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**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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24 **Abstract**

25 Lobanovite, $K_2Na(Fe^{2+}_4Mg_2Na)Ti_2(Si_4O_{12})_2O_2(OH)_4$, is a new mineral of the astrophyllite
26 supergroup from Mt. Yukspor, the Khibiny alkaline massif, Kola Peninsula Russia. It has been
27 previously known under the following names: *monoclinic astrophyllite*, *magnesium astrophyllite*,
28 *magnesiumastrophyllite* and *magnesoastrophyllite* but has never been formally proposed and
29 approved as a valid mineral species by the CNMNC-IMA. It has now been revalidated and
30 named *lobanovite* after Dr. Konstantin V. Lobanov, a prominent Russian ore geologist who
31 worked in Kola Peninsula for more than forty years (Nomenclature voting proposal 15-B).
32 Lobanovite has been described from pegmatitic cavities on Mt. Yukspor where it occurs as
33 elongated bladed crystals, up to 0.04 mm wide and 0.2 mm long, with straw yellow to orange
34 colour. Associated minerals are shcherbakovite, lamprophyllite, delindeite, wadeite, umbite and
35 kostylevite. Lobanovite is biaxial (–) with refractive indices ($\lambda = 589$ nm) $\alpha = 1.658$, $\beta_{calc.} = 1.687$,
36 $\gamma = 1.710$; $2V_{meas.} = 81.5–83^\circ$. Lobanovite is monoclinic, space group $C2/m$, a 5.3327(2), b
37 23.1535(9), c 10.3775(4) Å, β 99.615(1)°, V 1263.3(1) Å³, $Z = 2$. The six strongest reflections in
38 the X-ray powder diffraction data [d (Å), I , (hkl)] are: 3.38, 100, (003); 2.548, 90, (063); 10.1, 80,
39 (001); 3.80, 60, (042,131); 3.079, 50, (132,062); 2.763, 90, ($\bar{1}71$). The chemical composition of
40 lobanovite was determined by electron-microprobe analysis and the empirical formula
41 $(K_{1.97}Ba_{0.01})_{\Sigma 1.98}(Na_{0.65}Ca_{0.14})_{\Sigma 0.79}(Fe^{2+}_{3.18}Mg_{2.02}Na_{1.00}Mn_{0.72})_{\Sigma 6.92}(Ti_{1.99}Nb_{0.06})_{\Sigma 2.05}[(Si_{8.01}$
42 $Al_{0.06})_{\Sigma 8.07}O_{24}]O_2(OH)_{4.03}F_{0.19}$ was calculated on the basis of 30.2 (O + OH + F) anions, with H₂O
43 calculated from structure refinement, $D_{calc.} = 3.161$ g cm⁻³. In the structure of lobanovite, the
44 main structural unit is the HOH block, which consists of one close-packed O (Octahedral) and
45 two H (Heteropolyhedral) sheets. The M(1–4) octahedra form the O sheet and the T₄O₁₂
46 *astrophyllite* ribbons and [5]-coordinated Ti-dominant D polyhedra link through common vertices
47 to form the H sheet. The HOH blocks repeat along [001], and K and Na atoms occur at the
48 interstitial A and B sites. The simplified and endmember formulae of lobanovite are

49 $\text{K}_2\text{Na}[(\text{Fe}^{2+}, \text{Mn})_4\text{Mg}_2\text{Na}]\text{Ti}_2(\text{Si}_4\text{O}_{12})_2\text{O}_2(\text{OH})_4$ and $\text{K}_2\text{Na}(\text{Fe}^{2+}_4\text{Mg}_2\text{Na})\text{Ti}_2(\text{Si}_4\text{O}_{12})_2\text{O}_2(\text{OH})_4$,
50 respectively.

51

52 *Keywords:* lobanovite, magnesiumastrophyllite, astrophyllite supergroup, chemical composition,
53 crystal-structure refinement

54 **Introduction**

55 Lobanovite, $K_2Na(Fe^{2+}_4Mg_2Na)Ti_2(Si_4O_{12})_2O_2(OH)_4$, is a new mineral of the astrophyllite
56 supergroup from Mt. Yukspor, the Khibiny alkaline massif, Kola Peninsula Russia. It has been
57 previously known under the names *monoclinic astrophyllite*, *magnesium astrophyllite*,
58 *magnesiumastrophyllite* and *magnesioastrophyllite* (Peng and Ma, 1963; X-ray Laboratory,
59 Hubei Geologic College, 1974; Shi *et al.*, 1998; Piilonen *et al.*, 2003a; Sokolova and Cámara,
60 2008; Cámara *et al.*, 2010) but has never been formally proposed and approved as a valid
61 mineral species by the CNMNC-IMA, although it was discovered in the CNMNC era. It has now
62 been revalidated and named *lobanovite* after Dr. Konstantin Valentinovich Lobanov (Cyrillic:
63 Константин Валентинович Лобанов; b. 1952, Roslavl', Russia), a prominent Russian ore
64 geologist, DSc. (Doctor of Science, Geology and Mineralogy) and an expert in Precambrian
65 metallogeny. It is particularly appropriate to name this mineral from the Kola Peninsula after Dr.
66 Lobanov, as he worked in the Kola Peninsula for the last 40 years, focusing on the rocks of the
67 Kola superdeep borehole and their relation to the deep structure of ore districts (CNMNC-IMA:
68 Nomenclature voting proposal 15-B). The holotype specimen of lobanovite is the microprobe
69 mount of the single crystal that was used for structure refinement by Sokolova and Cámara
70 (2008) and it was deposited in the collections of the Fersman Mineralogical Museum, Russian
71 Academy of Sciences, Leninskii Prospekt, 18/2, 119071 Moscow, Russia, catalogue number
72 4708/1.

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

76

77 **Previous work**

78 Semenov (1959) reported on the *astrophyllite with unusually high content of MgO (6.39 wt.%)*
79 from the Khibiny alkaline massif, Kola Peninsula, Russia; the complete chemical analysis was

80 not given. Peng and Ma (1963) reported a chemical analysis, with the following simplified
81 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
82 a 10.43(2), b 23.00(5), c 5.35(1) Å, β 102°, and a preliminary crystal structure in space group
83 $A2/m$ (atom coordinates were not reported) for the *astrophyllite from Khibiny*. X-ray Laboratory,
84 Hubei Geologic College (1974) reported the X-ray powder-diffraction data, DTA data and optical
85 properties for the material mentioned above. The crystal structure of *monoclinic astrophyllite*
86 was refined by Shi *et al.* (1998) on sample no. 3086 provided by A. Khomyakov from Mt.
87 Yukspor, the Khibiny alkaline massif, Kola Peninsula, Russia. They gave a full description of the
88 crystal structure, an ideal formula $K_2NaNa(Fe,Mn)_4Mg_2Ti_2(Si_4O_{12})_2(OH)_4(OH,F)_2$, and unit-cell
89 parameters, a 10.370(3), b 23.129(5), c 5.322(1) Å, β 99.55(2)°, V 1258.8(5) Å³, space group
90 $A2$, $Z = 2$, $D_{calc.} = 3.173$ g/cm⁻³ (this formula has an excess charge of 2⁺). The structure data of
91 Shi *et al.* (1998) is in the International Crystal Structure Database (ICSD) under #52032. The
92 ICSD revised #52032 as #56848, with higher symmetry, space group $A2/m$, and a quite different
93 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).
94 The latter formula is neutral but it is chemically and structurally incorrect as H₂O groups do not
95 occur in *magnesium astrophyllite*. Piilonen *et al.* (2003a) considered the structure of *magnesium*
96 *astrophyllite* (space group $A2$) and re-wrote its formula as $K_2Na[Na(Fe,Mn)_4Mg_2]Ti_2Si_8O_{26}$
97 $(OH)_4$. Although the ICSD #56848 points out that the possible space group might be $A2/m$,
98 the crystal structure of *magnesium astrophyllite* has not been re-investigated since the work of
99 Shi *et al.* (1998). Following the inconsistency between the chemical composition and structure
100 for *magnesium astrophyllite* in the ICSD (see above), Sokolova and Cámara (2008) refined the
101 crystal structure of *magnesium astrophyllite* (see below) and reported the chemical composition
102 of the crystal of *magnesium astrophyllite* used for structure refinement. They confirmed the
103 general topology of the crystal structure described by Shi *et al.* (1998) and gave the ideal
104 formula of *magnesium astrophyllite* as follows: $K_2Na(Fe_4Mg_2Na)^{[5]}Ti_2Si_8O_{26}(OH)_4$. Cámara *et al.*
105 (2010) suggested writing the astrophyllite-ribbon component of the formula as $(Si_4O_{12})_2O_2$

106 versus Si_8O_{26} [Piilonen *et al.* (2003a)]. They emphasized that (1) the translational repeat
107 fragment of the ribbon has the formula Si_4O_{12} ; (2) there are two ribbons (corresponding to two H
108 sheets) attached to the central O sheet; (3) the O_2 anions do not link to Si, and this information
109 should be preserved in the chemical formula by writing them separately from the silicate radical.
110 Cámara *et al.* (2010) wrote the formula of *magnesiumastrophyllite* as $\text{K}_2\text{Na}(\text{Fe}_4$
111 $\text{Mg}_2\text{Na})\text{Ti}_2(\text{Si}_4\text{O}_{12})_2\text{O}_2(\text{OH})_4$. Burke (2008) renamed *magnesium astrophyllite and/or*
112 *magnesiumastrophyllite* as *magnesioastrophyllite*. Sokolova (2012) showed that the topology of
113 the HOH block in *magnesioastrophyllite* is different from all other structures of the astrophyllite-
114 supergroup minerals due to the different chemical composition of the O sheet ($\text{Fe}^{2+}_4\text{Mg}_2\text{Na}$),
115 particularly the dominance of Na^+ at the *M*(1) site which makes the *M*(1) polyhedron too large to
116 share edges with Si_2O_7 groups of astrophyllite ribbons and results in a different linkage of H and
117 O sheets, i.e. a different topology of the HOH block. She wrote the ideal formula of
118 *magnesioastrophyllite* as follows: $\text{K}_2\text{Na}(\text{Fe}^{2+}_4\text{Mg}_2\text{Na})\text{Ti}_2(\text{Si}_4\text{O}_{12})_2\text{O}_2(\text{OH})_4$ and emphasized that
119 the name *magnesioastrophyllite* is misleading as it is the dominance of Na^+ at the *M*(1) site that
120 results in the different topology of the HOH block [not the dominance of Mg^{2+} at the *M*(4) site].

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

123

124 **Occurrence and mineral association**

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

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

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135

136 **Physical properties**

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

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

151

152 **Chemical composition**

153 Sokolova and Cámara (2008) determined the chemical composition of lobanovite using a
154 Cameca SX100 electron microprobe (WDS mode, 15 kV, 20 nA, 10 μm beam diameter). Ta, Zr,
155 Sn, Zn, Cs, Rb, Sr and Pb were sought but not detected [for details, see Sokolova and Cámara

156 (2008)]. The content of H₂O (wt. %) was calculated by stoichiometry from the results of the
157 crystal-structure refinement. The chemical composition of lobanovite is given in Table 2 (mean
158 of 10 analyses) in comparison with that of the X-ray Laboratory, Hubei Geologic College (1974).
159 Sokolova and Cámara (2008) calculated the empirical formula on the basis of 30.2 (O + OH + F)
160 anions which include 30 (O + OH) p.f.u. and 0.2 F a.p.f.u. (atoms per formula unit). The
161 empirical, simplified and endmember formulae are (K_{1.97}Ba_{0.01})_{Σ1.98}(Na_{0.65}Ca_{0.14})_{Σ0.79}
162 (Fe²⁺_{3.18}Mg_{2.02}Na_{1.00}Mn_{0.72})_{Σ6.92}(Ti_{1.99}Nb_{0.06})_{Σ2.05}[(Si_{8.01}Al_{0.06})_{Σ8.07}O₂₄]O₂(OH)_{4.03}F_{0.19}, Z = 2,
163 K₂Na[(Fe²⁺, Mn)₄Mg₂Na]Ti₂(Si₄O₁₂)₂O₂(OH)₄ and K₂Na(Fe²⁺₄Mg₂Na)Ti₂(Si₄O₁₂)₂O₂(OH)₄,
164 respectively.

165

166 X-ray powder-diffraction data

167 X-ray powder-diffraction data are presented in Table 3.

168

169 Crystal structure

170 Sokolova and Cámara (2008) refined the crystal structure of lobanovite to $R_1 = 3.2\%$ on the
171 basis of 1861 unique reflections ($F_o > 4\sigma F$) collected on a Bruker AXS SMART APEX
172 diffractometer with a CCD detector and MoK α -radiation: space group $C2/m$, a 5.3327(2), b
173 23.1535(9), c 10.3775(4)Å, β 99.615(1)°, V 1263.3(1) Å³, $Z = 2$, $D_{\text{calc.}}$ 3.161 g.cm⁻³ (Table 4)
174 from Mt. Yukspor, Khibina alkaline massif, Kola Peninsula, Russia. The main structural unit in
175 the structure of lobanovite is the HOH block which consists of a central close-packed O
176 (Octahedral) and two adjacent H (Heteropolyhedral) sheets. In the O sheet, there are four [6]-
177 coordinated $M(1-4)$ sites occupied by Na, Fe²⁺_{1.25}Mn_{0.75}, Fe²⁺_{1.20}Mg_{0.80} and Mg_{1.25}Fe²⁺_{0.75}, with
178 $\langle M(1,2,3,4)-O \rangle = 2.372, 2.166, 2.113$ and 2.094 Å, respectively (Fig. 1a, Table 5). The ideal
179 composition of the O sheet is (Fe²⁺₄Mg₂Na)O₂(OH)₄ p.f.u. In the H sheet, there is one [5]-
180 coordinated D site occupied by Ti_{1.97}Nb_{0.03}, with $\langle D-O \rangle = 1.907$ Å, and there are two

181 tetrahedrally coordinated *T* sites occupied primarily by Si with minor Al, with $\langle T-O \rangle = 1.625 \text{ \AA}$.
182 TO_4 tetrahedra form T_4O_{12} *astrophyllite* ribbons extending along *a*. Astrophyllite ribbons and [5]-
183 coordinated *D* polyhedra connect through common vertices to form the *H* sheet. The ideal
184 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
185 through common vertices of TO_4 tetrahedra, *D* octahedra and *M* octahedra to form an HOH
186 block parallel to (001) (Fig. 1a). The HOH blocks alternate with *I* (Intermediate) blocks along *c*
187 (Fig. 1b). In the *I* block, there are two interstitial sites, a [10]-coordinated *A* site and an [8]-
188 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 $\langle A-O \rangle =$
189 3.120 and $\langle B-O \rangle = 2.536 \text{ \AA}$ (Table 5). The ideal composition of the *I* block is K_2Na a.p.f.u.
190 Cations at the *A* and *B* sites form a layer parallel to (001) (Fig. 1b). The presence of the partly
191 occupied *F* site makes 17% of the *A* and *B* sites [11]- and [10]-coordinated, respectively (Table
192 5).

193 The general topology of the lobanovite structure is in accord with Shi *et al.* (1998). The
194 topology of the HOH block in lobanovite differs from all other structures of the astrophyllite-
195 supergroup minerals (for the astrophyllite structure, see Fig. 2a in Sokolova *et al.*, 2015) due to
196 the chemical composition of the *O* sheet, $Fe^{2+}_4Mg_2Na$, where Na^+ is dominant at the *M*(1) site
197 (Sokolova, 2012). Hence the Na octahedron is too large to share edges with Si_2O_7 groups of
198 astrophyllite ribbons resulting in a different linkage of *H* and *O* sheets, i.e. a different topology of
199 the HOH block [*cf.* Si–Si distances associated with the Na octahedron (3.96 Å) and the Fe^{2+}
200 octahedron (3.06 Å), Fig. 1a].

201

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- 244

245 **Figure captions**

246

247 Fig. 1. The crystal structure of lobanovite: (a) the HOH block viewed perpendicular to the plane
248 of the block [after Fig. 6a of Sokolova (2012)]; (b) general view of the crystal structure of
249 lobanovite [after Fig. 2b of Sokolova (2012)]. The [5]-coordinated Ti polyhedra and Fe²⁺- and
250 Mg-dominant octahedra are pale yellow, green and pink; Na octahedra are navy blue; Si
251 tetrahedra are orange; K and Na atoms at the A and B sites are shown as green and blue
252 spheres; OH groups are shown as small red spheres. The position of the cation layer in the I
253 (Intermediate) block (m = 1, where m is a number of cation layers) is shown by a turquoise line.

254

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 | $C2/m$ | $P\bar{1}$ |
| 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 | 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) |
| $d_{obs.}$ (Å) (I) | | |
| 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.*, 2003b)

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 ₂ O ₅ | n.a | 0.64 | 0.29 – 1.22 | 0.31 | Ba ₂ NaNb ₅ O 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 ₂ O ₃ | 1.11 | 0.24 | 0.08 – 0.42 | 0.13 | andalusite |
| Fe ₂ O 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 ₂ O | 7.28 | 7.66 | 7.54 – 7.78 | 0.07 | orthoclase |
| Na ₂ O | 5.38 | 4.22 | 4.10 – 4.29 | 0.07 | jadeite |
| H ₂ O | 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*

| $I_{\text{obs.}}$ | $d_{\text{obs.}}$ (Å) | $d_{\text{calc.}}$ (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 |

* $I_{\text{obs.}}$ and $d_{\text{obs.}}$ (Å) taken from X-ray Laboratory, Hubei Geologic College (1974); $d_{\text{calc.}}$ (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 | $U_{\text{eq}} (\text{Å}^2)$ |
|------|------------|------------|------------|------------------------------|
| 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} .

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.) | $\langle X-\varphi \rangle_{\text{calc.}}$ [*] (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) | 1.96 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.

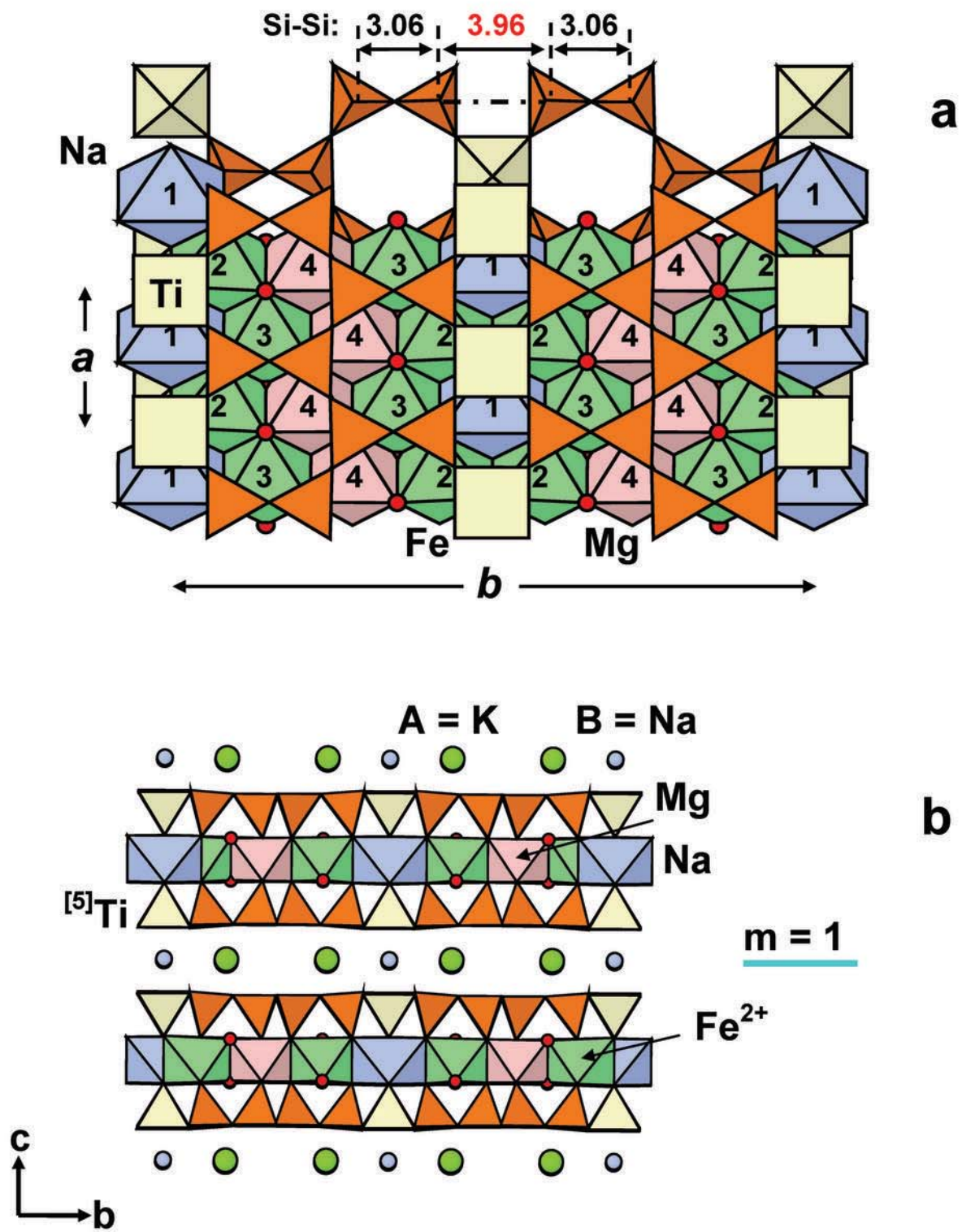


Fig. 1