

**MEGAKALSILITE, A NEW POLYMORPH OF KAISiO₄
FROM THE Khibina Alkaline Massif, Kola Peninsula, Russia:
Mineral Description and Crystal Structure**

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ABSTRACT

Megakalsilite, KAlSiO₄, hexagonal, a 18.1111(8), c 8.4619(4) Å, V 2403.7(2) Å³, $c/a = 0.4672$, space group $P6_3$, $Z = 24$, $R = 0.039$ (for 3255 observed reflections collected with a four-circle X-ray diffractometer), is a new mineral species from Mount Koashva, Khibina alkaline massif, Kola Peninsula, Russia. It is of pegmatitic origin. Associated minerals are K-feldspar, sodalite, cancrinite, natrolite, pectolite, aegirine, natrite, nacaphite, vitusite, fluorcaphite, belovite, umbite, lemmleinite-K, lomonosovite, lovozerite, phlogopite, sphalerite, and galena. The mineral was found in only one hand specimen of pegmatite rock as a corroded, irregularly shaped grain 2×3 mm across, intergrown with cancrinite, sodalite, and natrite. It is transparent, colorless with a white streak, a vitreous luster, and fluoresces pale whitish green under ultraviolet light. Megakalsilite has a Mohs hardness of 6, is brittle with a conchoidal fracture, and has no cleavage. D_{meas} is 2.58(2) g/cm³, D_{calc} is 2.62 g/cm³. Megakalsilite is uniaxial negative, non-pleochroic, ω 1.538(1), ε 1.531(1). The strongest five reflections in the X-ray powder-diffraction pattern [d in Å(hkl)] are: 3.091(100)(222), 2.612(70)(060), 1.240(60)(4.10.1,066,583), 3.18(50)(141), and 1.674(50)(173). An electron-microprobe analysis gives: K₂O 29.73, Na₂O 0.02, FeO 0.04, Al₂O₃ 32.38, SiO₂ 37.96, TiO₂ 0.01, sum 100.14 wt.%. The corresponding empirical formula is K_{0.997}Na_{0.001}Fe_{0.001}Al_{1.003}Si_{0.998}O₄ (based on O = 4), ideally KAlSiO₄. The name megakalsilite is derived from the Greek μέγας (great) and kalsilite, in allusion to the fact that megakalsilite shares the same chemical formula with kalsilite, but its unit cell is 12 times larger than that of kalsilite. The crystal structure of megakalsilite, KAlSiO₄, has been solved by direct methods and refined to an R_1 index of 3.82% based on 3255 observed [$F_o > 4\sigma(F_o)$] unique reflections measured with MoK α radiation on a conventional four-circle diffractometer. There are four Si sites, four Al sites, and six K sites in the structure. Megakalsilite is a tectosilicate with a framework consisting of six-membered rings of regularly alternating Si- and Al-centered tetrahedra; [9]- and [10]-coordinated K atoms are located in the large cavities. The six-membered rings of tetrahedra are present in two different conformations based on the following sequences of up (U) and down (D) tetrahedra: $UDUDUD$ and $UUUU$. The sequence of these two different rings along x (y) results in the unit cell parameter of 18.1111 Å. $UDUDUD$ rings are characteristic for the high tridymite topology. $UUUU$ rings have been reported for KAlSiO₄-01. Crystal structures of megakalsilite and the synthetic aluminogermanate KAlGeO₄ have the same framework topology.

Keywords: megakalsilite, new mineral species, polymorph, crystal structure, Khibina, Kola Peninsula, Russia.

SOMMAIRE

La mégakalsilite, KAlSiO₄, hexagonale, a 18.1111(8), c 8.4619(4) Å, V 2403.7(2) Å³, $c/a = 0.4672$, groupe spatial $P6_3$, $Z = 24$, $R = 0.039$ (pour 3255 réflexions observées, prélevées avec un diffractomètre à quatre cercles), est une nouvelle espèce minérale provenant du mont Koashva, complexe alcalin de Khibina, péninsule de Kola, en Russie. Elle a une origine pegmatitique. Lui sont associés feldspath potassique, sodalite, cancrinite, natrolite, pectolite, aegyrine, natrite, nacaphite, vitusite, fluorcaphite,

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bélovite, umbite, lemmleinite-K, lomonosovite, lovozérite, phlogopite, sphalerite, et galène. Le minéral a été découvert dans un seul échantillon de pegmatite comme grain corrodé, de forme irrégulière, 2×3 mm de taille, en intercroissance avec cancrinite, sodalite, et natrite. Il est transparent, incolore avec une rayure blanche, un éclat vitreux, et une fluorescence blanche à verdâtre pâle en lumière ultraviolette. La mégakalsilite a une dureté de Mohs de 6, est cassante avec une fracture conchoïdale, et ne montre aucun clivage. La densité mesurée est 2.58(2), et la densité calculée est 2.62 g/cm³. La mégakalsilite est uniaxe négative, non pléochroïque, ω 1.538(1), ε 1.531(1). Les cinq raies les plus intenses du spectre de diffraction, méthode des poudres [d en Å(I)(hkl)] sont: 3.091(100)(222), 2.612(70)(060), 1.240(60)(4.10.1,066,583), 3.18(50)(141), et 1.674(50)(173). Une analyse à la microsonde électronique a donné: K₂O 29.73, Na₂O 0.02, FeO 0.04, Al₂O₃ 32.38, SiO₂ 37.96, TiO₂ 0.01, somme 100.14% par poids. La formule empirique correspondante est K_{0.997}Na_{0.001}Fe_{0.001}Al_{1.003}Si_{10.998}O₄ (sur une base de O = 4) ou, idéalement, KAlSiO₄. Le nom, dérivé du grec $\mu\epsilon\gamma\alpha\varsigma$ (immense) et kalsilite, fait allusion au fait que la mégakalsilite partage la même formule chimique avec la kalsilite, mais la maille élémentaire est douze fois plus volumineuse que celle de la kalsilite. Nous avons résolu sa structure cristalline par méthodes directes, et nous l'avons affinée jusqu'à un résidu R_1 de 3.82% en utilisant 3255 réflexions uniques observées [$F_o > 4\sigma(F_o)$], mesurées avec rayonnement MoK α sur un diffractomètre conventionnel à quatre cercles. Il y a quatre sites Si, quatre sites Al, et six sites K dans la structure. La mégakalsilite est un tectosilicate dont la trame contient des anneaux à six membres de tétraèdres Si et Al en alternance; les atomes K, à coordinence [9] et [10], sont situés dans les cavités. Les anneaux de tétraèdres sont présents en deux agencements différents montrant les séquences suivantes de tétraèdres orientés vers le haut (U) ou le bas (D): $UDUDUD$ et $UUU\Delta$. La séquence de ces deux anneaux le long de x (y) mène à un paramètre réticulaire de 18.1111 Å. Les anneaux $UDUDUD$ sont caractéristiques de la topologie de la tridymite de haute température. Les anneaux $UUU\Delta$ sont aussi présents dans le KAlSiO₄-01. La mégakalsilite et de l'aluminogermanate synthétique KAlGeO₄ possèdent la même topologie de la trame.

(Traduit par la Rédaction)

Mots-clés: mégakalsilite, nouvelle espèce minérale, polymorphe, structure cristalline, Khibina, péninsule de Kola, Russie.

INTRODUCTION

In the context of a study of hyperagpaitic pegmatites on Mount Koashva in the Khibina alkaline massif, Kola Peninsula, Russia, one of us (APK) discovered an unusual mineral that is optically similar to nepheline and kalsilite, but differs from them in having a higher birefringence (0.007 *versus* 0.003–0.005). Its X-ray powder-diffraction characteristics also are distinctive. A detailed study of the mineral, including electron-microprobe and X-ray powder-diffraction and single-crystal analyses, shows that it is a potassium aluminosilicate, KAlSiO₄, virtually free of isomorphic substitutions of Na and other elements and substantially different in its structural features from the other natural phases with composition KAlSiO₄ or (K,Na)AlSiO₄, with potassium dominant over sodium: kaliophilite (Dana 1892), kalsilite (Bannister & Hey 1942), trikalsilite (Sahama & Smith 1957), and panunzite (Franco & De Gennaro 1988). The name megakalsilite is formed by adding the prefix mega (from the Greek $\mu\epsilon\gamma\alpha\varsigma$, meaning great) to the term kalsilite, which is the most common modification of KAlSiO₄ in nature, emphasizing the compositional similarity of the two minerals and the much larger cell volume of megakalsilite (2403.7 Å³) relative to kalsilite (200.4 Å³).

The new mineral species and its name have been approved by the Commission on New Minerals and Mineral Names of the International Mineralogical Association. The holotype specimen of megakalsilite is deposited at the Fersman Mineralogical Museum, catalogue #2624/1, Russian Academy of Sciences, in Moscow, Russia.

OCCURRENCE AND ASSOCIATED MINERALS

The Khibina alkaline massif in the Kola Peninsula, offers examples of differentiated agpaitic complexes comparable to those at such famous mineral localities as the other well known massif of Lovozero, also in the Kola Peninsula, Ilímaussaq (South Greenland), and Mont Saint-Hilaire (Quebec, Canada). Among these, Khibina is distinctive owing to the presence (in addition to the predominant perthitic minerals) of numerous high-K minerals (about 50 species). The list has recently been substantially extended with the discovery of altisite, Na₃K₆Ti₂Al₂Si₈O₂₆Cl, eršovite, (K,Na)₅Fe₇Si₂₀O₅₀(OH)₆•12H₂O, kalborsite, K₆Al₄BSi₆O₂₀(OH)₄Cl, lemmleinite-K, NaK₂(Ti,Nb)₂Si₄O₁₂(O,OH)₂•2H₂O, litsitsynite, KBSi₂O₆, lithosite, K₃(HAl₂Si₄O₁₃), sitinakitite, Na₂KTi₄Si₂O₁₃(OH)•4H₂O, umbite, K₂ZrSi₃O₉•H₂O, among others (Khomyakov *et al.* 1999, 2000). All of them, as well as the new mineral described here, were identified in investigations of hyperagpaitic pegmatites, the extreme alkaline differentiates of nepheline-bearing syenitic magmas (Khomyakov 1995). Most of the pegmatite bodies of this type occur within the central arc of the Khibina massif, composed mainly of rischorrite and ijolite–urtite. Megakalsilite was found in a large body of hyperagpaitic pegmatite in ijolite–urtite, near their contact with apatite–nepheline rocks. The subvertically dipping pegmatite body, up to 5 m thick, was traced along the quarry wall for about 100 m. Where the body swells, it is seen to consist of an intensely mineralized core composed mainly of water-soluble sodium fluoride (villiamite), carbonate (natrite and thermonatrite), and phosphate (natrophosphate), and a silicate rim consist-

ing of very large aegirine spherulites up to 1–1.5 mm across. Other minerals occurring mostly in the central zone of the body and at its contact with the aegirine-dominant rim are pectolite, microcline, sodalite, and lomonosovite; less common phases are chkalovite, vitusite, and REE,Sr-enriched fluorapatite, with sporadic cancrinite, natrolite, alkali amphibole, phlogopite (Ferraris *et al.* 2001), lamprophyllite, lovozerite, umbite, belovite, fluorcaphite, nacaphite, nefedovite, bonshtedtite, sphalerite, galena, and molybdenite. Lemleinite-K pseudomorphs after lomonosovite also were observed. A very characteristic feature of this and similar bodies of pegmatite in the Mount Koashva area is the presence of abundant solid bitumen. So far, only one hand specimen of pegmatite rock containing approximately 20 mg of megakalsilite has been collected.

PHYSICAL AND OPTICAL PROPERTIES

Megakalsilite occurs as a corroded, anhedral grain 2–3 mm across, intergrown with cancrinite, sodalite and natrite. It is vitreous, transparent and colorless, with a white streak. It fluoresces pale whitish green under ultraviolet light in the range 240–400 nm. It is brittle, with no cleavage, no parting, and it has a conchoidal fracture. It has a Mohs hardness of 6. The density of megakalsilite, measured by volumetric method, is 2.58(2) g/cm³, which compares satisfactorily with the calculated density, 2.62 g/cm³. On heating for two hours at 500°C, the mineral remains transparent and retains the original indices of refraction.

Megakalsilite is uniaxial negative, ω 1.538(1), ϵ 1.531(1) (λ 589 nm), and non-pleochroic.

A Gladstone–Dale calculation gives a compatibility index of 0.002, which is rated as superior (Mandarino 1981).

CHEMICAL COMPOSITION

The chemical composition of megakalsilite was determined by electron-microprobe analysis (Table 1). The analyses were done with a JEOL Superprobe 733 electron microprobe; six points on each of five grains were

TABLE 1. CHEMICAL COMPOSITION OF MEGAKALSILITE*

Oxide	wt. %	Range	Cation	<i>apfu</i>
SiO ₂	37.96	37.75–38.07	Si	0.998
TiO ₂	0.01	0.00–0.02	Ti	0.000
Al ₂ O ₃	32.38	32.21–32.54	Al	1.003
FeO	0.04	0.03–0.05	Fe ²⁺	0.001
Na ₂ O	0.02	0.01–0.03	Na	0.001
K ₂ O	29.73	29.44–30.04	K	0.997
Σ	100.14	99.98–100.42	Σ	3.000

*Cations were recalculated on the basis of four atoms of oxygen.

analyzed, with an excitation voltage of 15 kV and a specimen current of 15 nA. We used the following standards: albite (Na), synthetic K₂ZrSi₂O₇ (K), almandine (Fe), synthetic AlPO₄ (Al), diopside (Si), and synthetic SrTiO₃ (Ti). No evidence of H₂O or OH was found in the mineral as a result of the structure refinement. On the basis of four atoms of oxygen per formula unit, the following empirical formula was obtained for megakalsilite: K_{0.997}Na_{0.001}Fe_{0.001}Al_{1.003}Si_{0.998}O₄. The ideal formula is KAlSiO₄. When megakalsilite was put in a ceramic container with 10% HCl and HNO₃ solution, it readily decomposed at room temperature, yielding silica gel.

X-RAY CRYSTALLOGRAPHY

Powder X-ray-diffraction study

Two grains of megakalsilite were crushed in an agate mortar and rolled into a sphere with rubber cement. For this sample, X-ray powder-diffraction data were collected with a Debye–Scherrer camera (diameter 114.6 mm, FeK α radiation). Intensities were estimated by eye, no correction for shrinkage was carried out, and no internal standard was used. The following hexagonal unit-cell was obtained by least-square refinement: *a* 18.104(3), *c* 8.467(2) Å. The indexed powder pattern is presented in Table 2.

Single-crystal X-ray-diffraction study

A single crystal, which was previously studied with Weissenberg photographs, was selected for structural characterization. Intensity data were collected at room temperature with an Ital Structures conventional four-circle diffractometer. The intensities of three standard reflections, monitored every hundredth measurement, showed variations well within the estimated standard deviations. The absorption effects were empirically accounted for on the basis of ψ -scan measurements. The structure was solved with direct methods (SHELXS–86 package; Sheldrick 1985) and refined smoothly against squared structure amplitudes to $R_1 = 0.038$ (SHELXL–93 package; Sheldrick 1993). The refinement was completed with anisotropic-displacement parameters for all atoms. The greatest R_{\max}/R_{\min} value between radii of the thermal ellipsoids was 2.63 for O(6). Additional details of data collection and structure refinement are given in Table 3.

DESCRIPTION OF THE STRUCTURE

Coordination of the cations

Final atom position and displacement parameters are given in Table 4, selected interatomic distances in Table 5, and the bond-valence analysis in Table 6. In the crystal structure of megakalsilite, there are four Si

TABLE 2. POWDER X-RAY DIFFRACTION PATTERN FOR MEGAKALSILITE

l_{obs}	d_{obs}	d_{calc}	hkl	l_{obs}	d_{obs}	d_{calc}	hkl
30	6.19	6.18	111	10	1.328	1.330	284
20	4.21	4.23	002	30	1.308	1.306	0.12.0
20	3.99	3.99	221	30	1.290	1.289	393
20	3.41	3.42	140	"	"	1.289	474
50	3.18	3.17	141	10	1.280	1.278	771
100	3.091	3.092	222	10	1.250	1.248	0.12.2
10	2.960	2.963	240	60	1.240	1.242	4.10.1
20	2.874	2.876	042	"	"	1.242	066
70	2.612	2.613	060	"	"	1.240	583
40	2.498	2.497	061	10	1.229	1.230	256
30	2.405	2.407	251	"	"	1.228	664
20	2.262	2.263	440	50	1.204	1.204	4.10.2
10	2.225	2.224	062	"	"	1.204	285
10	2.157	2.159	252	40	1.175	1.176	2.11.3
30	2.117	2.117	004	"	"	1.176	773
20	2.063	2.061	333	"	"	1.173	475
10	1.998	1.996	442	30	1.147	1.147	4.10.3
30	1.917	1.917	063	10	1.134	1.132	880
"	"	1.917	224	30	1.117	1.118	1.10.5
30	1.875	1.876	253	10	1.113	1.112	0.12.4
10	1.810	1.810	550	20	1.104	1.104	774
20	1.767	1.770	551	"	"	1.104	2.11.4
"	"	1.765	443	10	1.097	1.097	5.11.1
10	1.712	1.711	280	20	1.089	1.090	257
50	1.674	1.673	173	10	1.080	1.080	4.10.4
20	1.646	1.645	064	"	"	1.079	1.14.0
20	1.619	1.618	363	"	"	1.079	167
50	1.585	1.586	282	30	1.072	1.072	1.13.3
"	"	1.586	225	20	1.058	1.057	3.12.3
30	1.544	1.546	444	10	1.052	1.051	7.10.1
50	1.516	1.518	145	30	1.045	1.045	0.15.0
"	"	1.509	660	"	"	1.045	177
30	1.465	1.466	1.10.1	"	"	1.043	694
"	"	1.463	283	50	1.031	1.031	666
20	1.422	1.421	662	"	"	1.031	228
20	1.405	1.404	255				

FeK α radiation ($\lambda = 1.93728 \text{ \AA}$)
 Debye-Scherrer camera ($r = 114.6 \text{ mm}$)
 Intensities from visual estimation on photographic film

sites, four Al sites, and six K sites. The average $\langle T-O \rangle$ bond distances indicate an ordered distribution of silicon and aluminum in neighboring tetrahedra, as expected in a framework with Si:Al ratio of 1:1. This is a feature shared with all other minerals of the kalsilite group. Five K atoms [all but K(4)] are 9-coordinated, with $\langle K-O \rangle$ ranging from 2.98 to 3.11 Å. The K(4) site can be considered as 10-coordinated, with a $\langle K(4)-O \rangle$ of 3.15 Å. Coordination polyhedra for K(1), K(2) and K(3) are regular tri-augmented antiprisms (point symmetry $3m$), with all K-O bonds between 2.86 and 3.09 Å. The same type of polyhedron was recently described for Na atoms in the crystal structure of topologically related malinkoite, NaBSiO₄ (Sokolova *et al.* 2001). Coordination polyhedra of K(4), K(5) and K(6) are less symmetrical than those surrounding K(1), K(2) and K(3), with K-O bonds distributed in two groups of four shorter and five (or six) longer bonds ($K-O < 2.80 \text{ \AA}$ and $K-O > 3.19 \text{ \AA}$, respectively). The coordination proposed for the cations is confirmed by bond-valence

analysis, presented in Table 6. Observed and calculated structure-factors may be obtained from The Depository of Unpublished Data, CISTI, National Research Council, Ottawa, Ontario K1A 0S2, Canada.

Topology of the structure

Megakalsilite is a tectosilicate with a structure consisting of six-membered rings of regularly alternating Si- and Al-centered tetrahedra, and K located in the large cavities (Fig. 1). Si- and Al-centered tetrahedra form six-membered rings of two different conformations based on the following sequences of up (*U*) and down (*D*) tetrahedra: *UDUDUD* and *UUUΔ*, in the proportion 1:3. The sequence of these two different rings along *x* (*y*) results in a unit-cell parameter equal to 18.1111 Å. *UDUDUD* rings are characteristic of the topology of high tridymite, first described more than 70 years ago (Gibbs 1927) and common to a number of (K,Na) AlSiO₄ structures (see below). *UUUΔ* rings have been described in a sulfate analogue, N₂H₅LiSO₄ (Brown 1964); in silicates, they were first reported in KAlSiO₄-O1 (Gregorkiewitz & Schäfer 1980).

There are two types of channels that extend along the *c* axis: (1) the stacking of *UDUDUD* rings produces channels that contain K in regular tri-augmented antiprisms; (2) the stacking of *UUUΔ* rings produces channels that contain K in [9]- and [10]-coordination.

It is worth noting that all *T-O-T* angles, with only one exception, fall within the range of 128.7 to 148.5° (Table 5), *i.e.*, close to the angle of 139° characteristic for unstrained bonds in framework silicates (Liebau 1985). In particular, atoms O(1) to O(4) link tetrahedra along [001]. For those atoms, the *T-O-T* angles are very close to 148°, with the exception of the Si(2)-O(2)-Al(2) angle, which is 174.9°. We assume that this angle differs from all others because of bond-valence requirements dependent on weak interactions with surrounding K atoms, and resulting in the shortest of all Si-O and Al-O bond distances.

An interesting feature of the megakalsilite framework emerges if we focus our attention on clusters of four tetrahedra pointing in the same direction (Fig. 2a) rather than on single tetrahedra that point upward (*U*) or downward (*D*). Such clusters, if projected down [001], can be schematically drawn as equilateral triangles. The distribution of such clusters is well ordered. In fact, each cluster of four *U* tetrahedra has, as closest neighbors, three clusters of four *D* tetrahedra, and *vice versa* (Fig. 2b). The same topology had been found in the S₁ sheet tetrahedra of reyerite (Merlino 1988).

Related compounds

The structure of megakalsilite can be described as characterized by a new type of framework if compared with the crystal structures of minerals with composition (K,Na)AlSiO₄: kalsilite, nepheline, trikalsilite,

TABLE 3. MISCELLANEOUS INFORMATION FOR MEGAKALSILITE

<i>a</i> (Å)	18.1111(8)	Radiation	MoK α ($\lambda = 0.71073$ Å)
<i>c</i> (Å)	8.4619(4)	Operating conditions	50 kV, 30 mA
<i>V</i> (Å ³)	2403.7(2)	2 θ range for data collection (°)	4–60
<i>c/a</i>	0.4672	Scan width in θ (°)	± 0.5
Space group	<i>P</i> 6 ₃	Scan speed (°/min ⁻¹)	2
Cell content	24 K Al Si O ₄		
No. of reflections and 2 θ range for cell refinement	24 (27° < 2 θ < 34°)	Range for indices	0 $\leq h \leq 21$ –6 $\leq k \leq 21$ –10 $\leq l \leq 11$
Absorption coefficient (mm ⁻¹)	1.72	Measured intensities	3620
<i>F</i> (000)	1872.0	<i>R</i> (int) from merging equivalents	0.0161
Crystal size (mm)	0.06 x 0.20 x 0.20	Unique reflections	3328
		Observed reflections [<i>F</i> _o > 4 σ (<i>F</i> _o)]	3255
		<i>R</i> (obs)	0.0382
		<i>R</i> (all data)	<i>R</i> _i = 0.0405 <i>wR</i> ₂ = 0.0963 Goof = 0.746
		Maximum/minimum in the final ΔF map (e/Å)	+0.53 / –0.58

TABLE 4. FINAL POSITIONAL AND DISPLACEMENT PARAMETERS FOR MEGAKALSILITE

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{6a}	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₂₃	<i>U</i> ₁₃	<i>U</i> ₁₂
Si(1)	0.8321(1)	0.8406(1)	0.1939(2)	0.0110(3)	0.0108(7)	0.0099(7)	0.0119(7)	0.0007(5)	–0.0006(5)	0.0049(6)
Si(2)	0.6655(1)	0.6652(1)	0.7939(2)	0.0106(3)	0.0106(8)	0.0104(8)	0.0109(7)	0.0004(5)	–0.0007(5)	0.0052(6)
Si(3)	0.6578(1)	0.4940(1)	0.1784(2)	0.0111(3)	0.0110(7)	0.0102(7)	0.0120(7)	–0.0004(5)	0.0010(5)	0.0052(6)
Si(4)	0.5039(1)	0.6775(1)	0.1778(2)	0.0116(3)	0.0118(7)	0.0103(7)	0.0126(7)	–0.0016(6)	0.0001(5)	0.0055(6)
Al(1)	0.8303(1)	0.8381(1)	0.8114(2)	0.0108(3)	0.0106(8)	0.0106(8)	0.0112(8)	0.0017(6)	0.0001(6)	0.0052(7)
Al(2)	0.6683(1)	0.6682(1)	0.1834(2)	0.0110(4)	0.0115(8)	0.0108(8)	0.0107(7)	0.0002(6)	–0.0002(6)	0.0055(7)
Al(3)	0.6554(1)	0.4915(1)	0.7961(2)	0.0109(3)	0.0122(8)	0.0111(8)	0.0105(8)	–0.0001(6)	0.0002(6)	0.0066(7)
Al(4)	0.5014(1)	0.6761(1)	0.7962(2)	0.0110(3)	0.0102(8)	0.0104(8)	0.0120(8)	0.0006(6)	0.0009(6)	0.0050(7)
K(1)	0	0	0.4862(3)	0.0201(4)	0.0206(5)	0.0206(5)	0.0192(10)	0	0	0.0103(2)
K(2)	2/3	1/3	0.5052(4)	0.0208(4)	0.0204(5)	0.0204(5)	0.0218(11)	0	0	0.0102(2)
K(3)	1/3	2/3	0.5048(4)	0.0217(4)	0.0209(5)	0.0209(5)	0.0233(11)	0	0	0.0105(2)
K(4)	0.4776(1)	0.0047(1)	0.4916(2)	0.0230(2)	0.0291(5)	0.0213(4)	0.0208(6)	0.0021(6)	–0.0007(6)	0.0141(4)
K(5)	0.6665(1)	0.8126(1)	0.4946(2)	0.0235(2)	0.0238(4)	0.0264(5)	0.0199(6)	0.0007(7)	0.0023(5)	0.0123(4)
K(6)	0.8049(1)	0.6675(1)	0.4956(2)	0.0233(2)	0.0229(5)	0.0229(4)	0.0240(6)	0.0072(6)	0.0039(7)	0.0113(4)
O(1)	0.8161(2)	0.8533(2)	0.0101(5)	0.0175(7)	0.0188(14)	0.0200(15)	0.0150(17)	–0.0008(16)	–0.0011(16)	0.0106(12)
O(2)	0.6699(2)	0.6650(2)	0.9824(6)	0.0198(6)	0.0278(16)	0.0201(15)	0.0121(15)	–0.0015(16)	–0.0003(18)	0.0125(14)
O(3)	0.6272(2)	0.4778(2)	0.9951(5)	0.0155(6)	0.0150(14)	0.0171(13)	0.0143(17)	0.0025(17)	–0.0003(17)	0.0078(11)
O(4)	0.5164(2)	0.7065(2)	0.9940(5)	0.0171(6)	0.0203(14)	0.0159(14)	0.0135(17)	–0.0023(17)	0.0003(18)	0.0079(11)
O(5)	0.9308(2)	0.8671(2)	0.2178(5)	0.0172(8)	0.0130(16)	0.0167(18)	0.0221(18)	0.0040(15)	–0.0022(14)	0.0074(14)
O(6)	0.7365(2)	0.4676(2)	0.7714(5)	0.0163(7)	0.0131(16)	0.0167(18)	0.0204(18)	0.0036(14)	0.0062(14)	0.0083(14)
O(7)	0.8009(2)	0.3960(2)	0.2724(5)	0.0151(7)	0.0152(18)	0.0115(16)	0.0193(17)	–0.0006(14)	0.0036(14)	0.0073(14)
O(8)	0.9075(2)	0.8084(2)	0.7999(5)	0.0183(8)	0.0199(18)	0.0231(19)	0.0166(21)	0.0038(15)	0.0053(14)	0.0142(15)
O(9)	0.5250(2)	0.7663(2)	0.6852(5)	0.0178(7)	0.0187(17)	0.0188(17)	0.0202(21)	0.0065(15)	0.0072(15)	0.0127(14)
O(10)	0.4361(2)	0.5771(2)	0.1895(5)	0.0193(8)	0.0198(17)	0.0116(15)	0.0227(22)	–0.0011(15)	0.0052(16)	0.0049(14)
O(11)	0.7702(2)	0.7420(2)	0.2507(4)	0.0155(8)	0.0148(18)	0.0128(17)	0.0173(20)	0.0002(12)	–0.0043(12)	0.0059(14)
O(12)	0.8981(2)	0.5948(2)	0.7519(4)	0.0160(8)	0.0138(17)	0.0162(18)	0.0137(19)	–0.0028(12)	0.0024(12)	0.0042(15)
O(13)	0.9256(2)	0.3585(3)	0.2558(4)	0.0151(8)	0.0156(18)	0.0228(20)	0.0119(18)	–0.0028(14)	–0.0029(13)	0.0135(15)
O(14)	0.3587(3)	0.9297(2)	0.7338(4)	0.0161(8)	0.0190(19)	0.0122(17)	0.0188(20)	0.0026(13)	0.0040(14)	0.0092(15)
O(15)	0.5944(2)	0.9066(2)	0.2253(4)	0.0155(7)	0.0108(16)	0.0131(16)	0.0175(17)	–0.0039(13)	0.0017(12)	0.0023(14)
O(16)	0.7348(3)	0.7584(2)	0.7258(4)	0.0168(7)	0.0172(18)	0.0150(17)	0.0159(17)	–0.0005(13)	–0.0024(13)	0.0062(15)

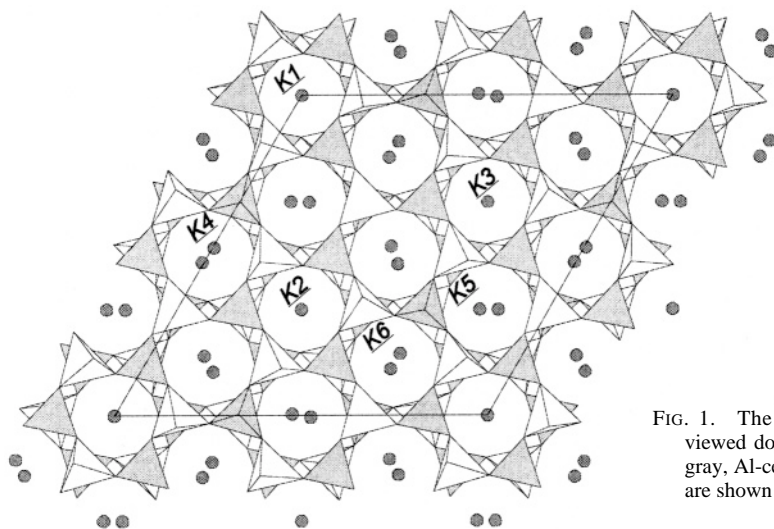


FIG. 1. The crystal structure of megakalsilite viewed down [001]. Si-centered tetrahedra are gray, Al-centered tetrahedra are white, K atoms are shown as spheres. The unit cell is outlined.

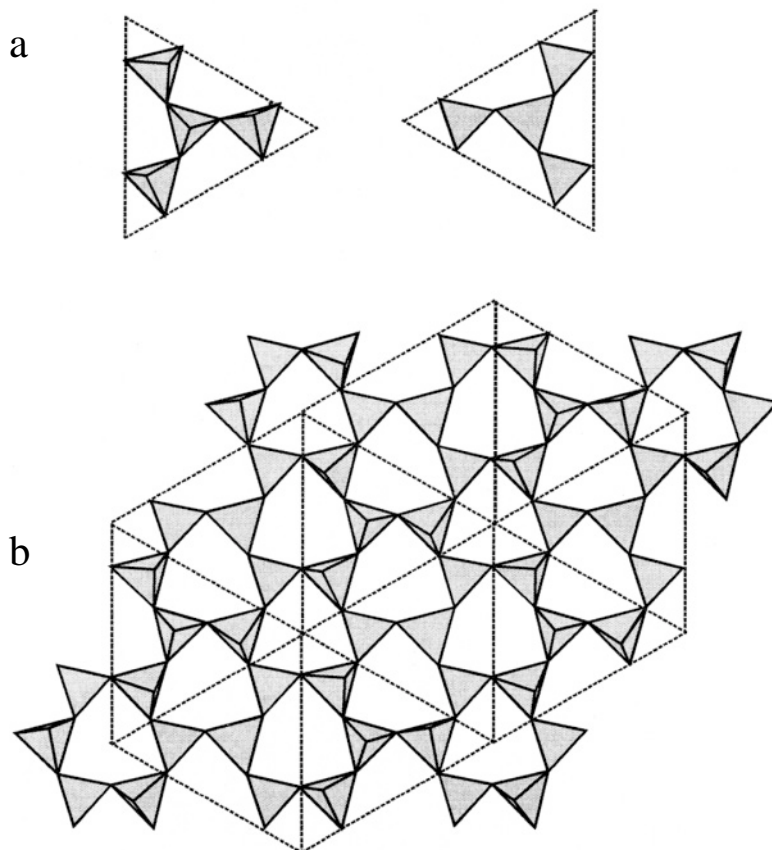


FIG. 2. a. Clusters of four *U*- and *D*-pointing tetrahedra. b. A (001) layer of tetrahedra emphasizing the mutual orientation of the clusters.

TABLE 5. SELECTED INTERATOMIC DISTANCES (Å) AND ANGLES (°) FOR MEGAKALSILITE

Si(1)–O(5)	1.616(4)	Si(2)–O(2)	1.597(5)	Si(3)–O(7)	1.617(4)	Si(4)–O(10)	1.611(4)
Si(1)–O(1)	1.619(4)	Si(2)–O(14)	1.623(4)	Si(3)–O(9)	1.621(4)	Si(4)–O(4)	1.621(5)
Si(1)–O(8)	1.627(4)	Si(2)–O(16)	1.623(4)	Si(3)–O(3)	1.625(4)	Si(4)–O(6)	1.621(4)
Si(1)–O(11)	1.635(4)	Si(2)–O(15)	1.632(4)	Si(3)–O(13)	1.632(4)	Si(4)–O(12)	1.629(4)
<Si(1)–O>	1.624	<Si(2)–O>	1.619	<Si(3)–O>	1.624	<Si(4)–O>	1.621
O(5)–Si(1)–O(1)	109.2(2)	O(14)–Si(2)–O(2)	111.0(2)	O(7)–Si(3)–O(3)	107.9(2)	O(6)–Si(4)–O(4)	107.9(2)
O(8)–Si(1)–O(1)	108.0(2)	O(15)–Si(2)–O(2)	108.8(2)	O(9)–Si(3)–O(3)	108.7(2)	O(10)–Si(4)–O(4)	109.2(2)
O(11)–Si(1)–O(1)	111.3(2)	O(16)–Si(2)–O(2)	110.1(2)	O(13)–Si(3)–O(3)	110.2(2)	O(12)–Si(4)–O(4)	109.7(2)
O(8)–Si(1)–O(5)	110.8(2)	O(15)–Si(2)–O(14)	108.7(2)	O(9)–Si(3)–O(7)	109.9(2)	O(10)–Si(4)–O(6)	109.7(2)
O(11)–Si(1)–O(5)	109.9(2)	O(16)–Si(2)–O(14)	109.3(2)	O(13)–Si(3)–O(7)	110.4(2)	O(12)–Si(4)–O(6)	110.6(2)
O(11)–Si(1)–O(8)	107.7(2)	O(16)–Si(2)–O(15)	108.9(2)	O(13)–Si(3)–O(9)	109.6(2)	O(12)–Si(4)–O(10)	109.6(2)
<O–Si(1)–O>	109.5	<O–Si(2)–O>	109.5	<O–Si(3)–O>	109.5	<O–Si(4)–O>	109.5
Al(1)–O(8)	1.735(4)	Al(2)–O(2)	1.702(6)	Al(3)–O(6)	1.740(4)	Al(4)–O(4)	1.741(5)
Al(1)–O(1)	1.744(4)	Al(2)–O(11)	1.746(4)	Al(3)–O(3)	1.741(5)	Al(4)–O(7)	1.742(4)
Al(1)–O(5)	1.745(4)	Al(2)–O(12)	1.751(4)	Al(3)–O(10)	1.745(4)	Al(4)–O(9)	1.743(4)
Al(1)–O(16)	1.762(4)	Al(2)–O(13)	1.752(4)	Al(3)–O(15)	1.755(4)	Al(4)–O(14)	1.749(4)
<Al(1)–O>	1.746	<Al(2)–O>	1.738	<Al(3)–O>	1.745	<Al(4)–O>	1.744
O(5)–Al(1)–O(1)	106.7(2)	O(11)–Al(2)–O(2)	108.8(2)	O(6)–Al(3)–O(3)	107.7(2)	O(7)–Al(4)–O(4)	108.0(2)
O(8)–Al(1)–O(1)	108.0(2)	O(12)–Al(2)–O(2)	111.6(2)	O(10)–Al(3)–O(3)	107.0(2)	O(9)–Al(4)–O(4)	107.1(2)
O(16)–Al(1)–O(1)	111.4(2)	O(13)–Al(2)–O(2)	108.4(2)	O(15)–Al(3)–O(3)	113.6(2)	O(14)–Al(4)–O(4)	112.2(2)
O(8)–Al(1)–O(5)	109.5(2)	O(12)–Al(2)–O(11)	109.5(2)	O(10)–Al(3)–O(6)	112.3(2)	O(9)–Al(4)–O(7)	112.2(2)
O(16)–Al(1)–O(5)	111.5(2)	O(13)–Al(2)–O(11)	108.7(2)	O(15)–Al(3)–O(6)	110.3(2)	O(14)–Al(4)–O(7)	110.2(2)
O(16)–Al(1)–O(8)	109.6(2)	O(13)–Al(2)–O(12)	109.7(2)	O(15)–Al(3)–O(10)	105.9(2)	O(14)–Al(4)–O(9)	117.0(2)
<O–Al(1)–O>	109.5	<O–Al(2)–O>	109.5	<O–Al(3)–O>	109.5	<O–Al(4)–O>	109.5
Si(1)–O(1)–Al(1)	148.5(2)	K(1)–O(5) x3	2.862(4)	K(2)–O(7) x3	2.885(4)	K(3)–O(6) x3	2.887(4)
Si(2)–O(2)–Al(2)	174.9(2)	K(1)–O(1) x3	3.057(3)	K(2)–O(4) x3	3.022(3)	K(3)–O(3) x3	3.038(3)
Si(3)–O(3)–Al(3)	148.1(2)	K(1)–O(5)′ x3	3.083(4)	K(2)–O(6) x3	3.084(5)	K(3)–O(7) x3	3.093(5)
Si(4)–O(4)–Al(4)	147.8(2)	<K(1)–O>	3.001	<K(2)–O>	2.997	<K(3)–O>	3.006
Si(1)–O(5)–Al(1)	139.9(3)	K(4)–O(13)	2.694(4)	K(5)–O(16)	2.745(4)	K(6)–O(15)	2.687(4)
Si(4)–O(6)–Al(3)	139.3(3)	K(4)–O(10)	2.774(4)	K(5)–O(12)	2.753(4)	K(6)–O(11)	2.713(4)
Si(3)–O(7)–Al(4)	139.3(2)	K(4)–O(14)	2.786(4)	K(5)–O(9)	2.780(4)	K(6)–O(4)	2.782(3)
Si(1)–O(8)–Al(1)	137.8(2)	K(4)–O(3)	2.792(3)	K(5)–O(8)	2.787(4)	K(6)–O(1)	2.784(3)
Si(3)–O(9)–Al(4)	137.1(2)	K(4)–O(15)	3.208(4)	K(5)–O(11)	3.308(4)	K(6)–O(16)	3.194(4)
Si(4)–O(10)–Al(3)	138.8(2)	K(4)–O(14)′	3.382(4)	K(5)–O(2)	3.321(3)	K(6)–O(13)	3.286(4)
Si(1)–O(11)–Al(2)	128.7(2)	K(4)–O(12)	3.423(4)	K(5)–O(14)	3.368(4)	K(6)–O(12)	3.393(4)
Si(4)–O(12)–Al(2)	130.3(2)	K(4)–O(10)′	3.443(4)	K(5)–O(11)′	3.438(4)	K(6)–O(8)	3.443(4)
Si(3)–O(13)–Al(2)	129.7(2)	K(4)–O(13)′	3.464(4)	K(5)–O(15)	3.488(4)	K(6)–O(9)	3.479(4)
Si(2)–O(14)–Al(4)	131.5(2)	K(4)–O(2)	3.484(4)	<K(5)–O>	3.108	<K(6)–O>	3.085
Si(2)–O(15)–Al(3)	129.1(2)	<K(4)–O>	3.146				
Si(2)–O(16)–Al(1)	129.6(2)						
<Si–O–Al>	139.4						

panunzite and kaliophilite. For the latter mineral, structural data are still lacking. All others, namely kalsilite, KAlSiO_4 (Perrotta & Smith 1965), nepheline, $\text{Na}_{0.75}\text{K}_{0.25}\text{AlSiO}_4$ (Hahn & Buerger 1955), trikalsilite, $\text{K}_{0.67}\text{Na}_{0.33}\text{AlSiO}_4$ (Bonaccorsi *et al.* 1988), and panunzite, $\text{K}_{0.7}\text{Na}_{0.3}\text{AlSiO}_4$ (Merlino *et al.* 1985) can be regarded as stuffed derivatives of tridymite (Buerger 1954). Although displaying the same topology, the structures of kalsilite, nepheline, trikalsilite and panunzite contain up to three types of $UDUDUD$ rings, with hexagonal, ditrigonal and oval shape, occurring in different proportions depending on the Na:K ratio.

Although new to the mineral kingdom, the framework of megakalsilite is already known among synthetic compounds, occurring in the potassium aluminogermanate, KAlGeO_4 (space group $P6_3$, a 18.429, c 8.599 Å; Sandomirskii *et al.* 1986), which is isostructural with megakalsilite.

Interestingly, all hexagonal minerals and synthetic phases whose a axis is an integer multiple of the a axis of kalsilite [kalsilite itself, nepheline ($2a$), trikalsilite ($3a$), panunzite ($4a$)] have the same framework topology as tridymite. On the contrary, this is not true for mineral and synthetic phases whose a axis is an integer multiple of $\sqrt{3}a$, either megakalsilite and synthetic KAlGeO_4 ($2\sqrt{3}a$: $UDUDUD$ and $UUUD$ 1:3; this study and Sandomirskii *et al.* 1986), or for synthetic KAlSiO_4 – $O1$ ($\sqrt{3}a$: $UUDDUD$ and $UUUD$ 2:1; Gregorkiewitz & Schäfer 1980), or for kaliophilite ($3\sqrt{3}a$). Although the structure of kaliophilite is still unknown, there is evidence that its framework is not based upon the tridymite topology (Gregorkiewitz 1986, Bonaccorsi 1988).

Comparison of megakalsilite with related minerals is presented in Table 7.

TABLE 6. BOND-VALENCE TABLE FOR MEGAKALSILITE *

	Si(1)	Si(2)	Si(3)	Si(4)	Al(1)	Al(2)	Al(3)	Al(4)	K(1)	K(2)	K(3)	K(4)	K(5)	K(6)	Σ
O(1)	1.01				0.78				0.08 ^{cs} _↓					0.17	2.04
O(2)		1.08				0.87						0.03	0.04		2.02
O(3)			1.00				0.78				0.09 ^{cs} _↓	0.17			2.04
O(4)				1.01				0.78		0.09 ^{cs} _↓				0.17	2.05
O(5)	1.02				0.78				0.14 ^{cs} _↓	0.08 ^{cs} _↓					2.02
O(6)				1.00			0.79		0.08 ^{cs} _↓	0.13 ^{cs} _↓					2.00
O(7)			1.02					0.78		0.13 ^{cs} _↓	0.07 ^{cs} _↓				2.00
O(8)	0.99				0.80								0.17	0.03	1.99
O(9)			1.01					0.78					0.17	0.03	1.99
O(10)				1.04				0.78				0.18			2.03
												0.03			
O(11)	0.97					0.77							0.04	0.21	2.02
													0.03		
O(12)				0.99		0.76						0.03	0.19	0.03	2.00
O(13)			0.98			0.76						0.22		0.04	2.03
												0.03			
O(14)		1.00						0.77					0.17	0.04	2.01
												0.03			
O(15)		0.98						0.75				0.05	0.03	0.22	2.03
O(16)		1.00			0.74								0.19	0.06	1.99
Σ	3.99	4.06	4.01	4.04	3.10	3.16	3.10	3.11	0.90	0.90	0.87	0.94	0.90	0.96	

*Parameters taken from Brese & O'Keeffe (1991)

TABLE 7. COMPARISON OF MEGAKALSILITE WITH RELATED MINERALS

	Megakalsilite	Kalsilite	Nepheline	Trikalsilite	Panunzite	Kaliophillite
Formula	K Al Si O ₄	K Al Si O ₄	(Na,K) Al Si O ₄	(K,Na) Al Si O ₄	(K,Na) Al Si O ₄	K Al Si O ₄
Space group	P6 ₃	P6 ₃	P6 ₃	P6 ₃	P6 ₃	P6 ₃ (?)
a (Å)	18.111	5.16	9.993	15.339	20.513	26.930
c (Å)	8.462	8.69	8.374	8.501	8.553	8.522
V (Å ³)	2403.7	200.4	724.2	1732.2	3116.8	5352.4
Z	24	2	8	18	32	54
D (g/cm ³)	2.58	2.59–2.62	2.55–2.66	2.64	2.59	2.49–2.65
Strongest lines in the powder pattern <i>d</i> _{meas} (Å)	3.091 (100)	3.118 (100)	3.027 (100)	3.076 (100)	3.071 (100)	3.09 (100)
	2.612 (70)	2.579 (50)	3.870 (60)	3.050 (95)	3.929 (70)	2.593 (30)
	1.240 (60)	3.973 (45)	3.294 (40)	2.558 (45)	2.558 (40)	2.131 (25)
	3.18 (50)	2.175 (17)	4.21 (35)	4.269 (35)	2.914 (30)	4.26 (15)
	1.674 (50)	2.472 (15)	2.905 (35)	2.410 (35)	4.277 (25)	3.76 (12)
	1.585 (50)	4.351 (12)	2.359 (30)	3.932 (30)	2.380 (20)	3.02 (12)
	1.515 (50)	2.432 (10)	2.593 (20)	3.384 (25)	2.268 (20)	2.814 (12)
ω	1.538	1.532–1.543	1.529–1.546	–	1.540	1.536
ε	1.531	1.527–1.537	1.526–1.542	–	1.535	1.531
ε – ω	0.007	0.004–0.006	0.003–0.005	–	0.005	0.005
Color	Colorless	Colorless	Colorless	White	Colorless	Colorless

DISCUSSION

In connection with the discovery of megakalsilite, it appears interesting to analyze its genetic relationship to other highly alkaline minerals of the Khibina massif. Kalsilite is fairly common within Khibina, but its geological environment is completely different from that of megakalsilite. Kalsilite is most typical of rischorrite and juvite of the central arc at Khibina, which includes Mount Koashva. These rocks are characterized by el-

evated concentrations of K and graphic intergrowths of kalsilite and K-feldspar. Such intergrowths are regarded as possible products of decomposition of leucite (KAlSi₂O₆) (Borutsky 1988). The greatest diversity of perpotassic minerals at Khibina (as already noted) is associated with hyperagpaitic pegmatites and hydrothermal veins. These minerals, as well as megakalsilite, are mineralogical rarities, whereas the dominant constituents of hyperagpaitic rocks are sodic rather than potassic minerals of various chemical classes. This scheme

is consistent with the principle of polarity of chemical bonds as defined by Kogarko (1977); as the agpaite alkaline magma crystallizes, the major portion of K is consumed to form K-feldspar and nepheline, whereas Na progressively accumulates in residual melts, producing its own compounds in late-stage and postmagmatic differentiates. This pronounced sodic *tendency* of hyperagpaite rocks is clearly manifested, for example, at Lovozero, Ilímaussaq, and Mont Saint-Hilaire. During the formation of the main rock-types along the central arc at Khibina, the partitioning of K between early products of crystallization and residual melts was manifested not as fully as in the aforementioned three massifs, as a result of which a substantial proportion of K was concentrated and passed into solid phases during and after the crystallization of most of the Na minerals. The outcome was the widespread development of exotic perpotassic mineralization in pegmatites and hydrothermal veins of the central arc, occasionally overprinting pre-existing mineral assemblages, including per sodic ones. Megakalsilite appears to have crystallized in such a way from a residual highly alkaline pegmatite-forming melt or solution. Evidence for this inference includes, in particular: (i) its discovery in the pegmatites of the axial zone, consisting mainly of water-soluble Na carbonates, phosphates, and fluorides, (ii) the secondary nature of many K-rich minerals encountered in the pegmatites of the axial zone, such as the titanoborosilicate lemmleinite-K, pseudomorphous after lomonosovite, and the zirconosilicate umbite, a fairly common product of hydrothermal alteration of eudialyte in the Mount Koashva pegmatites, and (iii) the fact that megakalsilite is a polymorphic modification of $KAlSiO_4$ that has a more highly ordered structure than kalsilite. Finally, it might be noted that the new orthorhombic borosilicate lisitsynite, discovered in this same pegmatite body (Khomyakov *et al.* 2000, Sokolova *et al.* 2001), is a more highly ordered phase of composition $KBSi_2O_6$ than its synthetic analogue “boroleucite”, whose symmetry is cubic (Mikloš *et al.* 1992).

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REFERENCES

- BANNISTER, F.A. & HEY, M.H. (1942): A chemical, optical, and X-ray study of nepheline and kaliophilite. *Mineral. Mag.* **22**, 569-608.
- BONACCORSI, E. (1988): *Relazioni strutturali tra le fasi naturali del sistema $NaAlSiO_4$ - $KAlSiO_4$* . Tesi di laurea, University of Pisa, Pisa, Italy.
- _____, MERLINO, S. & PASERO, M. (1988): Trikalsilite: its structural relationships with nepheline and tetrakalsilite. *Neues Jahrb. Mineral., Monatsh.*, 559-567.
- BORUTSKY, B. (1988): *Rock-Forming Minerals of the High-Alkaline Complexes*, Nauka, Moscow, Russia (in Russ.).
- BRESE, N.E. & O'KEEFFE, M. (1991): Bond-valence parameters for solids. *Acta Crystallogr.* **B47**, 192-197.
- BROWN, I.D. (1964): The crystal structure of lithium hydrazinium sulfate. *Acta Crystallogr.* **17**, 654-660.
- BUERGER, M.J. (1954): The stuffed derivatives of the silica structures. *Am. Mineral.* **39**, 600-614.
- DANA, E.S. (1892): *The System of Mineralogy of James Dwight Dana. Descriptive Mineralogy* (6th ed.). J. Wiley & Sons, New York, N.Y.
- FERRARIS, G., GULA, A., IVALDI, G., NESPOLO, M., SOKOLOVA, E., UVAROVA, YU. & KHOMYAKOV, A.P. (2001): First structure determination of an MDO-2O mica polytype associated with a 1M polytype. *Eur. J. Mineral.* **13**, 1013-1023.
- FRANCO, E. & DE GENNARO, M. (1988): Panunzite, a new mineral from Mt. Somma – Vesuvio, Italy. *Am. Mineral.* **73**, 420-421.
- GIBBS, R.E. (1927): The polymorphism of silicon dioxide and the structure of tridymite. *Proc. R. Soc. London* **113A**, 351-367.
- GREGORKIEWITZ, M. (1986): Alkali ion diffusion in $M(AlSiO_4)$ compounds with frameworks of the tridymite topology and its variations. *Solid State Ionics* **18-19**, 534-538.
- _____, & SCHÄFER, H. (1980): The structure of $KAlSiO_4$ – kaliophilite-O1: application of the subgroup–super group relations to the quantitative space group determination of pseudosymmetric crystals. *6th Eur. Crystallogr. Meeting (Barcelona)*, 155 (abstr.).
- HAHN, T. & BUERGER, M.J. (1955): The detailed structure of nepheline, $KNa_3Al_4Si_4O_{16}$. *Z. Kristallogr.* **106**, 308-338.
- KHOMYAKOV, A.P. (1995): *Mineralogy of Hyperagpaite Alkaline Rocks*. Clarendon Press, Oxford, U.K.
- _____, NECHELYUSTOV, G.N., RASTSVETAEVA, R.K. & DOROKHOVA, G.I. (1999): Lemleinite, $NaK_2(Ti,Nb)_2Si_4O_{12}(O,OH)_2 \cdot 2H_2O$, a new mineral of the labuntsovite–nenadkevichite family. *Zap. Vser. Mineral. Obshchest.* **128(5)**, 54-63 (in Russ.).
- _____, _____, SOKOLOVA, E.V. & HAWTHORNE, F.C. (2000): New borosilicates: malinkoite, $NaBSiO_4$, and lisitsynite, $KBSi_2O_6$, from alkaline pegmatites of the Khibina–Lovozero complex, Kola Peninsula. *Zap. Vser. Mineral. Obshchest.* **129(6)**, 35-42 (in Russ.).
- KOGARKO, L.N. (1977): *Problems of the Origin of Agpaite Magmas*. Nauka, Moscow, Russia (in Russ.).

- LIEBAU, F. (1985): *Structural Chemistry of Silicates: Structure, Bonding and Classification*. Springer-Verlag, Berlin, Germany.
- MANDARINO, J.A. (1981): The Gladstone–Dale relationship. IV. The compatibility concept and its application. *Can. Mineral.* **19**, 441-450.
- MERLINO, S. (1988): The structure of reyerite, $(\text{Na,K})_2\text{Ca}_{14}\text{Si}_{22}\text{Al}_2\text{O}_{58}(\text{OH})_8 \cdot 6\text{H}_2\text{O}$. *Mineral. Mag.* **52**, 247-256.
- _____, FRANCO, E., MATTIA, C.A., PASERO, M. & DE GENNARO, M. (1985): The crystal structure of panunzite (natural tetrakalsilite). *Neues Jahrb. Mineral. Monatsh.*, 322-328.
- MIKLOŠ, D., SMRČOK, Ľ., ŽUROVIČ, S., GYEPESOVÁ, D. & HANDLOVIČ, M. (1992): Refinement of the structure of boroleucite, $\text{K}(\text{BSi}_2\text{O}_6)$. *Acta Crystallogr.* **C48**, 1831-1832.
- PERROTTA, A.J. & SMITH, J.V. (1965): The crystal structure of kalsilite, KAlSiO_4 . *Mineral. Mag.* **35**, 588-595.
- SAHAMA, T.G. & SMITH, J.V. (1957): Tri-kalsilite, a new mineral. *Am. Mineral.* **42**, 286.
- SANDOMIRSKII, P.A., MESHALKIN, S.S., ROZHDESTVENSKAYA, I.V., DEM'YANETS, L.N. & UVAROVA, T.G. (1986): Crystal structures of the D-phase of $\text{K}\{\text{AlGeO}_4\}$ and the C-phase of $\text{Na}\{\text{AlGeO}_4\}$. *Sov. Phys. Crystallogr.* **31**, 522-527.
- SHELDRIK, G.M. (1985): *SHELXS-86, Program for the Solution of Crystal Structures*. University of Göttingen, Göttingen, Germany.
- _____. (1993): *SHELXL-93, Program for the Refinement of Crystal Structures*. University of Göttingen, Göttingen, Germany.
- SOKOLOVA, E.V., HAWTHORNE, F.C. & KHOMYAKOV, A.P. (2001): The crystal chemistry of malinkoite, NaBSiO_4 , and lisitsynite, KBSi_2O_6 from the Khibina–Lovozero complex, Kola Peninsula, Russia. *Can. Mineral.* **39**, 159-169.

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