

Recommended nomenclature for labuntsovite-group minerals*

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Abstract: The present report contains recommendations on the nomenclature of the labuntsovite-group (LG) minerals based on a crystal-structural classification. The labuntsovite group includes hydrous titanium and niobium silicates, both orthorhombic and monoclinic, with a structure characterized by a framework consisting of chains of (Ti,Nb)O-octahedra, linked by four-member rings of Si,O-tetrahedra. This framework contains open cavities occupied by H₂O molecules and extra-framework cations. Seven subgroups are distinguished, each corresponding to different structure types. In accordance with the nomenclature recommendations, LG minerals have different root names if they belong to different subgroups, or are characterized by different prevailing cations in the (Ti,Nb)-position. The species with doubled unit cell are distinguished by the prefix “para”. In the case of structurally ordered members (space groups *C2/m*, *I2/m*), separate species within each subgroup are recognized by different root names (to distinguish the members with Ti > Nb or Ti < Nb) and by a modifier (-K, -Mn, -Mg *etc.*, to distinguish the members with differently occupied “key” positions). Unlike zeolites, a complex substitution of extra-framework cations is possible in monoclinic LG minerals: 2C → D(H₂O)₂ where C = K, Ba; D = Fe, Mg, Mn or Zn. Only one of these coupled sites (C or D) can be more than 50 % occupied, whereas the other is more than 50 % vacant and is not considered as the “key” (species-forming) position. In the case of structurally disordered members (vuoriyarvite series) with space group *Cm* and a large number of extra-framework positions, separate species are recognized in which different extra-framework cations (K, Na, Ca, Sr, Ba) are the most abundant in atomic proportions.

Key-words: labuntsovite group, nomenclature, labuntsovite, nenadkevichite, korobitsynite, vuoriyarvite, lemmleinite, kuzmenkoite, organovaite, paralabuntsovite, tsepinite, karupmollerite, gutkovaite.

Introduction

The first brief description of labuntsovite (from the Khibiny massif), under the name “titanium elpidite”, was given by A.N. Labuntsov (1926). In 1955, this mineral and a related Nb-dominant species were described in more detail, and named, respectively, labuntsovite (Semenov & Burova, 1955) and nenadkevichite (Kuz'menko & Kazakova, 1955). Although the existence of an isomorphous series between these two minerals has been proposed (Semenov, 1959), a number of facts contradict this hypothesis (Chukanov *et al.*, 1999b).

Although more than sixty papers have been published so far on the mineralogy and crystal chemistry of labuntsovite and related species, the proliferating terminology became rather confusing. For example, the name “nenadkevichite” has been applied to orthorhombic and monoclinic members, as well as to minerals with Ti > Nb or Nb > Ti, and to minerals with Na > K or K > Na (Perrault *et al.*, 1973; Organova *et al.*, 1981; Rastsvetaeva *et al.*, 1994).

The evident need to clarify the nomenclature of these minerals prompted us to undertake a comprehensive investigation. This included the determination of the chemical compositions of more than 300 specimens (from 12 different massifs) by electron microprobe analysis. The results show remarkably wide ranges of the species-forming components (weight %): Na₂O 0.17–13.87, K₂O 0–14.90, CaO 0–7.28, SrO 0–8.24, BaO 0–16.90, MgO 0–2.29, MnO 0–7.37, FeO 0–4.96, ZnO 0–7.06, TiO₂ 0.81–27.10, Nb₂O₅ 0.14–38.89. Additionally, there are also variations of physical properties, IR spectra and crystal structures between the members of the group. Single-crystal structure analysis has been performed for a number of LG minerals with unusual physical properties and/or chemical compositions (Rastsvetaeva *et al.*, 1994, 1996, 1997a, 1997b, 1998, 2000a, 2000b, 2001; Golovina *et al.*, 1998). The results obtained in the above cited works demonstrate the existence of a number of structural types within the LG.

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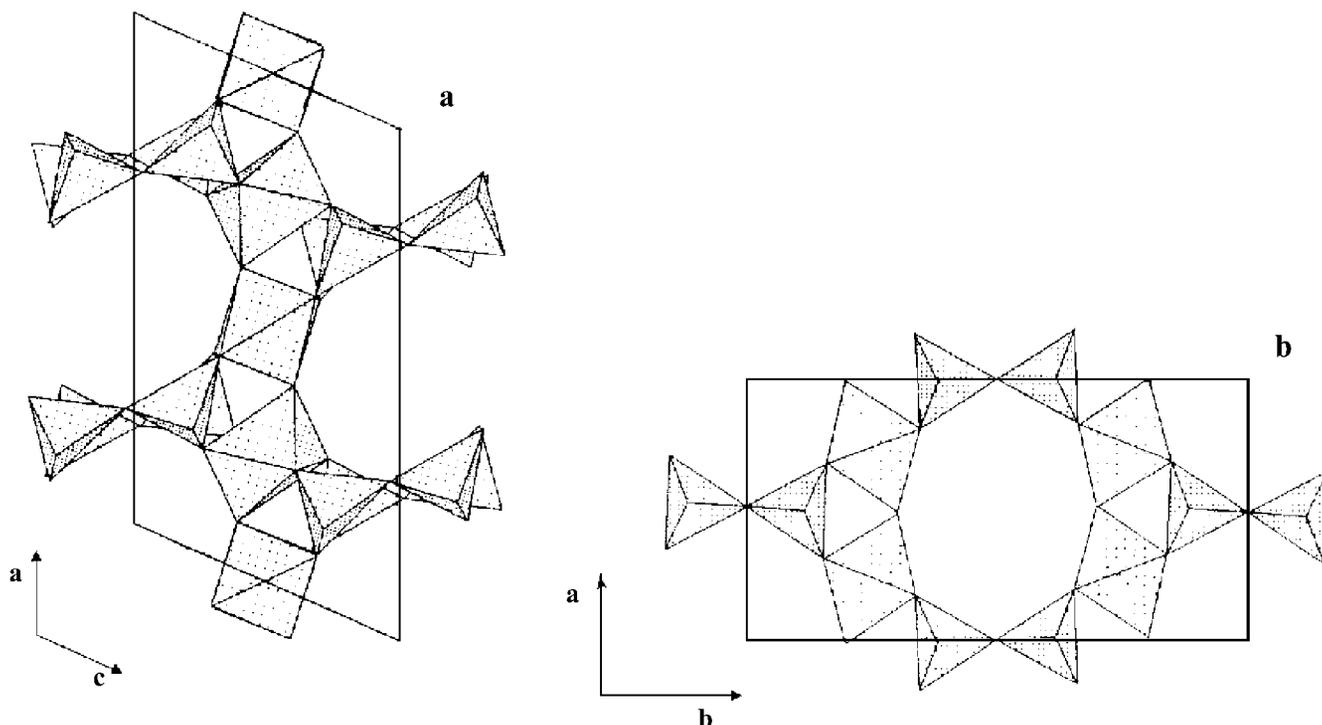


Fig. 1. Fragments of the labuntsovite (a) and nenadkevichite (b) crystal structures. Deformation of the framework causes a symmetry lowering in labuntsovite.

Definition

A labuntsovite-group mineral is a crystalline substance with a structure characterized by a framework consisting of chains of (Ti,Nb)O-octahedra having shared trans-vertices. The chains are linked by tetrahedral four-membered rings [Si₄O₁₂], forming a three-dimensional framework that contains cavities in the form of channels and cages. These channels and cages are usually occupied by H₂O and extra-framework cations. The labuntsovite group includes orthorhombic and monoclinic members. In monoclinic members, the chains of (Ti,Nb)O-octahedra can be linked additionally by DO-octahedra, where D is usually a bivalent cation such as Fe²⁺, Mn²⁺, Zn or Mg. The presence of vacancies in the positions of extra-framework and D cations is typical for the LG minerals.

Crystal structure

The labuntsovite group contains orthorhombic and monoclinic, hydrous titanium and niobium silicates. The basis of their structure (Fig. 1–3) is a framework consisting of chains of (Ti,Nb)O-octahedra (M) that are linked by four-membered rings of Si₄O-tetrahedra (T). Large low-valent cations (“extra-framework cations” hereafter) and H₂O are situated in open cavities of this zeolite-like framework. Some O-atoms bridging the (Ti,Nb)O-octahedra are substituted with OH. The symmetry of the LG minerals depends on the configuration of the octahedral chains (Fig. 1).

The (Ti,Nb)O-octahedral chains are straight in the structure of **orthorhombic** members of the LG (nenadkevichite

subgroup, space group *Pbam*, $a \approx 7.4$, $b \approx 14.2$, $c \approx 7.1$ Å; Fig. 3). Both A cation sites are relatively small and similar in size, so they are occupied mainly by Na. The general formula is: A₆M₄(T₄O₁₂)₂(O,OH)₄·*n*H₂O (*Z* = 1); T = Si; A = Na, □; M = Nb (**nenadkevichite**) or Ti (**korobitsynite**). The presence of vacancies up to 50 % is characteristic of the A sites. Minor amounts of larger cations can be present: a structurally investigated nenadkevichite (Perrault *et al.*, 1973) contained 0.24 K atoms and 0.11 Ca atoms per unit cell.

The crystal structures of **monoclinic** members of the LG contain corrugated chains of (Ti,Nb)O-octahedra (Fig. 2, 3). As a result, zeolite-like cavities are different in size and extra-framework sites are occupied with different cations. Monoclinic LG minerals can be subdivided into six subgroups:

1. **Labuntsovite-type structures** (including those of **labuntsovite** and **lemleinite** subgroups, space group *C2/m*; $a \approx 14.3$, $b \approx 13.8$, $c \approx 7.75$ Å, $\beta \approx 117^\circ$; see Table 1) are the commonest and best studied monoclinic structures (Golovastikov, 1973; Organova *et al.*, 1976, 1981; Rastsvetaeva *et al.*, 1996, 1997b, 1998). In this structure type, an additional octahedral position is located at the site where the distance between chains is minimal; this site is called “the linking octahedron” D and is distinct from the M octahedra present in the chains. Three non-equivalent, extra-framework cation sites (A, B, and C) are present in this structural type, and the general formula is: A₄B₄C₄D₂M₈(T₄O₁₂)₄(OH,O)₈·*n*H₂O (*Z*=1). The cations in the sites are: T = Si; M = Ti, Nb; D = small bivalent cations (M²⁺) such as Mn, Fe, Mg, Zn; A = Na; B = K, sometimes with minor Na; C = Ba, K. The distance between the sites C and D is short (~2.1 Å)

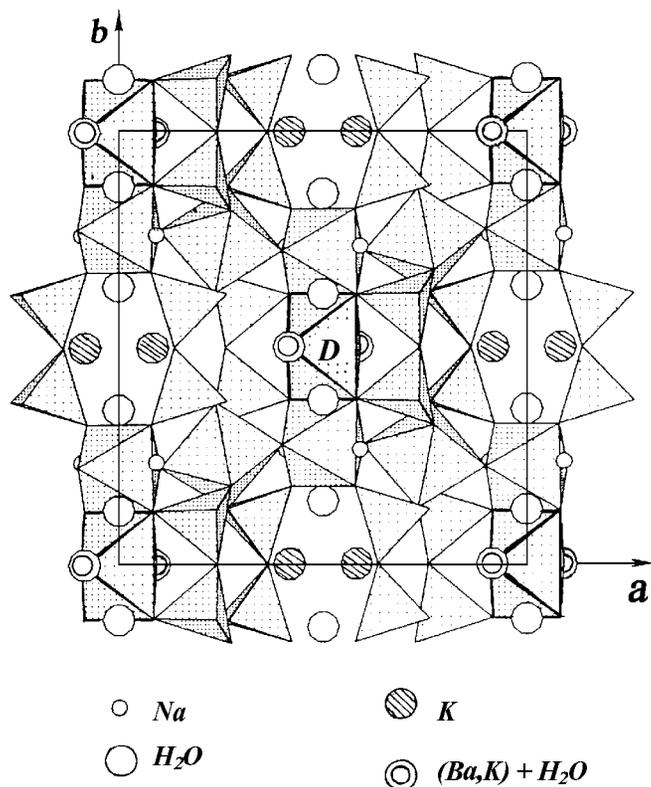


Fig. 2. The crystal structure of labuntsovite (D-octahedron is more than 50 % occupied).

and cations cannot occur in both sites at the same time. If the D site is occupied by cations, H_2O molecules occur in C and complete the octahedral coordination of the D cations; if $D = \square$, C can contain cations. The following mechanism governs the occupancy of C and D sites:

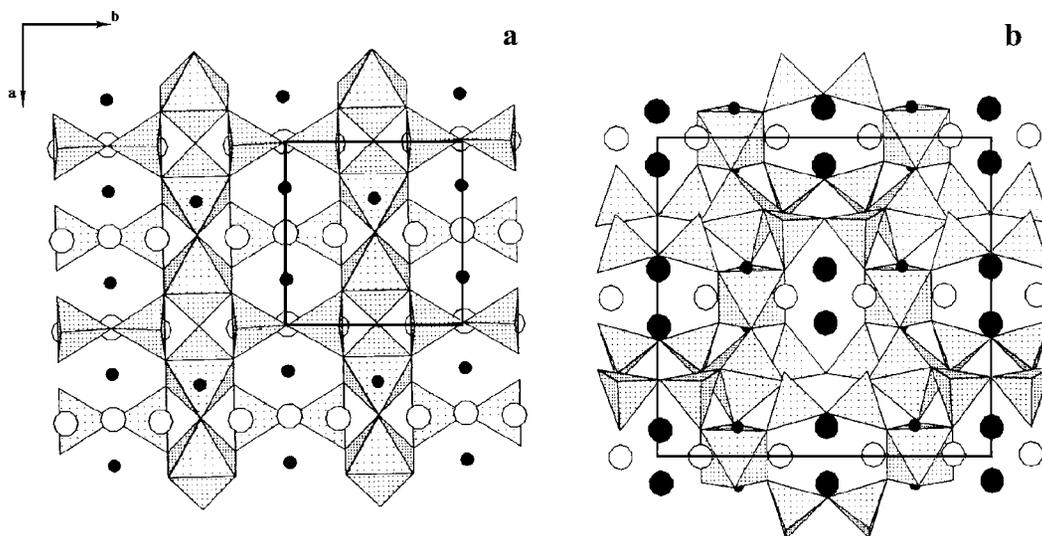
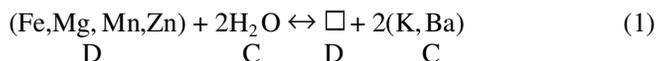


Fig. 3. The crystal structures (projection on ab -plane) of nenadkevichite (a) and lemmleinite (b). The black circles are: K (large) and Na (small ones). The open circles show the positions of water molecules.

The naming of labuntsovites and lemmleinites is according to the cation occupancy of the D site and the C site, respectively (see Tables 1 and 2).

2. Paralabuntsovite-type structure. Besides the original labuntsovite (space group $C2/m$ – Semenov, 1959), a dimorph with space group $I2/m$ and doubled unit cell ($a = 15.57$, $b = 13.75$, $c = 14.27$ Å, $\beta = 116.9^\circ$) has also been described (Milton *et al.*, 1958). The possible reason for the doubling of the unit cell is the ordering of the occupancies of the C and D sites (Organova *et al.*, 1981). In accordance with the IMA CNMMN guidelines (Nickel & Grice, 1998), the name **paralabuntsovite** was approved for the members of the corresponding subgroup.

3. Kuzmenkoite-type structure (space group $C2/m$, $a \approx 14.4$, $b \approx 13.9$, $c \approx 7.8$ Å, $\beta \approx 117^\circ$) differs from that of labuntsovite by the absence of the A cations. The B site is occupied mainly by K, and the C site is cation-deficient (Golovina *et al.*, 1998). Splitting of the B site can lower the symmetry to Cm (Rastsvetaeva *et al.*, 2000b). The idealized formula for the minerals with kuzmenkoite structure is: $K_4D_2M_8(Si_4O_{12})_4(OH,O)_8 \cdot nH_2O$ ($Z = 1$; $n = 10-12$). Two minerals, **kuzmenkoite-Mn** with $D = Mn^{2+}$, $M = Ti$, and **kuzmenkoite-Zn** with $D = Zn^{2+}$, $M = Ti$ have been described to date (Chukanov *et al.*, 1999b; Chukanov *et al.*, in press). A new mineral **karupmöllerrite-Ca** (see Table 2) is related to kuzmenkoite; it can be considered as B-vacant and Nb-dominant analog of hypothetical “kuzmenkoite-Ca”.

4. In the organovaite-type structure (space group $C2/m$, $a \approx 14.5$, $b \approx 14.0$, $c \approx 15.7$ Å, $\beta = 118^\circ$), the c parameter is doubled, due to the splitting of the K site. Two Nb-dominant members, **organovaite-Mn** (Chukanov *et al.*, 2001b) and **organovaite-Zn** (Pekov *et al.*, in press) and one Ti-dominant member, **parakuzmenkoite-Fe** (Chukanov *et al.*, 2001c) are known in this subgroup. The common formula is: $K_4D_2M_8(Si_4O_{12})_4(OH,O)_8 \cdot nH_2O$ ($Z = 2$; $n = 12-14$).

5. Vuoriyarvite-type structure. This structural type (Rastsvetaeva *et al.*, 1994) is characterized by the space group Cm ($a \approx 14.7$, $b \approx 14.2$, $c \approx 7.9$ Å, $\beta \approx 118^\circ$) and numerous

Table 1. Distinctive features of mineral series (root names are given) and mineral species in the labuntsovite group.

Symmetry	Number of non-equivalent extra-framework cation sites	Ideal occupancy of C-site	Ideal occupancy of D-site	Ideal formula, $Z = 1$	Series root name for the members with Ti > Nb in M-site	Series root name for the members with Nb > Ti in M-site	Rule for distinction of mineral species (use of modifiers)
Orthorhombic <i>Pbam</i>	2	C-site is absent	D-site is absent	$A_6M_4(Si_4O_{12})_2(O,OH)_4 \bullet nH_2O$	Korobitsynite	Nenadkevichite	No modifiers*
Monoclinic <i>Cm</i>	numerous, split (> 3)	Vacant	Vacant	$A_{12-x}\square_2M_8(Si_4O_{12})_4(OH,O)_8 \bullet nH_2O$	Tsepinite	Vuoriyarvite	By the prevailing A-cation
Monoclinic <i>C2/m</i>	2	Vacant	Occupied	$K_4\square_4D_2M_8(Si_4O_{12})_4(OH,O)_8 \bullet nH_2O$	Kuzmenkoite*		By the prevailing D-cation
Monoclinic <i>C2/m</i>	2	Vacant	Occupied	$\square_4\square_4D_2M_8(Si_4O_{12})_4(OH,O)_8 \bullet nH_2O$		Karupmöllerite	By the prevailing D-cation
Monoclinic <i>C2/m</i>	3	Occupied	Vacant	$Na_4K_4C_4\square_2M_8(Si_4O_{12})_4(OH,O)_8 \bullet nH_2O$	Lemleinite		By the prevailing C-cation**
Monoclinic <i>C2/m</i>	3	Vacant	Occupied or vacant	$Na_4K_4D_2M_8(Si_4O_{12})_4(OH,O)_8 \bullet nH_2O$	Labuntsovite***		By the prevailing D-cation
Monoclinic <i>I2/m****</i>	3	Vacant	Occupied or vacant	$Na_8K_8D_4M_{16}(Si_4O_{12})_8(OH,O)_{16} \bullet nH_2O$	Paralabuntsovite		By the prevailing D-cation
Monoclinic <i>C2/m</i>	2	Vacant	Occupied	$K_8D_4M_{16}(Si_4O_{12})_8(OH,O)_{16} \bullet nH_2O$	Parakuzmenkoite	Organovaite	By the prevailing D-cation
Monoclinic <i>Cm</i>	4	Vacant	Occupied	$Ca_2\square_2K_4D_4M_8(Si_4O_{12})_4(OH,O)_8 \bullet nH_2O$	Gutkovaite		By the prevailing D-cation

* – Nb-dominant mineral karupmöllerite is related to kuzmenkoite subgroup;

** – for the member with both D and C sites cation-deficient (< 50 % of maximum possible amount of cations in each position), the name “labuntsovite- \square ” is proposed;

*** – holotype specimen of labuntsovite by E.I. Semenov was described with such unit cell (Semenov, 1959);

**** – first description of this mineral was “labuntsovite” from Green River, Wyoming (Milton *et al.*, 1958).

split sub-sites. The **Vuoriyarvite-K** structure contains four sub-sites partly occupied by K, three sub-sites by Na, and five sub-sites by H_2O (Rastsvetaeva *et al.*, 1994). The general formula is: $A_{12-x}\square_2M_8(Si_4O_{12})_4(OH,O)_8 \bullet nH_2O$ ($Z = 1$) where $M = Nb, Ti$; the linking D octahedron is absent; “A” denotes the total combination of sub-sites of extra-framework cations similar to those in zeolites; $n = 12-16$. **Tsepinite-Na**, a new species, is a Ti- and Na-dominant analogue of vuoriyarvite-K (Rastsvetaeva *et al.*, 2000a; Shlyukova *et al.*, 2001).

6. Unlike labuntsovite-type structure, in the **gutkovaite-type structure** the A site is split into two non-equivalent

sites A_1 and A_2 ; as a result, the symmetry is lowered to *Cm*. In **gutkovaite-Mn** (Pekov *et al.*, in press) in A_1 prevails Ca, A_2 is vacant, D is occupied by Mn.

The occupancy of D and C by a competitive mechanism (1) is an important feature of the monoclinic LG mineral structures. The already stated site occupancy, is clearly correlated with compositional features. Separation of high-valent and bivalent octahedral cations between M and D sites has been reliably confirmed (Chukanov *et al.*, 1999b). In particular, the correlation on Fig. 4 demonstrates that the number of D cations per Si_{16} varies continuously from 0 to 2.

Table 2. Nomenclature for the minerals of the labuntsovite group.

Previous name	New name	Idealized formula (Z = 1); space group	Type locality	References	Notes
NENADKEVICHITE SUBGROUP					
Nenadkevichite	<i>Nenadkevichite</i>	$\text{Na}_{8-x}\text{Nb}_4(\text{Si}_4\text{O}_{12})_2$ (O,OH) ₄ ·8H ₂ O; <i>Pbam</i>	Karnasurt Mt., Lovozero, Kola, Russia	(1) Kuz'menko & Kazakova (1955) (2) Perrault <i>et al.</i> (1973)	Firstly described before the CNMMN IMA foundation (1955)
Korobitsynite	<i>Korobitsynite</i>	$\text{Na}_{8-x}\text{Ti}_4(\text{Si}_4\text{O}_{12})_2$ (O,OH) ₄ ·8H ₂ O; <i>Pbam</i>	Alluaiv and Karnasurt Mts., Lovozero, Kola, Russia	(1) Pekov <i>et al.</i> (1999) (2) Rastsvetaeva <i>et al.</i> (1997a)	Approved by CNMMN IMA 98–019
VUORIYARVITE SUBGROUP					
Vuoriyarvite*	<i>Vuoriyarvite-K</i>	(K,Na) _{12-x} Nb ₈ (Si ₄ O ₁₂) ₄ O ₈ ·nH ₂ O (x = 0–6, n = 12–16); <i>Cm</i>	Vuoriyarvi, Northern Karelia, Russia	(1) Subbotin <i>et al.</i> (1998) (2) Rastsvetaeva <i>et al.</i> (1994)	Approved by CNMMN IMA 95–031
None	<i>Tsepinite-Na</i>	(Na,H ₃ O,K,Sr,Ba) _{12-x} Ti ₈ [Si ₄ O ₁₂] ₄ (OH,O) ₈ ·nH ₂ O (x = 0–6, n = 12–16); <i>Cm</i>	Khibinpakchchorr Mt., Khibiny, Kola, Russia	(1) Shlyukova <i>et al.</i> (in press) (2) Rastsvetaeva <i>et al.</i> (2000a)	Approved by CNMMN IMA 2000–046
KUZMENKOITE SUBGROUP					
Kuzmenkoite**	<i>Kuzmenkoite-Mn</i>	$\text{K}_4\text{Mn}_2\text{Ti}_8$ (Si ₄ O ₁₂) ₄ (OH) ₈ ·nH ₂ O (n = 10–12); <i>C2/m</i>	Selsurt Mt., Lovozero, Kola, Russia	(1) Chukanov <i>et al.</i> (1999) (2) Golovina <i>et al.</i> (1998)	Approved by CNMMN IMA 98–058
None	<i>Kuzmenkoite-Zn</i>	$\text{K}_4\text{Mn}_2\text{Ti}_8$ (Si ₄ O ₁₂) ₄ (OH) ₈ ·nH ₂ O (n = 12–14); <i>C2/m</i>	Lepkhe-Nelm Mt., Lovozero, Kola, Russia	(1) Chukanov <i>et al.</i> (in press) (2) Chukanov <i>et al.</i> (in press)	Approved by CNMMN IMA 01–037
None	<i>Karupmøllerite-Ca</i>	(Na,Ca,K) ₄ Ca ₂ Nb ₈ (Si ₄ O ₁₂) ₄ (O,OH) ₈ ·14H ₂ O; <i>C2/m</i>	Ilimaussaq, Greenland	(1) (2) Yamnova <i>et al.</i> (2000)	Approved by CNMMN IMA 2001–028
LEMMLEINITE SUBGROUP					
Lemmleinite***	<i>Lemmleinite-K</i>	$\text{Na}_4\text{K}_4\text{K}_4\text{Ti}_8(\text{Si}_4\text{O}_{12})_4$ (O,OH) ₈ ·8H ₂ O; <i>C2/m</i>	Koashva Mt., Khibiny, Kola, Russia	(1) Khomyakov <i>et al.</i> (1999) (2) Rastsvetaeva <i>et al.</i> (1996)	Approved by CNMMN IMA 97–003
Labuntsovite	<i>Lemmleinite-Ba</i>	$\text{Na}_4\text{K}_4\text{Ba}_{2+x}\text{Ti}_8(\text{Si}_4\text{O}_{12})_4$ (O,OH) ₈ ·8H ₂ O; <i>C2/m</i>	Kukisvumchorr Mt., Khibiny, (1) Kola, Russia	Chukanov <i>et al.</i> (2001a) (2) Rastsvetaeva <i>et al.</i> (1997b)	Approved by CNMMN IMA 98–052a
LABUNTSOVITE SUBGROUP					
Labuntsovite****	<i>Labuntsovite-Mn</i>	$\text{Na}_4\text{K}_4\text{Mn}_2\text{Ti}_8(\text{Si}_4\text{O}_{12})_4$ (O, OH) ₈ ·nH ₂ O (n = 10–12); <i>C2/m</i>	Kuftn'yun Mt., Lovozero, Kola, Russia	(1) Semenov & Burova (1955) (2) Organova <i>et al.</i> (1981)	Firstly described before the CNMMN IMA foundation (1955)
Labuntsovite	<i>Labuntsovite-Mg</i>	$\text{Na}_4\text{K}_4\text{Mg}_2\text{Ti}_8$ (Si ₄ O ₁₂) ₄ (O, OH) ₈ ·nH ₂ O (n = 10–12); <i>C2/m</i>	Kovdor, Kola, Russia	(1) Khomyakov <i>et al.</i> (2001) (2) Khomyakov <i>et al.</i> (2001)	Approved by CNMMN IMA 98–050a
Labuntsovite	<i>Labuntsovite-Fe</i>	$\text{Na}_4\text{K}_4\text{Fe}_2\text{Ti}_8(\text{Si}_4\text{O}_{12})_4$ (O, OH) ₈ ·nH ₂ O (n = 10–12); <i>C2/m</i>	Kukisvumchorr Mt., Khibiny, Kola, Russia	(1) Khomyakov <i>et al.</i> (2001) (2) Khomyakov <i>et al.</i> (2001)	Approved by CNMMN IMA 98–051a
PARALABUNTSOVITE SUBGROUP					
Labuntsovite	<i>Paralabuntsovite-Mg</i>	$\text{Na}_8\text{K}_8\text{Mg}_4\text{Ti}_{16}(\text{Si}_4\text{O}_{12})_8$ (O,OH) ₁₆ ·nH ₂ O (n = 20–24); <i>I2/m</i>	Trona Mine, Sweetwater Co., Wyoming, USA	(1) Milton <i>et al.</i> (1958)	Approved by CNMMN IMA 00-A

Table 2. Nomenclature for the minerals of the labuntsovite group (cont.).

Previous name	New name	Idealized formula (Z = 1); space group	Type locality	References	Notes
ORGANOVAITE SUBGROUP					
None	<i>Organovaite-Mn</i>	$K_8Mn_4Nb_{16}(Si_4O_{12})_8O_{16} \cdot nH_2O$ ($n = 20-28$); <i>C2/m</i>	Karnasurt Mt., Lovoze-ro, Kola, Russia	(1) Chukanov <i>et al.</i> (2001b) (2) Chukanov <i>et al.</i> (2001b)	Approved by CNMMN IMA 2000-031
None	<i>Organovaite-Zn</i>	$K_8Zn_4Nb_{16}(Si_4O_{12})_8O_{16} \cdot nH_2O$ ($n = 20-28$); <i>C2/m</i>	Karnasurt Mt., Lovoze-ro, Kola, Russia	(1) Pekov <i>et al.</i> , (2001) (2) Pekov <i>et al.</i> (2001)	Approved by CNMMN IMA 2001-006
None	<i>Parakuzmenkoite-Fe</i>	$(K,Ba)_8Fe_4Ti_{16}(Si_4O_{12})_8(OH,O)_{16} \cdot nH_2O$ ($n = 20-28$); <i>C2/m</i>	Kedykverpakhk Mt., Lovozero, Kola, Russia	(1) Chukanov <i>et al.</i> (2001c) (2) Chukanov <i>et al.</i> (2001c)	Approved by CNMMN IMA 2001-007
GUTKOVAITE SUBGROUP					
None	<i>Gutkovaite-Mn</i>	$Ca_2K_4Mn_2Ti_8(Si_4O_{12})_4O_8 \cdot nH_2O$ ($n \approx 10$); <i>Cm</i>	Maly Mannepakhk Mt., Khibiny, Kola, Russia	(1) Pekov <i>et al.</i> (in press) (2) Rastsvetaeva <i>et al.</i> (2001)	Approved by CNMMN IMA 2001-038

* – The first described vuoriyarvite is K-dominant; it must be renamed vuoriyarvite-K in accordance with the new nomenclature;

** – The first described kuzmenkoite is Mn-dominant; it must be renamed kuzmenkoite-Mn in accordance with the new nomenclature;

*** – The first described lemmleinite is K-dominant; it must be renamed lemmleinite-K in accordance with the new nomenclature;

**** – The first described labuntsovite is Mn-dominant; it must be renamed labuntsovite-Mn in accordance with the new nomenclature.

In the column "References":

(1) – first mineralogical description;

(2) – publication on the crystal structure.

Principles of the labuntsovite-group nomenclature

The nomenclature of monoclinic LG minerals is based on the following principles and is in accordance with the rules recommended by IMA CNMMN (Nickel & Grice, 1998):

1. Members of a solid solution series are distinguished by the "50 % rule".

2. Mineral species are named using combinations of "root names" and modifiers. Each species name for monoclinic LG minerals consists of a root name and modifier.

3. Minerals have different "root names" if at least one of the following conditions is fulfilled:

– different structural type;

– octahedral M sites in the chains contain different cations – Ti or Nb;

– more (one case) or less (another case) than 50 % cations occur in the D site. Only in the latter case, the neighbouring C site can be more than 50 % occupied;

– different root names should also be given for representatives (not yet described) of labuntsovite-type members, when the dominant cation in A is not Na or in B is not K.

The first and principal rule for species distinction is the **50 % rule**. However, a serious problem is represented by the important role of vacancies in the D octahedron and extra-framework cation sites. Therefore, a second important rule is: **if a site is more than 50 % occupied by cations (i.e. $\Sigma cations > \square$), the component which predominates over any other must be considered as a species-forming cation**. This is

similar to Levinson's rule: if the sum of REE prevails over any other component in this site, the mineral is considered as a rare-earth species and the prevailing REE is used to suffix the root name of the mineral species. If the site is less than 50 % occupied with cations (i.e. $\Sigma cations < \square$, H_2O), this site is considered cation-deficient. Full occupancy of D site per 16Si is 2 atoms, and that of C site is 4 atoms, therefore the 50 % threshold is 1 atom per formula unit for D cations and 2 atoms per formula unit for C cations. **Only cations, not water molecules, are taken into account in the C site**. Using the last rule, we can identify mineral species on the basis of cation composition (e.g. from electron microprobe analysis).

In spite of the zeolite-like character of structurally ordered LG minerals (members with space groups *C2/m* and *I2/m*), all extra-framework cations occupy only two or three fixed, non-split positions. Furthermore, the occupancies obtained from structure analysis are in good agreement with real chemical compositions. **Mineral species within the corresponding series are distinguished by root-names (to distinguish the cases $Ti > Nb$ and $Ti < Nb$) and by modifiers denoting the most abundant cation in the species-forming, i.e. non-vacant, C or D position**. An analogue of labuntsovite has been described with vacancies predominating in both C and D positions (Bulakh & Evdokimov, 1973; Organova *et al.*, 1981). For this mineral, the name "**labuntsovite- \square** " (**not an approved name**) could be used.

In vuoriyarvite, we observe a condition close to that existing in zeolites: extra-framework cations are situated in

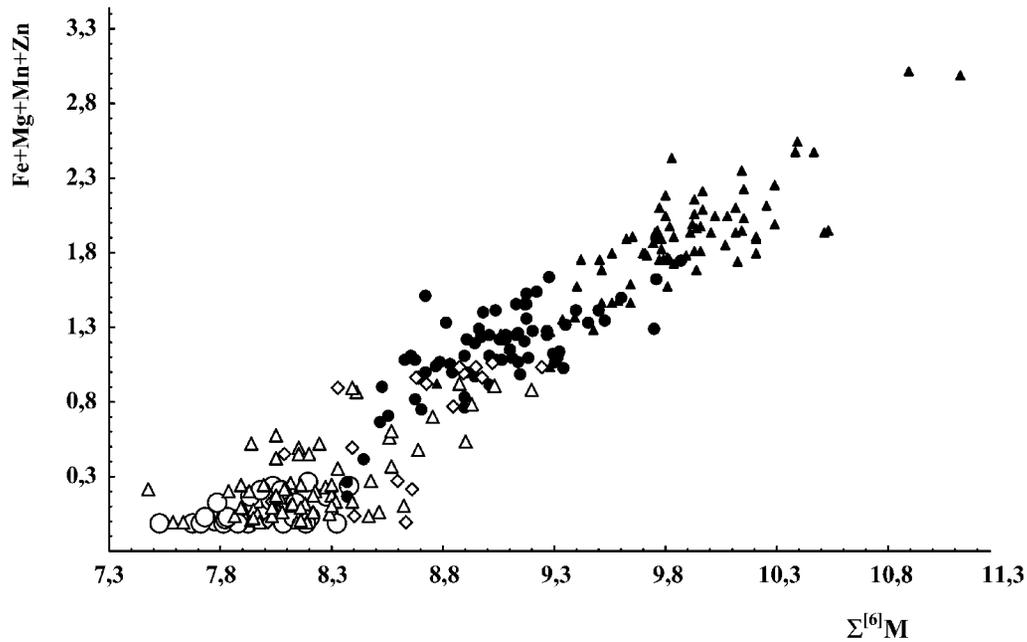


Fig. 4. Correlation between total amount of octahedral cations (per unit cell) and amount of bivalent octahedral cations (Mg, Mn, Fe, Zn) for minerals of labuntsovite group: labuntsovite subgroup (black circles), kuzmenkoite and organovaite subgroups (black triangles), vuoriyarvite subgroup (open triangles), lemmleinite subgroup (quadrangles), nenadkevichite subgroup (open circles).

numerous split sites (sub-sites) dominated by vacancies. For this reason, **mineral species with vuoriyarvite-like structures are distinguished by the prevailing extra-framework cation (without distinction of extra-framework sites)**, in a similar way to the accepted rules for zeolites (Coombs *et al.*, 1997) – see Table 1.

Non-approved and obsolete names for the labuntsovite-group minerals

The complex and variable chemical composition of the LG minerals and the similarity of their physical properties has resulted in the unnecessary proliferation of names, mainly derivatives of the “old” mineral names, labuntsovite and nenadkevichite. These non-approved and obsolete names are given here in italic type, with their corresponding accepted mineral species names under the present nomenclature.

Titanium elpidite, titano-elpidite (Labuntsov, 1926) = labuntsovite-Mn.

Labuntsovite I (Organova *et al.*, 1981), according to the new nomenclature rules it should be named labuntsovite-□.

Potassium labuntsovite, labuntsovite II (Organova *et al.*, 1981) = labuntsovite-Mn.

Labuntsovite III (Organova *et al.*, 1981), described also as *Potassium-rich labuntsovite* (Rastsvetaeva *et al.*, 1998) = lemmleinite-K.

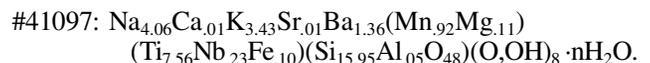
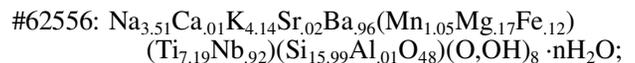
Monoclinic nenadkevichite, Ti-nenadkevichite (Organova *et al.*, 1976) = monoclinic member of LG with Ca as the most abundant D-cation (not approved yet).

K-rich nenadkevichite (Rastsvetaeva *et al.*, 1994) = vuoriyarvite-K.

K-dominant nenadkevichite (Petersen *et al.*, 1996) = vuoriyarvite-K?

According to the accepted nomenclature, the old names “vuoriyarvite”, “lemmleinite” and “kuzmenkoite” must be replaced with vuoriyarvite-K, lemmleinite-K and kuzmenkoite-Mn, respectively. The name “labuntsovite” has been applied to different minerals: labuntsovite-Mn (Semenov & Burova, 1955; Golovastikov, 1973; partly: Bulakh & Evdokimov, 1973; Organova *et al.*, 1981), labuntsovite-Mg (partly: Bulakh & Evdokimov, 1973), labuntsovite-□ (partly: Bulakh & Evdokimov, 1973; Organova *et al.*, 1981), lemmleinite-K (partly: Organova *et al.*, 1981), paralabuntsovite-Mg (Milton *et al.*, 1958).

Labuntsovite was first described in 1926 from the Khibiny massif, Kola, as “titanium elpidite” (Labuntsov, 1926). In 1955, the same mineral from the Lovozero massif, Kola, was studied and named “labuntsovite” (Semenov & Burova, 1955). We have examined both type specimens by electron microprobe analysis: Semenov’s holotype of labuntsovite from Kuftn’yun Mt., Lovozero massif, and Labuntsov’s “titanio-elpidite” type specimen from Yum’egor Pass, Khibiny massif, which are deposited in the Fersman Mineralogical Museum, Moscow (samples ## 62556 and 41097 respectively). Both samples are labuntsovite-Mn in accordance with the accepted nomenclature. Their empirical formulae are:



Rules for the calculation of crystal chemical formulae for structurally ordered monoclinic labuntsovite-group minerals (labuntsovite, lemmleinite, kuzmenkoite and paralabuntsovite subgroups)

In comparison to orthorhombic members, monoclinic LG minerals are characterized by more complicated and widely variable chemical compositions. It is necessary to take into consideration some important crystal chemical features of these minerals for the correct calculation of their formulae. The scheme of calculation given below for phases with labuntsovite structure is based on the following structure features:

1. Tetrahedral sites (T = Si with traces of Al) and chain octahedra (M = Ti, Nb plus some Fe³⁺) do not show vacancies. The theoretical ratio T:M=2 is close respected (Fig. 4).

2. The D octahedron is selectively occupied by small bivalent cations (Mn²⁺, Mg, Fe²⁺, Zn); its occupancy varies from 0 to 100 %.

3. The A site is fully occupied with Na.

4. The B site is occupied by K, with minor amounts of Na and vacancies (< 25 %).

5. Ba is selectively localized at the C site (*i.e.* no Ba has been found at the B position in the crystal structures of Ba-rich samples, see Organova *et al.*, 1981; Rastsvetaeva *et al.*, 1997b); K may be present at C site along with Ba.

6. The distance between C and D sites is short (~ 2.1 Å), and the mechanism of their cation occupancy is as discussed above.

Taking into account the structural data, we propose the following scheme of calculation for the crystal chemical formulae of LG minerals with space groups *C2/m* and *I2/m*:

1. Basis of calculation – [(Si₄Al)₄O₁₂]₄(OH, O)₈; Z = 2 for the paralabuntsovite series, and Z=1 for the other series, *i.e.* Si + Al = 16 apfu.

2. Place Ti, Nb into M; if (Ti+Nb) < 8, add Fe (as Fe³⁺). If (Ti+Nb) > 8, put redundant Ti into D.

3. Place Mn, Zn, Mg, and rest of Fe into D.

4. Place Na into A. Put redundant (over 4 apfu) Na into B.

5. Place Ba and Sr into C.

6. Fill the B site with excess (over 4 apfu) Na; add K up to 4 atoms in the B position. Place the rest of K into C (together with Ba and Sr) and check that the C site has a total number of water molecules and anions which is twice the number of cations at the D site.

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