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*

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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 previously known 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 CNMNC-IMA. It has now been revalidated and named *lobanovite* after Dr. Konstantin V. Lobanov, a prominent Russian ore geologist who worked in 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 straw yellow to orange colour. Associated minerals are shcherbakovite, lamprophyllite, delindeite, wadeite, umbite and kostylevite. Lobanovite is biaxial (–) with refractive indices (λ = 589 nm) α = 1.658, $\beta_{calc.}$ = 1.687, γ = 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, β 99.615(1)°, *V* 1263.3(1) Å^3, *Z* = 2. The six strongest reflections in the X-ray powder 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 $(K_{1.97}Ba_{0.01})_{\Sigma 1.98}(Na_{0.65}Ca_{0.14})_{\Sigma 0.79}(Fe^{2+}_{3.18}Mg_{2.02}Na_{1.00}Mn_{0.72})_{\Sigma 6.92}(Ti_{1.99}Nb_{0.06})_{\Sigma 2.05}[(Si_{8.01}Al_{0.06})_{\Sigma 8.07}O_{24}]O_2(OH)_{4.03}F_{0.19}$ 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 endmember 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 previously known 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 CNMNC-IMA, 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 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.

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

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

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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, β 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 X-ray powder-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, β 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) 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 $(Si_4O_{12})_2O_2$

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versus Si_8O_{26} [Piilonen *et al*. (2003a)]. 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* 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.

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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 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 luster 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 (–), α = 1.658, $\beta = 1.687_{\text{calc.}}$, γ = 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). 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 (WDS 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) p.f.u. and 0.2 F a.p.f.u. (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.

X-ray powder-diffraction data

X-ray powder-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, $Z = 2$, $D_{calc.}$ 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 $(Fe^{2+}_4Mg_2Na)O_2(OH)_4$ p.f.u. 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

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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 $Ti_2(Si_4O_{12})_2$ p.f.u. 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 $K_{1.96}Ba_{0.01}\square_{0.03}$ 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 a.p.f.u. Cations at the *A* and *B* sites form a layer parallel to (001) (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*., 2015) 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*].

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Figure captions

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.

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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*	$P\overline{1}$
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*)

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Table 2. Chemical composition of lobanovite

Constituent	wt.%		Range (wt.%)	SD (wt.%)	Probe Standard
	X-ray Lab., Hubei Geologic College (1974)	Sokolova and Cámara (2008)			
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 analyzed;
*calculated from structure refinement.

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	–1 3 3
50	2.763	2.764	–1 7 1
90	2.548	2.554	0 6 3
20	2.350	2.369	1 7 2
30	2.260	2.265	–1 7 3
30	2.040	2.047	0 0 5
50	1.818	1.805	1 11 1
50	1.727	1.727	–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	–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	–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.

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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_{iso}.

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

Site	Refined site-scattering (e.p.f.u.)	Assigned site-population (a.p.f.u.)	Calculated site-scattering (e.p.f.u.)	$\langle X–\varphi\rangle_{calc.}$* (Å)	$\langle X–\varphi\rangle_{obs.}$ (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)	1.96 K + 0.01 Ba + 0.03 □	37.8		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.

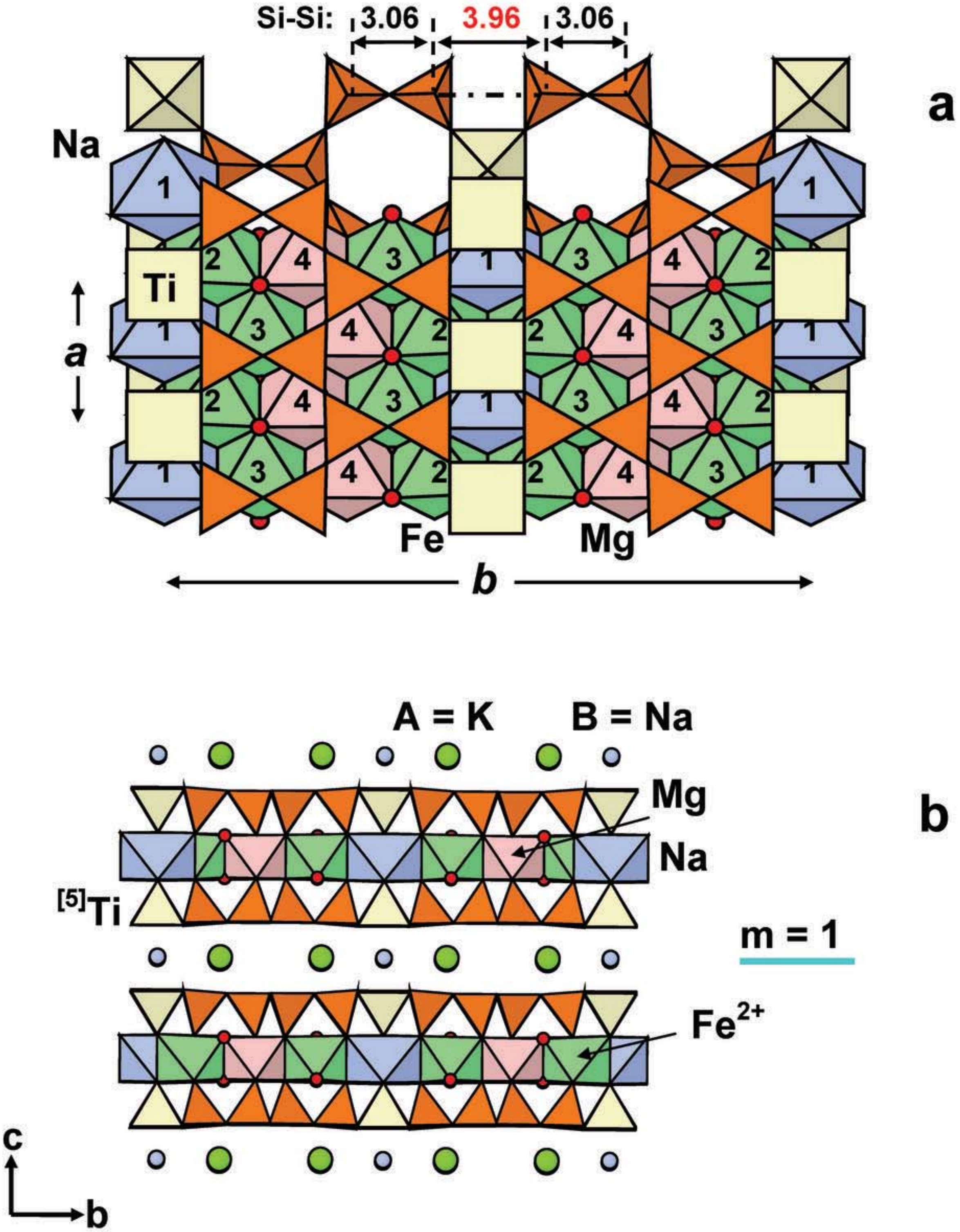

Fig. 1