

Noonkanbahite, BaKNaTi₂(Si₄O₁₂)O₂, a new mineral species: description and crystal structure

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ABSTRACT

Noonkanbahite, ideally BaKNaTi₂(Si₄O₁₂)O₂, is described as a new mineral species. At Liley [Löhley], Eifel Mountains, Germany (the holotype locality), it occurs as sprays of prismatic crystals (up to 8 mm) or single prismatic crystals (up to 4 mm) on walls of cavities in alkaline igneous rocks. At Murun, Siberia, Russia, noonkanbahite forms coarse lamellar crystals up to 0.05 cm × 0.7 cm × 1.5 cm embedded in kalsilite syenite. Noonkanbahite is brittle, $H = 6$, $D_{\text{obs.}} = 3.39(1)$, $D_{\text{calc.}} = 3.49 \text{ g/cm}^3$, has a vitreous lustre and does not fluoresce in ultraviolet light. It has poor cleavage on {010} and {100} and weak parting on {011}. Noonkanbahite is biaxial positive with $2V_{\text{obs.}} = 75(2)^\circ$, $2V_{\text{calc.}} = 72.7(9)^\circ$, $\alpha 1.730(5)$, $\beta 1.740(5)$ and $\gamma 1.765(5)$, dispersion is medium, $r < v$. In transmitted plane-polarized light, noonkanbahite is strongly pleochroic, with X colourless, Y yellowish, Z straw-yellow; $X = a$, $Y = b$, $Z = c$. Noonkanbahite is orthorhombic, space group *Imma*, $a = 8.0884(4)$, $b = 10.4970(5)$, $c = 13.9372(6) \text{ \AA}$, $V = 1183.3(1) \text{ \AA}^3$, $Z = 4$. The strongest ten X-ray diffraction lines in the powder pattern [d in $\text{\AA}(hkl)$] are: 2.907(100)(222), 8.353(50)(001), 3.196(50)(220), 2.097(50)(242), 2.241(40)(215), 2.179(40)(035), 3.377(30)(031), 2.694(30)(015), 2.304(30)(233), and 1.564(30)(064). Electron microprobe analysis gives SiO₂ 37.82, TiO₂ 15.54, ZrO₂ 0.42, Nb₂O₅ 3.18, Al₂O₃ 0.17, Fe₂O₃ (recalculated from FeO) 5.63, MnO 0.32, MgO 0.53, BaO 20.60, CaO 1.36, K₂O 5.32, Na₂O 6.14, F 0.78, H₂O 0.58, sum 98.39 wt.%, (H₂O determined by SIMS). The formula unit, calculated on the basis of 14 anions (O+OH+F), is

(Ba_{0.85}K_{0.13}) Σ 0.98(K_{0.59}Na_{0.26}Ca_{0.15}) Σ 1.00Na(Ti_{1.23}Fe³⁺_{0.45}Nb_{0.15}Mg_{0.08}Mn_{0.03}Zr_{0.02}Al_{0.01}) Σ 1.97(Si_{3.99}Al_{0.01}O₁₂)(O_{1.33}OH_{0.41}F_{0.26}) Σ 2.00, $Z = 4$.

The crystal structure was refined to $R_1 = 2.8\%$ for 970 unique ($F_0 > 4\sigma F$) reflections collected on a Bruker single-crystal P4 diffractometer with a CCD detector and MoK α X-radiation. The crystal structure of noonkanbahite is isostructural with that of batisite, ideally BaNa₂Ti₂(Si₄O₁₂)O₂, and scherbakovite, ideally K₂NaTi₂(Si₄O₁₂)O(OH). There are two octahedrally coordinated sites, $M(1)$ and $M(2)$, occupied by (Ti_{1.23}Fe³⁺_{0.45}Nb_{0.15}Mg_{0.08}Mn_{0.03}Zr_{0.02}Al_{0.01}), ideally Ti₂ a.p.f.u. There are three interstitial A sites, ^[9] $A(1)$, ^[8] $A(2)$ and ^[6] $A(3)$, occupied by Ba, K and Na, respectively. Si tetrahedra and M octahedra form a framework with interstitial cages occupied by Ba, K and Na atoms at the A sites. Noonkanbahite, BaKNaTi₂(Si₄O₁₂)O₂, is a K analogue of batisite, BaNa₂Ti₂(Si₄O₁₂)O₂, and a Ba analogue of scherbakovite, K₂NaTi₂(Si₄O₁₂)O(OH).

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KEYWORDS: noonkanbahite, new mineral species, crystal-structure refinement, shcherbakovite, batisite, end-member, Liley, Eifel Mountains, Germany, Murun, Russia.

Introduction

NOONKANBAHITE was first found near the Noonkanbah sheep station, Wolgidee Hills (18°18'S, 124°51'E), West Kimberley District, Australia (Prider, 1965). Prider (1965) introduced the name *noonkanbahite* but it was not approved as a new mineral species at that time. Here, we formally describe noonkanbahite from Liley [Löhley], Eifel Mountains, Germany, as a new mineral species and report its crystal structure. The species and name have been approved by the International Mineralogical Association Commission on New Minerals, Nomenclature and Classification (IMA 2009-059). Noonkanbahite was named after the Noonkanbah sheep station and we maintain the priority of its discoverer. Holotype material is deposited at the Royal Ontario Museum (Department of Earth Sciences) under catalogue # M54065.

The holotype locality of the mineral is confined to igneous rocks at Liley [Löhley] quarry, 800 m NE of Üdersdorf (50°9'48"N, 6°48'39"E), Eifel Mountains, Germany. The cotype locality of noonkanbahite is in kalsilite syenite at Tausonite Hill, Murun alkaline complex, Siberia, Russia. Noonkanbahite belongs to the shcherbakovite group of minerals which are common in agpaite pegmatites and hydrothermal veins in the Khibiny alkaline complex, Kola Peninsula, Russia (shcherbakovite, ideally $K_2NaTi_2(Si_4O_{12})O(OH)$; Khomyakov, 1995), peralkaline rocks of the Inagli complex, Aldan, Siberia (batisite, ideally $BaNa_2Ti_2(Si_4O_{12})O_2$; Kravchenko *et al.*, 1960), and Tertiary nephelinite-leucite volcanic rocks, West Eifel, Germany (Schmall and Tillmanns, 1987). The structure of these minerals is tolerant of a wide range of isomorphous substitutions at each cation site. This structural flexibility permits shcherbakovite-group minerals to be a sink for high-field-strength elements in parageneses ranging from mantle conditions to processes of post-magmatic evolution of peralkaline rocks in the upper lithosphere (Uvarova *et al.*, 2003).

Occurrence and mineral association

At Liley, noonkanbahite occurs in numerous cavities in igneous alkaline rocks. It forms

sprays of straw-yellow prismatic crystals (up to 8 mm) or free-standing single prismatic (up to 4 mm) crystals on walls of numerous cavities, or occurs as anhedral grains up to 1 cm. The paragenesis includes sanidine, richterite, perovskite, cristobalite, hematite, magnetite, analcime and phlogopite. At Murun, it forms coarse lamellar, typically slightly curved crystals up to 0.05 cm × 0.7 cm × 1.5 cm embedded in a coarse-grained kalsilite syenite. Usually, they are isolated, and only rarely combined in clusters up to 2 cm. At Murun, noonkanbahite is a rock-forming mineral in coarse-grained kalsilite syenite, and its content in the rock sporadically reaches 20–25%. It occurs in association with potassic feldspar, kalsilite, aegirine and galena.

Physical and optical properties

Noonkanbahite varies from pinkish orange (Liley) to brownish yellow to brown (Murun). It is brittle, Mohs' hardness is 6, $D_{obs.} = 3.39(1)$, $D_{calc.} = 3.49 \text{ g/cm}^3$, has a vitreous lustre and does not fluoresce in ultraviolet light. It has poor cleavage on {010} and {100} and a weak parting on {011}. Noonkanbahite is biaxial positive with $2V_{obs.} = 75(2)^\circ$, $2V_{calc.} = 72.7(9)^\circ$, $\alpha 1.730(5)$, $\beta 1.740(5)$ and $\gamma 1.765(5)$. The optical dispersion is medium, $r < v$. In transmitted, plane-polarized light, noonkanbahite is strongly pleochroic, with X colorless, Y yellowish and Z straw-yellow; $X = a$, $Y = b$, $Z = c$.

Chemical composition

The chemical composition of noonkanbahite from Liley was determined using a Cameca SX 100 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 counting times on peak and background of 20 and 10 s, respectively. The following standards were used for K or L X-ray lines: Na: $K\alpha$, albite; Si, Ca: $K\alpha$, diopside; Mg: $K\alpha$, olivine; Al: $K\alpha$, andalusite; K: $K\alpha$, orthoclase; Ti: $K\alpha$, titanite; Ba: $L\alpha$, barite; Mn: $K\alpha$, spessartine; Nb: $L\alpha$, $MnNb_2O_6$ (syn.); Zr: $L\alpha$, zircon; Fe: $K\alpha$, fayalite; F: $K\alpha$, fluor-riebeckite. Data were reduced using the X-PHI procedure (Merlet, 1992).

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Ion-microprobe analysis was performed using a Cameca IMS 7f instrument. An $^{16}\text{O}^-$ primary beam $<5\ \mu\text{m}$ in diameter, corresponding to a beam current of $\sim 1.5\text{--}2\ \text{nA}$, was used. The analytical

method for H was similar to that described by Ottolini *et al.* (2002). The sample and the H standards that were used for the calibration procedure were left in the ion-microprobe

TABLE 1. Chemical composition (wt.%) and unit formula (a.p.f.u.) for noonkanbahite.

	(1)	(2)	(3)	(4)	(5)	(6)
SiO ₂	37.82	43.25	38.18	39.55	40.21	39.28
Nb ₂ O ₅	3.18	—	—	b.d.l.	0.10	0.27
Al ₂ O ₃	0.17	0.07	—	0.15	0.12	0.05
TiO ₂	15.54	21.15	22.69	19.85	19.51	20.86
ZrO ₂	0.42	0.85	—	—	—	b.d.l.
Fe ₂ O ₃	5.63	1.70	2.41	4.36**	4.91**	4.78
FeO	—	0.61	—	—	—	—
MnO	0.32	—	—	0.26	0.25	0.16
MgO	0.53	—	—	—	—	—
BaO	20.60	14.47	23.50	21.00	19.32	20.11
CaO	1.36	1.77	0.12	0.46	1.20	0.65
SrO	—	—	0.03	b.d.l.	0.56	b.d.l.
K ₂ O	5.32	10.83	5.84	7.39	7.73	7.64
Na ₂ O	6.14	4.50	5.99	6.09	5.90	5.56
F	0.78	—	—	—	—	—
H ₂ O*	0.58	0.94	0.72	—	—	—
O=F	−0.33	—	—	—	—	—
Σ	98.06	100.14	99.48	99.11	99.81	99.36
Si	3.99	4.21	3.97	4.14	4.15	4.06
Al	0.01	0.01	—	0.02	0.01	0.01
ΣT	4.00	4.22	3.97	4.16	4.16	4.07
Ti ⁴⁺	1.23	1.55	1.78	1.56	1.51	1.63
Zr	0.02	0.04	—	—	—	—
Fe ³⁺	0.45	0.12	0.19	0.34	0.38	0.37
Fe ²⁺	—	0.05	—	—	—	—
Nb	0.15	—	—	—	—	0.01
Mg	0.08	—	—	—	—	—
Mn	0.03	—	—	0.02	0.02	0.01
ΣM	1.96	1.76	1.97	1.92	1.91	2.02
Ba	0.85	0.55	0.96	0.86	0.78	0.82
Sr	—	—	—	—	0.03	—
Ca	0.15	0.18	0.01	0.05	0.13	0.07
K	0.72	1.35	0.78	0.99	1.02	1.01
Na	1.26	0.85	1.21	1.24	1.18	1.12
ΣA	2.98	2.93	2.96	3.14	3.14	3.02
F	0.26	—	—	—	—	—
H ⁺	0.41	0.61	0.50	—	—	—

Localities: (1) Liley, Eifel Mountains, Germany; (2) Wolgidee Hills, Western Australia; (3) — (6) Murun, Siberia, Russia.

References: (1) this work; (2) Prider (1965); (3) Lazebnik and Makhotko (1983); (4) Konev *et al.* (1996); (5) Konev *et al.* (1996); (6) this work.

—: no data; b.d.l.: below detection limit; * determined by SIMS; ** recalculated from FeO. In analyses 1, and 3–6, all Fe is considered as Fe³⁺.

sample chamber for two days to reduce adsorbed H. The energy-filtering technique was used to eliminate any possible molecular interference and to reduce matrix effects affecting light-element ionization. Secondary positive-ion currents were measured at masses 1 (H) and 30 (Si was used as the reference element), and corrected for isotopic abundance. The results were put on a quantitative basis using empirical calibration curves based on standard silicate samples. For H quantification, we used the extrapolated regression line: IY(H/Si) vs. (Fe + Ti + Mn), derived for kornepupine (Ottolini and Hawthorne, 2001) and tested successfully on tourmaline standards. The accuracy of the H result, H_{0.41} p.f.u., is estimated to be in the order of 10% relative.

Table 1, analysis (1), gives the chemical composition and empirical formula unit of the holotype sample based on 14 anions (O + OH + F) as follows: (Ba_{0.85}K_{0.13})_{Σ0.98}(K_{0.59}Na_{0.26}Ca_{0.15})_{Σ1.00}Na(Ti_{1.23}Fe_{0.45}³⁺Nb_{0.15}Mg_{0.08}Mn_{0.03}Zr_{0.02}Al_{0.01})_{Σ1.97}(Si_{3.99}Al_{0.01}O₁₂)_{(O_{1.33}OH_{0.41}F_{0.26})_{Σ2.00}, Z = 4.}

The chemical composition of noonkanbahite from Murun was characterized using a Cameca SX50 electron microprobe (WDS, 20 kV, 20 nA, a beam size of 5 mm, count times on peak and background of 10 and 5 + 5 s, respectively). The following standards were used for K α or L α X-ray lines: Na: albite; K, Al: microcline; Si, Ca, Mg, Fe: amphibole; Ti, Mn: MnTiO₃; Ba: BaSO₄ (syn.); Nb: RbNb₄O₁₁ (syn.). Table 1 shows both the present and previously published chemical data on the mineral from Murun and the analysis of the original noonkanbahite from Noonkanbah; formulae were calculated as described above.

X-ray powder diffraction

The powder diffraction pattern was recorded with Ni-filtered Cu-K α X-radiation ($\lambda = 1.54178 \text{ \AA}$) and a 114.6 mm Gandolfi camera. Table 2 shows the X-ray powder diffraction data for noonkanbahite from Liley, together with the refined cell dimensions; these values are in reasonable agreement with those determined by single-crystal diffraction.

X-ray data collection and structure refinement

X-ray diffraction data for noonkanbahite from Liley were collected with a Bruker P4 diffractometer equipped with a CCD detector (Mo-K α radiation) from a single-crystal of noonkanbahite

TABLE 2. X-ray powder diffraction data for noonkanbahite.

<i>I</i>	<i>d</i> _{meas.} (\AA)	<i>d</i> _{calc.} (\AA)	<i>h k l</i>
70	8.353	8.373	0 1 1
20	5.219	5.241	0 2 0
15	4.042	4.024	1 0 3
15	3.487	3.484	0 0 4
30	3.377	3.390	0 3 1
50	3.196	3.200	2 2 0
100	2.907	2.908	2 2 2
30	2.694	2.693	0 1 5
20	2.623	2.624	0 4 0
30	2.304	2.300	2 3 3
40	2.241	2.242	2 1 5
40	2.179	2.179	0 3 5
50	2.097	2.098	2 4 2
15	2.011	2.013	2 0 6
20	1.676	1.676	0 5 5
20	1.590	1.591	2 3 7
30	1.564	1.564	0 6 4

Refined cell: $a = 8.102(17)$, $b = 10.443(7)$,
 $c = 13.950(14) \text{ \AA}$, $V = 1180.2(2.4) \text{ \AA}^3$.

(Strongest diffraction lines given in bold).

with dimensions 0.16 mm \times 0.06 mm \times 0.02 mm. The intensities of 4645 reflections with $-4 < h < 11$, $-14 < k < 14$, $-19 < l < 19$ were collected to 59.98 $^\circ$ 2 θ using 25 s per 0.125 $^\circ$ frame; an empirical absorption correction (SADABS, Sheldrick, 1998) was applied. The refined unit-cell parameters were obtained from 1608 reflections with $I > 10\sigma I$. Using atom coordinates of shcherbakovite (Uvarova *et al.*, 2003), the crystal structure of noonkanbahite was refined to $R_1 = 0.028$ and a GoF value of 1.159 for 970 independent reflections (73 refined parameters including extinction) with the Bruker SHELXTL version 5.1 system of programs. During the refinement, the *M* site had a high displacement parameter along the *a* axis ($U_{11} = 0.03$). A difference-Fourier map showed a maximum of 6.8 *e*/ \AA at a distance of 0.46 \AA from the *M* site. This maximum was included in the refinement as the *M*(2) site, *M* becoming the *M*(1) site. Site occupancies were refined for the two *M* sites (occupied primarily by Ti, Fe³⁺ and Nb) and three *A* sites (occupied primarily by Na, Ba and K). Details of the data collection and structure refinement are given in Table 3, final atom parameters are given in Table 4, selected

TABLE 3. Miscellaneous refinement data for noonkanbahite.

a (Å)	8.0884(4)
b	10.4970(5)
c	13.9372(6)
V (Å ³)	1183.3(1)
Space group	<i>Imma</i>
Z	4
Absorption coefficient (mm ⁻¹)	5.25
$F(000)$	1180.8
$D_{\text{calc.}}$ (g/cm ³)	3.496
Crystal size (mm)	0.16 × 0.06 × 0.02
Radiation/filter	Mo- $K\alpha$ /graphite
2 θ -range for data collection (°)	59.98
R_{int} (%)	1.66
Reflections collected	4645
Independent reflections	970
$ F_o > 4\sigma F$	961
Refinement method	Full-matrix least-squares on F^2 , fixed weights proportional to $1/\sigma F_o^2 $
Goodness of fit on F^2	1.157
Final R_{obs} (%)	$R_1 = 2.81$
$[F_o] > 4\sigma F$	
	$R_1 = 2.83$
R indices (all data) (%)	$wR_2 = 6.92$
	GoF = 1.159

interatomic distances and angles in Table 5, refined site-scattering values and assigned populations for selected sites are given in Table 6, and bond-valence values in Table 7. A list of observed and calculated structure factors has been deposited with the Principal Editor of *Mineralogical Magazine* and are available from www.minersoc.org/pages/e_journals/dep_mat.html.

Description of the structure

Cation sites

In the crystal structure of noonkanbahite, there is one site tetrahedrally coordinated by O atoms and solely occupied by Si with $\langle \text{Si}-\text{O} \rangle = 1.606$ Å. There are two sites partly occupied by Ti, Fe^{3+} and Nb, $M(1)$ and $M(2)$, with $M(1)-M(2) =$

TABLE 4. Final atom positions and displacement parameters (Å²) for noonkanbahite.

	x	y	z	U_{eq}	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
$M(1)$	0.2728(6)	¼	0.4713(1)	0.0089(5)	0.0114(14)	0.0066(3)	0.0087(6)	0	0.0003(6)	0
$M(2)$	0.2282(9)	¼	0.4695(4)	0.0089(5)	0.0114(14)	0.0066(3)	0.0087(6)	0	0.0003(6)	0
$A(1)$	0	¼	0.74487(3)	0.0131(2)	0.0128(2)	0.0119(2)	0.0147(2)	0	0	0
$A(2)$	0	¼	0.6819(2)	0.0271(20)	0.0176(8)	0.0155(7)	0.0481(11)	0	0	0
$A(3)$	0	½	½	0.0351(10)	0.0093(11)	0.0474(18)	0.0486(19)	-0.0365(15)	0	0
Si	-0.30317(9)	0.97420(6)	0.64500(5)	0.0097(2)	0.0114(4)	0.0074(3)	0.0103(3)	-0.0007(2)	0.0004(2)	-0.0001(2)
O(1)	-0.2207(3)	0.8831(2)	0.5673(1)	0.0156(4)	0.0230(10)	0.0107(8)	0.0132(8)	-0.0037(7)	0.0043(7)	0.0005(7)
O(2)	-0.2455(3)	0.1203(2)	0.6368(1)	0.0180(5)	0.0308(12)	0.0093(9)	0.0140(9)	0.0012(7)	0.0003(8)	-0.0041(8)
O(3)	-¼	0.9189(3)	¼	0.0336(10)	0.0784(30)	0.0111(14)	0.0111(13)	0	-0.0081(15)	0
O(4)	-½	0.9668(4)	0.6439(4)	0.0536(14)	0.0111(15)	0.0380(23)	0.1118(44)	-0.0187(26)	0	0
O(5)	0	¼	0.4574(3)	0.0133(7)	0.0128(17)	0.0157(18)	0.0115(16)	0	0	0
O(6)	½	¼	0.4704(3)	0.0221(9)	0.0236(22)	0.0173(20)	0.0255(22)	0	0	0

TABLE 5. Selected interatomic distances (Å) and angles (°) for noonkanbahite.

Si–O(1)	1.591(2)	M(1)–O(1) × 2	1.980(2)	M(2)–O(1) × 2	1.954(4)
Si–O(2)	1.607(2)	M(1)–O(2) × 2	2.043(2)	M(2)–O(2) × 2	2.016(4)
Si–O(3)	1.632(1)	M(1)–O(5)	2.215(5)	M(2)–O(5)	1.854(7)
Si–O(4)	1.594(1)	M(1)–O(6)	1.838(5)	M(2)–O(6)	2.198(7)
<Si–O>	1.606	<M(1)–O>	2.017	<M(2)–O>	1.999
		M(1)–M(2)	0.36		
A(1)–O(2) × 4	2.840(2)	A(2)–O(1) × 4	2.773(2)	A(3)–O(1) × 4	2.361(2)
A(1)–O(2) _a × 4	2.968(2)	A(2)–O(2) × 4	2.852(2)	A(3)–O(5) × 2	2.691(1)
A(1)–O(5)	2.819(4)	<A(2)–O>	2.813	<A(3)–O>	2.471
<A(1)–O>	2.895				

a: $x+1/2$, $-y+1/2$, $-z+3/2$

0.36 Å. The M(1) site is occupied by (Ti_{0.59}Fe_{0.45}³⁺Nb_{0.15}Mg_{0.08}Mn_{0.03}Zr_{0.02}Al_{0.01}□_{0.67}) with <M(1)–φ> = 2.017 Å, and the M(2) site is occupied by (Ti_{0.64}□_{1.36}) with <M(2)–φ> = 1.999 Å where φ = O, OH, F. Ideally, the M(1) and M(2) sites give Ti₂ a.p.f.u.

There are three interstitial A sites. The [9]-coordinated A(1) site is occupied by (Ba_{0.82}K_{0.16}□_{0.02}) with <A(1)–φ> = 2.895 Å, the [8]-coordinated A(2) site is occupied by (K_{0.56}Na_{0.26}Ca_{0.15}Ba_{0.03}) with <A(2)–O> = 2.813 Å, and the A(3) site is occupied by Na with <A(3)–φ> = 2.471 Å. The ideal aggregate composition of the A sites can be given as BaKNa p.f.u.

bond-valence for noonkanbahite gives incident bond-valence sums of 1.38 v.u. at O(5) and 1.47 v.u. at O(6) (Table 7) (v.u. = valence unit). These values indicate that these sites are both occupied by O²⁻, (OH)⁻ and F⁻, which agrees with chemical and SIMS analyses, (O_{1.33}OH_{0.41}F_{0.26}). Ideally, the O(5) and O(6) sites give O₂ a.p.f.u. There are hydrogen bonds to these atoms, but it was not possible to locate the H atoms in the structure, and H is not taken into consideration in the bond-valence calculations, accounting for the fact that the incident bond-valence at O(6) and O(5) is smaller than expected (Table 7). The total anion content is ideally O₁₄ a.p.f.u.

Anion considerations

The O(1)–O(4) anions coordinate Si atoms and are O atoms. They give O₁₂ a.p.f.u. Calculation of

Topology of the structure

In the structure of noonkanbahite, (SiO₄) tetrahedra link to form a batisite-like (Si₄O₁₂)⁸⁻ chain

TABLE 6. Refined site-scattering values (e.p.f.u.) and assigned site-populations (a.p.f.u.) for noonkanbahite.

	Refined site-scattering	Site population	Calculated site-scattering	<X–φ> _{calc.} *	<X–φ> _{obs.}
A(1)	47.2(2)	0.82 Ba + 0.16 K + 0.02 □	49.0	2.863	2.895
A(2)	16.4(1)	0.56 K + 0.26 Na + 0.15 Ca + 0.03 Ba	18.2	2.743	2.813
A(3)	11.0	1.00 Na	11.0	2.400	2.471
M(1)	35(3)	0.59 Ti ⁴⁺ + 0.45 Fe ³⁺ + 0.15 Nb + 0.08 Mg + 0.03 Mn + 0.02 Zr + 0.01 Al + 0.67 □	34	2.008	2.017
M(2)	14(3)	0.64 Ti ⁴⁺ + 1.36 □	14	1.985	1.999

* Calculated by summing constituent ionic radii (values from Shannon, 1976)

NOONKANBAHITE, $\text{BaKNaTi}_2(\text{Si}_4\text{O}_{12})\text{O}_2$, A NEW MINERAL SPECIES

TABLE 7. Bond-valence table for noonkanbahite.

	$A(1)^{**}$	$A(2)^{**}$	$A(3)^{**}$	$M(1)^*$	$M(2)^*$	Si*	Σ
O(1)		0.143×4	0.221×4	0.416×2	0.218×2	1.090	2.09
O(2)	0.209×4 0.148×4			0.346×2	0.188×2	1.047	1.94
O(3)		0.115×2 $\times 4$				0.979×2	2.19
O(4)						1.084×2	2.17
O(5)	0.222		0.091×2 $\times 2$	0.216×2	0.273×2		1.38
O(6)				0.615×2	0.120×2		1.47
Σ	1.650	1.032	1.066	2.355	1.205	4.200	

* bond-valence parameters (v.u.) from curves of Brown (1981)

** bond-valence parameters (v.u.) from curves of Brown and Altermatt (1985)

TABLE 8. Comparison of noonkanbahite, batisite and shcherbakovite.

	Noonkanbahite*	Batisite**	Shcherbakovite***
Formula	$\text{BaKNaTi}_2(\text{Si}_4\text{O}_{12})\text{O}_2$	$\text{BaNaNaTi}_2(\text{Si}_4\text{O}_{12})\text{O}_2$	$\text{KKNaTi}_2(\text{Si}_4\text{O}_{12})\text{O}(\text{OH})$
System	orthorhombic	orthorhombic	orthorhombic
Space group	<i>Imma</i>	<i>Imma</i> ^s	<i>Imma</i>
a (Å)	8.0884(4)	8.087(2)	8.1538(4)
b	10.4970(5)	10.499(2)	10.5569(5)
c	13.9372(6)	13.913(4)	13.9882(6)
V (Å ³)	1183.3(1)	1181.3(2)	1204.09(18)
Z	4	4	4
D_{meas} (g/cm ³)	3.39(1)	3.432	2.968
	8.353 (70)	3.39 (50)	3.39 (50)
	3.196 (50)	2.91 (100)	2.90 (100)
Strongest lines in the powder pattern d_{meas} (Å)	2.907 (100)	2.62 (30)	2.64 (70)
	2.241 (40)	2.16 (50)	2.10 (40)
	2.179 (40)	2.09 (40)	2.04 (50)
	2.097 (50)	1.68 (50)	1.69 (70)
Optical character	biaxial positive	biaxial positive	biaxial negative
n_α	1.730(5)	1.730(1)	1.707
n_β	1.740(5)	1.735(1)	1.745
n_γ	1.765(5)	1.791(1)	1.776
$n_\alpha - n_\gamma$	0.035	0.061	0.069
$2V$ (°)	75(2)	7	82
Orientation	$X = a, Y = b,$ $Z = c$	$X = a, Y = b,$ $Z = c$	$X = a, Y = b,$ $Z = c$
Colour	pinkish orange	dark brown	dark brown
Pleochroism	X – colourless Y – yellowish Z – straw-yellow	X – colourless Y – yellow brown Z – reddish	X – pale yellow Y – yellow Z – brownish yellow

* This work

** Kravchenko *et al.* (1960), Schmahl and Tillmanns (1987)

^s cell re-oriented to conform with other minerals of this group

*** Es'kova and Kazakova (1954), Uvarova *et al.* (2003)

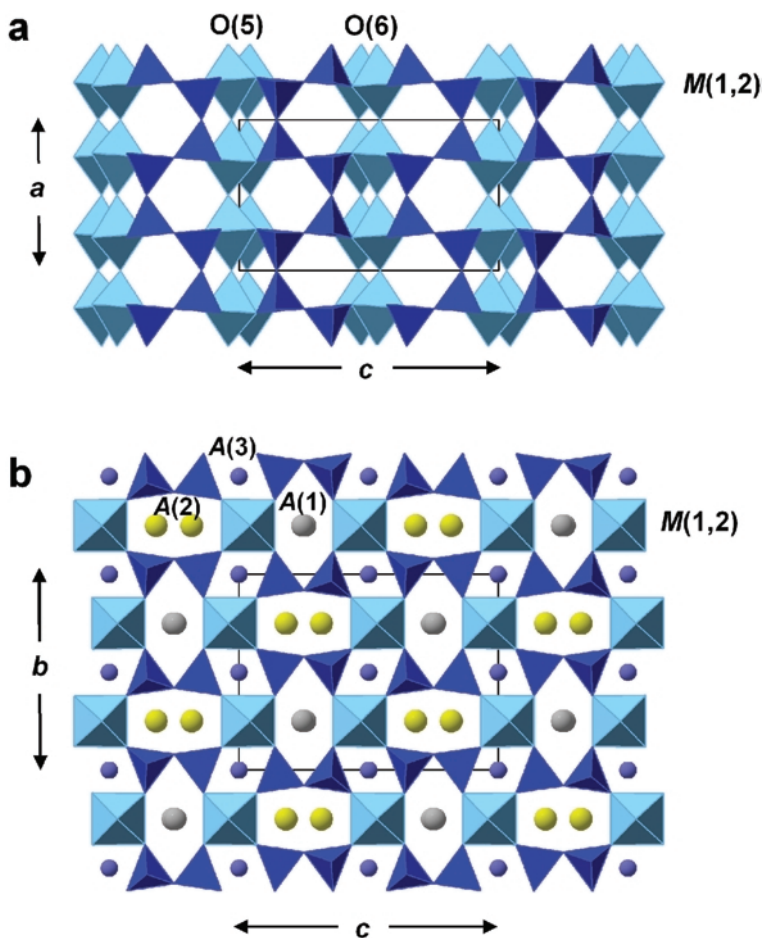


FIG. 1. The crystal structure of noonkanbahite: (a) a linkage of batisite-like $(\text{Si}_4\text{O}_{12})^{8-}$ chains and perovskite-like $(\text{M}\phi_5)^{6-}$ chains; (b) viewed down [100]: SiO_4 tetrahedra are light blue, $M(1,2)$ octahedra are blue; $A(1)$, $A(2)$ and $A(3)$ atoms are shown as grey, yellow and blue circles.

first described by Nikitin and Belov (1962). Ti-dominant $(\text{M}\phi_6)$ octahedra link *via* common vertices to form a perovskite-like $(\text{M}\phi_5)^{6-}$ chain. Both chains, $(\text{Si}_4\text{O}_{12})$ and $(\text{M}\phi_5)$, extend along the a axis (Fig. 1a). The $(\text{Si}_4\text{O}_{12})$ and $(\text{M}\phi_5)$ chains link to form a mixed tetrahedron-octahedron framework (Fig. 1b). Each $(\text{M}\phi_6)$ octahedron is connected through common vertices to four (SiO_4) tetrahedra, and each (SiO_4) tetrahedron is connected to two M octahedra and two Si tetrahedra.

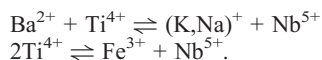
There are three types of interstitial cages (Fig. 1b), and cages are significantly different in size. The largest cage includes the $A(1)$ site and is

occupied by Ba and K. The intermediate-sized cage includes the $A(2)$ site, and is occupied by K and small amounts of Na, Ca and Ba. The smallest cage includes the $A(3)$ site which is populated by Na.

Summary

As was discussed by Uvarova *et al.* (2003), minerals of the shcherbakovite group form in a range of rocks from (K,Na)-rich to ultrapotassic silica-saturated rocks considered to be of mantle origin, and a very wide P - T range of stability can be expected for the members of this group. The

structure of shcherbakovite-group minerals is tolerant of a wide range of isomorphous substitutions at the cation sites, the main substitutions being



In Table 8, selected data for noonkanbahite, batisite and shcherbakovite are summarized. Structure refinements for batisite have been carried out in space groups *Ima2* and *Imam*. In this work, we have chosen the space group *Imma* (standard setting). All formulae are in accord with a general formula $A B C M_2 \phi_2 [\text{Si}_4\text{O}_{12}]$, where $A = \text{Ba}, \text{K}, \text{Na}, \text{Ca}$; $B = \text{K}, \text{Na}$; $C = \text{Na}$; $M = \text{Ti}^{4+}, \text{Nb}, \text{Fe}^{3+}, \text{Zr}$; $\phi = \text{O}, (\text{OH}), \text{F}$ (Uvarova *et al.*, 2003).

Noonkanbahite was originally described by Prider (1965) but was not approved as a new mineral species at the time. However, it is apparent from the above discussion that noonkanbahite should be a valid mineral species. In fact, prior to the approval of noonkanbahite, several minerals with a chemical composition similar to that of noonkanbahite were reported under the following names: (1) potassic batisite (Lazebnik and Makhotko, 1983), (2) batisite (Schmall and Tillmanns, 1987), (3) shcherbakovite (Mitchell, 1990), (4) K-batisite (Konev *et al.*, 1996), (5) K-containing batisite (Rastsvetaeva *et al.*, 1997), and (6) shcherbakovite-batisite (Hogarth, 1997), though they were not considered as possible new minerals.

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