{1.00}Mn_{0.72})_{\Sigma6.92}(Ti_{1.99}\ Nb_{0.06})_{\Sigma2.05}[(Si_{8.01}Al_{0.06})_{\Sigma8.07}O_{24}]$ $O_2(OH)_{4.03}F_{0.19}$ was calculated on the basis of 30.2 (O + OH + F) anions, with H_2O calculated from structure refinement, $D_{calc.} = 3.161$ g cm^{-3}. In the structure of lobanovite, the main structural unit is the HOH block, which consists of one close-packed O (Octahedral) and two H (Heteropolyhedral) sheets. The M(1–4) octahedra form the O sheet and the T_4O_{12} astrophyllite ribbons and [5]-coordinated Ti-dominant D polyhedra link through common vertices to form the H sheet. The HOH blocks repeat along [001], and K and Na atoms occur at the interstitial *A* and *B* sites. The simplified and end-member formulae of lobanovite are $K_2Na[(Fe^{2+},Mn)_4Mg_2Na]Ti_2(Si_4O_{12})_2O_2(OH)_4$ and $K_2Na(Fe^{2+}_4Mg_2Na)Ti_2(Si_4O_{12})_2O_2(OH)_4$, respectively.

Keywords: lobanovite, magnesiumastrophyllite, astrophyllite supergroup, chemical composition, crystal-structure refinement.

Introduction

Lobanovite, $K_2Na(Fe^{2+}_4Mg_2Na)Ti_2(Si_4O_{12})_2O_2(OH)_4$, is a new mineral of the astrophyllite supergroup from Mt. Yukspor, the Khibiny alkaline massif, Kola Peninsula, Russia. It has been known

---

[*] E-mail: elena_sokolova@umanitoba.ca

https://doi.org/10.1180/minmag.2016.080.088

previously under the names monoclinic astrophyllite, magnesium astrophyllite, magnesiumastrophyllite and magnesioastrophyllite (Peng and Ma, 1963; X-ray Laboratory, Hubei Geologic College, 1974; Shi *et al.*, 1998; Piilonen *et al.*, 2003*a*; Sokolova and Cámara, 2008; Cámara *et al.*, 2010) but has never been formally proposed and approved as a valid mineral species by the Commission on new Minerals, Nomenclature and Classification (CNMNC) of the International Mineralogical Association, although it was discovered in the CNMNC era. It has now been revalidated and named lobanovite after Dr. Konstantin Valentinovich Lobanov (Cyrillic: Константин Валентинович Лобанов; b. 1952, Roslavl', Russia), a prominent Russian ore geologist, DSc. (Doctor of Science, Geology and Mineralogy) and an expert in Precambrian metallogeny. It is particularly appropriate to name this mineral from the Kola Peninsula after Dr. Lobanov, as he has worked in the Kola Peninsula for the last 40 years, focusing on the rocks of the Kola superdeep borehole and their relation to the deep structure of ore districts (CNMNC-IMA: Nomenclature voting proposal 15-B). The holotype specimen of lobanovite is the microprobe mount of the single crystal that was used for structure refinement by Sokolova and Cámara (2008) and it was deposited in the collections of the Fersman Mineralogical Museum, Russian Academy of Sciences, Leninskii Prospekt, 18/2, 119071 Moscow, Russia, catalogue number 4708/1.

Here we give an overview of previous studies of lobanovite and report a compilation of data from the literature necessary for a description of lobanovite as a valid mineral species.

TABLE 1. Comparison of lobanovite and astrophyllite.

	Lobanovite*	Astrophyllite**
Formula	$K_2Na(Fe^{2+}_4Mg_2Na)Ti_2(Si_4O_{12})_2O_2(OH)_4$	$K_2NaFe^{2+}_7Ti_2(Si_4O_{12})_2O_2(OH)_4F$
System	Monoclinic	triclinic
Space group	*C*2/*m*	$P\bar{1}$
a (Å)	5.3327(2)	5.36–5.42
b	23.1535(9)	11.85–11.95
c	10.3775(4)	11.66–11.75
α (°)	90	112.03–113.13
β	99.615(1)	94.52–94.64
γ	90	103.08–103.14
V (Å^3)	1263.3(1)	652.9–668.5
Z	2	1
$D_{meas.}/D_{calc.}$ (g cm^{-3})	n.d./3.161	3.09–3.23/3.35
Strongest refl. in powder diffraction data $d_{obs.}$ (Å) (I)	3.38 (100), 2.548 (90), 10.1 (80), 3.80 (60), 3.079 (50), 2.763 (50)	10.6 (100), 3.51 (80), 2.77 (60), 2.64 (60), 2.57 (60), 1.76 (30)
Optical character	biaxial (–)	biaxial (+)
α	1.658	1.678–1.695
β	1.687	1.703–1.726
γ	1.710	1.733–1.758
$2V_{meas}$ (°)	81.5–83	66–84
Colour	Yellow to orange	Bronze yellow to golden yellow, brown to reddish brown
Pleochroism	*X* = bright yellow *Y* = pale yellowish grey *Z* = grey	*X* = deep orange red *Y* = orange yellow *Z* = lemon yellow

* All data are from Sokolova and Cámara (2008) except for powder diffraction data and optical properties (X-ray laboratory, Hubei Geologic College, 1974); **Data from Anthony *et al.* (1995) except for cell parameters (Piilonen *et al.*, 2003*b*).

TABLE 2. Chemical composition of lobanovite.

	X-ray Lab., HGC* (1974)	Sokolova and Cámara (2008)			
Constituent	wt.%	wt.%	Range (wt.%)	SD (wt.%)	Probe standard
Nb_2O_5	n.a	0.64	0.29–1.22	0.31	$Ba_2NaNb_5O_{15}$
TiO_2	12.18	13.11	12.47–13.48	0.31	titanite
SiO_2	37.98	39.72	39.43–39.92	0.18	diopside
Al_2O_3	1.11	0.24	0.08–0.42	0.13	andalusite
Fe_2O_3	2.95	n.d.			
BaO	n.a.	0.13	0.04–0.19	0.04	baryte
FeO	17.91	18.86	17.98–21.05	0.84	fayalite
MnO	4.00	4.21	3.10–4.59	0.45	spessartine
CaO	1.15	0.65	0.59–0.82	0.06	diopside
MgO	6.39	6.72	6.05–6.93	0.24	forsterite
K_2O	7.28	7.66	7.54–7.78	0.07	orthoclase
Na_2O	5.38	4.22	4.10–4.29	0.07	jadeite
H_2O	3.44	3.00**			
F	0.45	0.29	0.17–0.43	0.07	F- riebeckite
O = F	–0.19	–0.12			
Total	100.03	99.33			

n.d. – not detected; n.a. – not analysed; SD – standard deviation.
*HGC = Hubei Geologic College
**Calculated from structure refinement.

Previous work

Semenov (1959) reported on the "astrophyllite with unusually high content of MgO (6.39 wt.%)" from the Khibiny alkaline massif, Kola Peninsula, Russia; the complete chemical analysis was not given. Peng and Ma (1963) reported a chemical analysis, with the following simplified formula $K_2Na_2(Fe^{2+},Mn)_2(Fe^{2+},\ Fe^{3+})_3Mg_2Ti_2(Si_4O_{12})_2(O,OH)_3(OH,F)_4$, $Z = 2$, unit-cell parameters $a = 10.43(2)$, $b = 23.00(5)$, $c = 5.35(1)$ Å, $\beta = 102°$, and a preliminary crystal structure in space group *A*2/*m* (atom coordinates were not reported) for the 'astrophyllite from Khibiny'. X-ray Laboratory, Hubei Geologic College (1974) reported the powder X-ray diffraction data, DTA data and optical properties for the material mentioned above. The crystal structure of 'monoclinic astrophyllite' was refined by Shi *et al.* (1998) on sample no. 3086 provided by A. Khomyakov from Mt. Yukspor, the Khibiny alkaline massif, Kola Peninsula, Russia. They gave a full description of the crystal structure, an ideal formula $K_2NaNa(Fe,Mn)_4Mg_2Ti_2(Si_4O_{12})_2(OH)_4(OH,F)_2$, and unit-cell parameters, $a = 10.370(3)$, $b = 23.129(5)$, $c = 5.322(1)$ Å, $\beta = 99.55(2)°$, $V = 1258.8(5)$ Å^3, space group *A*2, $Z = 2$, $D_{calc.} = 3.173$ g cm^{-3} (this formula has an excess charge of 2^+). The structure data of Shi *et al.* (1998)

TABLE 3. Powder diffraction data for lobanovite*.

$I_{obs.}$	$d_{obs.}$ (Å)	$d_{calc.}$ (Å)	*h*	*k*	*l*
80	10.1	10.22	0	0	1
60	3.80	3.83	0	4	2
		3.82	1	3	1
100	3.38	3.41	0	0	3
50	3.079	3.11	1	3	2
		3.08	0	6	2
30	2.889	2.882	$\bar{1}$	3	3
50	2.763	2.764	$\bar{1}$	7	1
90	2.548	2.554	0	6	3
20	2.350	2.369	1	7	2
30	2.260	2.265	$\bar{1}$	7	3
30	2.040	2.047	0	0	5
50	1.818	1.805	1	11	1
50	1.727	1.727	$\bar{1}$	7	5
40	1.657	1.654	0	14	0
10	1.591	1.592	2	10	2
		1.586	1	7	5
20	1.525	1.517	$\bar{1}$	7	6
70	1.463	1.461	0	0	7
40	1.404	1.402	1	7	6
		1.400	2	14	0
10	1.373	1.379	$\bar{2}$	0	7
		1.371	2	14	1

*$I_{obs.}$ and $d_{obs.}$ (Å) taken from X-ray Laboratory, Hubei Geologic College (1974); $d_{calc.}$ (Å) and *hkl* – this work.

TABLE 4. Final atom coordinates and equivalent displacement parameters for lobanovite [from Sokolova and Cámara (2008)].

Atom	*x*	*y*	*z*	U_{eq} (Å^2)
M(1)	0	0	0	0.0129(3)
M(2)	½	0.07440(2)	0	0.0093(2)
M(3)	0	0.14505(2)	0	0.0091(2)
M(4)	½	0.21399(3)	0	0.0098(2)
D	0.43702(8)	0	0.28713(4)	0.0064(2)
T(1)	0.07901(9)	0.21773(2)	0.73587(5)	0.0073(1)
T(2)	0.07573(9)	0.08555(2)	0.72932(5)	0.0076(1)
A	½	0.13847(4)	1/2	0.0267(3)
B	0	0	1/2	0.0103(3)
O(1)	0.4035(4)	0	0.1178(2)	0.0107(4)
O(2)	0.1393(3)	0.08202(7)	0.8868(1)	0.0109(3)
O(3)	0.2982(3)	0.05764(7)	0.6609(1)	0.0152(3)
O(4)	0.1966(3)	0.05755(7)	0.3287(2)	0.0170(3)
O(5)	0.0537(3)	0.15325(6)	0.6769(2)	0.0161(3)
O(6)	0.1298(3)	0.21770(6)	0.8930(1)	0.0096(3)
O(7)	0.8141(3)	0.74859(7)	0.6781(1)	0.0139(3)
O(8)	0.3656(3)	0.14762(6)	0.1030(1)	0.0115(3)
H	0.386(6)	0.142(1)	0.191(1)	0.0138(0)*
F	1/2	0	1/2	0.009(4)*

*$U_{\text{iso.}}$

is in the International Crystal Structure Database (ICSD) under #52032. The ICSD revised #52032 as #56848, with higher symmetry, space group *A*2/*m*, and a quite different formula: $K_{1.96}Na_{2.06}Fe_{3.72}Mg_{2.28}Ti_2(Si_8O_{28})(H_2O)_2$, based on the same work of Shi *et al.* (1998). The latter formula is neutral but it is chemically and structurally incorrect as H_2O groups do not occur in magnesium astrophyllite. Piilonen *et al.* (2003*a*) considered the structure of magnesium astrophyllite (space group *A*2) and re-wrote its formula as $K_2Na[Na(Fe,Mn)_4Mg_2]Ti_2Si_8O_{26}(OH)_4\square$. Although the ICSD #56848 points out that the possible space group might be *A*2/*m*, the crystal structure of magnesium astrophyllite has not been re-investigated since the work of Shi *et al.* (1998). Following the inconsistency between the chemical composition and structure for magnesium astrophyllite in the ICSD (see above), Sokolova and Cámara (2008) refined the crystal structure of magnesium astrophyllite (see below) and reported the chemical composition of the crystal of magnesium astrophyllite used for structure refinement. They confirmed the general topology of the crystal structure described by Shi *et al.* (1998) and gave the ideal formula of magnesium astrophyllite as follows: $K_2Na(Fe_4Mg_2Na)^{[5]}Ti_2Si_8O_{26}(OH)_4$. Cámara *et al.* (2010) suggested writing the astrophyllite-ribbon component of the formula as $(Si_4O_{12})_2O_2$ versus Si_8O_{26} [Piilonen *et al.* (2003*a*)]. They emphasized that (1) the translational repeat fragment of the ribbon has the formula Si_4O_{12}; (2) there are two ribbons (corresponding to two H sheets) attached to the central O sheet; (3) the O_2 anions do not link to Si, and this information should be preserved in the chemical formula by writing them separately from the silicate radical. Cámara *et al.* (2010) wrote the formula of magnesiumastrophyllite as $K_2Na(Fe_4Mg_2Na)Ti_2(Si_4O_{12})_2O_2(OH)_4$. Burke (2008) renamed magnesium astrophyllite and/or magnesiumastrophyllite as magnesioastrophyllite. Sokolova (2012) showed that the topology of the HOH block in magnesioastrophyllite is different from all other structures of the astrophyllite-supergroup minerals due to the different chemical composition of the O sheet ($Fe^{2+}_4Mg_2Na$), particularly the dominance of Na^+ at the *M*(1) site which makes the M(1) polyhedron too large to share edges with Si_2O_7 groups of astrophyllite ribbons and results in a different linkage of H and O sheets, i.e. a different topology of the HOH block. She wrote the ideal formula of magnesioastrophyllite as follows: $K_2Na(Fe^{2+}_4Mg_2Na)Ti_2(Si_4O_{12})_2O_2(OH)_4$ and emphasized that the name magnesioastrophyllite

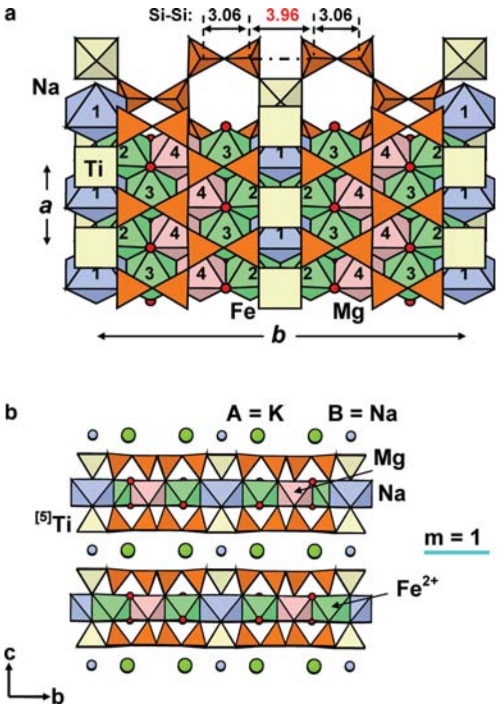

FIG. 1. The crystal structure of lobanovite: (*a*) the HOH block viewed perpendicular to the plane of the block [after fig. 6*a* of Sokolova (2012)]; (*b*) general view of the crystal structure of lobanovite [after fig. 2*b* of Sokolova (2012)]. The [5]-coordinated Ti polyhedra and Fe^{2+}- and Mg-dominant octahedra are pale yellow, green and pink; Na octahedra are navy blue; Si tetrahedra are orange; K and Na atoms at the *A* and *B* sites are shown as green and blue spheres; OH groups are shown as small red spheres. The position of the cation layer in the **I** (Intermediate) block (*m* = 1, where *m* is a number of cation layers) is shown by a turquoise line.

is misleading as it is the dominance of Na^+ at the *M*(1) site that results in the different topology of the HOH block [not the dominance of Mg^{2+} at the *M*(4) site].

Further on in the paper, we will use only the name lobanovite and compare its properties and structure to those of astrophyllite (Table 1).

Occurrence and mineral association

Sokolova and Cámara (2008) refined the crystal structure and determined the chemical composition of lobanovite on the same single crystal taken from the sample of delindeite in the collection of minerals of Adriana and Renato Pagano, Milan, Italy (Collezione Mineralogica, sample #6270). This sample came from Alexander Khomyakov and was described in Khomyakov (1995). Hence we use his description for the occurrence and associated minerals.

Lobanovite was found in pegmatite cavities at Mt. Yukspor, the Khibiny alkaline massif, Kola Peninsula, Russia. Associated minerals are shcherbakovite, lamprophyllite, delindeite, wadeite, umbite, kostylevite and other species [taken from Khomyakov (1995), p. 151].

Physical properties

Lobanovite occurs as elongated bladed crystals, with a straw yellow (Anthony *et al.*, 1995) to orange colour (Sokolova and Cámara, 2008) up to 0.04 mm wide and 0.2 mm long, with a vitreous lustre and a white to yellowish-white streak. The mineral has Mohs hardness of 3, perfect cleavage parallel to (001) and moderate cleavage parallel to (010). Twinning, parting and fracture have not been observed (Anthony *et al.*, 1995). Lobanovite does not fluoresce under SW or LW ultraviolet light, $D_{\text{calc.}} = 3.161$ g cm^{-3} (from the empirical formula of Sokolova and Cámara, 2008). Lobanovite is optically biaxial (–), $\alpha = 1.658$, $\beta = 1.687_{\text{calc.}}$, $\gamma = 1.710$ (589 nm), with $2V_{\text{meas.}} = 81.5$–83°. The pleochroism: X = bright yellow, Y = pale yellowish grey, Z = grey, with the absorption scheme: $Z < Y < X$ and orientation Y = b, $Z \wedge a = -5$ to $-6°$ (X-ray Laboratory, Hubei Geological College, 1974). The DTA curve shows endothermic peaks at 835°C (strong, escape of OH) and 900°C (weak) (X-ray Laboratory, Hubei Geologic College, 1974).

The compatibility index was calculated using the chemical analysis and unit-cell parameters of Sokolova and Cámara (2008) and optical properties from X-ray Laboratory, Hubei Geological College (1974): $1 - (K_p/K_c)$ is 0.057 and is rated as good (Mandarino, 1981).

Chemical composition

Sokolova and Cámara (2008) determined the chemical composition of lobanovite using a Cameca SX100 electron microprobe (wavelength-dispersive spectroscopy mode, 15 kV, 20 nA, 10 μm beam diameter). Ta, Zr, Sn, Zn, Cs, Rb, Sr and Pb were sought but not detected [for details, see Sokolova and Cámara (2008)]. The content of H_2O (wt.%) was calculated by stoichiometry from the results of the crystal-structure refinement. The chemical composition of lobanovite is given in Table 2 (mean of 10 analyses) in comparison with that of the X-ray Laboratory, Hubei Geologic College (1974). Sokolova and Cámara (2008) calculated the empirical formula on the basis of 30.2 (O + OH + F) anions which include 30 (O + OH) pfu and 0.2 F apfu (atoms per formula unit). The empirical, simplified and endmember formulae are $(K_{1.97}Ba_{0.01})_{\Sigma 1.98}(Na_{0.65}Ca_{0.14})_{\Sigma 0.79}(Fe^{2+}_{3.18}Mg_{2.02}Na_{1.00}Mn_{0.72})_{\Sigma 6.92}(Ti_{1.99}Nb_{0.06})_{\Sigma 2.05}[(Si_{8.01}Al_{0.06})_{\Sigma 8.07}O_{24}]O_2(OH)_{4.03}F_{0.19}$, $Z = 2$, $K_2Na[(Fe^{2+},Mn)_4Mg_2Na]Ti_2(Si_4O_{12})_2O_2(OH)_4$ and $K_2Na(Fe^{2+}_4Mg_2Na)Ti_2(Si_4O_{12})_2O_2(OH)_4$, respectively.

Powder X-ray diffraction data

Powder X-ray diffraction data are presented in Table 3.

Crystal structure

Sokolova and Cámara (2008) refined the crystal structure of lobanovite to $R_1 = 3.2\%$ on the basis of 1861 unique reflections ($F_o > 4\sigma F$) collected on a Bruker AXS SMART APEX diffractometer with a CCD detector and Mo*K*α radiation: space group *C*2/*m*, *a* = 5.3327(2), *b* = 23.1535(9), *c* = 10.3775(4) Å, β = 99.615(1)°, *V* = 1263.3(1) Å^3, *Z* = 2, $D_{\text{calc.}} = 3.161$ g cm^{-3} (Table 4) from Mt. Yukspor, Khibina alkaline massif, Kola Peninsula, Russia. The main structural unit in the structure of lobanovite is the HOH block which consists of a central close-packed O (Octahedral) and two adjacent H (Heteropolyhedral) sheets. In the O sheet, there are four [6]-coordinated *M*(1–4) sites occupied by Na, $Fe^{2+}_{1.25}Mn_{0.75}$, $Fe^{2+}_{1.20}Mg_{0.80}$ and $Mg_{1.25}Fe^{2+}_{0.75}$, with <M(1,2,3,4)–O> = 2.372, 2.166, 2.113 and 2.094 Å, respectively (Fig. 1*a*, Table 5). The ideal composition of the O sheet is $(Fe^{2+}_4Mg_2Na)O_2(OH)_4$ pfu. In the H sheet, there is one [5]-coordinated *D* site occupied by $Ti_{1.97}Nb_{0.03}$, with <D–O> = 1.907 Å, and there are two tetrahedrally coordinated *T* sites occupied primarily by Si with minor Al, with <T–O> = 1.625 Å. TO_4 tetrahedra form T_4O_{12} astrophyllite ribbons extending along **a**. Astrophyllite ribbons and [5]-coordinated D polyhedra connect through common vertices to form the H sheet. The ideal composition of the two H sheets is $Ti_2(Si_4O_{12})_2$ pfu. An O sheet and two adjacent H sheets link through common vertices of TO_4 tetrahedra, D octahedra and M octahedra to form an HOH block parallel to (001) (Fig. 1*a*). The HOH blocks alternate with **I** (Intermediate) blocks along **c** (Fig. 1*b*). In the **I** block, there are two interstitial sites, a [10]-coordinated *A* site and an [8]-coordinated *B* site occupied by $K_{1.97}Ba_{0.01}\square_{0.02}$ and $Na_{0.65}Ca_{0.14}\square_{0.21}$, respectively, with <A–O> = 3.120 and <B–O> = 2.536 Å (Table 5). The ideal composition of the **I** block is K_2Na apfu. Cations at the *A* and *B* sites form a layer parallel to (001)

TABLE 5. Refined site-scattering and assigned site-populations for lobanovite [from Sokolova and Cámara (2008)].

Site	Refined site scattering (epfu)	Assigned site population (apfu)	Calculated site scattering (epfu)	$\langle X–\varphi \rangle_{\text{calc.}}$* (Å)	$\langle X–\varphi \rangle_{\text{obs.}}$ (Å)
$^{[6]}M(1)$	11.0(4)	1.00 Na	11.0	2.400	2.372
$^{[6]}M(2)$	50.0(1)	1.25 Fe^{2+} + 0.75 Mn	51.3	2.169	2.166
$^{[6]}M(3)$	39.7(1)	1.20 Fe^{2+} + 0.80 Mg	40.8	2.126	2.113
$^{[6]}M(4)$	34.1(1)	1.25 Mg + 0.75 Fe^{2+}	34.5	2.090	2.094
$^{[5]}D$	44.4(1)	1.97 Ti + 0.03 Nb	44.6	1.891	1.907
$^{[6]}D$**				1.975	1.952
$^{[10]}A$	37.8(2)	1.97 K + 0.01 Ba + 0.02 □	38.0		3.120
$^{[11]}A$**					3.127
$^{[8]}B$	12.4(2)	0.65 Na + 0.14 Ca + 0.21 □	10.0		2.536
$^{[10]}B$**					2.562
F	1.5(1)	0.83 □ + 0.17 F	1.5		

*Calculated by summing constituent ionic radii; values from Shannon (1976), φ = O, OH, F.
**F atom is considered a ligand.

(Fig. 1*b*). The presence of the partly occupied *F* site makes 17% of the *A* and *B* sites [11]- and [10]-coordinated, respectively (Table 5).

The general topology of the lobanovite structure is in accord with Shi *et al.* (1998). The topology of the HOH block in lobanovite differs from all other structures of the astrophyllite-supergroup minerals (for the astrophyllite structure, see fig. 2*a* in Sokolova *et al.*, 2017) due to the chemical composition of the O sheet, $Fe^{2+}_4Mg_2Na$, where Na^+ is dominant at the *M*(1) site (Sokolova, 2012). Hence the Na octahedron is too large to share edges with Si_2O_7 groups of astrophyllite ribbons resulting in a different linkage of H and O sheets, i.e. a different topology of the HOH block [*cf.* Si–Si distances associated with the Na octahedron (3.96 Å) and the Fe^{2+} octahedron (3.06 Å), Fig. 1*a*].

Acknowledgements

Authors are grateful to two anonymous reviewers for their comments and Principal Editor Pete Williams for handling the manuscript. We thank the vice president of the CNMNC-IMA Frédéric Hatert and members of the Commission for useful comments and suggestions. FC acknowledges support by the University of Torino "Progetti di ricerca finanziati dall'Università degli Studi di Torino (ex 60%)" – year 2014. This work was also supported by a Canada Research Chair in Crystallography and Mineralogy and by a Discovery grant from the Natural Sciences and Engineering Research Council of Canada to FCH, and by Innovation Grants from the Canada Foundation for Innovation to FCH.

References

Anthony, J.W., Bideaux, R.A., Bladh, K.W. and Nichols, M.C. (1995) *Handbook of Mineralogy. II. Silica, Silicates.* Mineral Data Publishing, Tucson, pp. 505.

Burke, E.A.J. (2008) Tidying up mineral names: an IMA-CNMNC scheme for suffixes, hyphens and diacritical marks. *Mineralogical Record*, **39**, 131–135.

Cámara, F., Sokolova, E., Abdu, Y. and Hawthorne, F.C. (2010) The crystal structures of niobophyllite, kupletskite-(Cs) and Sn rich astrophyllite; revisions to the crystal chemistry of the astrophyllite-group minerals. *The Canadian Mineralogist*, **48**, 1–16.

Khomyakov, A.P. (1995) *Mineralogy of Hyperagpaitic Alkaline Rocks.* Clarendon Press, Oxford, UK, pp. 151.

Mandarino, J.A. (1981) The Gladstone-Dale relationship. Part IV. The compatibility concept and its application. *The Canadian Mineralogist*, **19**, 441–450.

Peng, S. and Ma. Z. (1963) The discovery of a new type of an Si–O ribbon – crystal-structure analysis of astrophyllite. *Scientica Sinica*, **12**, 272–276 [in Russian].

Piilonen, P.C., LaLonde, A.E., McDonald, A.M., Gault, R.A. and Larsen, A.O. (2003*a*) Insights into astrophyllite-group minerals. I. Nomenclature, composition and development of a standardized general formula. *The Canadian Mineralogist*, **41**, 1–26.

Piilonen, P.C., McDonald, A.M. and LaLonde, A.E. (2003*b*) Insights into astrophyllite-group minerals. II. Crystal chemistry. *The Canadian Mineralogist*, **41**, 27–54.

Semenov, E.I. (1959) Lithian and other micas and hydromicas in alkaline pegmatites of Kola Peninsula. *Trudy Mineralogicheskogo Muzeya, N9*, 107–137 [in Russian].

Shannon, R.D. (1976) Revised effective ionic radii and systematic studies of interatomic distances in halides and chalcogenides. *Acta Crystallographica*, **A32**, 751–767.

Shi, N., Ma, Z., Li, G., Yamnova, N.A. and Pushcharovsky, D.Y. (1998) Structure refinement of monoclinic astrophyllite. *Acta Crystallographica*, **B54**, 109–114.

Sokolova, E. (2012) Further developments in the structure topology of the astrophyllite-group minerals. *Mineralogical Magazine*, **76**, 863–882.

Sokolova, E. and Cámara, F. (2008) Re-investigation of the crystal structure of magnesium astrophyllite. *European Journal of Mineralogy*, **20**, 253–260.

Sokolova, E., Cámara, F., Hawthorne, F.C. and Ciriotti, M. E. (2017) The astrophyllite supergroup: nomenclature and classification. *Mineralogical Magazine*, **81**, 143–150.

X-ray Laboratory, Hubei Geologic College (1974) The crystal chemistry of astrophyllite group minerals. *Scientica Sinica*, **1**, 18–33 [in Chinese].