

8.1.2.5 Götzenite, labuntsovite, andremeyerite and related silicates

The sorosilicates from groups VIIIB09 - VIIIB10 are listed in Table 1 [91N1]. In addition to the classification given by [91N1], the nenadkevichite, classified in group VIII B11, will be also included in this section. According to recent data [02C1], the nenadkevichite was considered as a member of the labuntsovite group.

8.1.2.5.1 Crystal structure. Lattice parameters

Götzenite, $(\text{Ca},\text{Na})_6\text{Ti}(\text{Si}_2\text{O}_7)_2(\text{F},\text{OH},\text{O})_4$; rosenbuschite, $(\text{Ca},\text{Na})_6\text{TiZr}(\text{Si}_2\text{O}_7)_2(\text{F},\text{OH})_4$; seidozerite, $(\text{Na},\text{Ca})_4\text{MnTiZr}(\text{Si}_2\text{O}_7)_2\text{O}_2(\text{F},\text{OH})_2$

The silicate götzenite crystallizes in a triclinic lattice having space group $P\bar{1}$ [53S1, 60S1, 62N1, 64S1, 66S1, 72C1]. The same space group was reported for rosenbuschite [64S1, 66S1]. The seidozerite crystallizes in a monoclinic-type structure having space group Pc or P2/c [58S1, 60S1]. The main feature of the structure of götzenite is the presence of walls of octahedra and eight-cornered polyhedra parallel to (100) which are connected by “ribbons” of octahedra parallel to [001] and by Si_2O_7 groups [72C1]. This description corresponds also to that of the structure of rosenbuschite and seidozerite. The coordination polyhedra of Ti and Ca are octahedra; that of Na is an eight-cornered polyhedron which can be described as a hexagonal bipyramid. The oxygen O1, which is shared by two silicon atoms, is involved in this coordination polyhedron. The hexagonal bipyramid around Ca or Na is also present in rosenbuschite and seidozerite. In götzenite and rosenbuschite two successive “walls” are equivalent by translation, while in seidozerite (monoclinic) they are related by a glide plane. The arrangement of the cations in the “ribbons” of the three silicates is shown in Fig. 1 [72C1]. The above silicates are isostructural and could be considered as terms of an isomorphous series only if the minor differences in symmetry, bond distances and coordinations of the cations are neglected. In this case götzenite would be the Zr-free term, seidozerite the Zr-rich term and rosenbuschite as an intermediate phase. In the structure of götzenite, the positions occupied by the atoms are nearly consistent with a monoclinic symmetry - Table 2. However O1, Si1 and Si2 occupy only one half of their respective sets of “monoclinic” positions, thus lowering the symmetry. In the twinned crystals, the mentioned atoms occupy one half of their “monoclinic” positions in one individual and the other half in the second individual of the twin. This fact appears as a shift of $(1/2)c$ of Si_2O_7 groups and as an interchange of the positions of Na and Ti (Fig. 2 bottom). The remaining atoms maintained their positions through the boundary between the individuals of the twin as it is shown in Fig. 2 top, by the Ca-octahedra. The above features explain the pseudo-monoclinic cell reported by some groups. In rosenbuschite this type of twinning would produce a greater distortion of the structure owing to the presence of Zr. However, it has been observed that this silicate can be twinned in the same way as götzenite [72C1].

Fersmanite, $(\text{Ca},\text{Na})_8(\text{Ti},\text{Nb})_4(\text{Si}_2\text{O}_7)_8\text{O}_8\text{F}_3$

According to [77M1] fersmanite crystallizes in a triclinic lattice having space group P1 or $P\bar{1}$. Later on, [84S1] has reported that the structure is monoclinic with space group B2/b or Bb. The structural analysis was performed in the acentric space group Bb [84S1].

The structural units of fersmanite are Na polyhedra (with eight vertices), Ca polyhedra (with six vertices), fairly regular Ti octahedra and diortho groups [84S1]. The sodium polyhedra are deformed cubes; those of one of the two independent Na atoms are more twisted. As well as the six oxygen atoms, the coordination of sodium includes two fluorine atoms, in the *trans* position (along the solid diagonal). The coordination polyhedron of the calcium atoms can be described as a bent octahedron in which two faces lie almost in the same plane. One vertex of Ca polyhedron is occupied by a fluorine atom. For both the independent atoms the Ti octahedra have the same shape and size. The diortho group has the characteristic structures of diorthosilicates. Both tetrahedra are inscribed in a trigonal prism. The structure of fersmanite is based on perforated (checkerwise) networks of two types [84S1]. The first is formed from Na polyhedra (with eight vertices) and Ti octahedra such that occupied “cells” alternate with empty ones - Fig. 3a. The Ti octahedra of two crystallographically independent types are joined at their vertices into chains parallel to the $[10\bar{1}]$ diagonal of the unit cell. The chains of Na polyhedra are parallel to the Ti chains, and the polyhedra are joined together and to the Ti octahedra via common edges. The networks of the second type are made up to chains linked via the edges of the Ca polyhedra which are connected

together by the diortho groups - Fig. 3b. Two networks of the first type, related by a rotation axis, give a two layer Na, Ti packet - Fig. 3c. In the packet, the Ti octahedra are related to one another and to the screw axis so that it is converted to a single pitch pseudo-axis of the fourth order, while the octahedra are linked via their vertices into a spiral along the axis. The Na polyhedra joined via common edges form a similar spiral which is displaced relative to the first through the half period $c/2$. Networks of other type, related by the center of inversion, form a two layer Ca, Si packet in which two vertices of each diortho group of one network span the edge of the Ca polyhedron of the adjacent network. In the crystal structure, the Na, Ti packets are transposed from the Ca, Si packets parallel to the (010) plane. The networks are superimposed over one another so that the empty "cells" fit over occupied ones and viceversa, i.e. gaps are formed in a 1:1 ratio with the populated ones.

Rinkite, $(\text{Na,Ca})_3(\text{Ca,Ce})_4\text{Ti}_4(\text{Si}_2\text{O}_7)_2(\text{O,F})_4$

The crystallography of the silicate rinkite has been studied by various authors, and different symmetries (from triclinic to orthorhombic) have been ascribed. The first determination [63K1] is based on the triclinic cell of [57S1], in the space group $P\bar{1}$. The second [65L1] is topologically equivalent to the first but is based on a monoclinic (pseudo-orthorhombic) cell in space group $P2_1$ with $\beta \approx 90^\circ$. The third [67S1], with space group $P2_1$ and $\beta = 101^\circ$, is topologically equivalent to the above two structures. In [66G1] has been suggested how the monoclinic pseudo-orthorhombic character of the silicate could produce such disparate results. Two types of monoclinic cell (space group $P2_1/m$ or $P2_1$) were proposed. In [71G1] the data of [66G1] were confirmed but with the values of a and c interchanged with respect to those of [65L1, 66G1, 67S1]. The crystal has been shown to be monoclinic with space group $P2_1/c$. The above difference in the data was attributed to the fact that the measurements made by [66G1, 67S1] were probably performed on a twin.

A general view of the rinkite structure in (010) projection is shown in Fig. 4 [71G1]. The structure is based on sheets of octahedra parallel to the (001) plane with the Si_2O_7 groups and some metal ions between them. There are two symmetrically dependent octahedral sheets in the unit cell, containing gaps which are only statistically occupied. There are also two independent cations in sevenfold coordination.

Mosandrite, $(\text{Ca,Na,Fe})_{12}(\text{Ti,Zr})_2\text{Si}_7\text{O}_{25}(\text{OH})_6\text{F}_4$

Different symmetries, as in case of rinkite, were proposed for the crystal structure of mosandrite. According to [57S2] the silicate crystallizes in a monoclinic type structure, while in [57S1] a triclinic one was proposed. Probably the discussion concerning the structure of rinkite is valuable also in case of mosandrite.

Ilmajokite, $(\text{Na,Ca,Ba})_{10}\text{Ti}_5\text{Si}_{14}\text{O}_{22}(\text{OH})_{44}\cdot n\text{H}_2\text{O}$

Ilmajokite crystallizes, probably, in a monoclinic-type structure [72B1, 73F1].

Labuntsovite and nenadkevichite

According to [91N1] the labuntsovite minerals were classified in group VIII B9 and nenadkevichite in the group VIIIB11. Later on, in [02C1] the labuntsovite and nenadkevichite were analyzed together as the labuntsovite - nenadkevichite family. The presence of labuntsovite mineral was reported by [37L1]. The crystal structures of labuntsovite and related Nb-dominant species were described by [55S1] and that of nenadkevichite by [55K1]. Although the existence of an isomorphous series between these two minerals has been proposed [59S2], the detailed analysis of crystal structures contradicted the above hypothesis [99C1]. A recommended nomenclature of the labuntsovite group was presented by [02C1]. In addition, some new minerals of this group have been also reported later.

The crystal structure of the labuntsovite group of minerals is characterized by columns formed by (Nb,Ti)O octahedra with shared trans-vertices. The octahedral columns are linked by tetrahedral four-membered rings (Si_4O_{12}) forming a three-dimensional framework that contains cavities in the form of channels and cages. The channels and cages are usually occupied by H_2O and extra-framework low valent cations. Some O-atoms, bridging the (Ti,Nb)O octahedra, are substituted by OH. The silicates from the labuntsovite group crystallize in an orthorhombic or monoclinic-type structures, the crystal symmetry depending on the configuration of the octahedral chains - Fig. 5 [02C1]. The (Ti,Nb)O-octahedral chains are straight in the structure of orthorhombic

members (*nenadkevichite* subgroup, space group Pbam) - Fig. 5d. The general formula of this subgroup is $A_6M_4(T_4O_{12})_2(O,OH)_4 \cdot nH_2O$ where $T = Si$; $A = Na, \square$; $M = Nb$ (*nenadkevichite*) or Ti (*korobitsynite*) - Table 1b. Both A cation sites are relatively small and similar in size, so they are occupied mainly by Na. Minor amounts of larger cations can be also present. Characteristic for the A site is also the presence of vacancies, up to 50 %.

The crystal structures of monoclinic silicates have the chains of $(Ti,Nb)O$ octahedra that can be linked additionally by DO octahedra where D is usually a bivalent cation (Fe^{2+} , Mn^{2+} , Zn^{2+} , Mg^{2+}). The monoclinic structure contains corrugated chains of $(Ti,Nb)O$ octahedra - Fig. 5c, e [02C1]. As a result, zeolite-like cavities, which are different in size, and extra-framework sites are occupied by different cations. The various subgroups of labuntsovite minerals are given in Table 1b. According to [02C1] the monoclinic silicates can be divided into six subgroups. Then another subgroup was added (*paratsepinite*) [03C1].

Labuntsovite-type structures (labuntsovite, lemmleinite) crystallize in the space group C2/m [73G1, 76O1, 96R1, 98R1, 02C1]. 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 nonequivalent extra-framework cations sites (A, B, C) are present in this structure type and the general formula is $A_4B_4C_4D_2M_8(T_4O_{12})_4(OH,O)_8 \cdot nH_2O$. The occupancy of sites are: $T = Si$, $M = Ti, Nb$, $D = Mn^{2+}, Fe^{2+}, Mg^{2+}, Zn^{2+}$ etc; $A = Na$; $B = K$ and small content of Na, and $C = Ba, K$ [02C1]. The distance between the sites C and B is short and cations cannot occur in both sites at the same time. If the D site is occupied by cations, H_2O molecule occur in C and complete the octahedral coordination of the D cations. If $D = \square$, the C site can contain cations. According to [02C1], the mechanism which determines the occupancy of C and D sites is: $D(Fe,Mg,Mn,Zn) + C(2H_2O) \leftrightarrow D(\square) + C(2(K,Ba))$. The labuntsovites and lemmleinites can be classified according to the cation occupancy of D and C sites, respectively - Table 1b.

Paralabuntsovite crystallizes in space group I2/m, having doubled unit cell, as compared to labuntsovite [58M1]. The possible reason for doubling of the unit cell is the ordering of cations in C and D sites [81O1].

Kuzmenkoite-type silicates crystallize in space group C2/m. In this structure, unlike labuntsovite, the A cations are missing. The B site is occupied mainly by K and the C site is cation deficient [98G1]. Splitting of the B site can lower the symmetry to Cm [00R1]. According to the dominant cation in D site, kuzmenkoite-Mn and kuzmenkoite-Zn have been described [99C2, 02C2]. The *karupmøllerite*-Ca is a B-vacant and Nb-dominant analog of an hypothetical "kuzmenkoite-Ca" [00Y1, 02P3].

Organovaite-type silicates crystallize also in C2/m-type structure, the *c*-parameter being doubled due to the splitting of the K-site. Two Nb-dominant members were reported: organovaite-Mn [01C3] and organovaite-Zn [02P1] as well as one Ti-dominant member parakuzmenkoite-Fe [01C2].

The *Vuoriyarvite*-type structure was described in space group Cm and is characterized by numerous split sites [94R1]. The structure of vuoriyarvite-K contains four sub-sites partly occupied by K, three sub-sites by Na and five sub-sites by H_2O [94R1] - Table 2e. The linking D octahedron is absent - Table 1b. In this case A denotes the total combination of subsites of extra-framework cations similar to those of zeolites. *Tsepinite*-Na is a Ti- and Na-dominant analog of vuoriyarvite-K [00R2, 01S1]. *Tsepinite*-K and -Ca was also reported and denoted according to the dominant cations in A site [03C1, 03P1].

In case of the *gutkovaite*-type structure, the A site is split into two non-equivalent sites A1 and A2. As a result, the symmetry is lowered to Cm. In gutkovaite-Mn, Ca prevails in A1 site, A2 site is vacant and D is occupied by Mn [02P2]. In *alsakharovite*-Zn the Zn prevails in D site [03P2].

Paratsepinites crystallize in the C2/m-type structure [03C1]. The Ba or Na atoms are distributed in A, B and C sites and D sites are vacant.

The occupancy of D and C sites by a competitive mechanism, mentioned already, is an important feature of monoclinic structures. The site occupancy may be correlated with the composition. The separation of high-valent and bivalent octahedral cations between M and D sites was reported [99C1]. The number of D cations per Si_{16} can vary continuously from 0 to 2.

Andremeyerite, $BaFe(Fe,Mn,Mg)Si_2O_7$

The first crystal study of andremeyerite shows that the silicate crystallizes in $P2_1/c$ space group and the crystals show multiple (100) twinning [73S1]. Later on, in [88C1] the monoclinic-type lattice was confirmed. The pseudo-orthorhombic lattice parameters (transformation matrix 201/010/001) were also given - Table 3. The atomic positions are related by a pseudo-symmetry in the space group Bmcb as shown by the [001] projection of

the crystal structure - Fig. 6. Apart from the real monoclinic symmetry elements (i.e., the (010) c glide planes and the [010] screw axes, which separately relate the A and B sites of Si, O1, O2 and O3 atoms), Fig. 6 shows the additional pseudo-elements of symmetry that relate A sites to B sites – in particular, the (100) mirror plane on which the Ba and O4 atoms lie on the two sets of diad axes, one parallel to c through the Fe1 sites and the other parallel to [201] (orthorhombic a) through the Fe2 sites. The Si_2O_7 groups are held together by Fe and Ba cations; each of these is connected to the oxygens of four differing silicate radicals. The atomic arrangement in Si_2O_7 is near to an ideal, in which the atoms of the paired tetrahedra are related by $\text{mm}2$ symmetry. The Fe atoms lie in two independent sites whose coordinations with oxygens from the Si_2O_7 groups show some differences. Fe1 is bonded to four oxygens, which are arranged at the vertices of markedly flattened tetrahedron. If one neglects the fifth greatest bond distance, Fe2 shows a tetrahedral coordination, which is more regular than that around Fe1. However, when also considering the fifth bond, the Fe2 polyhedron becomes a distorted trigonal dipyramid. Alternate Fe1 and Fe2 polyhedra connected by O3A and O3B vertices form sets of chains running along [010]. Each Si_2O_7 group bridges four of these chains and shares all its oxygens but O4. In this way, a three-dimensional tetrahedral framework is formed and Ba occupies its cavities between four Si_2O_7 groups - Fig. 6. The Ba polyhedron approximates a trigonal prism with a centered lateral face. The crystal structure of andremeyerite, resembles to some extent a barylite [70C1, 77R1] - section 8.1.2.3. For instance, the scheme of the connections between the chains of the Be tetrahedra and the Si_2O_7 group is analogous to that between the chains of the Fe tetrahedra and silicate radicals in andremeyerite. However, because of a different topological arrangement of its atoms, the space group and the cell dimensions of barylite are not comparable with those of andremeyerite [88C1].

Taikanite, $(\text{Ba}, \text{Sr})_3\text{Mn}_2^{3+}\text{O}_2[\text{Si}_4\text{O}_{12}]$

In the original description of taikanite [85K1], the idealized formula $\text{Sr}_3\text{BaMn}_2\text{Si}_4\text{O}_{14}$ was given. The silicate was shown to crystallize in a monoclinic lattice having space group $\text{C}2/\text{m}$ [85K1, 87H1]. In [93A1] was shown that the silicate $\text{BaSr}_2\text{Mn}_2^{3+}\text{O}_2[\text{Si}_4\text{O}_{12}]$ is identical to taikanite and attributed the space group $\text{C}2$. The taikanite structure is composed of zig-zag chains of edge-sharing Mn^{3+}O_6 octahedra running parallel to [001] in which shared edges within each octahedron are connected in a semiadjoined way [93A1]. This type of arrangement was referred as a *cis-cis*-type. These octahedral chains are interwoven with undulating “vierer” single chains $[\text{Si}_4\text{O}_{12}]$ running parallel to [010]. Si1 tetrahedra share two corners with MnO_6 tetrahedra. Two types of channels occur along [001]. The larger channels are occupied by eightfold-coordinated Ba and the smaller ones by eightfold-coordinated Sr. The Mn^{3+}O_6 octahedra are strongly distorted. The Mn2 octahedron has four short and two long $\text{Mn}^{3+}\text{-O}$ distances leading to an elongated octahedron. The Mn1 octahedron has four intermediate and two short $\text{Mn}^{3+}\text{-O}$ bonds (compressed pseudotetragonal). Both octahedral distortions are in agreement with bond valence requirement dictated by the structural topology and by Jahn-Teller effect [93A1].

The synthetic silicate $\text{Ca}_3\text{Mn}_2^{3+}\text{O}_2[\text{Si}_4\text{O}_{12}]$ [77A1] was shown to have a related structure to that of $\text{BaSr}_2\text{Mn}_2^{3+}\text{O}_2[\text{Si}_4\text{O}_{12}]$ [93A1]. For crystal structures of nenadkevichite-labuntsovite see [76O2, 00Y1]. For crystal structure of fersmanite see [90Y1]. The lattice parameters are also given in Table 3.

Lamprophyllite, $(\text{Na}, \text{Ca})(\text{Na}, \text{Mn})_2(\text{Sr}, \text{Ba})_2\text{Ti}_3(\text{Si}_2\text{O}_7)_2(\text{O}, \text{OH}, \text{F})_4$; barytolamprophyllite, $\text{Na}_6\text{Ba}_3\text{Ti}_7\text{O}_4(\text{Si}_2\text{O}_7)_4(\text{F}, \text{OH}, \text{O})_4$

Lamprophyllite crystallizes in a monoclinic structure with $\text{C}2/\text{m}$ space group [83S1]. The above report corrected a previously proposed structure [64W1]. According to [83S1] the structure of lamprophyllite consists of three layer stacks parallel to (100) - Fig. 7a. The solid core of the stack is made of three kinds of octahedra - Fig. 7b. Threaded onto the rotation axis 2_y at the level $z = 0$ is a chain of alternating M2 (Na, Ca) and M4 (Ti, Fe) octahedra, while at the level $z = 1/2$ is a chain of M3 (Na, Mn, Ca, Fe) octahedra. The octahedra are linked into a wall along shared edges. The M2 octahedron is slightly larger than the M3 octahedron. The core of the stack is dressed on both sides in an anionic Ti, Si chain mail - Fig. 7c. Two Si tetrahedra, related by a mirror plane, form the diorthogroup Si_2O_7 . The Ti is in 5-fold coordination. The shape of the M1 polyhedron can be described as follows: six oxygen atoms, lying in one plane, form a hexagon that is slightly removed from the cation; a tetragon, on one side of the plane and an O6 atom, on the other side, complete the coordination of M1.

The presence of strontium free lamprophyllite was reported [98L1]. As for lamprophyllite, the above silicate crystallizes in a monoclinic lattice having space group C2/m.

Barytolamprophyllite is the Ba analogue of lamprophyllite. The silicate crystallizes into a monoclinic lattice having space group Cm or C2/m [65P1, 66F1].

Ericssonite, $\text{BaFeMn}_2\text{O}(\text{Si}_2\text{O}_7)(\text{OH})$; orthoericssonite, $(\text{Ba},\text{Sr})(\text{Fe},\text{Ti})(\text{Mn},\text{Fe})\text{Si}_2\text{O}_7(\text{O},\text{OH})_2$

The orthoericssonite silicate crystallizes in a orthorhombic-type lattice having space group Pnmm [71M1]. Ericssonite is monoclinic with space group C2/m. The crystal structure is closely related to lamprophyllite and barytolamprophyllite [66F1].

Bafertisite, $\text{Ba}(\text{Fe},\text{Mn})_2\text{Ti}(\text{Si}_2\text{O}_7(\text{O},\text{OH},\text{F}))_2$

The composition and crystal structure of bafertisite have been determined by various groups [59S1, 63P1, 65S1, 71G2, 72F1]. The silicate belongs to the sorosilicates characterized by double tetrahedral group $(\text{Si}_2\text{O}_7)^{6-}$, and crystallizes in space group C2/m. The crystal structure is shown in Fig. 8. A three-layer packet unbounded in two dimensions consists of a central layer of the Fe-octahedra surrounded by heterogeneous layers of the paired Si-tetrahedra and Ti-octahedra [63P1]. Ba atoms lie between these packets. The vertices of the Ti-octahedra penetrate somewhat into the space between layers. There are two kinds of Fe sites: Fe1 and Fe2-octahedra. Since a perfect crystal of bafertisite was not available and heavy atoms as Ba exist in bafertisite, the atom parameters obtained by [63P1] were not accurate. According to [98S1], Fe1 and Fe2 sites largely deviate from the perfect octahedron and the Fe2 sites are much more distorted than the Fe1 sites.

Delindeite, $(\text{Na},\text{K})_{2.7}(\text{Ba},\text{Ca})_4\text{Ti}_6\text{Si}_8\text{O}_{26}(\text{OH})_{14}$

The silicate delindeite crystallizes in a monoclinic cell having space group C2/m [87A1].

8.1.2.5.2 Nuclear gamma resonance (NGR) data

Bafertisite

According to [82K1], the ^{57}Fe NGR spectra of bafertisite were fitted assuming three Fe^{2+} doublets. These were assigned to Fe1, Fe2 and Ti sites. They concluded that 6% of the total iron occupy Ti sites. Later on, only the presence of two doublets was considered, in agreement with two types of Fe sites present in the structure [98S1] - Fig. 9. The doublet with smaller quadrupole splitting, ΔQ , was assigned to Fe2 sites and that with higher ΔQ values to Fe1 sites. The isomer shifts, at 95 K, are by ~ 0.1 mm/s larger than those at 298 K - Table 4. This behaviour was ascribed to a second order Doppler effect. The ΔQ values, at 95 K, increase by ~ 0.3 mm/s as compared with those at 298 K. No magnetic hyperfine splitting was observed at $T = 77$ K, showing that the magnetic ordering temperature is lower than above mentioned. We note that the possible presence of Fe^{2+} in the Ti sites could not be excluded, as reported in [82K1].

8.1.2.5.3 Nuclear magnetic resonance (NMR) data

Nenadkevichite

The ^{29}Si solid state MAS NMR spectra of synthetic nenadkevichite having molar ratios Ti/Nb = 0.8; 2.0; 4.1 and 12.3 were analyzed [96R2]. The main peak at $\delta \cong -90.8$ ppm shows the presence of Si (2Si, 2Ti) environments [95A1]. When increasing the Ti content, a second fainter peak grows at $\delta \cong -96$ ppm. The assignment of this resonance is not conclusive, although the resonance intensity increases upon Na^+ -ion exchange. The ^{93}Nb MAS NMR spectra display a single resonance at $\delta \cong 0$, as referred to Nb_2O_5 , consistent with the presence of six-coordinated niobium. The sideband MAS NMR pattern associated with this resonance indicates that the local niobium environment in nenadkevichite is more distorted than in Nb_2O_5 .

8.1.2.5.4 Optical properties

Ilmajokite

An infrared study showed the presence of both OH groups and molecular water [72B1, 73F1].

Nenadkevichite

The Raman spectra of the Ti/Nb = 0.8 synthetic nenadkevichite - Fig. 10 - displays two main bands at 668 and 226 cm^{-1} which was attributed to NbO_6 octahedra [96R2]. With increasing Ti content, the Raman contribution of these bands decrease dramatically while simultaneously two other strong bands grow at $\approx 764 \text{ cm}^{-1}$ and 290 cm^{-1} . These bands were assigned to TiO_6 octahedra. The bands at 940, 878 and 520 cm^{-1} also increase in intensity. In [96R2] these bands were compared with those of niobium silicate glasses [88F1] and titanosilicate glasses [92F1]. It was concluded that octahedral Nb^{5+} is substituted by octahedral Ti^{4+} in the framework of synthetic nenadkevichite.

The UV diffuse reflectance spectra confirmed that titanium is in octahedral environment [96R2].

The IR studies were performed on labuntsovites as korobitsynite [99P1], tsepinite-Na [01S1], kuzmenkoite-Zn [02C2], lemmleinite-Ba [01C1], organovaite-Zn [02P1], organovaite-Mn [01C3], lepkhenelmitite-Zn [04P1], alsakharovite-Zn [03P2], neskevaaraite-Fe [03C1].

The refractive indices for some silicates are given in Table 5.

Tables and figures

Table 1.

a) Silicate minerals from groups VIIIB09 – VIIIB10 [91N1].

Silicate	Ideal composition	Group
Götzenite	$(\text{Ca}, \text{Na})_6\text{Ti}(\text{Si}_2\text{O}_7)_2(\text{F}, \text{OH}, \text{O})_4$	VIIIB09
Rosenbuschite	$(\text{Ca}, \text{Na})_6\text{TiZr}(\text{Si}_2\text{O}_7)_2(\text{F}, \text{OH})_4$	VIIIB09
Seidozerite	$(\text{Na}, \text{Ca})_4\text{MnTiZr}(\text{Si}_2\text{O}_7)_2\text{O}_2(\text{F}, \text{OH})_2$	VIIIB09
Fersmanite	$(\text{Ca}, \text{Na})_8(\text{Ti}, \text{Nb})_4(\text{Si}_2\text{O}_7)_8\text{O}_8\text{F}_3$	VIIIB09
Rinkite	$(\text{Na}, \text{Ca})_3(\text{Ca}, \text{Ce})_4\text{Ti}_4(\text{Si}_2\text{O}_7)_2(\text{O}, \text{F})_4$	VIIIB09
Nacareniobsite-(Ce)	$\text{Na}_3\text{Ca}_3(\text{Ce}, \text{La})\text{Nb}(\text{Si}_2\text{O}_7)_2\text{OF}_3$	VIIIB09
Mosandrite	$(\text{Ca}, \text{Na}, \text{Ce})_{12}(\text{Ti}, \text{Zr})_2\text{Si}_7\text{O}_{25}(\text{OH})_6\text{F}_4$	VIIIB09
Ilmajokite	$(\text{Na}, \text{Ce}, \text{Ba})_{10}\text{Ti}_5\text{Si}_{14}\text{O}_{22}(\text{OH})_{44} \cdot n\text{H}_2\text{O}$	VIIIB09
Laplandite-(Ce)	$\text{Na}_4\text{CeTiPSi}_7\text{O}_{22} \cdot 5\text{H}_2\text{O}$	VIIIB09
Zirsinalite	$\text{Na}_6(\text{Ca}, \text{Mn}, \text{Fe})\text{ZrSi}_6\text{O}_{18}$	VIIIB09
Labuntsovite	$\text{A}_4\text{B}_4\text{C}_4\text{D}_2\text{M}_8(\text{T}_4\text{O}_{12})_4(\text{OH}, \text{O})_8 \cdot n\text{H}_2\text{O}$ [02C1] T = Si; M = Ti, Nb; D a small bivalent cation (Mn^{2+} , Fe^{2+} , Mg^{2+} , Zn^{2+}); A = Na; B = K and sometimes with minor Na; C = Ba, K	VIIIB09
Nenadkevichite ¹⁾	$\text{A}_6\text{M}_4(\text{T}_4\text{O}_{12})_2(\text{O}, \text{OH})_4 \cdot n\text{H}_2\text{O}$	VIIIB11
Andremeyerite	$\text{BaFe}(\text{Fe}, \text{Mn}, \text{Mg})\text{Si}_2\text{O}_7$	VIIIB10
Taikanite	$(\text{Sr}, \text{Ba})_4\text{Mn}_2(\text{Si}_2\text{O}_7)_2$ ²⁾	VIIIB10
Lamprophyllite	$(\text{Na}, \text{Ca})(\text{Na}, \text{Mn})_2(\text{Sr}, \text{Ba})_2\text{Ti}_3(\text{Si}_2\text{O}_7)_2(\text{O}, \text{OH}, \text{F})_4$	VIIIB10
Barytolamprophyllite	$\text{Na}_6\text{Ba}_3\text{Ti}_7\text{O}_4(\text{Si}_2\text{O}_7)_4(\text{F}, \text{OH}, \text{O})_4$	VIIIB10
Ericssonite	$\text{BaFeMn}_2\text{O}(\text{Si}_2\text{O}_7)\text{OH}$	VIIIB10
Orthoericssonite	$(\text{Ba}, \text{Sr})(\text{Fe}, \text{Ti})(\text{Mn}, \text{Fe})\text{Si}_2\text{O}_7(\text{O}, \text{OH})_2$	VIIIB10
Bafertisite	$\text{Ba}(\text{Fe}, \text{Mn})_2\text{Ti}(\text{Si}_2\text{O}_7)(\text{O}, \text{OH}, \text{F})_2$	VIIIB10
Delindeite	$(\text{Na}, \text{K})_{2.7}(\text{Ba}, \text{Ca})_4\text{Ti}_6\text{Si}_8\text{O}_{26}(\text{OH})_{14}$	VIIIB10
Synthetic silicate	$\text{Ca}_3\text{Mn}_2^{3+}\text{O}_2[\text{Si}_4\text{O}_{12}]$	

¹⁾ According to [02C1] the nenadkevichite was included in the labuntsovite group.

²⁾ According to [93A1] formula is $\text{BaSr}_2\text{Mn}_2^{3+}\text{O}_2[\text{Si}_4\text{O}_{12}]$

Table 1 (continued)

b) Labuntsovite group of minerals [02C1].

Silicate	Idealized formula	Ideal occupancy of		Space group	Number of non-equivalent extra-framework cation sites	Refs.
		C-site	D-site			
<i>Nenadkevichite subgroup</i>	$A_6M_4(Si_4O_{12})_2(O,OH)_4 \cdot nH_2O$	absent	absent		2	
Nenadkevichite	$Na_{8-x}Nb_4(Si_4O_{12})(O,OH)_4 \cdot nH_2O$			Pbam		55K1, 73P1
Korobitsynite	$Na_{8-x}Ti_4(Si_4O_{12})(O,OH)_4 \cdot nH_2O$ ³⁾			Pbam		97R1, 99P1
<i>Vuoriyarvite subgroup</i>	$A_{12-x}\square_2M_8(Si_4O_{12})_4(O,OH)_8 \cdot nH_2O$	vacant	vacant		numerous split (> 3)	
Vuoriyarvite-K	$(K,Na)_{12-x}Nb_8(Si_4O_{12})_4O_8 \cdot nH_2O$ (x = 0...6; n = 12...16)			Cm		94R1, 98S2
Tsepenite-Na	$(Na,H_3O,K,Sr,Ba)_{12-x}Ti_8[Si_4O_{12}]_4(OH,O)_8 \cdot nH_2O$; (x = 0...6; n = 12...16)			Cm		01S1
Tsepenite-K ²⁾	$(K,Ba,Na)_2(Ti,Nb)_2(Si_4O_{12})(OH,O)_2 \cdot 3H_2O$			Cm		03C1
Tsepenite-Ca ²⁾	$(Ca,K,Na,\square)_2(Ti,Nb)_2(Si_4O_{12})(OH,O)_2 \cdot 4H_2O$			C2/m		03P1
<i>Paratsepenite subgroup</i>	$A_2B_2C_2M_4(Si_4O_{12})_2(O,OH)_4 \cdot nH_2O$	occupied	vacant			
Paratsepenite-Ba ²⁾	$(Ba,Na,K)_{2-x}(Ti,Nb)_2(Si_4O_{12})(OH,O)_2 \cdot 4H_2O$			C2/m		03C1
Paratsepenite-Na ²⁾	$(Na,B,K)_{2-x}(Ti,Nb)(Si_4O_{12})(OH,O)_2 \cdot 4H_2O$			C2/m		
<i>Kuzmenkoite subgroup</i>	$K_4\square_4D_2M_8(Si_4O_{12})_4(OH,O)_8 \cdot nH_2O$	vacant	occupied		2	
Kuzmenkoite-Mn	$K_4Mn_2Ti_8(Si_4O_{12})_4(OH)_8 \cdot nH_2O$; (n = 10...12)			C2/m or Cm		98G1, 99C2
Kuzmenkoite-Zn	$K_4Zn_2Ti_8(Si_4O_{12})_4(OH)_8 \cdot nH_2O$; (n = 12...17)			Cm		02C2
Karupmöllerite	$\square_4\square_4D_2M_8(Si_4O_{12})_4(OH,O)_8 \cdot nH_2O$	vacant	occupied		2	
	$(Na,Ca,K)_4Ca_2Nb_8(Si_4O_{12})_4(O,OH)_8 \cdot 14H_2O$			C2/m		01Y1, 02P3
Lepkhenelmitite-Zn ²⁾	$Ba_2Zn(Ti,Nb)_4(Si_4O_{12})_2(O,OH)_4 \cdot 7H_2O$			Cm		04P1
<i>Lemleinite subgroup</i>	$Na_4K_4C_4\square_2M_8(Si_4O_{12})_4(O,OH)_8 \cdot nH_2O$	occupied	vacant		3	
Lemleinite-K	$Na_4K_4K_4Ti_8(Si_4O_{12})_4(O,OH)_8 \cdot 8H_2O$			C2/m		99K1
Lemleinite-Ba	$Na_4K_4Ba_{2+x}Ti_8(Si_4O_{12})_4(O,OH)_8 \cdot 8H_2O$			C2/m		96R1

Table 1 (continued)

Silicate	Idealized formula	Ideal occupancy of		Space group	Number of non-equivalent extra-framework cation sites	Refs.
		C-site	D-site			
<i>Labuntsovite subgroup</i>	$\text{Na}_4\text{K}_4\text{D}_2\text{M}_8(\text{Si}_4\text{O}_{12})_4(\text{OH},\text{O})_8 \cdot n\text{H}_2\text{O}$	vacant	occupied or vacant	C2/m	3	55S1, 81O1 01K1 01K1
Labuntsovite-Mn	$\text{Na}_4\text{K}_4\text{Mn}_2\text{Ti}_8(\text{Si}_4\text{O}_{12})_4(\text{O},\text{OH})_8 \cdot n\text{H}_2\text{O}$; (n = 10...12)					
Labuntsovite-Mg	$\text{Na}_4\text{K}_4\text{Mg}_2\text{Ti}_8(\text{Si}_4\text{O}_{12})_4(\text{O},\text{OH})_8 \cdot n\text{H}_2\text{O}$; (n = 10...12)					
Labuntsovite-Fe	$\text{Na}_4\text{K}_4\text{Fe}_2\text{Ti}_8(\text{Si}_4\text{O}_{12})_4(\text{O},\text{OH})_8 \cdot n\text{H}_2\text{O}$; (n = 10...12)					
<i>Paralabuntsovite subgroup</i>	$\text{Na}_8\text{K}_8\text{D}_4\text{M}_{16}(\text{Si}_4\text{O}_{12})_8(\text{O},\text{OH})_{16} \cdot n\text{H}_2\text{O}$	vacant	occupied or vacant	I2/m	3	58M1
Paralabuntsovite-Mg	$\text{Na}_8\text{K}_8\text{Mg}_4\text{Ti}_{16}(\text{Si}_4\text{O}_{12})_8(\text{O},\text{OH})_{16} \cdot n\text{H}_2\text{O}$; (n = 20...24)					
<i>Organovaite subgroup</i>	$\text{K}_8\text{D}_4\text{M}_{16}(\text{Si}_4\text{O}_{12})_8(\text{OH},\text{O})_{16} \cdot n\text{H}_2\text{O}$	vacant	vacant	C2/m	2	01C3 02P1 01C2
Organovaite-Mn	$\text{K}_8\text{Mn}_4\text{Nb}_{16}(\text{Si}_4\text{O}_{12})_8\text{O}_{16} \cdot n\text{H}_2\text{O}$; (n = 20...28)					
Organovaite-Zn	$\text{K}_8\text{Zn}_4\text{Nb}_{16}(\text{Si}_4\text{O}_{12})_8\text{O}_{16} \cdot n\text{H}_2\text{O}$; (n = 20...28)					
Parakuzmenkoite-Fe	$(\text{K},\text{Ba})_8\text{Fe}_4\text{Ti}_{16}(\text{Si}_4\text{O}_{12})_8(\text{OH},\text{O})_{16} \cdot n\text{H}_2\text{O}$; (n = 20...28)					
<i>Gutkovaite subgroup</i>	$\text{Ca}_2\Box_2\text{K}_4\text{D}_4\text{M}_8(\text{Si}_4\text{O}_{12})_4(\text{OH},\text{O})_8 \cdot n\text{H}_2\text{O}$	vacant	occupied	Cm	4	02P2
Gutkovaite-Mn	$\text{Ca}_2\text{K}_4\text{Mn}_2\text{Ti}_8(\text{Si}_4\text{O}_{12})_4\text{O}_8 \cdot n\text{H}_2\text{O}$; (n ≈ 10)					
Alsakharovite-Zn ²⁾	$\text{NaSrKZn}(\text{Ti},\text{Nb})_4(\text{Si}_4\text{O}_{12})_2(\text{O},\text{OH})_4 \cdot 6\text{H}_2\text{O}$			Cm		03P2
Neskevaaraite-Fe ²⁾	$\text{NaK}_3\text{Fe}(\text{Ti},\text{Nb})_4(\text{Si}_4\text{O}_{12})_2(\text{O},\text{OH})_4 \cdot 6\text{H}_2\text{O}$			Cm		03C1

¹⁾ The idealized formula of silicates were given after [02C1]; ²⁾ for these silicates the idealized formula was given according to original papers supplied by Dr. N.V. Chukanov; ³⁾ In [99P1] reported composition $\text{Na}_{3-x}(\text{Ti},\text{Nb})_2[\text{Si}_4\text{O}_{12}](\text{O},\text{OH})_2 \cdot 3 \dots 4\text{H}_2\text{O}$.

Table 2. Atomic coordinates and thermal parameters.a) Götzenite, $\text{Ca}_4(\text{Ca}_{1.2}\text{Na}_{0.8})\text{NaTi}(\text{Si}_2\text{O}_7)_2(\text{F},\text{OH},\text{O})_4$, having triclinic structure, space group $\text{P}\bar{1}$ [72C1].

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{eq} [Å ²]
Ca1	0.6389(7)	0.2115(11)	0.9097(8)	0.07(14)
Ca2	0.9859(8)	0.4955(15)	0.2418(12)	0.57(13)
Ca3	0.6305(7)	0.2268(11)	0.4075(9)	0.17(15)
Na	0.0	0.0	0.5	1.21(47)
Ti	0.0	0.0	0.0	0.93(27)
Si1	0.7197(6)	0.7475(11)	0.6460(14)	0.74(14)
Si2	0.7210(6)	0.7471(10)	0.2100(12)	0.27(12)
O1	0.762(2)	0.784(4)	0.443(3)	2.33(35)
O2	0.619(2)	0.927(3)	0.673(3)	0.02(28)
O3	0.614(2)	0.925(4)	0.127(3)	1.45(43)
O4	0.636(2)	0.472(4)	0.665(3)	2.09(41)
O5	0.676(2)	0.465(3)	0.162(3)	1.09(32)
O6	0.879(2)	0.819(3)	0.778(3)	1.72(30)
O7	0.881(2)	0.830(3)	0.171(3)	1.47(28)
O8	0.884(2)	0.256(3)	0.969(3)	0.28(29)
O9=F	0.890(2)	0.313(3)	0.475(3)	0.53(32)

b) Fersmanite⁶⁾ having monoclinic unit cell, space group B2/b [84S1].

Atom	Multiplicity	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{eq} [Å ²]
Ti1	9.4(2)	0.1083(1)	0.18702(5)	0.0629(1)	0.78(3)
Ti2	9.4(2)	0.1401(1)	0.31278(5)	0.3110(1)	0.70(3)
Ca1	7.2(3)	0.1690(2)	0.4363(1)	0.0650(2)	1.72(5)
Ca2	7.2(3)	0.4233(2)	0.4333(1)	0.8099(2)	1.75(6)
Na1	10.1(4)	0.3847(2)	0.3055(1)	0.0585(2)	1.80(7)
Na2	10.1(4)	0.1426(2)	0.3057(1)	0.8166(2)	1.85(7)
Si1	8	0.4312(2)	0.4169(1)	0.2980(2)	1.52(6)
Si2	8	0.6530(2)	0.4174(1)	0.0761(2)	1.67(6)
O1	8	0.2898(6)	0.3823(3)	0.2424(6)	2.71(18)
O2	8	0.4780(6)	0.3823(3)	0.4322(6)	2.88(20)
O3	8	0.4358(6)	0.4938(3)	0.3113(6)	3.21(21)
O4	8	0.5366(6)	0.3978(3)	0.1879(6)	3.17(21)
O5	8	0.5874(6)	0.3812(3)	0.9429(6)	2.72(19)
O6	8	0.6843(6)	0.4939(3)	0.0640(6)	3.34(23)
O7	8	0.7779(6)	0.3817(3)	0.1326(6)	2.88(20)
O8	8	0.2409(5)	0.2161(3)	0.9365(6)	2.24(19)
O9	8	0.1915(5)	0.2500(3)	0.1871(5)	2.26(17)
O10	8	−0.0257(6)	0.1472(3)	0.1870(5)	2.19(17)
O11	4	0	1/4	0.9951(8)	2.19(25)
O12	4	0	1/4	0.3782(8)	2.06(24)
F1	8	0.2792(5)	0.3690(3)	0.9390(5)	1.78(16)
F2	4	0	1/4	0.6866(8)	2.09(23)

⁶⁾ for composition see footnote in Table 3.

Table 2 (continued)c) Rinkite⁸⁾ having monoclinic structure, space group $P2_1/c$ [71G1].

Atom	x	y	z	$\beta_{ij} \cdot 10^4$					
				β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
M1	0.0000	0.0000	0.0000	27(3)	286(36)	13(1)	−23(4)	6(1)	−40(2)
M2	0.5000	0.0000	0.0000	99(11)	162(45)	4(2)	2(13)	1(3)	−6(5)
M3	0.7500(5)	0.5012(9)	0.0004(2)	86(7)	97(40)	21(1)	6(8)	10(2)	16(3)
M4	0.0938(2)	0.6605(3)	0.1918(1)	38(2)	113(34)	10(1)	0(2)	3(1)	4(1)
M5	0.5969(2)	0.6630(3)	0.1902(1)	54(2)	190(34)	11(1)	3(3)	5(1)	3(1)
Si1	0.3515(4)	0.1541(7)	0.1403(2)	39(5)	132(38)	6(1)	−3(6)	1(1)	−1(2)
Si2	0.7831(4)	0.1530(7)	0.1379(1)	41(5)	109(37)	6(1)	−7(6)	3(1)	1(2)
O1	0.2172(11)	0.1488(17)	0.0609(4)	93(14)	122(51)	11(2)	−19(17)	−8(4)	1(7)
O2	0.8306(11)	0.1410(19)	0.0578(4)	88(14)	289(55)	8(2)	15(19)	7(4)	9(7)
O3	0.3379(11)	0.3971(17)	0.1849(5)	86	16	21	5	15	−15
O4	0.8436(12)	0.3949(18)	0.1797(5)	89(15)	125(54)	22(3)	−16(18)	13(5)	−22(8)
O5	0.3355(11)	0.9311(18)	0.1918(4)	87(14)	139(59)	11(2)	14(17)	7(4)	3(7)
O6	0.8559(11)	0.9365(17)	0.1903(4)	87(15)	116(51)	12(2)	6(17)	3(5)	5(7)
O7	0.5581(11)	0.1413(20)	0.1206(5)	70(14)	324(57)	15(3)	2(2)	7(5)	−14(8)
OF(1)	0.0308(10)	0.7052(17)	0.0617(4)	115(14)	296(53)	14(2)	−41(18)	6(4)	0(7)
OF(2)	0.5303(11)	0.6546(16)	0.0642(4)	156(16)	155(51)	14(2)	17(19)	8(5)	3(7)

⁸⁾ for composition see footnote in Table 3.d) Nenadkevichite¹⁰⁾, having orthorhombic-type structure, space group $Pbam$ [73P1].

Atom	Site	x	y	z	$B_{eq} [\text{\AA}^2]$	Occupation
Nb ⁵⁺	4h	0.28640(7)	0.25956(3)	1/2	0.62	0.986(2)
Na1	4g	0.2586(7)	0.2500(4)	0	1.92	0.526(9)
Na2	4h	0.1952(9)	0.0227(5)	1/2	3.13	0.54(1)
Si ⁴⁺	8i	0.0085(1)	0.38978(5)	0.2247(1)	0.63	1 ^{a)}
O1	4g	0.0091(8)	0.3820(3)	0	1.76	1 ^{a)}
O2	4f	0.0	1/2	0.2854(6)	2.17	1 ^{a)}
O3	8i	0.1922(4)	0.3449(2)	0.3039(4)	1.47	1 ^{a)}
O4	8i	0.3316(4)	0.1619(2)	0.3044(4)	1.41	1 ^{a)}
O5	4h	0.0131(4)	0.1983(2)	1/2	0.81	1 ^{a)}
H ₂ O1	4g	0.015(2)	0.1609(6)	0	5.51	1.02(2)
H ₂ O2	4e	0.0	0	0.267(2)	6.54	1.01(2)

¹⁰⁾ for composition see footnote in Table 3;^{a)} fixed value.

Table 2 (continued)e) Vuoriharvite-K¹³⁾ having monoclinic structure, space group Cm [94R1].

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{eq} [Å ²]	Site occupancy
Si1	0.2170(5)	0.8920(3)	0.7800(9)	1.5(1)	1
Si2	0.6918(7)	0.8916(5)	0.736(1)	2.0(1)	1
Si3	0.8055(5)	0.8901(3)	0.186(1)	0.9(1)	1
Si4	0.3287(5)	0.8914(5)	0.230(1)	1.0(1)	1
M1	0.0 ^{a)}	0.7691(1)	0.5 ^{a)}	0.32(4)	1
M2	0.7434(3)	0.7480(1)	0.4644(6)	0.53(4)	1
K1	0.5001(9)	0.8194(4)	0.983(2)	3.4(1)	0.76(1)
K2	0.432(2)	0.0	0.705(3)	6.8(3)	0.53(2)
K3	0.910(2)	0.0	0.648(4)	3.0(5)	0.44(2)
K4	0.081(2)	0.0	0.288(3)	3.7(3)	0.49(2)
Na1	0.009(2)	0.0	0.468(3)	1.9(5)	0.58(3)
Na2	0.796(6)	0.0	0.529(10)	8.8(6)	0.39(5)
Na3	0.006(9)	0.0	0.109(16)	13.9(1.1)	0.25(5)
O1	0.911(2)	0.766(1)	0.586(3)	3.2(1)	1
O2	0.925(1)	0.873(3)	0.308(2)	1.8(3)	1
O3	0.268(1)	0.867(1)	0.341(2)	1.7(3)	1
O4	0.274(2)	0.823(1)	0.702(3)	3.3(4)	1
O5	0.429(1)	0.8256(8)	0.285(2)	1.4(3)	1
O6	0.375(2)	0.0	0.280(4)	2.9(5)	1
O7	0.2512(8)	0.879(1)	0.003(2)	2.0(4)	1
O8	0.227(2)	0.0	0.730(4)	1.8(5)	1
O9	0.104(1)	0.7682(8)	0.372(2)	0.6(2)	1
O10	0.092(1)	0.870(1)	0.665(2)	2.3(4)	1
O11	0.747(1)	0.8652(9)	0.601(2)	2.1(3)	1
O12	0.732(1)	0.8244(8)	0.245(2)	0.9(2)	1
O13	0.591(1)	0.826(1)	0.672(2)	2.3(4)	1
O14	0.656(2)	0.0	0.711(3)	1.5(4)	1
O15	0.771(1)	0.872(1)	0.956(2)	2.9(4)	1
O16	0.777(2)	0.0	0.204(4)	1.7(5)	1
H ₂ O1	0.030(2)	0.880(2)	0.982(4)	2.7(6)	0.56(3)
H ₂ O2	0.564(4)	0.0	0.212(8)	4.2(1.0)	0.61(5)
H ₂ O3	0.299(6)	0.0	0.513(1)	2.6(1.8)	0.32(5)
H ₂ O4	0.036(5)	0.872(5)	0.025(11)	12.5(1.4)	0.37(5)
H ₂ O5	0.514(7)	0.0	0.891(13)	6.1(1.9)	0.36(6)

¹³⁾ for composition see footnote in Table 3; in original paper was named K-rich nenadkevichite;^{a)} chosen to fix the origin in space group Cm.

Table 2 (continued)f) Andremeyerite³⁰⁾ having monoclinic unit cell, space group $P2_1/c$ [88C1].

Atom	<i>x</i>	<i>y</i>	<i>z</i>	Site population	$B_{eq} [\text{\AA}^2]$
Ba	0.4893(1)	0.1434(0)	0.2940(1)	Ba 1.00	0.96(1)
Fe1	−0.0024(2)	0.2439(1)	0.3058(2)	Fe 1.0	0.78(3)
Fe2	−0.0380(2)	0.5016(1)	0.2115(2)	Fe 0.92; Mg 0.08 ^{a)}	0.86(4)
Si A	0.2765(3)	0.3908(2)	0.2023(4)		0.75(6)
Si B	0.7241(3)	0.3833(2)	0.3877(4)		0.65(6)
O1 A	0.2262(9)	0.5001(5)	0.1055(9)		1.04(16)
O1 B	0.7251(10)	0.4833(5)	0.2737(11)		1.39(19)
O2 A	0.2573(9)	0.3118(5)	0.0249(10)		1.17(17)
O2 B	0.7270(9)	0.2903(5)	0.2481(11)		1.34(19)
O3 A	0.1229(9)	0.3714(4)	0.3016(11)		1.21(18)
O3 B	0.9090(9)	0.3763(5)	0.6290(10)		1.24(17)
O4	0.5104(8)	0.3784(4)	0.4021(9)		0.76(15)

³⁰⁾ for composition see footnote in Table 3;^{a)} The site population in Fe2 could also be due to 0.07 Mg, 0.08 Mn and 0.85 Fe determined with microprobe analysis.g) Lamprophyllite³⁴⁾ having monoclinic unit cell, space group $C2/m$ [83S1].

Atom	Multiplicity	<i>x</i>	<i>y</i>	<i>z</i>	$B_{eq} [\text{\AA}^2]$
M1(Sr,Ba,K)	4.3(1)	0.2841(1)	0.0	0.2629(3)	0.85(4)
M2(Na,Ca)	2.7(3)	0.0	0.0	0.0	1.22(26)
M3(Na,Mn,Ca,Fe)	4.7(3)	0.0	0.2591(5)	0.5	1.24(9)
M4(Ti,Fe)	2.5(2)	0.0	0.5	0.0	1.11(10)
Ti	4	0.1493(1)	0.0	0.7069(6)	0.03(4)
Si	8	0.1425(1)	0.2839(3)	0.2045(7)	0.05(5)
O1	8	0.0597(3)	0.295(1)	0.172(2)	0.34(15)
O2	8	0.1739(4)	0.189(1)	0.467(2)	0.41(16)
O3	8	0.1741(4)	0.187(1)	0.971(2)	0.63(18)
O4	4	0.1749(5)	0.50	0.217(3)	0.35(21)
O5	4	0.0621(7)	0.0	0.665(7)	0.94(31)
O,OH,F ₆	4	0.4433(7)	0.0	0.273(3)	0.86(30)

³⁴⁾ for composition see footnote in Table 3.

Table 3. Crystal structures and lattice parameters.

Silicate	<i>T</i> [K]	Space group	Lattice parameters				Refs.
			<i>a</i> [Å]	<i>b</i> [Å]	<i>c</i> [Å]	α, β, γ	
Götzenite ¹⁾	RT	$P\bar{1}$	9.667	5.731	7.334	$\alpha = 90^\circ$ $\beta = 101.05^\circ$ $\gamma = 101.31^\circ$	66S1, 72C1
Götzenite ²⁾	RT		10.93(5)	7.32(3)	5.74(3)	$\alpha = 90^\circ$ $\beta = 100(1)^\circ$ $\gamma = 120(1)^\circ$	53S1
Rosenbuschite ³⁾	RT	$P\bar{1}$	10.14	11.41	7.28	$\alpha = 91^\circ 21'$ $\beta = 99^\circ 38.5'$ $\gamma = 111^\circ 54.5'$	66S1
Seidozerite ⁴⁾	RT	Pc or P2/c	5.53(3)	7.10(4)	18.30(1)	$\beta = 102^\circ 43'$	58S1, 58S2
Fersmanite ⁵⁾	RT	P1 or $P\bar{1}$	7.210(1)	7.213(2)	20.451(3)	$\alpha = 95.13(3)^\circ$ $\beta = 95.60(2)^\circ$ $\gamma = 89.04(5)^\circ$	77M1
Fersmanite ⁶⁾	RT	B2b	10.212(6)	20.450(20)	10.198(9)	$\beta = 97.22(5)^\circ$	84S1
Ilmajokite ⁷⁾	RT	monoclinic?	≈ 23	≈ 24.4	≈ 37		72B1, 73F1
Rinkite ⁸⁾	RT	P2 ₁ /c	7.437(2)	5.664(2)	18.843(3)	$\beta = 101^\circ 23(1)'$	71G1
Rinkite ⁹⁾	RT	P2 ₁ /m or P2 ₁	18.83	5.66	7.44	$\beta = 101^\circ 22'$	66G1
Rinkite ⁹⁾	RT	monoclinic	18.47	5.67	7.46	$\beta = 91^\circ 13'$	57S2
Rinkite ⁹⁾	RT	triclinic	18.51(1)	7.45(3)	5.64(3)	$\alpha = 90^\circ$ $\beta = 91^\circ$ $\gamma = 101^\circ$	57S1
Mosandrite ⁹⁾	RT	monoclinic	18.37	5.63	7.42	$\beta = 93^\circ 4'$	57S2
Mosandrite ⁹⁾	RT	triclinic	18.45(6)	7.44(3)	5.63(2)	$\alpha = 90.2^\circ$ $\beta = 91.0^\circ$ $\gamma = 100.9^\circ$	57S1
Nenadkevichite ¹⁰⁾ (natural, Quebec)	RT	Pbam	7.408(2)	14.198(3)	7.148(2)		73P1
Korobitsynite ¹¹⁾	RT	Pbam	7.349(2)	14.164(2)	7.130(1)		99P1
Labuntsovite ¹²⁾	RT		15.57	13.74	14.25	$\beta = 116^\circ 55'$	76O1
Vuoriyarvite ¹³⁾	RT	Cm	14.692(4)	14.164(4)	7.859(3)	$\beta = 117.87(2)^\circ$	94R1
Tsepenite-Na ¹⁴⁾	RT	Cm	14.604(7)	14.274(8)	7.933(2)	$\beta = 117.40(3)^\circ$	01S1
Tsepenite-Ca ¹⁵⁾	RT	C2/m	14.484(4)	14.191(4)	7.907(2)	$\beta = 117.26(2)^\circ$	03P1
Kuzmenkoite-Mn ¹⁶⁾	RT	C2/m	14.369(3)	13.906(8)	7.812(1)	$\beta = 117.09(2)^\circ$	99C2
Kuzmenkoite-Zn ¹⁷⁾	RT	Cm	14.400	13.851	7.781	$\beta = 117.33^\circ$	02C2
Tsepenite-K ¹⁸⁾	RT	Cm	14.327(3)	13.802(2)	7.783(3)	$\beta = 116.95(1)^\circ$	03C1
Paratsepenite-Ba ¹⁹⁾	RT	C2/m	14.551(2)	14.001(2)	15.702(3)	$\beta = 117.58(1)^\circ$	03C1
Lemleinite-Ba ²⁰⁾	RT	C2/m	14.216(2)	13.755(3)	7.767(5)	$\beta = 116.7(1)^\circ$	96R1, 01C1
Organovaite-Mn ²¹⁾	RT	C2/m	14.551(2)	14.001(2)	15.702(3)	$\beta = 117.584(2)^\circ$	01C3
Organovaite-Zn ²²⁾	RT	C2/m	14.535	13.927	15.665	$\beta = 117.6^\circ$	02P1
Parakuzmenkoite ²³⁾	RT	C2/m	14.410(2)	13.880(2)	15.587(2)	$\beta = 117.53(1)^\circ$	01C2
Gutkovaite-Mn ²⁴⁾		Cm	14.30	13.889	7.760	$\beta = 117.51^\circ$	02P2
Lepkhenelmitite-Zn ²⁵⁾		Cm	14.381(3)	13.889(3)	7.793(2)	$\beta = 117.52(3)^\circ$	04P1
Karupmøllerite-Ca ²⁶⁾		C2/m	14.641(1)	14.214(1)	7.9148(2)	$\beta = 117.36(1)^\circ$	02P3
Alsakharovite-Zn ²⁷⁾		Cm	14.495(10)	13.945(10)	7.838(8)	$\beta = 117.75(7)^\circ$	03P2
Neskevaaraite-Fe ²⁸⁾		Cm	14.450(6)	13.910(6)	7.836(4)	$\beta = 117.42(1)^\circ$	03C1
Andremeyerite ²⁹⁾	RT	P2 ₁ /c	7.464(8)	13.794(5)	7.093(5)	$\beta = 118.15(10)^\circ$	73S1, 74F1

Table 3 (continued)

Silicate	<i>T</i> [K]	Space group	Lattice parameters				Refs.
			<i>a</i> [Å]	<i>b</i> [Å]	<i>c</i> [Å]	α, β, γ	
Andremeyerite ³⁰⁾	RT	P2 ₁ /c	7.488(1)	13.785(1)	7.085(1)	$\beta = 118.23(1)^\circ$	88C1
Andremeyerite ³⁰⁾	RT	pseudo-orth (Bmcb)	13.195(2)	13.785(1)	7.085(1)	$\beta = 89.99(1)^\circ$	88C1
Taikanite ³¹⁾	RT	C2/m	7.82(3)	14.60(3)	5.15(4)	$\beta = 92.50^\circ$	85K1, 87H1
Taikanite ³²⁾	RT	C2	14.600(2)	7.759(4)	5.142(1)	$\beta = 93.25(2)^\circ$	93A1
Ericssonite ³³⁾	RT	C2/m	20.46	7.03	5.34	$\beta = 95^\circ 30'$	71M1
Orthoericssonite ³³⁾	RT	Pnmm	20.37	7.03	5.34		71M1
Lamprophyllite ³⁴⁾	RT	C2/m	19.431(3)	7.086(1)	5.392(1)	$\beta = 96.75(5)^\circ$	83S1
Sr-free lamprophyllite ³⁵⁾	RT	C2/m	5.43(1)	7.12(1)	19.80(2)	$\beta = 96.4(1)^\circ$	98L1
Barytolamprophyllite ³⁶⁾	RT	Cm or C2/m	19.96(6)	7.07(2)	5.43(1)	$\beta = 96^\circ 30'$	65P1, 66F1
Bafertsite ³⁷⁾	RT	C2/m	10.98	6.80	5.36	$\beta = 94^\circ$	63P1
Barium titanosilicate ³⁸⁾	RT	P1 or P $\bar{1}$	10.764(7)	13.858(9)	32.996(6)	$\alpha = 90.2(1)^\circ$ $\beta = 94.6(1)^\circ$ $\gamma = 89.96(5)^\circ$	89S1
Delindeite ³⁹⁾	RT	C2/m	21.617(13)	6.814(5)	5.383(3)	$\beta = 94.03(5)^\circ$	87A1
Ca ₃ Mn ₂ ³⁺ O ₂ [Si ₄ O ₁₂]	RT	I2/c	14.263(28)	7.620(13)	10.025(4)	$\beta = 93.27(5)^\circ$	77A1

1) Ca₄(Ca_{1.2}Na_{0.8})NaTi(Si₂O₇)₂(F,OH,O)₄;

2) (Ca,Na)_{6.66}(Ti,Al,etc.)_{1.66}(Si₄O₁₄)(F,OH)_{3.49};

3) Ca_{3.5}Na_{2.5}(Ti,Mn)Zr(Si₂O₇)₂(O,OH,F)₄;

4) Na_{1.79}Ca_{0.19}Mn_{0.23}Mg_{0.17}Fe_{0.06}²⁺Fe_{0.13}³⁺Al_{0.10}Zr_{0.72}Ti_{0.63}Nb_{0.02}Si₂O₈(F_{0.72}O_{0.28}); the above formula should be written Na₆MnTi(Zr_{1.5}Ti_{0.5})(Si₂O₇)₂O₂(F,OH)₂;

5) (Ca,Na)₄(Ti,Nb)₂O₄(Si₂O₇)(F,OH)₂;

6) Ca_{4.72}Na_{3.28}Ti_{3.20}Nb_{0.80}(Si₂O₇)₂O₈F₃;

7) (Na_{8.8}Ba_{0.5}R_{0.7})Ti₅(Si_{13.9}Al_{0.1})O₂₂(OH)₄₄ · nH₂O;

8) Ca_{3.35}Na_{2.11}K_{0.06}Ce_{1.05}Th_{0.04}Nb_{0.33}Zr_{0.07}Ti_{0.52}Fe_{0.09}Mg_{0.08}Al_{0.09}(Si₂O₇)₂OF₃;

9) natural sample, composition not mentioned;

10) (Na_{3.76}K_{0.24}Ca_{0.11}Mn_{0.03}□_{3.86})(Nb_{2.76}Ti_{1.18}Fe_{□0.06})(O_{2.80}OH_{1.20})Si₈O₂₄ · 8H₂O;

11) (Na_{2.62}Ba_{0.02})(Ti_{1.57}Nb_{0.45})[Si₄O₁₂](OH_{1.13}O_{1.03}) · 3.4H₂O;

12) (Na_{8.79}Ca_{0.1}K_{7.31}Ba_{2.90})(Ti_{15.39}(Nb, Ta)_{0.09}Fe_{0.25}³⁺Mg_{2.20})(Si_{31.67}Al_{0.33})O₄₈ and H_{49.4}⁺;

13) Na_{0.6}K_{1.5}(Nb_{0.6}Ti_{0.4})(Nb_{0.5}Ti_{0.5})(Si₄O₁₂)(O,OH)₂ · 1.6H₂O;

14) H_{34.83}(Na_{4.21}K_{0.80}Sr_{0.54}Ba_{0.41}Ca_{0.08}Zr_{0.01})(Ti_{4.22}Nb_{3.71}Fe_{0.07}³⁺)Si₁₆O_{70.78};

15) {(Na_{1.40}K_{1.11}(H₂O_{0.35}□_{1.14})[Ba_{0.35}(H₂O)_{3.65}]}{[Ca_{0.52}Sr_{0.40}(H₂O)_{2.60}□_{0.48}][Ba_{0.19}(H₂O)_{3.81}]}{[Sr_{0.28}(H₂O)_{3.72}][Ca_{0.84}□_{3.16}]}(Ca_{0.85}Mn_{0.05}Fe_{0.01}Zn_{0.03}□_{1.06})[Ti_{6.4}Nb_{1.60}](Si_{15.98}Al_{0.02}O₄₈)[O_{3.44}(OH)_{4.56}];

16) (K_{3.43}Na_{0.46}Ba_{0.17})(Mn_{1.26}Fe_{0.36}Mg_{0.17})(Ti_{7.11}Nb_{0.81})[Si₄O₁₂]₄[(OH)_{7.70}O_{0.30}] · 9.54H₂O;

17) (K_{3.00}Ca_{0.97}Na_{0.39}Ba_{0.32}Sr_{0.05})(Zn_{1.14}Mn_{0.73}Fe_{0.19}Mg_{0.02})(Ti_{5.50}Nb_{2.35})(Si_{15.79}Al_{0.21})O₄₈[(OH)_{4.07}O_{3.93}] · 17H₂O;

18) (K_{0.86}Ba_{0.46}Na_{0.43}Mn_{0.10})(Ti_{1.66}Nb_{0.33}Fe_{0.03}³⁺)Si₄O₁₂(OH)_{1.21}O_{0.79} · 2.94H₂O;

19) (Ba_{0.46}Na_{0.37}K_{0.23}Sr_{0.12}Mn_{0.10}Ca_{0.06})(Ti_{1.40}Nb_{0.55})(Si_{3.97}Al_{0.03}O₁₂)(OH)_{1.58}O_{0.42} · 3.7H₂O;

20) Na_{4.34}K_{3.74}(Ba_{2.08}Sr_{0.03})(□_{1.07}Mn_{0.56}Mg_{0.24}Fe_{0.13})[(Ti_{7.94}Nb_{0.08}Zr_{0.02})O_{6.40}(OH)_{1.60}][Si₄O₁₂]₄ · 10.46H₂O;

21) (K_{2.27}Zn_{0.62}Ca_{0.47}Na_{0.41}Ba_{0.21})(Mn_{1.77}Fe_{0.08}²⁺)(Nb_{5.23}Ti_{2.76})[Si_{15.86}Al_{0.14}O₄₈][O_{6.03}(OH)_{1.97}] · 12.79H₂O;

22) (K_{1.93}Na_{0.52}Ca_{0.49}Ba_{0.35}Sr_{0.04})(Zn_{1.60}Mn_{0.24}Fe_{0.08}Mg_{0.06})(Nb_{4.79}Ti_{3.17})[(Si_{15.79}Al_{0.21})O₄₈][O_{4.59}(OH)_{3.41}] · 11.97H₂O;

Table 3 (continued)

- 23) $(K_{1.56}Na_{0.36}Ba_{1.47}Sr_{0.11}Ca_{0.11}Zn_{0.07})(Fe_{1.58}^{2+}Mn_{0.65}Mg_{0.09})(Ti_{4.44}Nb_{3.41}Fe_{0.16}^{3+})[Si_4O_{12}][O_{6.40}(OH)_{1.60}] \cdot 14.29H_2O$;
- 24) $(Ca_{2.00}Na_{0.14})(K_{3.24}Ba_{0.16}Sr_{0.12})(Mn_{1.63}^{2+}Fe_{0.20}Mg_{0.10}Zn_{0.04})(Ti_{7.14}Nb_{0.90}Zr_{0.02})[(Si_{15.92}Al_{0.08})O_{48}][O_{4.94}(OH)_{3.06}] \cdot 9.7H_2O$;
- 25) $(Ba_{0.92}K_{0.54}Ca_{0.26}Na_{0.24}Sr_{0.22})(Zn_{0.58}Mn_{0.15}Fe_{0.04}Mg_{0.01})(Ti_{2.97}Nb_{1.02})(Si_{7.89}Al_{0.11})O_{24}[O_{2.01}(OH)_{1.99}] \cdot 7.39H_2O$;
- 26) $(Na_{1.68}Ca_{1.28}K_{0.88}Ba_{0.04}Sr_{0.02})(Ca_{1.28}Mn_{0.01}Zn_{0.02})(Nb_{5.39}Ti_{2.55}Fe_{0.14}^{3+})(Si_{15.88}Al_{0.12})O_{48}[O_{5.49}(OH)_{2.51}] \cdot 13.80H_2O$;
- 27) $(Na_{0.68}Ca_{0.32})(Sr_{0.53}Na_{0.12})(K_{0.63}Ba_{0.29})(Zn_{0.75}Fe_{0.04}Mn_{0.02}Mg_{0.01})(Ti_{2.88}Nb_{1.15})(Si_{7.96}Al_{0.04})O_{24}[O_{2.58}(OH)_{1.42}] \cdot 6.80H_2O$;
- 28) $Na_{1.22}K_{2.29}Ba_{0.26}(Fe_{0.31}Mg_{0.23}Mn_{0.09})(Ti_{2.31}Nb_{1.65})(Si_{8.00}O_{24})[O_{2.78}(OH)_{1.22}] \cdot 5.68H_2O$;
- 29) $(Ba_{0.85}K_{0.06}Ca_{0.03}Na_{0.01})(Fe_{1.75}Al_{0.08}Mn_{0.08}Mg_{0.08})Si_{2.15}O_{7.24}$;
- 30) $BaFe(Fe_{0.85}Mn_{0.08}Mg_{0.07})Si_2O_7$;
- 31) $(Sr_{2.78}Ca_{0.07}Na_{0.05}Mg_{0.03})Ba_{1.03}Mn_{2.34}Si_{3.86}O_{14}$;
- 32) $Ba_{0.91}Sr_{1.81}Pb_{0.05}Ca_{0.04}Na_{0.02}Mn_{2.04}^{3+}Al_{0.01}Si_{4.06}O_{14}$;
- 33) SiO_2 -20.83, As_2O_5 -1.23, BaO -29.81, PbO -1.40, MnO -24.38, Fe_2O_3 -14.47, H_2O -1.52; sum 93.64 %; ideal formula $BaMn_2(Fe^{3+}O)Si_2O_7OH$;
- 34) $(Sr,Ba,K)_2(Na,Ca)(Na,Mn,Ca,Fe^{2+})_2(Ti,Fe^{3+})Ti_2O_2(Si_2O_7)_2(O,OH,F)_2$;
- 35) $(Na_{0.94}Ca_{0.06})(Na_{1.66}Mn_{0.13}Mg_{0.07}Al_{0.07})(Ba_{1.33}Na_{0.44}K_{0.17}Sr_{0.06})(Ti_{0.94}Fe_{0.06}^{3+})Ti_2O_2[Si_{4.05}O_{14}][O_{1.72}Fe_{0.52}O_{0.30}]$;
- 36) $(Na_{4.96}K_{1.06})(Ba_{2.10}Sr_{0.23}Ca_{0.49}Mn_{0.18})(Mn_{0.22}Mg_{0.40}Fe_{0.57}^{2+}Fe_{0.55}^{3+}Ti_{5.35})(Al_{0.35}Si_{7.65})O_{32}(O_{1.14}OH_{1.24}F_{1.35}Cl_{0.27})$;
- 37) $(Ba_{0.933}Na_{0.075}K_{0.012}Ca_{0.019})(Mg_{0.059}Mn_{0.109}Fe_{1.563}^{2+}Nb_{0.030})Ti_{0.826}(Si_{1.881}Al_{0.026}Ti_{0.093})_2O_7O(O_{0.042}(OH)_{0.875}Cl_{0.083})$;
- 38) $(Ba_{0.96}Na_{0.03}Ca_{0.01}Cs_{0.002})(Mn_{1.70}Fe_{0.17}Mg_{0.05}Al_{0.08})(Ti_{0.93}Sn_{0.07}Nb_{0.015})(Si_{1.97}Al_{0.02})O_7O_{20} \cdot 0.25H_2O$;
- 39) $(Na_{2.16}K_{0.55})(Ba_{3.80}Ca_{0.19})(Ti_{5.08}Fe_{0.56}Al_{0.34})(Si_{7.96}Al_{0.04})[(H_2O)_{7.12}O_{32.83}]$;
- 40) $Ba(Fe_{0.76}^{2+}Fe_{0.33}^{3+}Mn_{0.90})TiSi_2O_7(O,OH,F)_2$;
- 41) $(K,Ba,Na,Ca,Mn)(Ti,Nb)(Si,Al)_2(O,OH)_7 \cdot 0.6H_2O$.

Table 4. Data obtained by ^{57}Fe NGR.

Silicate	<i>T</i> [K]	Site	δ^a [mm/s]	ΔQ [mm/s]	<i>DH</i> [mm/s]	<i>A</i> [%]	Refs.
Bafertisite ³⁷⁾	95	Fe ²⁺ 1	1.26(1)	2.49(8)	0.41(2)	58	98S1
		Fe ²⁺ 2	1.25(1)	2.15(5)	0.32(3)	42	
	298	Fe ²⁺ 1	1.12(1)	2.17(5)	0.59(2)	51	
		Fe ²⁺ 2	1.12(1)	1.82(3)	0.33(2)	49	
Bafertisite ⁹⁾	77	Fe ²⁺		2.59			82K1
		Fe ²⁺		2.17			
		Fe ²⁺		1.81			
	298	Fe ²⁺		2.29			
		Fe ²⁺		1.88			
		Fe ²⁺		1.66			

a) relative to α -Fe; ^{9, 37)} for composition see Table 3

Table 5. Refractive indices.

Silicate ^{a)}	n_α	n_β	n_γ	$2V$			Refs.
				calc.	meas.		
Götzenite ²⁾	1.660	1.662	1.670	53.5°	52°	biaxial, positive	53S1
Seidozerite ⁴⁾	1.725	1.758	1.830		68°	biaxial, positive	58S1, 58S2
Fersmanite ⁹⁾	1.886	1.930	1.939				37L1
Fersmanite ⁵⁾	1.872		1.914		0...7°	biaxial, negative	77M1
Ilmajokite ⁷⁾	1.573	1.576	1.579		90°	biaxial, positive	72B1, 73F1
Labuntsovitte ⁴¹⁾	1.689	1.702	1.795		41°	axial plane	55S1
Korobitsynite ¹¹⁾	1.646...1.650	1.654... 1.658	1.763...1.780	30(1)°		biaxial, positive	99P1
Tsepinite-Na ¹⁴⁾	1.658(1)	1.668(1)	1.770(5)	36°	19°...31°	biaxial, positive	01S1
Tsepinite-Ca ¹⁵⁾	1.666(2)	1.676(2)	1.780(4)	36°	30(10)°	biaxial, positive	03P1
Kuzmenkoite-Mn ¹⁶⁾	1.683(1)	1.687(2)	1.775(2)	26(9)°		biaxial, positive	99C2
Kuzmenkoite-Zn ¹⁷⁾	1.680...1.683	1.686... 1.688	1.783...1.787		25(10)°	biaxial, positive	02C2
Tsepinite K ¹⁸⁾	1.689	1.700(3)	1.775(5)		25°...40°	biaxial, positive	03C1
Paratsepinite-Ba ¹⁹⁾	1.667(2)	1.674(2)	1.770(5)		25°...40°	biaxial, positive	03C1
Lemmleinite-Ba ²⁰⁾	1.684(2)	1.690(2)	1.820(5)		37(10)°	biaxial, positive	01C1
Organovaite-Mn ²¹⁾	1.683(2)	1.692(3)	1.775(5)			biaxial, positive	01C3
Organovaite-Zn ²²⁾	1.683	1.688	1.785		45(15)°	biaxial, positive	02P1
Parakuzmenkoite ²³⁾	1.687(1)	1.689(2)	1.805(5)		22(10)°	biaxial, positive	01C2
Gutkovaite-Mn ²⁴⁾	1.688	1.700	1.805		35(10)°	biaxial, positive	02P2
Lepkhenelmitte-Zn ²⁵⁾	1.683	1.692	1.795	34.5°	25(10)°	biaxial, positive	04P1
Karupmöllerrite-Ca ²⁶⁾	1.656(2)	1.662(2)	1.755(3)	29.7°	30(15)°	biaxial, positive	02P3
Alsakharovite-Zn ²⁷⁾	1.680	1.687	1.785		25(10)°	biaxial, positive	03P2
Neskevaaraite-Fe ²⁸⁾	1.677(1)	1.684(2)	1.790(5)		25(10)°	biaxial, positive	03C1
Andremeyerite ²⁹⁾	1.740(5)	1.740(5)	1.760(5)		dispersion very strong	biaxial, positive	73S1, 74F1
Taikanite ³¹⁾	1.775(3)	1.792(calc.)	1.814(2)		74°...80°	biaxial, positive	85K1, 87H1
Orthoericssonite ³³⁾	1.807(5)	1.833(5)	1.89(1)		43°	biaxial, positive	71M1
Sr-free lamprophyllite ³⁵⁾	1.750		1.779		40(5)°	biaxial, positive	98L1
Barytolamprophyllite ³⁶⁾	1.742...1.743	1.754(calc.)	1.776...1.778		29°...30°	biaxial, positive	65P1, 66F1
Bafertisitite ⁴⁰⁾	1.786(calc.)	1.813	1.852		80°		71G1, 72F1
Delindeite ³⁹⁾	1.790(5)	1.825(5)				biaxial, positive	87A1

^{a)} composition according to Table 3.

Götzenite

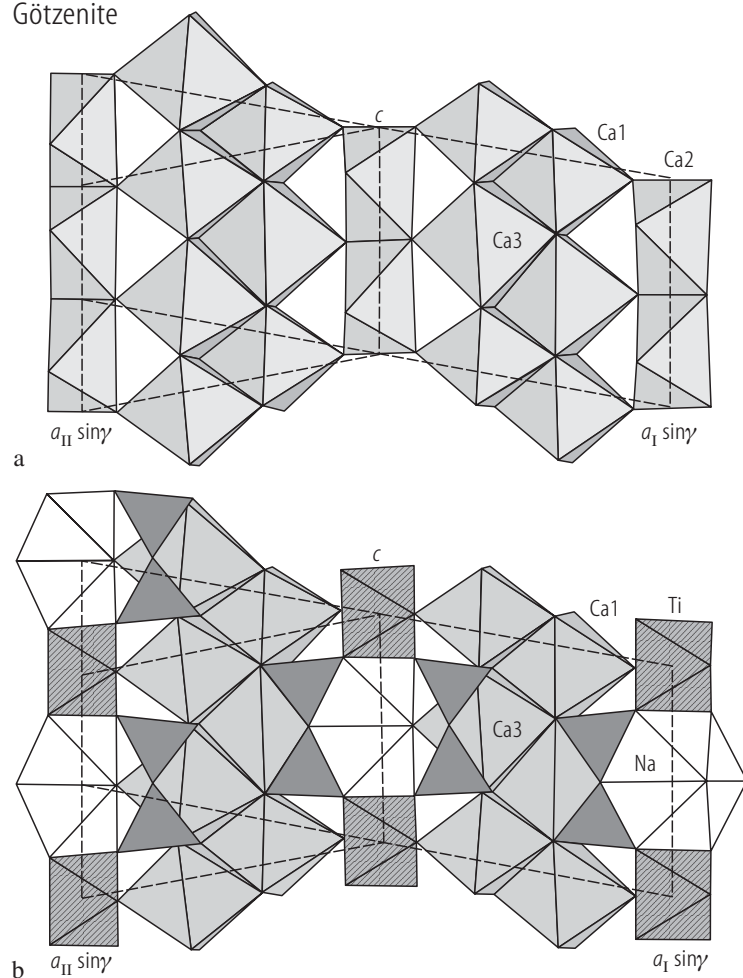


Fig. 1. Götzenite. The structural aspects of the twin. **(a)** Arrangement of Ca-polyhedra which maintain their positions through the boundary between the individuals of the twin; **(b)** the shift of $c/2$ of the Si_2O_7 groups and the consequent interchange between Na and Ti polyhedra caused by twinning [72C1].

Götzenite

Rosenbuschite

Seidozerite

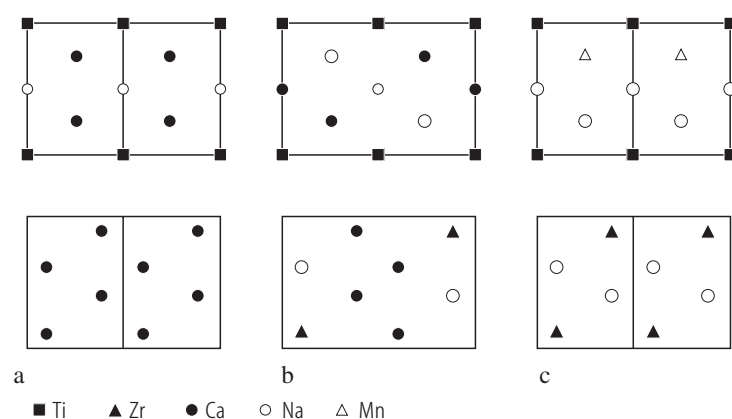


Fig. 2. Götzenite **(a)**, rosenbuschite **(b)**, seidozerite **(c)**. Schematic view of the cations in the "walls" (top) and in the "ribbons" (bottom). The plane of projection is normal to a in götzenite and to equivalent directions in rosenbuschite and seidozerite [72C1].

Fersmanite

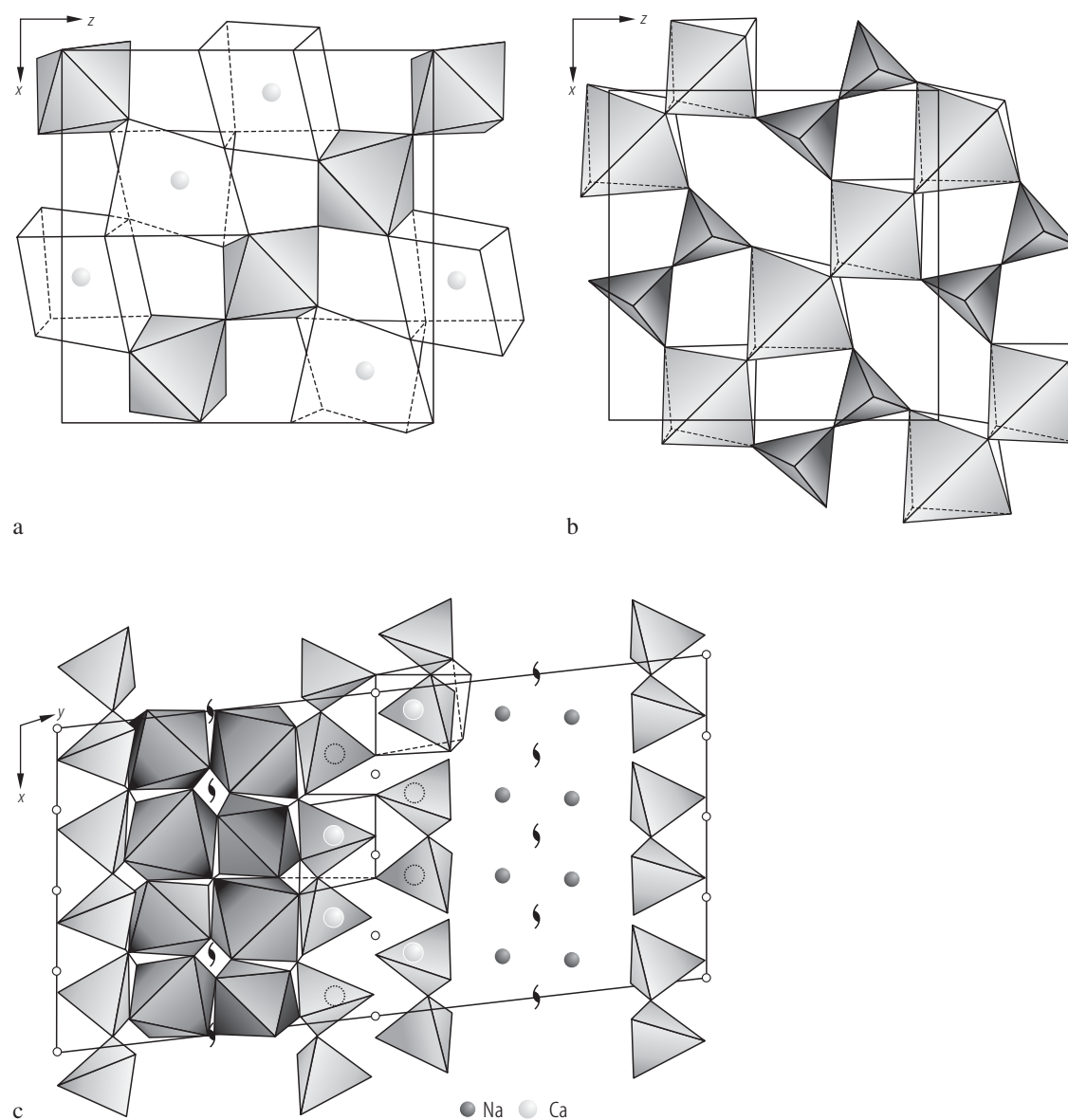


Fig. 3. Fersmanite, crystal structure. **(a)** Ti octahedra and Na polyhedra at mean level $x = 0.19$; **(b)** Ca polyhedra and diortho groups at mean level $y = 0.43$; **(c)** fragment of structure showing Ti octahedra and diortho groups (see text) [84S1].

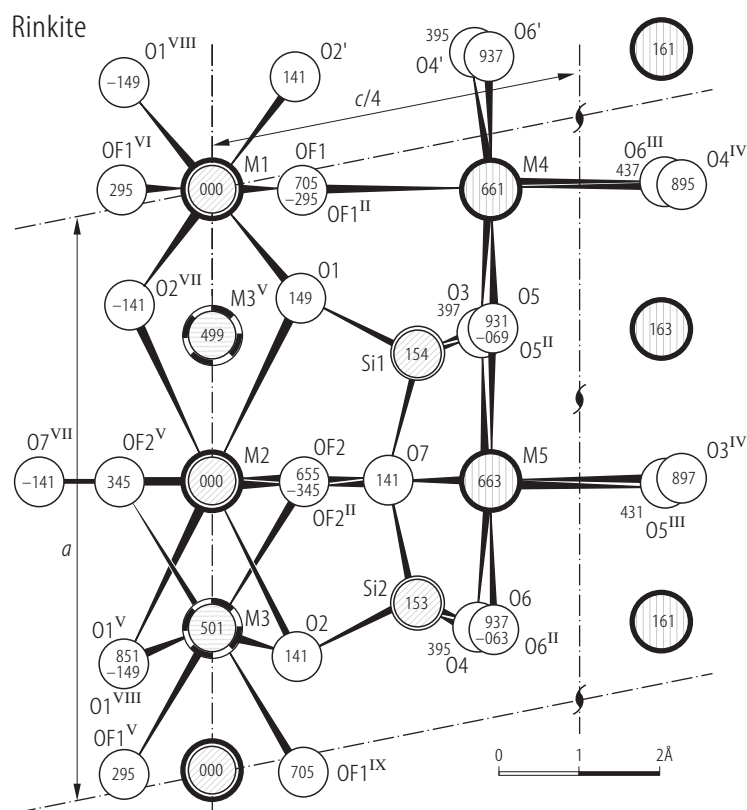


Fig. 4. Rinkite. Projection of the structure on (010) plane. Numbers inside the circles give the heights of the atoms in thousandths of the cell edge [71G1]. The superscripts refer to the symmetry code: i- $(x-1, y, z)$; ii- $(x, y-1, z)$; iii- $(1-x, y-1/2, 1/2-z)$; IV- $(1-x, y+1/2, 1/2-z)$; V- $(1-x, 1-y, -z)$; VI- $(-x, 1-y, -z)$; VII- $(1-x, -y, -z)$; VIII- $(-x, -y, -z)$; IX- $(x+1, y, z)$; X- $(x, y, z-1)$.

For Fig. 5 see next page

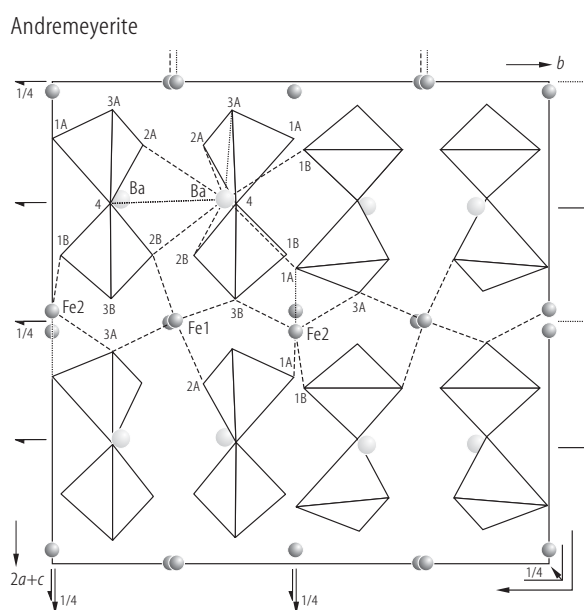
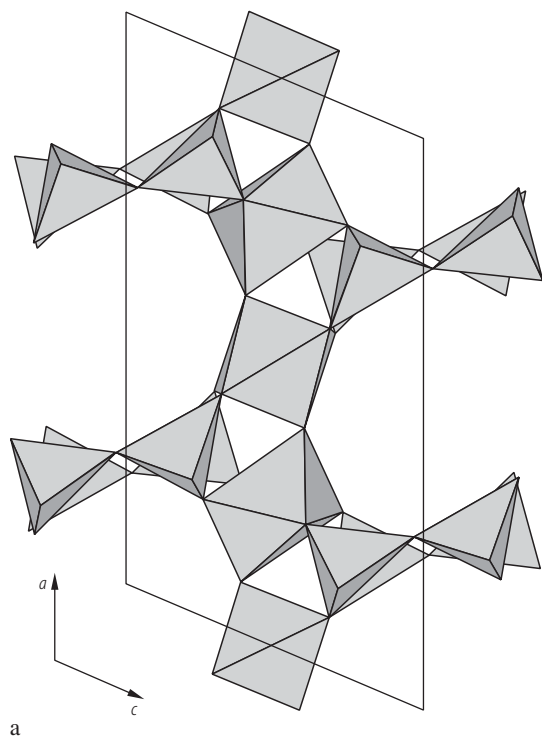
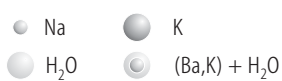
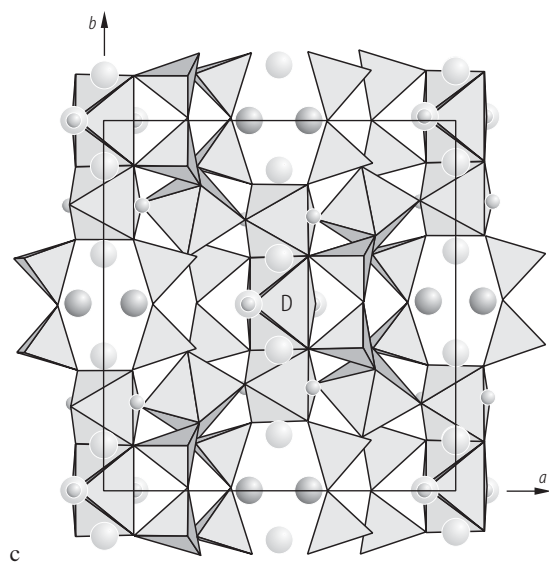


Fig. 6. Andremeyerite. Crystal structures in the "orthorhombic" unit cell as seen along [001] [88C1]. Dotted lines represent the greatest Ba-O and Fe2-O bond distances [88C1].

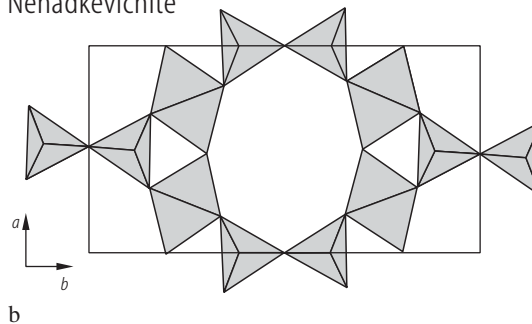
Labuntsovite



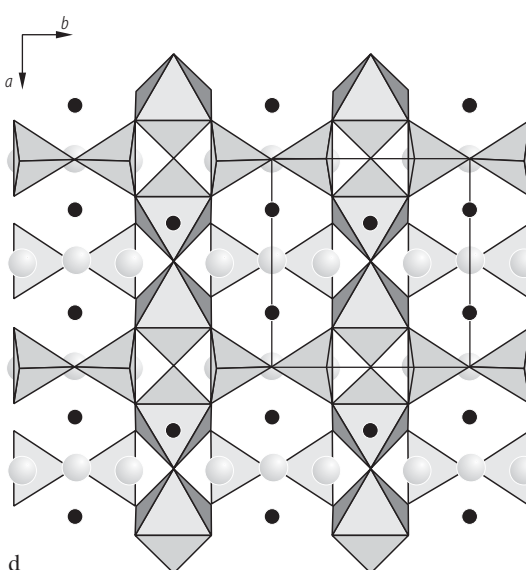
Labuntsovite



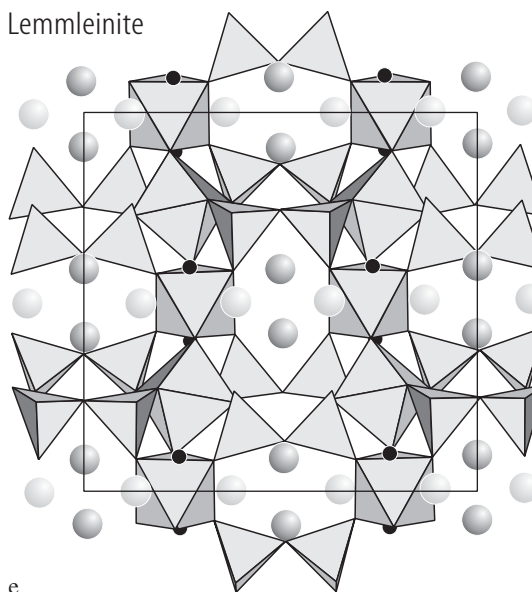
Nenadkevichite



Nenadkevichite



Lemmleinite



←

Fig. 5. Labuntsovite **(a)**, nenadkevichite **(b)**. Fragments of crystal structures. Deformation of the framework causes a symmetry lowering in labuntsovite. In **(c)** the crystal structure of labuntsovite is shown, where the D-octahedron is more than 50 % occupied. The projections on the (ab) plane of nenadkevichite **(d)** and lemmleinite **(e)** are also plotted. The small black circles in **(d)** and **(e)** are Na atoms, the dark larger circles are K atoms. The light (large) circles show the position of water molecules [02C1].

Lamprophyllite

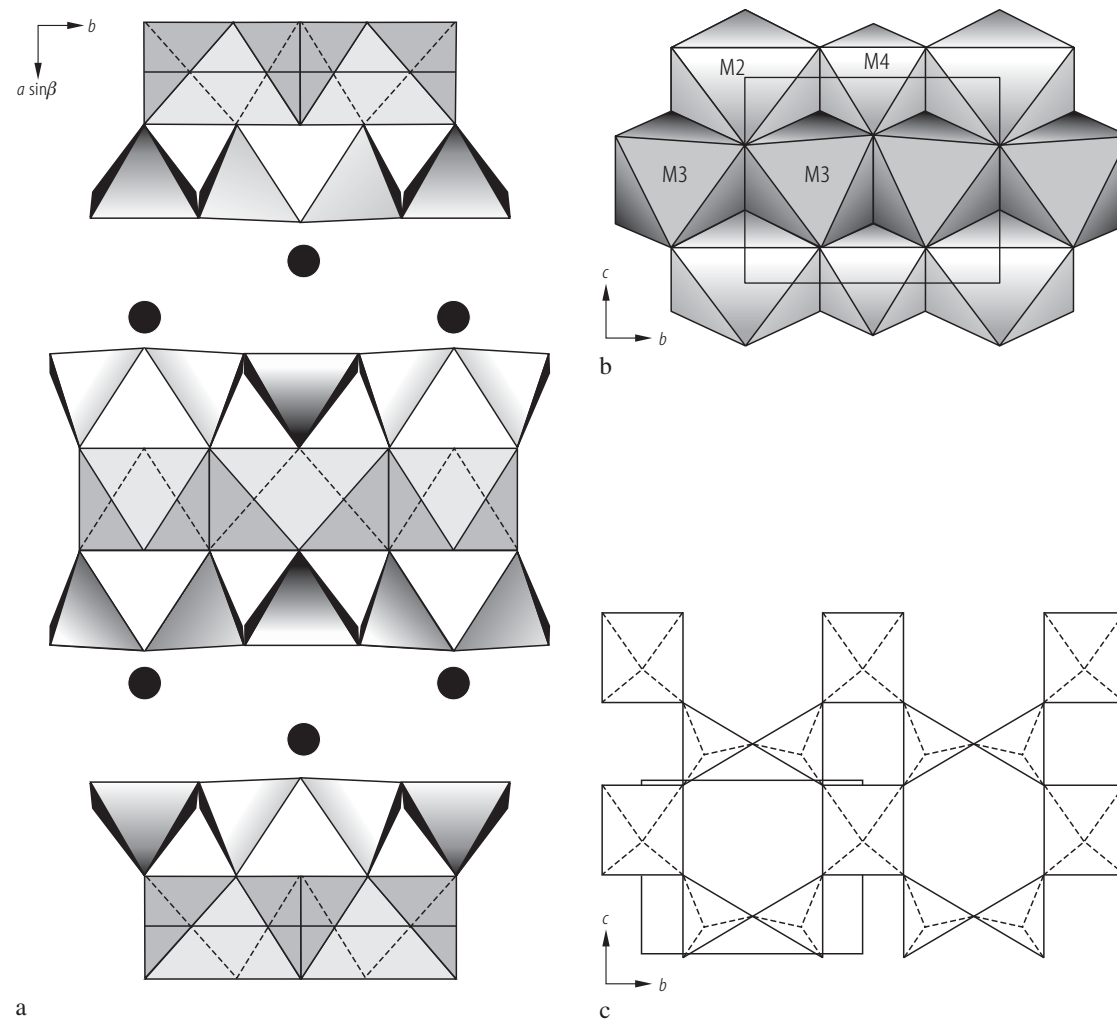
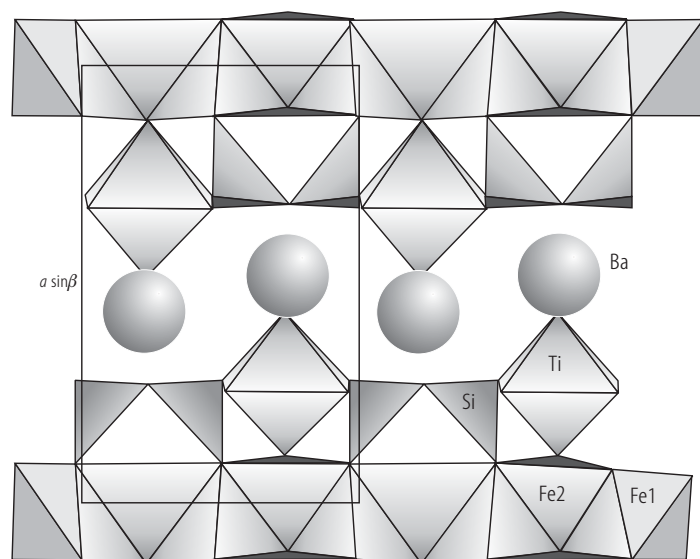
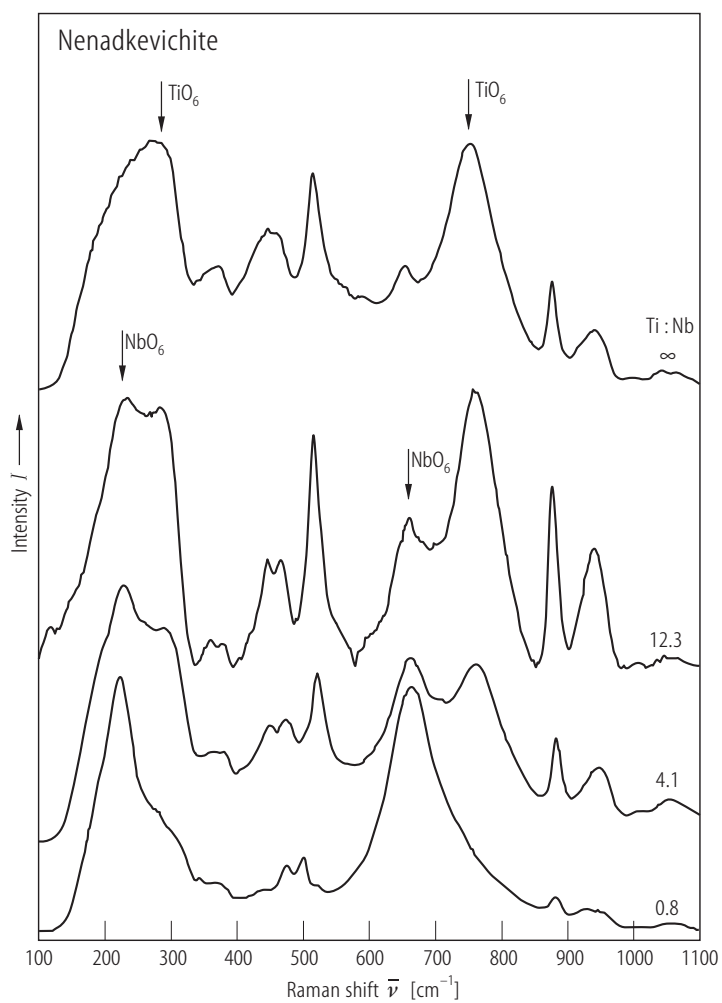


Fig. 7. Lamprophyllite. **(a)** Projection of the crystal structure. The circles denote Sr atoms; **(b)** core of three-layer stack: M2(Na,Ca), M3(Na,Mn,Ca,Fe), M4(Ti,Fe); **(c)** Ti, Si anion network [83S1].

Bafertisite

**Fig. 8.** Bafertisite. Crystal structure [63P1].

For Fig. 9 see next page

**Fig. 10.** Nenadkevichite (synthetic). Selected Stokes shifted Raman spectra, at room temperature. The Ti/Nb molar ratios are indicated [96R2].

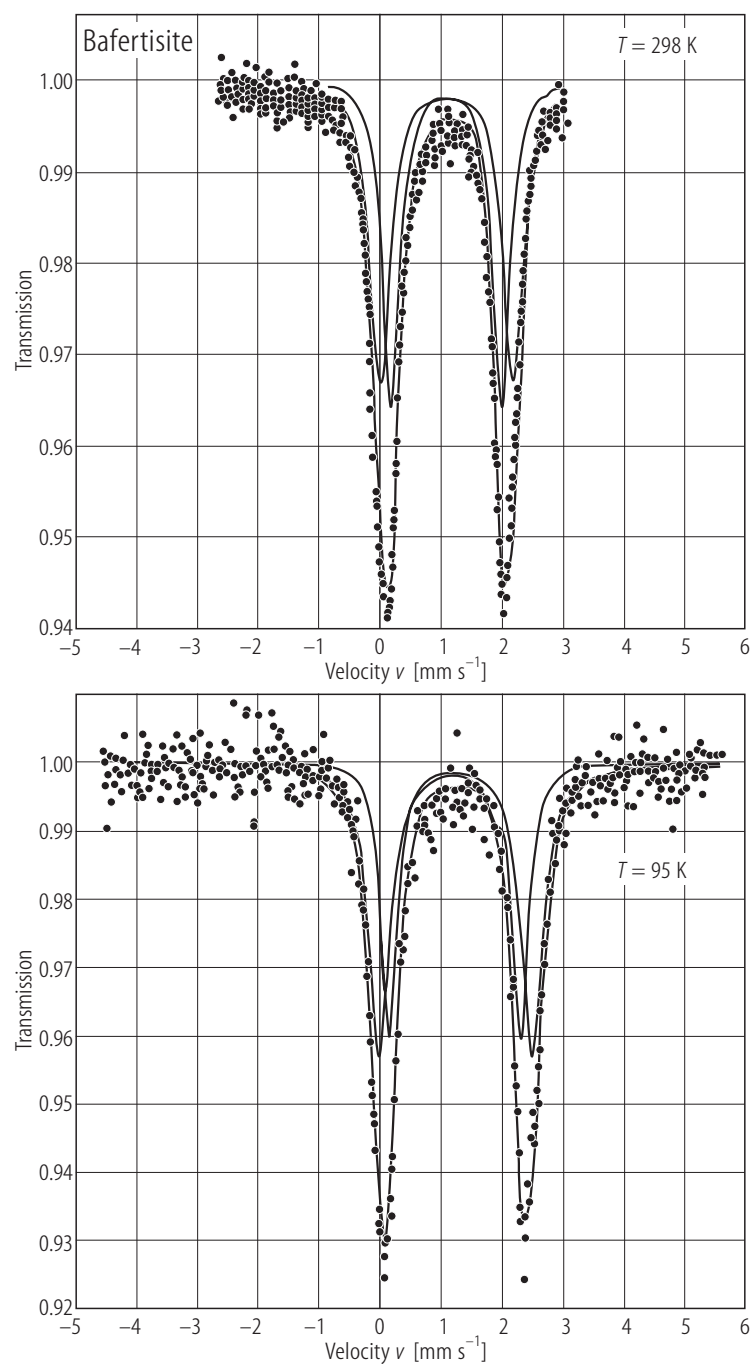


Fig. 9. Bafertisite. ^{57}Fe NGR spectra at (a) 298 K and (b) 95 K [98S1].

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