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THE CRYSTAL CHEMISTRY OF FAIZIEVITE, K_2 Li_6 Na (Ca_6Na) Ti_4 $[Si_6O_{18}]_2$ $[Si_{12}O_{30}]$ F_2, A NOVEL STRUCTURE BASED ON INTERCALATED BLOCKS OF THE BARATOVITE AND BEREZANSKITE STRUCTURES

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ABSTRACT

The crystal structure of faizievite, ideally K_2 Li_6 Na (Ca_6Na) Ti_4 $[Si_6O_{18}]_2$ $[Si_{12}O_{30}]$ F_2, *a* 9.8156(9), *b* 9.8249(9), *c* 17.3087(16) Å, α 99.209(2), β 94.670(2), γ 119.839(1)°, *V* 1403.7(4) Å^3, space group $P\overline{1}$, $Z = 1$, $D_{calc.}$ 2.846 g/cm^3, has been solved and refined to an R_1 index of 7.5% based on 5044 unique ($F_o > 4\sigma F$) reflections collected on a Bruker single-crystal *P*4 diffractometer with a 4K CCD detector and Mo*K*α X-radiation. Electron-microprobe analysis gave SiO_2 60.65, TiO_2 13.44, Nb_2O_5 0.11, CaO 14.52, K_2O 3.93, Na_2O 1.99, SrO 0.72, Rb_2O 0.13, F 1.30, Li_2O 3.76, sum 100.24 wt.%. Concentrations of Li_2O, Rb_2O, SrO and BaO were determined by ICP–OES. There are fifteen tetrahedrally coordinated sites: twelve sites are occupied by Si, with a grand <*Si*–O> of 1.613 Å; three sites are occupied by Li, with a grand <*Li*–O> distance of 1.928 Å. There are six octahedrally coordinated sites. The two *Ti*(1) and *Ti*(2) sites are occupied by $Ti_{2.00}$ with <*Ti*–O> = 1.937 and 1.934 Å, respectively. The four *M* sites are occupied by Ca with minor Sr and Na: the *M*(1) site (= $Ca_{2.00}$), with <*M*(1)–O> = 2.441 Å, the *M*(2) site [= $(Ca_{1.87}\,Sr_{0.13})$], with <*M*(2)–O> = 2.424 Å, the *M*(3) site [= $(Ca_{1.56}\,Na_{0.40}\,Sr_{0.04})$], with <*M*(3)–O> = 2.415 Å, and the *M*(4) site [= $(Ca_{0.73}\,Na_{0.27})$], with <*M*(4)–O> = 2.418 Å. There are two interstitial *A* sites: the *A*(1) site is [12]-coordinated and is occupied by $(K_{1.93}\,Ba_{0.04}\,Rb_{0.03})$, with <*A*(1)–O> = 3.092 Å; the *A*(2) site is [9]-coordinated and is occupied by $(Na_{0.86}\,\square_{0.14})$, with <*A*(2)–O> = 2.718 Å. The crystal structure of faizievite consists of four types of (001) sheets. The Si tetrahedra form two types of six-membered rings: a single (Si_6O_{18}) ring, as in baratovite, and a double $(Si_{12}O_{30})$ ring, as in milarite-group minerals, in the ratio 2:1. Each type of ring forms a distinct sheet (Na atoms occur in a sheet of milarite double rings). Two other sheets are: a sheet of corner-sharing (LiO_4) tetrahedra and (TiO_6) octahedra with K atoms in large voids, and a sheet of edge-sharing *M* octahedra (*M* = Ca >> Na). Each sheet is characterized by a planar cell based on translation vectors, $\mathbf{t_1}$ and $\mathbf{t_2}$, with $t_1 \approx t_2 \approx 9.8$ Å and $\mathbf{t_1} \wedge \mathbf{t_2}$ close to 120°. The composition of the four individual sheets within the planar cell $\mathbf{t_1},\mathbf{t_2}$ is: (1) (Si_6O_{18}), (2) $(Si_{12}O_{30})Na$, (3) KLi_3Ti_2, (4) $(Ca_6Na)F_2$. The crystal structure of faizievite is a hybrid of the structures of baratovite, $KLi_3Ca_7Ti_2(Si_6O_{18})_2F_2$, and berezanskite, $KLi_3Ti_2(Si_{12}O_{30})$ (milarite group). The *baratovite* block of composition $[KLi_3(Ca_6Na)Ti_2(Si_6O_{18})_2F_2]$ comprises sheets (3)(1)(4)(1). The *berezanskite* block of composition $[KNaLi_3Ti_2(Si_{12}O_{30})]$ comprises sheets (3)(2). In the faizievite structure, baratovite and berezanskite blocks alternate along [001] and sum to the following sequence: (3)(1)(4)(1)(3)(2). There are minor differences between the chemical compositions of baratovite and berezanskite and analogous blocks in the crystal structure of faizievite. Baratovite, K Li_3 Ca_7 Ti_2 $(Si_6O_{18})_2$ F_2, and the *baratovite* block in faizievite, $KLi_3(Ca_6Na)Ti_2(Si_6O_{18})_2F_2$, are related by the substitution: $^{[6]}Ca^{2+} \Leftrightarrow {}^{[6]}Na^{+}$. Berezanskite, $K^{[9]}\,\square\,Li_3\,Ti_2\,(Si_{12}O_{30})$, and the *berezanskite* block in faizievite, $K^{[9]}NaLi_3Ti_2(Si_{12}O_{30})$, are related by the substitution: $^{[9]}\square \Leftrightarrow {}^{[9]}Na^{+}$. Assembly of faizievite from baratovite and berezanskite components is accompanied by the following substitution: $^{[6]}Ca^{2+} + {}^{[9]}\square \Leftrightarrow {}^{[6]}Na^{+} + {}^{[9]}Na^{+}$.

Keywords: faizievite, new mineral species, crystal-structure refinement, baratovite, berezanskite, intercalated framework.

SOMMAIRE

Nous avons résolu la structure cristalline de la faizievite, de composition idéale K_2 Li_6 Na (Ca_6Na) Ti_4 $[Si_6O_{18}]_2$ $[Si_{12}O_{30}]$ F_2, *a* 9.8156(9), *b* 9.8249(9), *c* 17.3087(16) Å, α 99.209(2), β 94.670(2), γ 119.839(1)°, *V* 1403.7(4) Å^3, groupe spatial $P\overline{1}$, $Z = 1$, $D_{calc.}$ 2.846 g/cm^3, et nous l'avons affiné jusqu'à un résidu R_1 de 7.5% en utilisant 5044 réflexions uniques ($F_o > 4\sigma F$) prélevées sur monocristal avec un diffractomètre Bruker *P*4 muni d'un détecteur CCD 4K et avec rayonnement Mo*K*α. Une analyse par microsonde électronique a donné SiO_2 60.65, TiO_2 13.44, Nb_2O_5 0.11, CaO 14.52, K_2O 3.93, Na_2O 1.99, SrO 0.72, Rb_2O 0.13, F 1.30, Li_2O 3.76, pour un total de 100.24% (poids). La concentration de Li_2O, Rb_2O, SrO et BaO a été déterminée par ICP–OES. Il y a quinze sites ayant une coordinence tétraédrique: douze contiennent Si, avec une moyenne globale <*Si*–O>

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de 1.613 Å; trois sites contiennent Li, avec une moyenne globale <*Li*–O> de 1.928 Å. La structure contient six sites à coordinence octaédrique. Les deux sites *Ti*(1) et *Ti*(2) contiennent $Ti_{2.00}$, avec <*Ti*–O> = 1.937 et 1.934 Å, respectivement. Les quatre sites *M* contiennent Ca et des quantités moindres de Sr et Na: le site *M*(1) (= $Ca_{2.00}$), avec <*M*(1)–O> = 2.441 Å, le site *M*(2) [= $(Ca_{1.87}Sr_{0.13})$], avec <*M*(2)–O> = 2.424 Å, le *M*(3) site [= $(Ca_{1.56}\,Na_{0.40}\,Sr_{0.04})$], avec <*M*(3)–O> = 2.415 Å, et le site *M*(4) [= $(Ca_{0.73}\,Na_{0.27})$], avec <*M*(4)–O> = 2.418 Å. La structure contient deux sites *A* interstitiels: Le site *A*(1), à coordinence [12], contient $(K_{1.93}\,Ba_{0.04}\,Rb_{0.03})$, avec <*A*(1)–O> = 3.092 Å; le site *A*(2), à coordinence [9], contient $(Na_{0.86}\,\square_{0.14})$, avec <*A*(2)–O> = 2.718 Å. La structure cristalline de la faizievite est faite de quatre types de feuillets (001). Les tétraèdres Si sont disposés en deux types d'anneaux à six membres, un anneau (Si_6O_{18}) simple, et un anneau ($Si_{12}O_{30}$) double, tout comme dans les minéraux du groupe de la milarite, dans une proportion 2:1. Chaque type d'anneau forme un feuillet distinct (les atomes Na se trouvent dans le feuillet à anneaux doubles de type milarite). Les deux autres feuillets contiennent les tétraèdres (LiO_4) à coins partagés et les octaèdres (TiO_6) avec les atomes K situés dans les larges trous, et un feuillet d'octaèdres *M* (*M* = Ca >> Na) à arêtes partagées. Chaque feuillet possède une maille planaire fondée sur les vecteurs de translation $\mathbf{t_1}$ et $\mathbf{t_2}$, avec $t_1 \approx t_2 \approx 9.8$ Å et $\mathbf{t_1} \wedge \mathbf{t_2}$ voisin de 120°. La composition des quatre feuillets individuels au sein de la maille planaire $\mathbf{t_1},\mathbf{t_2}$ est: (1) (Si_6O_{18}), (2) ($Si_{12}O_{30}$)Na, (3) KLi_3Ti_2, (4) (Ca_6Na)F_2. La structure de la faizievite est un hybride des structures de la baratovite, $KLi_3Ca_7Ti_2(Si_6O_{18})_2F_2$, et de la berezanskite, $KLi_3Ti_2(Si_{12}O_{30})$ (groupe de la milarite). Le bloc *baratovite*, de composition [$KLi_3(Ca_6Na)Ti_2(Si_6O_{18})_2F_2$], est constitué des feuillets (3)(1)(4)(1). Le bloc *berezanskite*, de composition [$KNaLi_3Ti_2(Si_{12}O_{30})$], est constitué des feuillets (3)(2). Dans cette structure, les blocs de baratovite et de berezanskite alternent le long de [001] et définissent la séquence (3)(1)(4)(1)(3)(2). Il existe de légères différences entre les compositions de la baratovite et de la berezanskite et les blocs analogues faisant partie de la structure de la faizievite. La baratovite, $K\,Li_3\,Ca_7\,Ti_2\,(Si_6O_{18})_2\,F_2$, et le bloc *baratovite* dans la faizievite, $KLi_3(Ca_6Na)Ti_2(Si_6O_{18})_2F_2$, sont apparentés selon la substitution: $^{[6]}Ca^{2+} \Leftrightarrow {}^{[6]}Na^{+}$. La berezanskite, $K^{[9]}\square\,Li_3\,Ti_2\,(Si_{12}O_{30})$, et le bloc *berezanskite* dans la faizievite, $K^{[9]}NaLi_3Ti_2(Si_{12}O_{30})$, sont apparentés selon la substitution: $^{[9]}\square \Leftrightarrow {}^{[9]}Na^{+}$. L'assemblage des composantes baratovite et berezanskite pour constituer la faizievite se fait selon la substitution $^{[6]}Ca^{2+} + {}^{[9]}\square \Leftrightarrow {}^{[6]}Na^{+} + {}^{[9]}Na^{+}$.

(Traduit par la Rédaction)

Mots-clés: faizievite, nouvelle espèce minérale, affinement de la structure, baratovite, berezanskite, trames intercalées.

Introduction

Faizievite, $K_2\,Li_6\,Na\,(Ca_6Na)\,Ti_4\,[Si_6O_{18}]_2\,[Si_{12}O_{30}]\,F_2$, is a new mineral species from the moraine of the Dara-i-Pioz glacier, the Alai mountain ridge, Tien-Shan Mountains, northern Tajikistan (Agakhanov *et al*. 2008). In a quartz–pectolite boulder, faizievite forms a rim around grains of baratovite, $K\,Li_3\,Ca_7\,Ti_2\,(Si_6O_{18})_2\,F_2$, and occurs in association with aegirine, fluorite, polylithionite, neptunite, hyalotekite, baratovite, sokolovaite, pectolite, senkevichite and a Ti-rich mica. Here, we report the crystal structure of faizievite as an assemblage of intercalated blocks of the structures of baratovite, $K\,Li_3\,Ca_7Ti_2\,(Si_6O_{18})_2\,F_2$ (Sandomirskii *et al*. 1976), and berezanskite, $K\,Li_3\,Ti_2\,(Si_{12}O_{30})$ (milarite group) (Pautov & Agakhanov 1997). Both baratovite and berezanskite were first described as accessory minerals in quartz – albite – aegirine pegmatitic veinlets in quartz–aegirine syenites and albitites of the Dara-i-Pioz massif, northern Tajikistan (Dusmatov *et al*. 1975, and Pautov & Agakhanov 1997, respectively). The crystal structure of baratovite was solved by Sandomirskii *et al*. (1976) and refined by Menchetti & Sabelli (1979). Sandomirskii *et al*. (1976) gave the formula of baratovite as $K\,Li_3\,Ca_7\,Ti_2\,(Si_6O_{18})_2\,F_2$. Menchetti & Sabelli (1979) wrote the formula of baratovite as $K\,Li_3\,Ca_7\,(Ti_{0.87}Zr_{0.13})_2\,[Si_6O_{18}]_2\,(OH,F)_2$ without realizing that the OH-dominant site makes it another mineral. An OH-dominant analogue of baratovite, katayamalite, $K\,Li_3\,Ca_7\,Ti_2\,[Si_6O_{18}]_2\,(OH)_2$, was described by Murakami *et al*. (1983). Its structure was described by Kato & Murakami (1985) as triclinic and related to the structure of baratovite. However, Baur & Kassner (1992) showed that: (1) there is not enough fluorine in baratovite to justify 2 atoms of F per formula unit, and therefore, the formula of baratovite should be written as $K\,Li_3\,Ca_7\,Ti_2\,[Si_6O_{18}]_2\,(OH,F)_2$, and (2) baratovite and katayamalite are both monoclinic and are structurally identical. In this work, we will use the structure data of Sandomirskii *et al*. (1976). The crystal structure of berezanskite has not yet been refined. Berezanskite is a Li-bearing member of the milarite group with a vacancy at the *B* site; we can write its formula as $K\,{}^{[9]}\square\,Li_3\,Ti_2\,(Si_{12}O_{30})$.

Chemical Composition

The crystal of faizievite, for which the X-ray single-crystal diffraction data were collected, was placed on an aluminum disk, carbon-coated and analyzed with a Cameca SX100 electron microprobe operating in wavelength-dispersion mode with an accelerating voltage of 15 kV, a specimen current of 20 nA, a beam size of 10 μm, and count times on peak and background of 20 and 10 s, respectively. The following standards were used for *K* and *L* X-ray lines: Na: albite, Si, Ca: diopside, K: orthoclase, Ti: titanite, Nb: $LiNbO_3$, and F: fluorite. Magnesium, aluminum, chlorine, iron, manganese, and chromium were sought, but not detected. Data were

reduced using the X–PHI procedure (Merlet 1992). The contents of Li_2O, Rb_2O, SrO and BaO were determined by inductively coupled plasma – optical emission spectroscopy (ICP–OES). Table 1 gives the chemical composition; the empirical formula based on (O + F) = 68 atoms per formula unit (*apfu*) is $(K_{1.97}Ba_{0.04}Rb_{0.03})_{\Sigma 2.05}$ $Li_{6.00}$ $(Na_{0.86}\square_{0.14})_{\Sigma 1.00}$ $(Ca_{6.16}Na_{0.67}Sr_{0.17})_{\Sigma 7.00}$ $(Ti_{4.00}Nb_{0.02})_{\Sigma 4.02}$ $Si_{24.01}$ O_{66} $(F_{1.63}O_{0.37})_{\Sigma 2}$.

X-Ray Data Collection and Structure Refinement

Crystals of faizievite, polylithionite, baratovite, sokolovaite and a Ti-rich mica form complex aggregates of thin platy flakes of similar white to slightly yellowish color. It was extremely difficult to find a suitable single crystal for structure work. A small flake with dimensions of 0.04 × 0.04 × 0.01 mm was selected for a single-crystal determination of the structure.

X-ray-diffraction data for faizievite were collected with a Bruker *P*4 diffractometer equipped with a 4K CCD detector (Mo*K*α radiation). The intensities of 13758 reflections with $-13 < h < 13$, $-13 < k < 13$, $-24 < l < 24$ were collected to 59.99° 2θ using 15 s per 0.2° frame; an empirical absorption-correction (SADABS, Sheldrick 1998) was applied. The refined unit-cell parameters were obtained from 1823 reflections with $I > 20\sigma I$. During the refinement, the data were truncated at 2θ = 50° as there was no significant diffracted intensity at higher 2θ values. The crystal structure of faizievite was solved by direct methods and refined to $R_1 = 0.075$ and a Go*F* value of 1.147 for 6452 independent reflections (514 refined parameters including extinction) with the Bruker SHELXTL version 5.1 system of programs (Sheldrick 1997). Site occupancies were refined for two *Ti* sites, four *M* sites (primarily occupied by Ca with minor Na and Sr), and two *A* sites (primarily occupied by K and Na with minor Rb and Ba).

Details of the data collection and structure refinement are given in Table 2, final parameters of the atoms in Table 3, selected interatomic distances and angles in Table 4, refined site-scattering values and assigned populations for selected sites in Table 5, and bond-valence values in Table 6. A table of structure factors is available from the Depository of Unpublished Data on the Mineralogical Association of Canada website [document Faizievite CM46_163].

TABLE 1. CHEMICAL COMPOSITION AND UNIT FORMULA OF FAIZIEVITE

SiO_2 wt.%	60.65	Si *apfu*	24.01	K *apfu*	1.98
Li_2O*	3.76	Σ*T*	24.01	Rb	0.03
TiO_2	13.44			Ba	0.04
Nb_2O_5	0.11	Li	6.00	Σ*A*(1)	2.05
CaO	14.52	Σ	6.00		
SrO*	0.72				
Na_2O	1.99	Ti^{4+}	4.00	Na	0.86
K_2O	3.93	Nb	0.02	Σ*A*(2)	0.86
Rb_2O*	0.13	Σ*D*	4.02		
BaO*	0.24				
F	1.30	Ca	6.16	F	1.63
O=F	–0.55	Sr	0.17		
		Na	0.67		
Total	100.24	Σ*M*	7.00		

* determined by ICP–OES.

Description of the Structure

Cation sites

There are fifteen tetrahedrally coordinated sites. Twelve [4]-coordinated sites are occupied solely by Si, with a grand <*Si*–O> of 1.613 Å. Three [4]-coordinated sites are solely occupied by Li, with a grand <*Li*–O> distance of 1.928 Å. There are six octahedrally coordinated sites. Two sites are occupied by Ti, and four *M* sites are occupied by Ca with minor Na and Sr. The two *Ti*(1) and *Ti*(2) sites are occupied by $Ti_{2.00}$ with <*Ti*–O> = 1.937 and 1.934 Å, respectively. The four *M* sites are occupied by Ca with minor Na and Sr: the *M*(1) site is occupied solely by $Ca_{2.00}$, with <*M*(1)–O> = 2.441 Å, the *M*(2) site is occupied by $(Ca_{1.87}Sr_{0.13})$, with <*M*(2)–O> = 2.424 Å, the *M*(3) site is occupied by $(Ca_{1.56}Na_{0.40}Sr_{0.04})$, with <*M*(3)–O> = 2.415 Å, and the *M*(4) site is occupied by $(Ca_{0.73}Na_{0.27})$, with <*M*(4)–O> 2.418 Å. There are two interstitial *A* sites: the [12]-coordinated *A*(1) site is occupied by $(K_{1.93}Ba_{0.04}Rb_{0.03})$, with <*A*(1)–O> = 3.092 Å; the [9]-coordinated *A*(2) site is occupied by $(Na_{0.86}\square_{0.14})$, with <*A*(2)–O> = 2.718 Å. The bond-valence sums around both cations and anions (Table 6) are in accord with the assigned site-populations.

Structure topology

The crystal structure of faizievite consists of four types of sheet, all of which are parallel to (001). Sheets (1) and (2) are composed of two distinct types of six-membered rings of Si tetrahedra: a single (Si_6O_{18}) ring (Fig. 1a), as in beryl and baratovite, K Li_3 Ca_7

TABLE 2. MISCELLANEOUS STRUCTURE-REFINEMENT DATA FOR FAIZIEVITE

a (Å)	9.8156(9)	α (°)	99.209(2)
b	9.8249(9)	β	94.670(2)
c	17.3087(16)	γ	119.839(1)
V (Å^3)	1403.7(4)		
Space group	$P\bar{1}$	*Z*	1
Absorption coefficient (mm^{-1})			2.03
F(000)	1188.0	D_{calc} (g/cm^3)	2.846
Crystal size (mm)	0.04 × 0.04 × 0.01	Radiation/filter	Mo*K*α/graphite
2θ range for data collection (°)		59.99	
R(int) (%)		5.59	
Reflections collected		24778	
Unique reflections		13758	
Independent reflections		6452	
$F_o > 4\sigma F_o$		5044	
Refinement method		Full-matrix least-squares on F^2, fixed weights proportional to $1/\sigma F_o^2$	
Goodness of fit on F^2		1.147	
Final $R_{(obs)}$ (%) [$F_o > 4\sigma F_o$]		R_1 = 7.45	
R indices (all data) (%)		R_1 = 9.79	
		wR_2 = 14.39	
		Go*F* = 1.147	

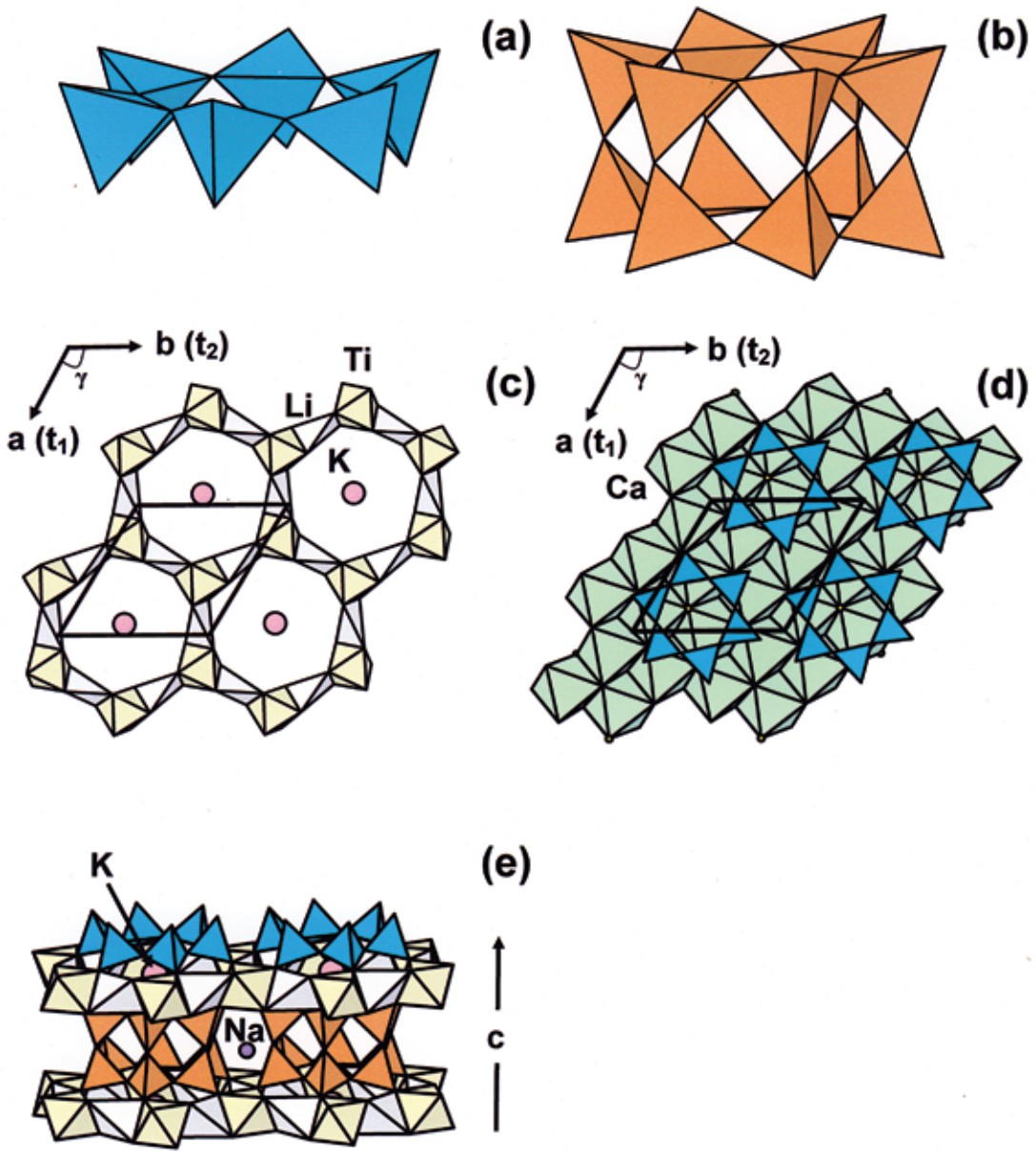

FIG. 1. Fragments of the crystal structure of faizievite: (a) a six-membered single *beryl* ring [Si_6O_{18}]; (b) a six-membered double *milarite* ring [$Si_{12}O_{30}$]; (c) a sheet of (LiO_4) tetrahedra and (TiO_6) octahedra and K atoms in large voids viewed down [001]; (d) a sheet of Ca-dominant *M*(1,2,3,4) octahedra and adjacent [Si_6O_{18}] rings viewed down [001]; (e) linkage of ($Si_{12}O_{30}$) and (Si_6O_{18}) rings and a sheet of (LiO_4) tetrahedra and (TiO_6) octahedra viewed down [110]. The (SiO_4) tetrahedra of milarite and beryl rings are orange and blue, the (LiO_4) tetrahedra are grey, the (TiO_6) octahedra are honey yellow; the *M*(1,2,3,4) octahedra are green, *A*(1) (= Na), *A*(2) (= K) and F atoms are shown as large pink, medium purple and small yellow circles, respectively.

TABLE 3. FINAL POSITIONS AND DISPLACEMENT PARAMETERS (Å^2) OF ATOMS IN FAIZIEVITE

	x	*y*	*z*	U_{eq}*	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ti(1)	0.4153(1)	0.2695(1)	0.21637(6)	0.0024(4)	0.0019(6)	0.0026(6)	0.0028(5)	0.0006(4)	−0.0000(4)	0.0014(5)
Ti(2)	−0.2525(1)	−0.0651(1)	0.21454(6)	0.0033(4)	0.0019(6)	0.0032(6)	0.0051(6)	0.0012(4)	0.0005(4)	0.0016(5)
M(1)	0.2884(2)	0.3543(2)	0.49983(8)	0.0074(4)	0.0072(7)	0.0075(7)	0.0091(7)	0.0025(5)	0.0026(5)	0.0047(6)
M(2)	0.1489(2)	0.9347(2)	0.51649(7)	0.0084(4)	0.0059(7)	0.0075(7)	0.0116(7)	0.0024(5)	0.0016(5)	0.0032(6)
M(3)	0.4259(2)	0.7867(2)	0.50910(8)	0.0090(5)	0.0076(8)	0.0094(8)	0.0103(7)	0.0008(5)	0.0015(5)	0.0050(6)
M(4)	0	1/2	1/2	0.0110(7)	0.0084(12)	0.0098(13)	0.0150(12)	0.0003(9)	0.0012(8)	0.0057(10)
Li(1)	0.0806(13)	0.1015(15)	0.2129(7)	0.0114(23)	0.0018(54)	0.0144(61)	0.0245(62)	0.0092(49)	0.0041(45)	0.0073(50)
Li(2)	−0.4128(14)	−0.3992(15)	0.2143(7)	0.0128(25)	0.0103(59)	0.0127(61)	0.0093(52)	0.0008(45)	0.0075(43)	0.0013(51)
Li(3)	−0.4225(15)	0.0952(15)	0.2119(7)	0.0140(25)	0.0200(67)	0.0119(61)	0.0193(60)	0.0089(48)	0.0049(49)	0.0133(56)
Si(1)	0.7618(2)	0.4199(2)	0.3383(1)	0.0062(4)	0.0058(9)	0.0057(9)	0.0068(8)	−0.0013(7)	−0.0010(6)	0.0039(8)
Si(2)	0.5077(2)	0.0979(2)	0.6625(1)	0.0058(4)	0.0069(9)	0.0066(9)	0.0073(8)	0.0022(7)	0.0027(7)	0.0055(8)
Si(3)	0.3974(2)	0.6639(2)	0.0932(1)	0.0066(4)	0.0067(9)	0.0070(9)	0.0066(8)	0.0014(7)	−0.0009(7)	0.0041(8)
Si(4)	0.3730(2)	0.5384(2)	0.3392(1)	0.0059(4)	0.0055(9)	0.0039(9)	0.0080(8)	0.0008(7)	0.0019(6)	0.0024(8)
Si(5)	0.1552(2)	0.3031(2)	0.0932(1)	0.0068(4)	0.0056(9)	0.0081(9)	0.0070(8)	0.0033(7)	0.0005(6)	0.0033(8)
Si(6)	0.2516(2)	0.0291(2)	0.3403(1)	0.0061(4)	0.0054(9)	0.0061(9)	0.0078(8)	0.0024(7)	0.0019(6)	0.0034(8)
Si(7)	0.6721(2)	0.4225(2)	0.0924(1)	0.0068(4)	0.0082(9)	0.0065(9)	0.0067(8)	0.0014(7)	0.0029(7)	0.0043(8)
Si(8)	−0.1130(2)	−0.2157(2)	0.3392(1)	0.0058(4)	0.0047(9)	0.0050(9)	0.0075(8)	0.0021(7)	0.0019(6)	0.0020(8)
Si(9)	0.2757(2)	−0.0953(2)	0.0935(1)	0.0073(4)	0.0073(9)	0.0082(9)	0.0065(8)	−0.0009(7)	0.0000(7)	0.0049(8)
Si(10)	0.0089(2)	0.2956(2)	0.3378(1)	0.0062(4)	0.0036(9)	0.0073(9)	0.0072(8)	0.0000(7)	0.0010(6)	0.0029(8)
Si(11)	−0.2075(2)	0.1811(2)	0.0921(1)	0.0066(4)	0.0069(9)	0.0083(9)	0.0066(8)	0.0022(7)	0.0015(7)	0.0052(8)
Si(12)	0.9132(2)	0.7840(2)	0.0925(1)	0.0069(4)	0.0062(9)	0.0066(9)	0.0061(8)	−0.0010(7)	0.0018(6)	0.0026(8)
A(1)	0.9146(2)	0.3924(2)	0.7745(1)	0.0249(6)	0.0199(10)	0.0228(10)	0.0342(11)	0.0081(8)	0.0065(7)	0.0121(8)
A(2)	0.3337(11)	0.1676(11)	0.0032(5)		0.0350(32)					
O(1)	0.5993(5)	0.2869(6)	0.2751(3)	0.0090(10)	0.0030(23)	0.0091(24)	0.0136(23)	0.0032(18)	−0.0016(18)	0.0025(20)
O(2)	0.4539(6)	0.4686(6)	0.2789(3)	0.0091(10)	0.0095(24)	0.0078(24)	0.0118(22)	0.0008(18)	0.0057(18)	0.0058(21)
O(3)	−0.2345(5)	−0.1966(6)	0.2795(3)	0.0095(10)	0.0051(23)	0.0077(24)	0.0144(23)	0.0066(19)	−0.0014(18)	0.0018(20)
O(4)	−0.0649(5)	0.1255(6)	0.2744(3)	0.0094(10)	0.0044(23)	0.0064(24)	0.0131(23)	−0.0027(18)	−0.0005(18)	0.0015(20)
O(5)	0.2723(6)	0.1450(6)	0.2796(3)	0.0086(10)	0.0098(24)	0.0115(25)	0.0094(21)	0.0059(18)	0.0050(18)	0.0078(21)
O(6)	0.2231(6)	0.2278(6)	0.1483(3)	0.0092(10)	0.0102(24)	0.0088(24)	0.0108(22)	0.0074(18)	0.0029(18)	0.0049(21)
O(7)	0.5431(6)	0.4017(6)	0.1463(3)	0.0106(10)	0.0135(26)	0.0089(24)	0.0102(22)	0.0003(18)	0.0037(19)	0.0067(22)
O(8)	0.3966(5)	0.0783(5)	0.1480(3)	0.0086(10)	0.0044(23)	0.0044(23)	0.0124(22)	−0.0007(18)	−0.0007(18)	−0.0001(20)
O(9)	−0.3883(5)	−0.0281(6)	0.2761(3)	0.0078(9)	0.0069(23)	0.0091(24)	0.0134(22)	0.0075(18)	0.0081(18)	0.0062(21)
O(10)	−0.1101(6)	−0.0857(6)	0.1469(3)	0.0108(10)	0.0081(24)	0.0124(25)	0.0127(23)	−0.0000(19)	0.0027(18)	0.0066(22)
O(11)	−0.2932(6)	0.0562(6)	0.1451(3)	0.0114(10)	0.0110(25)	0.0092(25)	0.0167(24)	0.0053(19)	0.0059(19)	0.0061(22)
O(12)	−0.4335(5)	−0.2676(6)	0.1475(3)	0.0101(10)	0.0063(24)	0.0057(24)	0.0154(23)	0.0014(19)	−0.0031(18)	0.0019(21)
O(13)	0.2609(6)	0.5686(6)	0.5708(3)	0.0144(11)	0.0158(27)	0.0148(27)	0.0096(23)	0.0043(20)	0.0015(19)	0.0056(23)
O(14)	0.8321(6)	0.5950(6)	0.3150(3)	0.0108(10)	0.0110(25)	0.0059(23)	0.0163(24)	0.0065(19)	0.0053(19)	0.0035(21)
O(15)	0.8994(6)	0.3758(6)	0.3251(3)	0.0147(11)	0.0125(27)	0.0155(27)	0.0267(27)	0.0083(22)	0.0050(21)	0.0139(24)
O(16)	0.4194(6)	0.0216(6)	0.5713(3)	0.0130(11)	0.0132(26)	0.0171(27)	0.0092(22)	0.0012(19)	0.0024(19)	0.0087(23)
O(17)	0.6479(6)	0.0575(6)	0.6820(3)	0.0099(10)	0.0114(25)	0.0138(26)	0.0134(23)	0.0042(19)	0.0070(19)	0.0120(22)
O(18)	0.5990(6)	0.2941(6)	0.6817(3)	0.0124(10)	0.0132(26)	0.0056(24)	0.0185(25)	0.0041(19)	0.0018(20)	0.0048(22)
O(19)	0.4104(7)	0.6381(7)	0.0001(3)	0.0227(13)	0.0239(32)	0.0296(33)	0.0086(24)	−0.0004(22)	−0.0010(21)	0.0116(28)
O(20)	0.2677(6)	0.4966(6)	0.1122(3)	0.0168(11)	0.0126(27)	0.0068(25)	0.0274(28)	0.0092(21)	0.0002(21)	0.0014(22)
O(21)	0.3270(6)	0.7810(6)	0.1134(3)	0.0164(11)	0.0162(28)	0.0113(26)	0.0207(26)	−0.0006(21)	−0.0002(21)	0.0081(24)
O(22)	0.4401(6)	0.5655(6)	0.4314(3)	0.0142(11)	0.0195(28)	0.0168(27)	0.0085(23)	0.0013(20)	0.0020(19)	0.0115(24)
O(23)	0.1791(5)	0.4189(6)	0.3157(3)	0.0094(10)	0.0013(22)	0.0096(24)	0.0141(23)	0.0023(19)	0.0020(17)	0.0006(20)
O(24)	0.1387(7)	0.2279(7)	0.0002(3)	0.0216(13)	0.0329(34)	0.0350(35)	0.0043(22)	0.0024(22)	0.0029(21)	0.0235(30)
O(25)	−0.0152(6)	0.2697(7)	0.1116(3)	0.0176(12)	0.0117(27)	0.0242(31)	0.0223(27)	0.0059(21)	0.0037(21)	0.0130(25)
O(26)	0.3022(6)	0.1221(6)	0.4326(3)	0.0119(10)	0.0102(25)	0.0133(26)	0.0118(23)	−0.0005(19)	−0.0008(18)	0.0073(22)
O(27)	0.0658(6)	−0.1211(6)	0.3186(3)	0.0120(10)	0.0057(24)	0.0102(25)	0.0178(22)	0.0029(20)	0.0036(19)	0.0024(21)
O(28)	0.8145(6)	0.6089(6)	0.1118(3)	0.0174(11)	0.0158(28)	0.0104(26)	0.0240(27)	0.0072(21)	0.0087(22)	0.0038(23)
O(29)	0.7594(6)	0.3259(7)	0.1120(3)	0.0180(12)	0.0213(30)	0.0202(30)	0.0281(29)	0.0121(23)	0.0131(23)	0.0189(26)
O(30)	0.0962(6)	−0.1685(6)	0.1119(3)	0.0182(12)	0.0080(26)	0.0174(28)	0.0259(28)	−0.0002(22)	0.0040(21)	0.0055(23)
O(31)	0.1125(6)	0.1578(6)	0.5684(3)	0.0115(10)	0.0148(26)	0.0153(26)	0.0054(21)	0.0025(19)	0.0025(18)	0.0085(23)
O(32)	0.2714(7)	−0.0902(7)	0.0009(3)	0.0228(13)	0.0304(34)	0.0214(31)	0.0071(23)	−0.0012(21)	−0.0011(22)	0.0086(28)
O(33)	0.0306(6)	0.2819(6)	0.4280(3)	0.0139(11)	0.0155(27)	0.0137(26)	0.0104(23)	0.0050(19)	0.0004(19)	0.0056(23)
F	0.1739(5)	0.7233(6)	0.4533(3)	0.0209(10)	0.0195(24)	0.0243(25)	0.0202(22)	0.0029(19)	0.0039(18)	0.0130(22)

Ti_2 $(Si_6O_{18})_2$ F_2 (Sandomirskii *et al.* 1976), and a double $(Si_{12}O_{30})$ ring (Fig. 1b), as in the milarite-group minerals, in the ratio 2:1. Sheet (3) consists of corner-sharing (LiO_4) tetrahedra and (TiO_6) octahedra with K atoms in large voids (Fig. 1c). Sheet (4) consists of edge-sharing *M* octahedra (*M* = Ca >> Na > Sr) (Fig. 1d). The [9]-coordinated Na atoms occur in small cages between the milarite rings in sheet (2) (Fig. 1e). Figure 1e shows the large cages occupied by [12]-coordinated K atoms; these cages are formed by (LiO_4) tetrahedra, (TiO_6) octahedra and (Si_6O_{18}) and $(Si_{12}O_{30})$ rings. Each sheet is characterized by a planar cell based on transla-

tion vectors, $\mathbf{t_1}$ and $\mathbf{t_2}$, and $\mathbf{t_1} \wedge \mathbf{t_2}$ (= γ). We may write the composition of the four individual sheets within the planar cell **a**, **b**: (1) (Si_6O_{18}), (2) $(Si_{12}O_{30})Na$, (3) KLi_3Ti_2, and (4) $(Ca_6Na)F_2$. In the crystal structure of faizievite, four types of sheets alternate along [001] and give a sequence (2)(3)(1)(4)(1)(3), the repeat distance of which corresponds to the *c* unit-cell parameter (Fig. 2). The heteropolyhedral sheet (3) of composition KLi_3Ti_2 has two different adjacent sheets: sheet (1) consists of (Si_6O_{18}) rings, and sheet (2) consists of $(Si_{12}O_{30})$ rings and [9]-coordinated Na atoms (Figs. 2, 1e). The sheet of octahedra (4) of composition $(Ca_6Na)F_2$ has two identical adjacent sheets (1) composed of (Si_6O_{18}) rings (Figs. 2, 1d). We may write the ideal formula of faizievite as a sum of six sheets (2)(3)(1)(4)(1)(3) (see above): $2 \times (1) + (2) + 2 \times (3) + (4) = 2 \times (Si_6O_{18}) + (Si_{12}O_{30})Na + 2 \times KLi_3Ti_2 + (Ca_6Na)F_2 = K_2\,Li_6\,Na\,(Ca_6Na)\,Ti_4\,[Si_6O_{18}]_2\,[Si_{12}O_{30}]\,F_2$, Z = 1.

The Faizievite Structure: An Assemblage of Intercalated Blocks of the Baratovite and Berezanskite Structures

The crystal structure of faizievite is a hybrid of the structures of baratovite, $K\,Li_3\,Ca_7Ti_2\,(Si_6O_{18})_2\,F_2$ (Sandomirskii *et al.* 1976), and berezanskite, $K\,Li_3\,Ti_2\,(Si_{12}O_{30})$ (milarite group) (Pautov & Agakhanov 1997) (Table 7). There is a strong similarity between faizievite, baratovite and berezanskite: (1) they are ring silicates of K, Li and Ti, (2) they occur as associated minerals in the same unique locality, the moraine of the Dara-i-Pioz glacier, (3) their structure topology is based on an alternation of analogous sheets, and (4) each sheet is characterized by a planar cell based on translation vectors, $\mathbf{t_1}$ and $\mathbf{t_2}$, with $t_1 \approx t_2 \approx 9.8$ Å and $\mathbf{t_1} \wedge \mathbf{t_2}$ close to 120°.

The crystal structure of faizievite comprises structural fragments of both the baratovite and berezanskite structures. Consider the crystal structures of baratovite (Fig. 3) and berezanskite (Fig. 4). For the diagram of a hypothetical structure of berezanskite, we use atom coordinates of the crystal structure of sogdianite, $K\,^{[9]}\square\,Li_3\,Zr_2\,(Si_{12}O_{30})$, as the crystal structure of berezanskite has not been yet refined. Sogdianite is a Zr-analogue of berezanskite, with *a* 10.1240(3), *c* 14.3198(5), space group *P*6/*mcc*, *Z* = 2 (Sokolova *et al.* 2000).

We may consider the crystal structure of baratovite as an assemblage of three different sheets: (1) a sheet of Ca-octahedra, (2) a sheet of (Si_6O_{18}) single rings, and (3) a sheet of (LiO_4) tetrahedra, (TiO_6) octahedra and K atoms (Fig. 3). These three sheets of the baratovite structure correspond to sheets (4), (1) and (3) in the structure of faizievite (*cf.* Figs. 3, 2 and 1c, d). We relate the structures of baratovite and faizievite and identify a specific sequence of five sheets, (3)(1)(4)(1)(3), as the *baratovite* block of the faizievite structure. As the two outer sheets, (3), are shared between the *baratovite* block and the adjacent berezanskite block, they are counted accordingly in deriving the composition of the *baratovite* block: (3)(1)(4)(1) = $K_2Li_3(Ca_6Na)Ti_2(Si_6O_{18})_2F_2$. There is a minor difference between the chemical compositions of baratovite and its block in the crystal structure of faizievite. Sheet (4) has the composition Ca_7F_2 (Fig. 3) and $(Ca_6Na)F_2$ (Fig. 2) in baratovite and faizievite, respectively. Therefore, baratovite, $K\,Li_3\,Ca_7\,Ti_2\,(Si_6O_{18})_2\,(OH)_2$, and the *baratovite* block in faizievite, $K_2(Ca_6Na)Li_6Ti_4(Si_6O_{18})_2F_2$, are related by the substitution: $^{[6]}Ca^{2+} \Leftrightarrow {}^{[6]}Na^{+}$.

We may consider the crystal structure of berezanskite as a combination of two sheets: (1) a sheet of

TABLE 4. SELECTED INTERATOMIC DISTANCES (Å) AND ANGLES (°) IN FAIZIEVITE

Si(1)–O(1)	1.623(5)	*Si*(2)–O(9)	1.616(5)	*Si*(3)–O(12)	1.588(5)
Si(1)–O(13)	1.602(5)	*Si*(2)–O(16)	1.599(5)	*Si*(3)–O(19)	1.617(5)
Si(1)–O(14)	1.639(5)	*Si*(2)–O(17)	1.636(5)	*Si*(3)–O(20)	1.609(5)
Si(1)–O(15)	1.632(5)	*Si*(2)–O(18)	1.630(5)	*Si*(3)–O(21)	1.620(5)
<*Si*(1)–O>	1.624	<*Si*(2)–O>	1.620	<*Si*(3)–O>	1.609
Si(4)–O(2)	1.623(5)	*Si*(5)–O(6)	1.586(5)	*Si*(6)–O(5)	1.622(5)
Si(4)–O(18)	1.635(5)	*Si*(5)–O(20)	1.611(5)	*Si*(6)–O(17)	1.625(5)
Si(4)–O(22)	1.604(5)	*Si*(5)–O(24)	1.619(5)	*Si*(6)–O(26)	1.608(5)
Si(4)–O(23)	1.632(5)	*Si*(5)–O(25)	1.607(5)	*Si*(6)–O(27)	1.637(5)
<*Si*(4)–O>	1.624	<*Si*(5)–O>	1.606	<*Si*(6)–O>	1.623
Si(7)–O(7)	1.585(5)	*Si*(8)–O(3)	1.616(5)	*Si*(9)–O(8)	1.580(5)
Si(7)–O(19)	1.605(5)	*Si*(8)–O(14)	1.625(5)	*Si*(9)–O(21)	1.601(5)
Si(7)–O(28)	1.613(5)	*Si*(8)–O(27)	1.630(5)	*Si*(9)–O(30)	1.621(5)
Si(7)–O(29)	1.617(5)	*Si*(8)–O(31)	1.608(5)	*Si*(9)–O(32)	1.611(5)
<*Si*(7)–O>	1.605	<*Si*(8)–O>	1.620	<*Si*(9)–O>	1.603
Si(10)–O(4)	1.612(5)	*Si*(11)–O(11)	1.585(5)	*Si*(12)–O(10)	1.588(5)
Si(10)–O(15)	1.639(5)	*Si*(11)–O(25)	1.613(5)	*Si*(12)–O(24)	1.611(5)
Si(10)–O(23)	1.625(5)	*Si*(11)–O(29)	1.603(5)	*Si*(12)–O(28)	1.608(5)
Si(10)–O(33)	1.595(5)	*Si*(11)–O(32)	1.612(5)	*Si*(12)–O(30)	1.604(5)
<*Si*(10)–O>	1.618	<*Si*(11)–O>	1.603	<*Si*(12)–O>	1.603
Li(1)–O(4)	1.932(12)	*Li*(2)–O(2)	1.914(13)	*Li*(3)–O(1)	1.922(13)
Li(1)–O(5)	1.936(12)	*Li*(2)–O(3)	1.947(13)	*Li*(3)–O(8)	1.931(13)
Li(1)–O(6)	1.928(13)	*Li*(2)–O(7)	1.934(13)	*Li*(3)–O(9)	1.896(13)
Li(1)–O(10)	1.935(13)	*Li*(2)–O(12)	1.938(14)	*Li*(3)–O(11)	1.917(13)
<*Li*(1)–O>	1.933	<*Li*(2)–O>	1.933	<*Li*(3)–O>	1.917
M(1)–O(13)	2.409(5)	*M*(2)–O(16)	2.398(5)	*M*(3)–O(13)	2.432(5)
M(1)–O(22)	2.434(6)	*M*(2)–O(26)	2.493(5)	*M*(3)–O(16)	2.420(5)
M(1)–O(22)a	2.496(5)	*M*(2)–O(31)	2.437(5)	*M*(3)–O(16)c	2.475(5)
M(1)–O(26)	2.462(5)	*M*(2)–O(31)b	2.491(5)	*M*(3)–O(22)	2.438(5)
M(1)–O(31)	2.422(5)	*M*(2)–O(33)	2.399(5)	*M*(3)–O(26)	2.416(5)
M(1)–O(33)	2.422(5)	*M*(2)–F	2.323(5)	*M*(3)–F	2.308(5)
<*M*(1)–O>	2.441	<*M*(2)–O,F>	2.424	<*M*(3)–O,F>	2.415
Ti(1)–O(1)	1.913(5)	*Ti*(2)–O(3)	1.904(5)	*M*(4)–O(13) ×2	2.454(5)
Ti(1)–O(2)	1.913(5)	*Ti*(2)–O(4)	1.899(5)	*M*(4)–O(33) ×2	2.466(5)
Ti(1)–O(5)	1.906(5)	*Ti*(2)–O(9)	1.905(5)	*M*(4)–F ×2	2.334(5)
Ti(1)–O(6)	1.957(5)	*Ti*(2)–O(10)	1.959(5)	<*M*(4)–O,F>	2.418
Ti(1)–O(7)	1.965(5)	*Ti*(2)–O(11)	1.970(5)		
Ti(1)–O(8)	1.969(5)	*Ti*(2)–O(12)	1.967(5)		
< *Ti*(1)–O>	1.937	< *Ti*(2)–O>	1.934		
A(1)–O(14)	2.996(5)	*A*(2)–O(6)	2.906(10)	*Si*(1)–O(14)–*Si*(8)	149.8(3)
A(1)–O(15)	3.020(6)	*A*(2)–O(7)	2.880(10)	*Si*(1)–O(15)–*Si*(10)	158.4(4)
A(1)–O(17)	3.050(5)	*A*(2)–O(8)	2.903(10)	*Si*(2)–O(17)–*Si*(6)	153.6(3)
A(1)–O(18)	2.970(5)	*A*(2)–O(10)	2.976(10)	*Si*(2)–O(18)–*Si*(4)	151.6(3)
A(1)–O(20)	3.173(6)	*A*(2)–O(11)	2.955(10)	*Si*(3)–O(19)–*Si*(7)	150.4(4)
A(1)–O(21)	3.175(6)	*A*(2)–O(12)	3.001(11)	*Si*(3)–O(20)–*Si*(5)	153.8(4)
A(1)–O(23)	3.018(5)	*A*(2)–O(19)	2.290(11)	*Si*(3)–O(21)–*Si*(9)	153.6(4)
A(1)–O(25)	3.195(6)	*A*(2)–O(24)	2.267(11)	*Si*(4)–O(23)–*Si*(10)	151.1(3)
A(1)–O(27)	2.987(5)	*A*(2)–O(32)	2.283(11)	*Si*(5)–O(24)–*Si*(12)	149.5(4)
A(1)–O(28)	3.184(6)	<*A*(2)–O>	2.718	*Si*(5)–O(25)–*Si*(11)	154.1(4)
A(1)–O(29)	3.192(6)			*Si*(6)–O(27)–*Si*(8)	151.0(3)
A(1)–O(30)	3.148(6)			*Si*(7)–O(29)–*Si*(11)	153.1(4)
<*A*(1)–O>	3.092			*Si*(7)–O(28)–*Si*(12)	154.0(4)
				Si(9)–O(32)–*Si*(11)	150.3(4)
				Si(9)–O(30)–*Si*(12)	153.4(4)

a: $-x + 1, -y + 1, -z + 1$; b: $-x, -y + 1, -z + 1$; c: $-x + 1, -y + 2, -z + 1$.

(LiO_4) tetrahedra, (TiO_6) octahedra and K atoms, and (2) a sheet of ($Si_{12}O_{30}$) double rings. These two sheets correspond to sheets (3) and (2) of the faizievite structure (*cf.* Figs. 4, 2 and 1e). We identify the *berezanskite* block in the crystal structure of faizievite as the sequence of sheets: (3)(2)(3) (Figs. 2, 4). As the two outer sheets (3) belong to both the *berezanskite* block and the baratovite block, they are counted accordingly, and the *berezanskite* block has a composition (3)(2) = K Na $Li_3Ti_2(Si_{12}O_{30})$. There is a minor difference between the chemical composition of berezanskite and its block in the crystal structure of faizievite. Sheet (2) has a composition $(Si_{12}O_{30})^{[9]}\square$ (Fig. 4) and $(Si_{12}O_{30})^{[9]}$ Na (Fig. 2) in berezanskite and faizievite, respectively. Therefore, berezanskite, $K^{[9]}\square Li_3Ti_2(Si_{12}O_{30})$, and the *berezanskite* block in faizievite, $K^{[9]}NaLi_3Ti_2(Si_{12}O_{30})$, are related by the substitution: $^{[9]}\square \Leftrightarrow {}^{[9]}Na^+$.

In the faizievite structure, *baratovite* and *berezanskite* blocks alternate along [001], and share a common sheet (3) of composition KLi_3Ti_2. We write the ideal formula of faizievite as an intercalation of *baratovite* and *berezanskite* blocks: sheets (3)(1)(4)

TABLE 5. REFINED SITE-SCATTERING VALUES (*epfu*) AND ASSIGNED SITE-POPULATIONS (*apfu*) FOR FAIZIEVITE

Site	Refined site-scattering	Assigned site-population	Calculated site-scattering	<X-φ>$_{calc}$*	<X-φ>$_{obs}$
Ti(1)	43.8(2)	2.00 Ti^{4+}	44.0	1.985	1.937
Ti(2)	43.3(2)	2.00 Ti^{4+}	44.0	1.985	1.934
M(1)	40.1(2)	2.00 Ca	40.0	2.380	2.441
M(2)	42.4(2)	1.87 Ca + 0.13 Sr	42.4	2.392	2.424
M(3)	37.7(2)	1.56 Ca + 0.40 Na + 0.04 Sr	37.1	2.411	2.415
M(4)	17.6(2)	0.73Ca + 0.27 Na	17.6	2.385	2.418
A(1)	38.9(3)	1.93 K + 0.03 Rb + 0.04 Ba	40.0	3.021	3.092
A(2)	4.5(1)	0.86 Na + 0.14 □	9.5	2.620	2.718

* Calculated by summing constituent ionic radii; values from Shannon (1976).
φ: unspecified anions.

TABLE 6. BOND-VALENCE* TABLE FOR FAIZIEVITE

	Ti(1)	*Ti*(2)	*M*(1)	*M*(2)	*M*(3)	*M*(4)	*Li*(1)	*Li*(2)	*Li*(3)	*Si*(1)	*Si*(2)	*Si*(3)	*Si*(4)	*Si*(5)	*Si*(6)	*Si*(7)	*Si*(8)	*Si*(9)	*Si*(10)	*Si*(11)	*Si*(12)	*A*(2)	*A*(1)	Σ
O(1)	0.77								0.29	1.01														2.07
O(2)	0.76							0.30					1.01											2.07
O(3)		0.79						0.27									1.02							2.08
O(4)		0.80					0.29												1.04					2.13
O(5)	0.78						0.28								1.01									2.07
O(6)	0.68						0.28							1.11								0.02		2.09
O(7)	0.67							0.29								1.11						0.02		2.09
O(8)	0.66								0.28									1.13				0.02		2.09
O(9)		0.79							0.32		1.02													2.13
O(10)		0.69					0.28														1.10	0.02		2.09
O(11)		0.67							0.29											1.11		0.02		2.09
O(12)		0.67						0.28				1.09										0.02		2.06
O(13)			0.30		0.28	0.27 ×2↓			1.06														1.91	
O(14)										0.96							1.00						0.10	2.06
O(15)										0.99									0.95				0.09	2.03
O(16)				0.31	0.26 0.29						1.07													1.93
O(17)											0.98				0.99								0.08	2.05
O(18)											0.98		0.98										0.10	2.06
O(19)												1.03				1.05						0.10		2.18
O(20)												1.04		1.03									0.06	2.13
O(21)												1.01						1.07					0.06	2.14
O(22)			0.24 0.28		0.28								1.06											1.86
O(23)													0.97						1.01				0.09	2.07
O(24)														1.01							1.04	0.11		2.16
O(25)														1.06						1.02			0.06	2.14
O(26)			0.26	0.24	0.30										1.05									1.85
O(27)															0.97		0.98						0.10	2.05
O(28)																1.03					1.04		0.06	2.13
O(29)																1.01				1.06			0.06	2.13
O(30)																		1.01			1.05		0.06	2.12
O(31)			0.29	0.28 0.25													1.04							1.86
O(32)																		1.02		1.04		0.11		2.17
O(33)			0.29	0.31		0.26 ×2↓													1.09					1.95
F				0.27	0.28	0.27 ×2↓																		0.82
Σ	4.32	4.41	1.66	1.66	1.69	1.60	1.13	1.14	1.18	4.02	4.05	4.17	4.02	4.21	4.02	4.20	4.04	4.23	4.09	4.23	4.23	0.44	0.92	

* bond-valence parameters (*vu*) from Brown & Altermatt (1985).

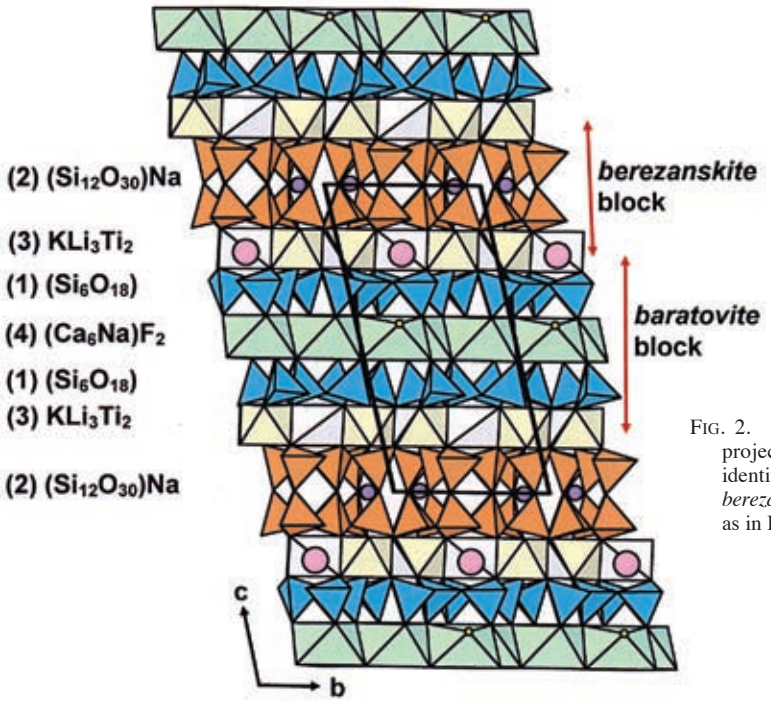

FIG. 2. The crystal structure of faizievite projected onto (011). Sheets (1)–(4) are identified; red double-headed arrows show *berezanskite* and *baratovite* blocks. Legend as in Figure 1.

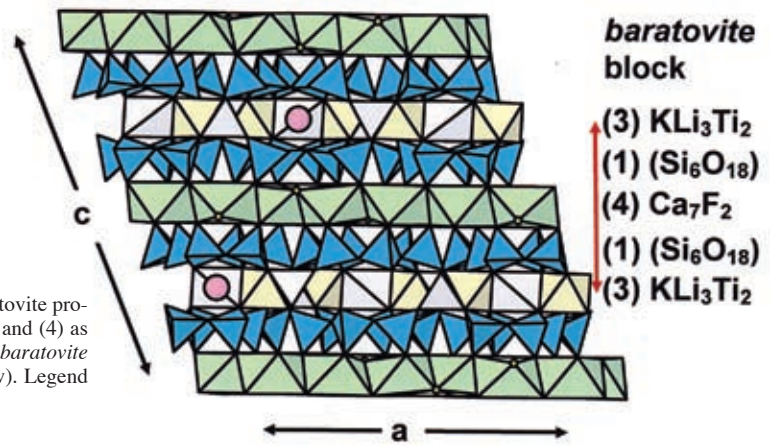

FIG. 3. The crystal structure of baratovite projected onto (011). Sheets (1), (3) and (4) as in faizievite are shown within the *baratovite* block (a red double-headed arrow). Legend as in Figure 1.

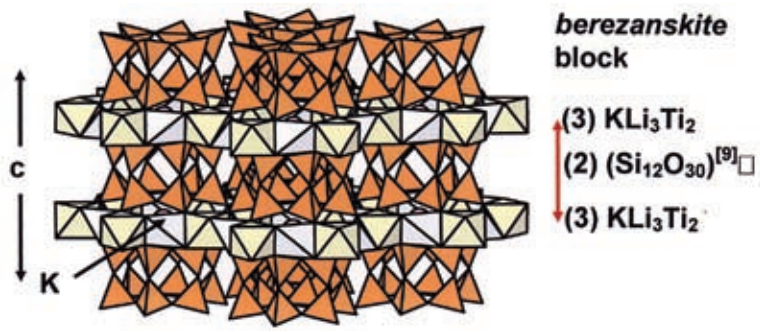

FIG. 4. General view of the crystal structure of berezanskite [drawn using atom coordinates of the sogdianite end-member, $K^{[9]}\square Li_3 Zr_2 (Si_{12}O_{30})$, from Sokolova *et al.* (2000)]. Sheets (2) and (3) as in faizievite are shown within the *berezanskite* block (a red double-headed arrow). Legend as in Figure 1.

TABLE 7. STRUCTURAL FORMULAE AND UNIT-CELL PARAMETERS FOR FAIZIEVITE, BARATOVITE AND BEREZANSKITE

Mineral and structural formula	*a* (Å) α (°)	*b* (Å) β (°)	*c* (Å) γ (°)	Space group	Z	$t_{1,2}$* (Å)	Ref.
faizievite $^{[12]}K_2\,^{[9]}Na\,^{[4]}Li_6\,^{[6]}(Ca_6Na)\,^{[6]}Ti_4\,(Si_6O_{18})_2\,(Si_{12}O_{30})\,F_2$	9.8156 99.209	9.8249 94.670	17.309 119.839	$P\bar{1}$	1	9.82(**a**) 9.82(**b**)	(1)
baratovite $^{[12]}K\,^{[4]}Li_3\,^{[6]}Ca_7\,^{[6]}Ti_2\,(Si_6O_{18})_2\,F_2$	16.953 90	9.752 112.46	20.916 90	*C*2/*c*	4	9.75(**b**) 9.78[(**b**-**a**)/2]	(2)
berezanskite $^{[12]}K\,^{[9]}\square\,^{[4]}Li_3\,^{[6]}Ti_2\,(Si_{12}O_{30})$	9.903 90	9.903 90	14.3198 120	*P*6/*mcc*	2	9.90(**a**) 9.90(**b**)	(3)

* translations of the planar cell characteristic for all sheets, $\mathbf{t}_1 \wedge \mathbf{t}_2$ close to 120°, corresponding unit-cell vectors, are given in brackets.
References: (1) this work, (2) Sandomirskii *et al.* (1976), (3) Pautov & Agakhanov (1997).

(1) + sheets (3)(2) = $K_2Li_3(Ca_6Na)Ti\,(Si_6O_{18})_2\,F_2$ + $KNaLi_3Ti_2(Si_{12}O_{30})$ = $K_2\,Li_6\,Na\,(Ca_6Na)\,Ti_4\,(Si_6O_{18})_2\,(Si_{12}O_{30})\,F_2$. Faizievite occurs as platy crystals attached to large crystals of baratovite (Agakhanov *et al.* 2008). We speculate that the assembly of the faizievite structure from *baratovite* and *berezanskite* blocks is probably a process of epitactic growth of berezanskite on a substrate of baratovite, accompanied by the following conceptual coupled substitution: $^{[6]}Ca^{2+} + {}^{[9]}\square \Leftrightarrow {}^{[6]}Na^{+} + {}^{[9]}Na^{+}$.

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