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The crystal structure of tokkoite and its relation to the structure of tinaksite

I. V. Rozhdestvenskaya
LNPO "Burevestnik", Leningrad, 195196, USSR

L. V. Nikishova, Yu. D. Lazebnik and K. A. Lazebnik
Institute of Geology, Yakut Branch, Siberian Department,
USSR Academy of Sciences, Yakutsk, 677891, USSR

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Abstract. Tokkoite, $K_2Ca_4[Si_7O_{18}(OH)](F,OH)$, a new mineral from Murun massif, South Yakutia, USSR, is triclinic with unit-cell dimensions $a = 1.0438(3)$ nm, $b = 1.2511(3)$ nm, $c = 0.7112(2)$ nm, $\alpha = 89.92(2)°$, $\beta = 99.75(2)°$, $\gamma = 92.89(2)°$, space group $P\bar{1}$, $Z = 2$. The crystal structure has been determined by the Patterson method and difference Fourier maps followed by a least-squares refinement to an R factor of 0.032 for 906 ($I > 1.96\ \sigma_I$) reflections measured on an automatic single-crystal X-ray diffractometer.

The structure consists of corrugated walls of calcium octahedra parallel to (100), between which bands of silicon–oxygen tetrahedra are situated. One of the non-bridging end anions is a OH group. K atoms are located within zig-zag channels formed by curved silicate bands.

Tokkoite and tinaksite, $K_2Ca_2NaTi\ [Si_7O_{18}(OH)]O$, are isostructural. These two structures are related by the substitution $2Ca^{2+} \rightleftharpoons Ti^{4+} + Na^+$ and $(F,OH)^- \rightleftharpoons O^{2-}$ which occurs simultaneously in kationic and anionic parts of minerals. Common structural details of tokkoite, miserite and canasite are also considered.

Introduction

The new mineral tokkoite was found in charoitites, rocks of unusual composition and appearance which occur in the Murun massif, south western Yakutia, USSR (Lazebnik et al., 1986). It is close in composition to potassic calcic silicates such as apophyllite and miserite and similar in appearance to the latter. The X-ray diffraction pattern and unit-cell parameters of tokkoite are similar to tinaksite, a mineral also found for the first time in charoitites. Tinaksite, however, contains substantial amounts of Na and Ti: $K_2NaTiCa_2Si_7O_{19}(OH)$ (Petrunina et al., 1973). In the formula $K_2Ca_4Si_7O_{17}(O,F,OH)_4$ suggested for tokkoite (Lazebnik et al., 1986) the silicon–oxygen radical is similar, though not identical, to that of tinaksite. Finding the true position of tokkoite among alcalic calcic silicates of charoitites is interesting in terms of both mineralogy and crystal chemistry.

It is the purpose of the present paper to report the crystal structure of tokkoite, obtained by means of single-crystal X-ray diffraction analysis and to compare it with that of tinaksite, miserite, and canasite.

Determination and refinement of the crystal structure

A single crystal of tokkoite in the form of a needle, measuring 0.025 × 0.05 × 0.15 mm was selected for the investigation. The unit-cell dimensions (Table 1) were determined by least-squares refinement of 2θ values of 16 reflections measured on a single-crystal diffractometer. The real composition of tokkoite corresponds to the formula

$$K_{1.85}Na_{0.15}Ca_{3.45}Mg_{0.06}Mn_{0.08}Fe_{0.15}Ti_{0.13}Si_{7.13}O_{17}$$
$$\times (O_{1.63}F_{0.61}OH_{2.02})\text{ (Lazebnik et al., 1986).}$$

A set of intensities was collected on the same $P2_1$ four-circle single-crystal X-ray diffractometer using Mo$K\alpha$ radiation, graphite monochromator, $\theta/2\theta$ method, variable scan rate of 2 to 30°/min. A total of 906

Table 1. Crystallographic data of tokkoite and tinaksite.

	Tokkoite $K_2Ca_4[Si_7O_{18}(OH)](F,OH)$ Present study	Tinaksite $K_2Ca_2NaTi[Si_7O_{18}(OH)]O$ Bissert (1980)
a (nm)	1.0438(3)	1.0377(3)
b (nm)	1.2511(3)	1.2166(3)
c (nm)	0.7112(2)	0.7059(1)
α (°)	89.92(2)	90.91(1)
β (°)	99.75(2)	99.30(1)
γ (°)	92.89(2)	92.76(1)
Z	2	2
Space group	$P\bar{1}$	$P\bar{1}$
d_m (g/cm^3)	2.76	2.821
d_c (g/cm^3)	2.77	2.84
μ (cm^{-1})	21.7	21.2

independent reflections with $I > 1.96\ \sigma_I$ were obtained within one hemisphere of the reciprocal space in the 2ϑ-range of 0° to 32°. The number of reflections is limited because of a very small sample size. Larger samples generally yielded patterns of circular textures or highly diffuse spots due to extremely fine twinning. The intensities were corrected for Lorentz and polarization factors. No absorption correction was applied at this stage.

Inititially, we performed the determination and refinement of the crystal structure in the acentric space group $P1$. Ca atom coordinates were obtained by interpretation of the Patterson function, those for Si, K and O from Fourier difference syntheses. Both were performed on a Nova 1200 computer using the XTL programs. A structure model was refined on a CM-4 computer. The atomic scattering factors for neutral atoms were taken from the *International Tables for X-ray Crystallography (1974)*. After several cycles of refinement of the atomic positional parameters and site occupancies defined by K and Ca atoms ($\sin\theta/\lambda < 0.45$, 906 reflections), the correction for an absorption was applied using the program (DIFABS) (Wolkers and Stewart, 1983). A few final cycles of site occupancy, atomic coordinate and isotropic temperature factor refinement (66 atoms, 262 variables, 906 reflections) were carried out, resulting in $R = 0.040$ ($R_w = 0.039$, weighing scheme $W = 1/\sigma(F^2)$. After removal of weak reflections with $F < 20$ ($F_{\max} = 297$), the unweighed and weighed R factors for 875 reflections were 0.036 and 0.035, respectively. However, three oxygen atoms have negative B_{iso} values. Hence, a similar procedure of refinement in the space group $P\bar{1}$ was attempted since the atomic coordinates and the positions of the cations suggested a centrosymmetrical structure model. At the final refinement stages the hydrogen atom position was determined by difference Fourier syntheses. The refinement with isotropic temperature factors (34 atoms, 137 variables, 875 reflections with $F > 20$) led to $R = 0.041$ ($R_w = 0.041$). Though the above values for the space group $P1$ were somewhat better owing to a larger number of variables, we preferred the latter values. They gave more acceptable values of B_{iso}, lower standard deviations and made it possible to locate a hydrogen atom. The refinement of all atomic coordinates and anisotropic temperature factors gave $R = 0.032$. The final atomic positional parameters and B_{iso} are listed in Table 2. Lists of the anisotropic temperature coefficients, the interatomic distances and O–Si–O angles have been deposited.[1]

Description of the crystal structure

In general, the crystal structure of tokkoite can be considered as composed of the following structural units: (1) corrugated walls parallel to (100), and

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[1] Additional material to this paper can be ordered referring to the no CSD 53517, names of the authors and citation of the paper at the Fachinformationszentrum Energie-Physik-Mathematik, D-7514 Eggenstein-Leopoldshafen 2, FRG.

Table 2. Atomic coordinates (standard deviation) and isotropic thermal parameters.

Atom	P^a	x	y	z	B (Å^2)
K(1)	0.84	0.3189(4)	0.1155(3)	0.2080(6)	2.80(10)
K(2)	0.96	0.4419(3)	0.3564(2)	0.7323(4)	1.63(8)
Ca(1)	1.015	0.0244(2)	−0.1176(2)	−0.1151(4)	1.10(6)
Ca(2)	0.94	0.0077(3)	−0.1188(2)	0.3748(4)	0.95(7)
Ca(3)	1.024	0.1208(2)	0.5872(2)	−0.0920(3)	0.76(6)
Ca(4)	1.01	0.1241(2)	0.5831(2)	0.4042(3)	0.87(6)
Si(1)	1.0	0.3196(3)	0.8096(3)	0.4191(5)	0.91(8)
Si(2)	1.0	0.3241(3)	−0.1891(3)	−0.0104(5)	0.94(9)
Si(3)	1.0	0.1355(3)	0.3134(3)	−0.1203(5)	0.82(8)
Si(4)	1.0	0.1328(3)	0.3119(3)	0.4347(5)	0.73(8)
Si(5)	1.0	0.3178(3)	0.4211(3)	0.2018(5)	0.74(8)
Si(6)	1.0	0.2842(4)	−0.0167(3)	0.6949(5)	1.05(8)
Si(7)	1.0	0.4010(3)	0.6484(3)	0.7248(5)	0.85(8)
O(1)	1.0	0.3405(9)	0.1073(6)	0.7022(13)	1.72(22)
O(2)	1.0	0.2778(7)	0.3500(6)	0.0062(11)	0.92(20)
O(3)	1.0	0.2727(7)	0.3460(6)	0.3716(11)	0.98(20)
O(4)	1.0	0.4753(7)	0.4274(6)	0.2467(11)	0.66(19)
O(5)	1.0	0.0936(8)	0.1938(6)	−0.0674(12)	1.56(22)
O(6)	1.0	0.1730(7)	0.7656(6)	0.3941(10)	0.68(20)
O(7)	1.0	0.1311(7)	−0.0258(6)	0.6599(12)	1.48(22)
O(8)	1.0	0.3487(8)	−0.0724(6)	−0.1023(11)	1.39(22)
O(9)	1.0	0.3428(7)	−0.0743(6)	0.5220(11)	1.00(20)
O(10)	1.0	0.3811(7)	0.8234(6)	0.2204(11)	1.14(21)
O(11)	1.0	0.4186(7)	0.7263(6)	0.5426(11)	1.07(21)
O(12)	1.0	0.4205(8)	0.7277(6)	0.9129(11)	1.45(22)
O(13)	1.0	0.1714(8)	0.3058(6)	0.6690(11)	1.40(22)
O(14)	1.0	0.1777(7)	0.7688(6)	−0.0626(11)	1.33(22)
O(15)	1.0	0.0830(8)	0.1948(6)	0.3646(11)	1.52(22)
O(16)	1.0	0.0334(6)	0.4052(6)	0.8847(10)	0.60(19)
O(17)	1.0	0.0315(7)	0.4036(6)	0.3786(11)	0.94(20)
O(18)	1.0	0.2697(7)	0.5780(6)	0.6945(10)	0.81(20)
O(19)	1.0	0.2610(7)	0.5352(6)	0.1891(10)	0.99(20)
O(20)	1.0	0.1001(7)	0.9810(6)	0.1504(10)	2.37(20)
H(1)		0.403(8)	0.104(6)	0.73(1)	3.40

[a] Occupancy.

Table 3. Si–O–Si angles (°) in the pyroxenoid chains for selected calcic silicates of charoitit

Tokkoite Present study		Miserite Scott, 1976		Canasite^a Rozhdestvenskaya et al., 19	
Si(5)–O(3)–Si(4)	134.4	Si(3)–O(10)–Si(8)	137.2	Si(1)–O(2)–Si(3)	130.5
Si(4)–O(13)–Si(3)	151.8	Si(8)–O(22)–Si(6)	149.6	Si(1)–O(17)–Si(1)^b	151.9
Si(3)–O(2)–Si(5)	131.8	Si(6)–O(11)–Si(3)	131.0	Si(1)^b–O(2)–Si(3)	130.5
Si(4)–O(11)–Si(1)	131.4	Si(4)–O(14)–Si(7)	135.9	Si(4)–O(5)–Si(2)	135.0
Si(1)–O(10)–Si(2)	135.7	Si(7)–O(17)–Si(5)	149.6	Si(2)–O(18)–Si(2)^b	148.6
Si(2)–O(12)–Si(7)	132.1	Si(5)–O(13)–Si(4)	143.1	Si(2)^b–O(5)–Si(4)	135.0

[a] Values for two of the four independent sub-chains are given.
[b] Symmetry-identical atoms.

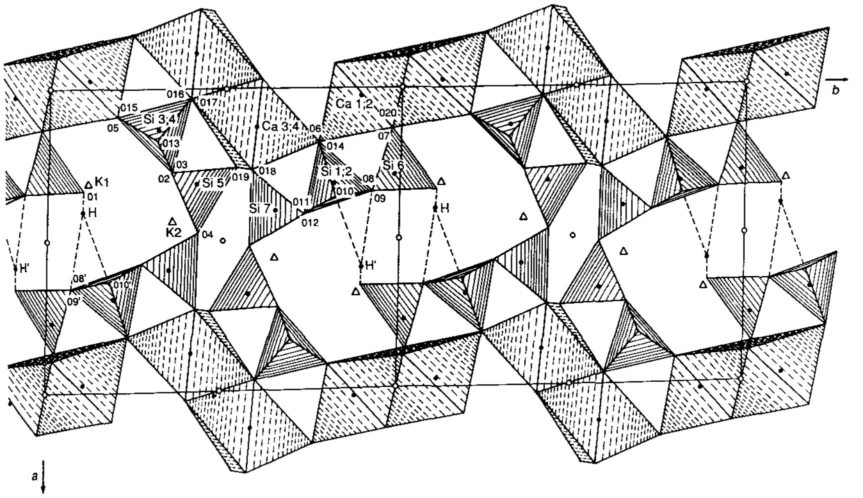

Fig. 1. Projection of the tokkoite structure along the *c* axis. The shortest hydrogen bonds are shown as dashed lines.

(2) curved bands with the composition $[Si_7O_{18}(OH)]^{-9}$ consisting of a hybrid three-repeat double chain (hybrid dreier double chain, Liebau, 1978) with four- and eight-membered rings.

These structural units are connected by corner sharing and alternate along the *a* axis, as illustrated in Figures 1 and 3. K and H atoms occur in large zig-zag channels between the silicon – oxygen bands. A general design of the tokkoite structure is identical to tinaksite (Bissert, 1980).

Silicate bands

The silicon – oxygen radical $[Si_7O_{18}(OH)]_\infty$ is analogous to that of tinaksite (Bissert, 1980) and can be considered as two polymerized chains of wollastonite-type with an additional tetrahedron or condensed chains of wollastonite and vlasovite-type (Petrunina et al., 1973), that form a curved band with eight- and four-member rings. Bands of silicon – oxygen tetrahedra are connected to the octahedral wall on both sides by sharing oxygen atoms. Three tetrahedra [Si(3), Si(4), Si(5)] join one octahedral wall, whereas the Si(1)′, Si(2)′, Si(6)′, Si(7)′ tetrahedra join the parallel wall causing the bands to curve into a semicircle (Fig. 1).

In order to adjust to the different edges of the Ca(1) and Ca(2) octahedra, the three-repeat wollastonite-type chain is easily deformed by tilting and turning of the tetrahedra of the Si(3), Si(4)-diorthogroup. The latter shares the O(16) and O(17) oxygens with the Ca(4) octahedron. The other part of the tetrahedral band, consisting of the Si(1), Si(2)-diorthogroup and

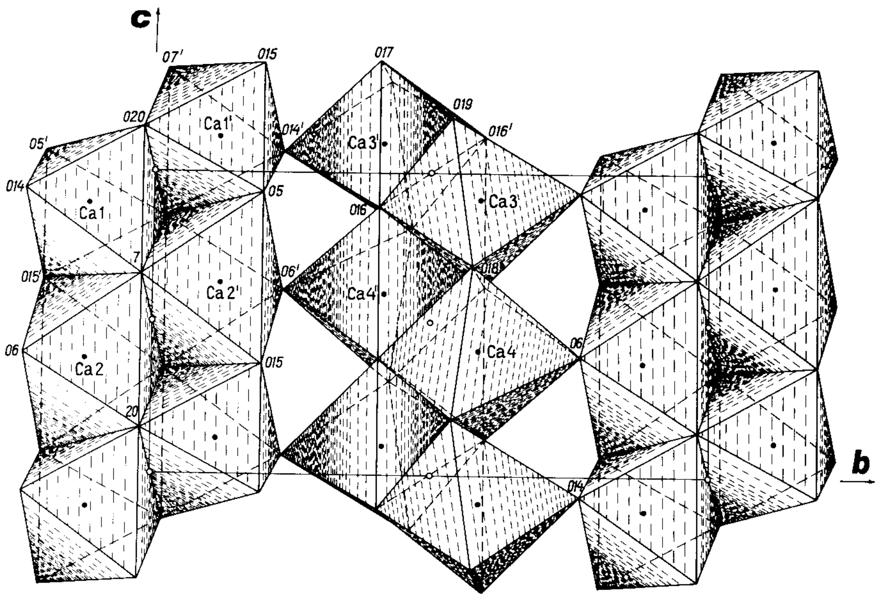

Fig. 2. Corrugated calcium wall consisting of Ca(1), Ca(2) and Ca(3), Ca(4)-octahedral bonds.

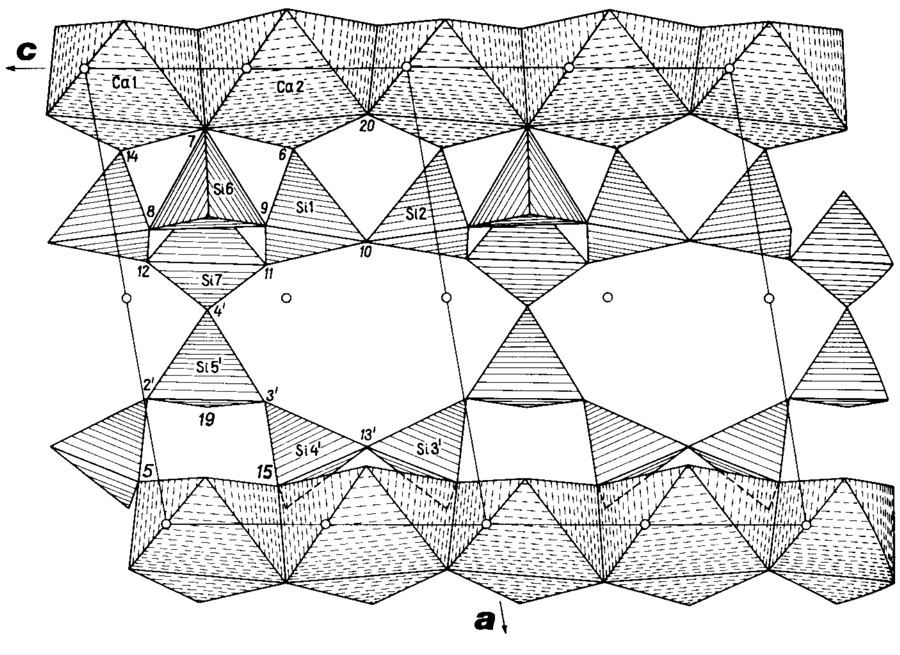

Fig. 3. The connection between silicate tetrahedral bond (hybrid dreier double chain) and octahedral walls. Partial view of the tokkoite structure down the *b* axis. Labelled cations at $y > 0.7$.

the Si(6) and Si(7) tetrahedron, links to the octahedral wall by sharing oxygens O(6), O(14) and O(7), O(18) respectively (Fig. 3). As a result the pyroxenoid period of the chains in tokkoite reduces to 0.7112 nm relative to undistorted 0.731 nm in wollastonite (Ohashi and Finger, 1978).

The mean Si—O bond lengths in the tetrahedra are similar ranging within 0.1616—0.1626 nm; the mean O—Si—O angles are close to an ideal value of 109.4° (Table 2). Si atoms are shifted towards non-bridging oxygens in all of the tetrahedra. These Si—O distances are reduced and range between 0.157 nm and 0.161 nm; mean O—Si—O angles for the non-bridging oxygens are larger (112.8°) than those fo the bridging ones (105.9°).

Potassium and hydrogen positions

K(1) and K(2) atoms are located in a zig-zag channel between two centrosymmetrical tetrahedral bands (Fig. 1) and have tenfold coordination with mean K—O distances of 0.3233 nm at K(1) and 0.2974 nm at K(2). Lower occupancy (0.84) and longer mean K—O of the K(1) position evidence for weaker bonding of this alcalic cation in the structure. This suggests its easier removal from the structure compared with the atom at K(2). The K(2) coordination sphere includes, apart from O(1), six oxygen atoms from the silicon—oxygen band and three atoms from the symmetrical adjacent one [O(4), O(18), O(19), Fig. 1]. K(1)—O(20) = 0.274 nm is the shortest among the K—O bond lengths. Hence the valency of the cation at K(1) is largely compensated at the expense of the anion at O(20).

It should be noted that among the oxygen atoms of the tenfold alkali cation coordination only O(1) does not form bonding with the octahedral cations. This nonbridging oxygen atom O(1) involved in the Si(6) tetrahedron is the most charge-deficient oxygen. The Si(6)—O(1) bond length (0.1628 nm) is larger than other Si—O ones with non-bridging anions. Its interaction with K(1) and K(2) in addition to Si(6) also fails to compensate its charge completely. This strongly suggests that the O(1) position is most likely occupied by a hydroxyl group.

Indeed, a difference synthesis revealed a peak at a distance of 0.065 nm from O(1), which is consistent with the hydrogen position. H and K(1) are located in a half-translation along the *c* axis and on both sides of O(1) in the *ab* plane (Fig. 1). In addition, protons connect two silicon—oxygen bands by hydrogen bonds. The shortest among them are (nm): H—O(10) = 0.236, H—O(9) = 0.267, H—O(8) = 0.258.

Valency balance and the crystal-chemical formula of tokkoite

The local valency balance was calculated according to the method proposed by Pyatenko (1972) taking into account interatomic distances and cation site occupancies, O(20) was assumed to be F. The results confirm that the local geometry and anion bond-valence requirements are highly satisfied. The deviations from the formal valence of anions are no more than 0.1 v.u. for most oxygens but one. Only the O(5) anion has a bond-valence sum of 1.832. The O(1) anion receives a sum of bond strengths of about 1.13 v.u. from Si(6), K(1), K(2) and 0.83 valency units due to hydrogen. The value of balance "quality" according to Pyatenko (1972) is 2.98% on the whole and indicates good refinement of the tokkoite structure.

Thus one of the oxygens in the tokkoite radical represents a hydroxyl group: $Si_7O_{18}(OH)$, which is identical to tinaksite (Bissert, 1980). Entry of an OH group (instead of an oxygen) into a silicon – oxygen radical has been reported, for instance, in the structure of lovozerite, $Na_2ZrSi_6O_{12}(OH)_6$, wherein 6 of the 18 anions being nonbridging link to one silicon atom only (Ilykhin and Belov, 1960). The positions of the OH group and F have been refined in the course of the present study, but the chemical analyses indicate F deficit to occupy the O(20) structural position completely, OH being in excess. Therefore the crystalchemical formula for tokkoite should be written as:

$$K_{1.85}(Ca_{0.87}Ti_{0.13})(Ca_{0.85}Na_{0.15})(Ca_{1.71}Fe_{0.15}Mn_{0.08}Mg_{0.06})$$
$$\times [Si_7O_{18}(OH)](F_{0.61}, OH_{0.39}),$$

or in a generalized form

$$K_2Ca_4[Si_7O_{18}(OH)](OH,F).$$

Comparison of the crystal structures of tokkoite and tinaksite

The present structure determination has corroborated the idea (Lazebnik et al., 1986) of a structural similarity of tokkoite and tinaksite (see Table 1). The details of both structures are all identical, the octahedral walls being geometrically similar. But tokkoite has a band of the Ca(1), Ca(2) octahedra instead of the Na + Ti polyhedra in tinaksite (Bissert, 1980). Mean distances in calcium octahedra are similar in both structures: 0.2366 nm, 0.2379 nm in tokkoite and 0.2323 nm, 0.2378 nm in tinaksite. Mean Ti – O is shorter than that in the smallest Ca(1) octahedron of tokkoite (0.1982 nm vs. 0.221 nm), whereas the mean distance in the Na polyhedron of tinaksite is longer than that in the Ca(2) octahedron of tokkoite (0.2497 nm vs. 0.2388 nm).

The silicon – oxygen band are identical in both minerals. Like the atom at O(1) in tokkoite, the O(18) terminal oxygen atom of tinaksite links to the H, one Si and the nearest K atoms. There are analogous O(20) positions in both structures but they are largely occupied by fluorine ions in tokkoite.

Discussion

The structural similarity of tinaksite and tokkoite strongly suggests they are the end members of the hypothetical isomorphous series $K_2Ca_4[Si_7O_{18}(OH)](O,OH,F)-K_2Ca_2NaTi[Si_7O_{18}(OH)]O$, when replacement such as $2Ca^{2+} \rightleftharpoons Ti^{4+} + Na^{+}$ take place. Ca substitution in the octahedral walls should apparently be correlated with the replacement $(F,OH)^{-} \rightleftharpoons O^{2-}$ in the above mentioned O(20) special position at the junction of the octahedra (Figs. 1, 2). Alkali calcic silicates of charoitites are quite suitable for such an isomorphism to take place because crystalchemical conditions favouring isomorphic entry of Ti into crystal structures are met (Pyatenko et al., 1976).

It is however noteworthy that chemical analyses of tinaksite from charoite rocks show constantly high concentrations of Ti and Na while samples containing intermediate amounts of these elements are lacking. Tokkoite contains only small amounts of Ti and Na. But they are distributed in an orderly fashion over the same polyhedra which are occupied by Na and Ti in the structure of tinaksite. It should be noted that a high fluorine content of tokkoite decreases the structure stability, hence its crystals are small and imperfect compared with those of tinaksite.

One more fact deserves mentioning. The fragment of the tokkoite structure including all tetrahedra of two silicon – oxygen bands, except Si_6, and protrusions of a calcium wall (Fig. 1, central part) are observed in the structures of miserite and canasite, the latter being compared in detail elsewhere (Rozhdestvenskaya et al., 1988). The Si – O – Si angles of the tetrahedra in two pseudowollastonite chains which compose both a tokkoite band, and half of the tubular radical $Si_{12}O_{30}$ in the structure of miserite and canasite are shown in Table 3. Si(2) – Si(1) – Si(7) and Si(3) – Si(4) – Si(5) are the repeat units in the two independent, linear, single-wollastonite-type chains with three tetrahedra per chain period for tokkoite. Those for miserite and canasite are Si(6) – Si(3) – Si(8) and Si(7) – Si(4) – Si(5); Si(3) – Si(1) – Si(1)′ and Si(4) – Si(2) – Si(2)′, respectively. The inter-tetrahedral Si – O – Si angles of the above minerals are in fact very close to each other.

Similar angles in the linear single chain (unbranched dreier single chain, Liebau, 1978) for wollastonite and pectolite are 139°, 149°, 140° (Prewitt and Buerger, 1963) and 136.4°, 147.8°, 135.0° (Prewitt, 1967), respectively. The Si – O – Si angle values of the examined minerals are closer to those of pectolite.

K atoms located at a bond of the silicon – oxygen radical in the structures of the minerals compared have remarkably similar position and role, namely K(2) in tokkoite, K(1) in miserite, K(2) and K(3) in canasite (Rozhdestvenskaya et al., 1988). They strengthen the structures through bonding to three oxygens of the adjacent silicon – oxygen radicals. Thus, the alcalic-calic silicates show another example of "synthesis" of silicates from large, "ready-made" parts (Belov, 1976) and the charoitites themselves composed almost entirely (up to 90%) of these minerals can be regarded as a manifestation of metasomatic processes which accompanied the formation of the unique Murun massif.

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References

Belov, N. V.: *Essays on structural mineralogy*. Moscow: Nedra 1976, p. 344.

Bissert, G.: Verfeinerung der Struktur von Tinaksit. $Ca_2K_2NaTiO[Si_7O_{18}(OH)]$. Acta Crystallogr. **B36** (1980) 259–263.

Ilyukhin, V. V., Belov, N. V.: The crystal structure of lovozerite. Dokl. Acad. Nauk SSSR **131** (1960) 176–179.

Lazebnik, K. A., Nikishova, L. V., Lazebnik, Yu. D.: Tokkoite, a new mineral of charoitites. Mineral. Zhurn. **8** (1986) 85–89.

Liebau, F.: Silicates with branched anions: a crystallochemically distinct class. Am. Mineral. **63** (1978) 918–923.

Ohashi, Y., Finger, L. W.: The role of octahedral cations in pyroxinoid crystal chemistry. I. Bustamite, wollastonite, and the pectolite-schizolite-serandite series. Am. Mineral. **63** (1978) 274–288.

Petrunina, A. A., Ilyukhin, V. V., Belov, N. V.: On the crystal structure of tinaksite. In: *Constitution and features of minerals* (Eds. E. K. Lazarenko, A. S. Povarennykh) p. 10–18. Kiev, Naukova Dumka 1973.

Prewitt, C. T.: Refinement of the structure of pectolite, $Ca_2NaHSi_3O_9$. Z. Kristallogr. **125** (1967) 298–316.

Prewitt, C. T., Buerger, M. J.: Comparison of the crystal structure of wollastonite and pectolite. Mineral. Soc. Spec. P. **1** (1963) 293–302.

Pyatenko, Yu. A.: On a single approach to the analysis of valency local balance in inorganic structures. Crystallographiya **17** (1972) 773–779.

Pyatenko, Yu. A., Voronkov, A. A., Pudovkina, Z. V.: *Mineralogical crystal chemistry of titanum*. p. 155, Moscow: Nauka 1976.

Rozhdestvenskaya, I. V., Nikishova, L. V., Bannova, I. I., Lazebnik, Yu. D.: Canasite – refinement and characteristics of the structure, structural typomorphism. Mineral. Zhurn. **10** (1988) 31–41.

Scott, J. D.: Crystal structure of miserite, a Zoltai type 5 structure. Can. Mineral. **14** (1976) 515–528.

Wolkers, N., Stewart, D.: An empirical method for correcting diffractometer date for absorption effects. Acta Crystallogr. **A39** (1983) 158–165.