

Cámaraite, $\text{Ba}_3\text{NaTi}_4(\text{Fe}^{2+}, \text{Mn})_8(\text{Si}_2\text{O}_7)_4\text{O}_4(\text{OH}, \text{F})_7$. I. A new Ti-silicate mineral from the Verkhnee Espe Deposit, Akjailyautas Mountains, Kazakhstan

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[Received 5 June 2009; Accepted 5 August 2009]

ABSTRACT

Cámaraite, ideally $\text{Ba}_3\text{NaTi}_4(\text{Fe}^{2+}, \text{Mn})_8(\text{Si}_2\text{O}_7)_4\text{O}_4(\text{OH}, \text{F})_7$, is a new mineral from the Verkhnee Espe deposit, Akjailyautas Mountains, Kazakhstan. It occurs as intergrowths with bafertisitite and jinshajiangite in separate platy crystals up to 8 mm × 15 mm × 2 mm in size, or as star-shaped aggregates of crystals with different orientations. Individual crystals are orange-red to brownish-red, and are platy on {001}. Cámaraite is translucent and has a pale-yellow streak, a vitreous lustre, and does not fluoresce under cathode or ultraviolet light. Cleavage is {001} perfect, no parting was observed, and Mohs hardness is <5; the mineral is brittle. The calculated density is 4.018 g cm⁻³. In transmitted light, cámaraite is strongly pleochroic, X = light brown, Y = reddish-brown, Z = yellow-brown, with Z < X < Y. Cámaraite is biaxial +ve and 2V_{meas.} = 93(1)°. All refractive indices are greater than 1.80. Cámaraite is triclinic, space group $C\bar{1}$, $a = 10.678(4)$ Å, $b = 13.744(8)$ Å, $c = 21.40(2)$ Å, $\alpha = 99.28(8)^\circ$, $\beta = 92.38(5)^\circ$, $\gamma = 90.00(6)^\circ$, $V = 3096(3)$ Å³, $Z = 4$, $a:b:c = 0.7761:1:1.5565$. The seven strongest lines in the X-ray powder-diffraction pattern are as follows: [d (Å), (h), (k), (l)]: 2.63, (100), (401); 2.79, (90), ($\bar{2}43$, $\bar{2}41$, $2\bar{2}6$, 225); 1.721, (70), ($\bar{2}411$, $\bar{2}49$, 082); 3.39, (50), ($2\bar{2}4$, 223); 3.18, (50), ($\bar{2}25$, $\bar{2}24$); 2.101, (50), ($\bar{4}42$, $\bar{4}40$); 1.578, (50), ($\bar{6}41$, $\bar{6}42$, $\bar{6}41$, $\bar{6}40$). Chemical analysis by electron microprobe gave: Nb₂O₅ 1.57, SiO₂ 25.25, TiO₂ 15.69, ZrO₂ 0.33, Al₂O₃ 0.13, Fe₂O₃ 2.77, FeO 16.54, MnO 9.46, ZnO 0.12, MgO 0.21, CaO 0.56, BaO 21.11, Na₂O 1.41, K₂O 0.84, H₂O 1.84, F 3.11, less O ≡ F 1.31, total 99.63 wt.%, where the valence state of Fe was determined by Mössbauer spectroscopy [$\text{Fe}^{3+}/(\text{Fe}^{2+} + \text{Fe}^{3+}) = 0.13(8)$] and the H₂O content was derived by crystal-structure determination. The resulting empirical formula on the basis of 39 anions is $(\text{Ba}_{2.61}\text{K}_{0.34})_{\Sigma 2.95}(\text{Na}_{0.86}\text{Ca}_{0.14})_{\Sigma 1}(\text{Ti}_{3.72}\text{Nb}_{0.22}\text{Al}_{0.05})_{\Sigma 3.99}(\text{Fe}_{4.36}^{2+}\text{Fe}_{0.66}^{3+}\text{Mn}_{2.53}\text{Mg}_{0.10}\text{Zr}_{0.05}\text{Zn}_{0.03}\text{Ca}_{0.05})_{\Sigma 7.78}\text{Si}_{7.97}\text{O}_{35.89}\text{H}_{3.88}\text{F}_{3.11}$. Cámaraite is a Group-II TS-block mineral in the structure hierarchy of Sokolova (2006). The mineral is named cámaraite after Fernando Cámara (born 1967) of Melilla, Spain, in recognition of his contribution to the fields of mineralogy and crystallography. The new mineral and mineral name have been approved by the Commission on New Minerals, Nomenclature and Classification, International Mineralogical Association (IMA 2009-11).

KEYWORDS: cámaraite, new mineral species, titanium silicate, Verkhnee Espe deposit, Akjailyautas Mountains, Kazakhstan, TS block.

Introduction

CÁMARAITE was originally discovered at the Verkhnee Espe deposit in Kazakhstan by A.V. Stepanov in the 1980s. The mineral was separated from a concentrate of bafertisitite and its chemical

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DOI: 10.1180/minmag.2009.073.5.847

composition was determined with a JXA 733 electron microprobe operated in energy-dispersive mode. Fernando Cámara and Elena Sokolova obtained a sample of bafertisite from this locality (originally collected by A.V. Stepanov) from the Fersman Mineralogical Museum in order to work on bafertisite, as this locality has the best crystals of the mineral (Yakovlevskaya and Mineev, 1965). During this work, they re-discovered cámaraite. Leonid Pautov (of the Fersman Mineralogical Museum) was aware of the unpublished work of Stepanov and his colleagues and informed ES that A.V. Stepanov had found this mineral twenty-five years earlier. The current paper is a collaboration of these two groups.

The mineral is named cámaraite after Fernando Cámara (born 1967) of Melilla, Spain (who discovered the mineral and solved its crystal structure), in recognition of his contribution to the fields of mineralogy and crystallography, particularly with respect to Ti-silicate minerals, amphiboles, arrojadite-group minerals and cancrinite-group minerals. The new mineral and mineral name have been approved by the Commission on New Minerals, Nomenclature and Classification, International Mineralogical Association (IMA 2009-11). The holotype specimen of cámaraite has been deposited at the Fersman Mineralogical Museum, Moscow, Russia, registration number 3828/1 and 3828/2.

Occurrence

The mineral occurs in the Verkhnee Espe deposit (48°03'–48°10'N, 81°26'–81°29'E), which is related spatially to two small oval outcrops of alkaline granite at the northern exo-contact of the large Akjailyautas granite massif in the northern part of the Tarbagatai mountain range, eastern Kazakhstan (Stepanov and Bekenova, 2009). Both these small intrusions are part of a belt of alkaline-granite dykes which extend 5 km NNE and more than 20 km SSW from these outcrops, and almost coincide with the western exo- and endo-contacts of the Akjailyautas granite massif. The Verkhnee Espe rare-element (Zr, Nb, REEs, Th, etc.) deposit formed probably during the later stages of the intrusion of the Akjailyautas massif.

Cámaraite was found at one locality in the deposit where fenites are most enriched in alkalis and have been extensively recrystallized. The accumulation of post-magmatic fluids and their contamination by host-rock fluids resulted in intense reworking of the granites and the host

rocks. The granites were intensely recrystallized with significant enrichment in F, Li and rare elements, with loss of the typical hypidiomorphic texture and development of granoblastic texture. Primary quartz and microcline inclusions partially survived, but primary platy albite and tartan-twinned microcline recrystallized extensively. Primary biotite and sodic-calcic amphiboles were replaced by Li-bearing riebeckite, aegirine and astrophyllite. Secondary feldspars differ from primary feldspars in that they lack perthite or antiperthite textures, do not contain micro-flakes of hematite, and show no sign of alteration or replacement. Due to the freshness of these secondary feldspars, the resulting fenitized granite has a white or bluish-white colour.

Crystals of riebeckite, aegirine and albite are oriented NW–SE irrespective of the orientation of the contact, suggesting recrystallization was accompanied by strong NE–SW stress. The associated pegmatites were extensively albitized or microclinized, with sporadic introduction of Zr, Th, Nb and REEs. Subsequent greisenization was very heterogeneous and weak, and was accompanied by partial to complete breakdown of riebeckite, aegirine, elpidite, astrophyllite and formation of polythionite, quartz, rutile and fluorite. Cámaraite is of hydrothermal origin and occurs with bafertisite (Peng, 1959) and jinshajiangite (Hong and Fu, 1982) in a zone of fenites. The source of Ba for these minerals (also for other Ba minerals: capellenite, barylite and bazirite) may have been the adjacent tuffaceous aleurolites and dykes of basic and intermediate rocks. Cámaraite is associated with various rare-metal minerals: bafertisite, jinshajiangite, zircon, pyrochlore-group minerals, thorite, monazite, xenotime etc., and formed at the exo-contact zone of the fenitized and granitized host rocks.

Physical properties

Cámaraite occurs on fracture surfaces (Fig. 1) as intergrowths with jinshajiangite (Fig. 2a) and bafertisite (Fig. 2b). Both these intergrowths resemble separate platy crystals up to 8 mm × 15 mm × 2 mm in size. Cámaraite also occurs as star-shaped aggregates of crystals with different orientations. Individual crystals are orange-red to brownish-red (paler than bafertisite), platy on {001} and show no twinning. Cámaraite is translucent and has a pale-yellow streak, a vitreous lustre, and does not fluoresce under cathode or ultraviolet light. Cleavage is {001}

CáMARAITE, A NEW TI-SILICATE

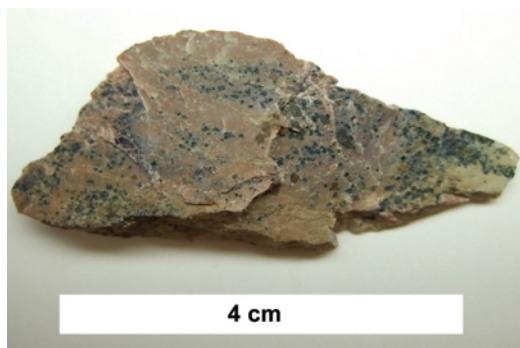


FIG. 1. Fenitized rock consisting of K-feldspar and albite with disseminated alkali amphiboles, astrophyllite, aegirine, cámaraites, bafertisite, jinshajiangite etc.

perfect, no parting is observed, and Mohs hardness is <5 (less than bafertisite); the mineral is brittle. The measured density (obtained by weighing 10 grains of cámaraites in air and in alcohol) is 3.871(1) and the calculated density is 4.018 g cm⁻³ (from the empirical formula and unit-cell parameters of the single crystal used for the crystal-structure determination). The measured density is less than the calculated density because the grains of cámaraites are intergrown with bafertisite and jinshajiangite (Fig. 2).

In transmitted light, cámaraites is strongly pleochroic, X = light brown, Y = reddish-brown, Z = yellow-brown, with Z < X < Y. The relation

between the optic axes (X, Y, Z) and crystallographic axes (*a*, *b*, *c*) is as follows:

	<i>a</i>	<i>b</i>	<i>c</i>
X	90.4°	3.2°	96.2°
Y	73.6°	86.9°	164.7°
Z	163.6°	89.5°	103.9°

where the entries in the matrix denote the angles between the corresponding directions. Cámaraites is biaxial +ve and 2*V*_{meas.} = 93(1)°. All refractive indices are greater than 1.80 but we were unable to measure their exact values due to safety restrictions. The calculated mean refractive index is 1.866, and measurement of the birefringence confirmed that all refractive indices are above 1.80. We were unable to measure the dispersion due to the combination of optic orientation and crystal shape.

Chemical composition

Crystals were analysed with a Cameca SX100 electron microprobe operating in wavelength-dispersive mode with an accelerating voltage of 15 kV, a probe current of 20 nA, and a final beam diameter of 10 µm. The following standards were used in the analysis: fluor-riebeckite (F-*Kα*); albite (Na-*Kα*); forsterite (Mg-*Kα*); andalusite (Al-*Kα*); diopside (Si-*Kα*, Ca-*Kα*); orthoclase (K-*Kα*); titanite (Ti-*Kα*); spessartine (Mn-*Kα*); fayalite (Fe-*Kα*); gahnite (Zn-*Kα*); zircon (Zr-*Lα*); synthetic Ba₂NaNb₅O₁₅ (Nb-*Lα*); and baryte (Ba-*Lα*). The elements Rb, Sr, Cs, Ta and Pb were sought but not detected. The data were

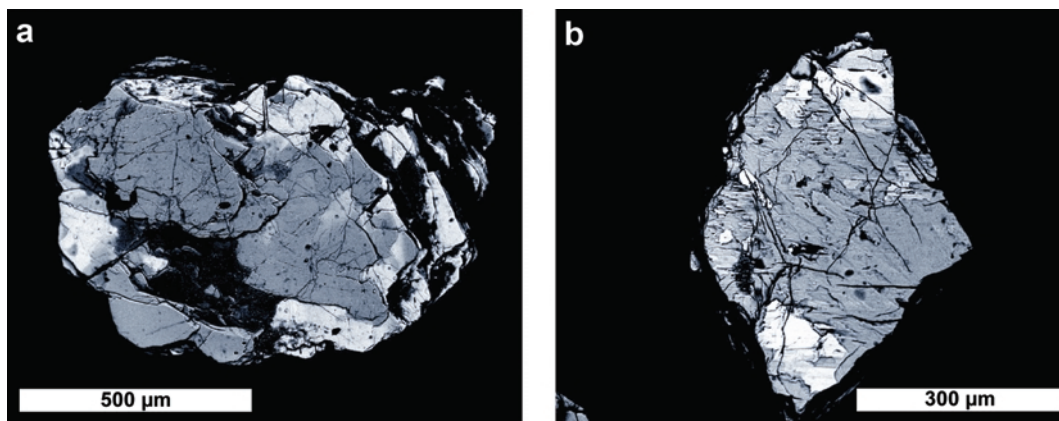


FIG. 2. Backscattered electron images of cámaraites intergrown with other Ti-silicate minerals; (a) cámaraites (white) and jinshajiangite (grey); (b) cámaraites (grey) and bafertisite (white); note the parallel intergrowth of all minerals.

TABLE 1. Chemical composition (wt.%) and formula (a.p.f.u.) for cámaraité¹.

	1	2			1	2
		Average	Range			
Nb ₂ O ₅	1.51	1.57	1.36–1.82	Si	8.14	7.97
SiO ₂	26.04	25.25	25.09–25.40			
TiO ₂	15.86	15.69	15.41–15.88	Ti	3.73	3.72
ZrO ₂	n.a.	0.33	0.22–0.52	Nb	0.21	0.22
Al ₂ O ₃	n.a.	0.13	0.09–0.22	Al	–	0.05
Fe ₂ O ₃ ²	n.a.	2.77		Σ	3.94	3.99
FeO	22.29	16.54	18.76–19.37 ³			
MnO	7.12	9.46	9.34–9.60	Fe ²⁺	5.82	4.36
ZnO	n.a.	0.12	0.09–0.17	Mn	1.88	2.53
MgO	n.a.	0.21	0.20–0.22	Fe ³⁺	–	0.66
CaO	0.57	0.56	0.48–0.70	Mg	–	0.1
BaO	22.51	21.11	20.60–21.66	Zr	–	0.05
Na ₂ O	1.41	1.41	1.32–1.48	Ca	0.04	0.05
K ₂ O	0.8	0.84	0.80–0.89	Zn	–	0.03
H ₂ O ⁴	3.36	1.84		Σ	7.74	7.78
F	n.a.	3.11	2.93–3.33			
sub total		100.94		Na	0.85	0.86
less O≡F	–	1.31		Ca	0.15	0.14
Total	101.47	99.63		Σ	1	1
				Ba	2.76	2.61
				K	0.32	0.34
				Σ	3.08	2.95
				O	35	35.89
				H	7	3.88
				F	–	3.11

¹ 1: Original EMP analysis (A.V. Stepanov); 2: EMPA for single crystal used for structure solution and optics.

² determined by Mössbauer spectroscopy.

³ for Fe total measured as Fe²⁺.

⁴ calculated from structure solution and refinement.

n.a. = not analysed.

reduced and corrected by the ‘PAP’ method of Pouchou and Pichoir (1985). The presence and quantity of (OH) groups were established by crystal-structure solution and refinement. The H₂O content was calculated by stoichiometry on the basis that (OH + F) = 7 a.p.f.u. Table 1 gives the chemical composition (mean of 13 determinations). Milli-Mössbauer spectroscopy on the same crystal used for the X-ray data collection (Fig. 3) gave Fe³⁺/Fe_{total} = 0.13(8). The unit-formula (analysis 2, Table 1) calculation was based on 39 anions per formula unit (p.f.u.). The general formula may be written as Ba₃NaTi₄(Fe²⁺, Mn)₈(Si₂O₇)₄O₄(OH, F)₇. There is very close correspondence between the original analysis of cámaraité (analysis 1, Table 1) and the

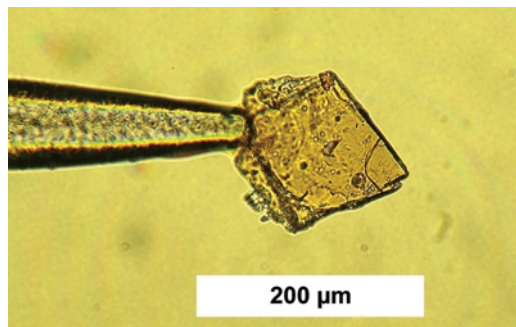


FIG. 3. A single crystal of cámaraité on a glass fibre, note the platy nature of the mineral.

composition of the crystal used for the structural analysis (analysis 2, Table 1). Comparison between analyses 1 and 2 indicates that cámaraita shows some variation in the amounts of Fe^{2+} and Mn but that all other constituents are in very close correspondence. Cámaraita is a Group-II TS-block mineral in the structure hierarchy of Sokolova (2006).

Mössbauer spectroscopy

The Mössbauer spectrum was collected at room temperature (RT) on a single crystal ($140 \text{ mm} \times 140 \text{ mm} \times 30 \text{ }\mu\text{m}$, Fig. 3) using a $^{57}\text{Co}(\text{Rh})$ point source. Due to the small size of the sample and the low signal-to-noise ratio, the collection time was about five weeks. Of course, these conditions are not optimal, but one must work with whatever amount of sample is available for new minerals. The off-resonance background of the folded spectrum is ~ 3.3 megacounts. The spectrometer was calibrated using the spectrum of $\alpha\text{-Fe}$ at room T . The cámaraita spectrum (Fig. 4) is fitted with two sites (each with one Gaussian component) due to Fe^{2+} (solid line) and Fe^{3+} (dashed line), using a Voigt-based quadrupole-splitting-distribution (QSD) analysis. Assuming equal recoil-free fractions for Fe^{2+} and Fe^{3+} , the $\text{Fe}^{3+}/\text{Fe}_{\text{tot}}$ ratio is 0.13(8). The ratio of the spectral areas of the low-velocity peak to the high-velocity peak ($A-/A+$) was allowed to vary for the Fe^{2+}

site, whereas it was constrained to be equal to unity for the minor Fe^{3+} . The Lorentzian line-width of the elemental doublet of the QSD was fixed at 0.1 mm s^{-1} , and the Gaussian width was fixed at 0.3 mm s^{-1} for both Fe^{2+} and Fe^{3+} components. Furthermore, the centre shift (CS) and the quadrupole splitting (QS) for Fe^{3+} were constrained to 0.4 mm s^{-1} and 0.7 mm s^{-1} respectively. The refined parameters for Fe^{2+} are: CS = $1.13(2) \text{ mm s}^{-1}$; QS = $1.94(5) \text{ mm s}^{-1}$ – characteristic of high-spin Fe^{2+} in octahedral coordination.

X-ray powder diffraction

The powder-diffraction pattern was recorded with monochromated $\text{Co-K}\alpha$ X-radiation ($\lambda = 1.79021 \text{ \AA}$) and a 57.3 mm diameter Debye-Scherrer camera. Table 2 shows the X-ray powder-diffraction data for cámaraita. The unit-cell parameters were refined, giving the following values: $a = 10.678(4) \text{ \AA}$, $b = 13.744(8) \text{ \AA}$, $c = 21.40(2) \text{ \AA}$, $\alpha = 99.28(8)^\circ$, $\beta = 92.38(5)^\circ$, $\gamma = 90.00(6)^\circ$, $V = 3096(3) \text{ \AA}^3$. Cámaraita is triclinic, space group $C\bar{1}$, $Z = 4$. Unit-cell dimensions were also determined on a Bruker diffractometer using graphite-monochromated $\text{Mo-K}\alpha$ X-radiation ($a = 10.6965(7) \text{ \AA}$, $b = 13.7861(9) \text{ \AA}$, $c = 21.478(2) \text{ \AA}$, $\alpha = 99.345(1)^\circ$, $\beta = 92.315(2)^\circ$, $\gamma = 89.993(2)^\circ$, $V = 3122.6(4) \text{ \AA}^3$) and are close to the values determined by powder diffraction.

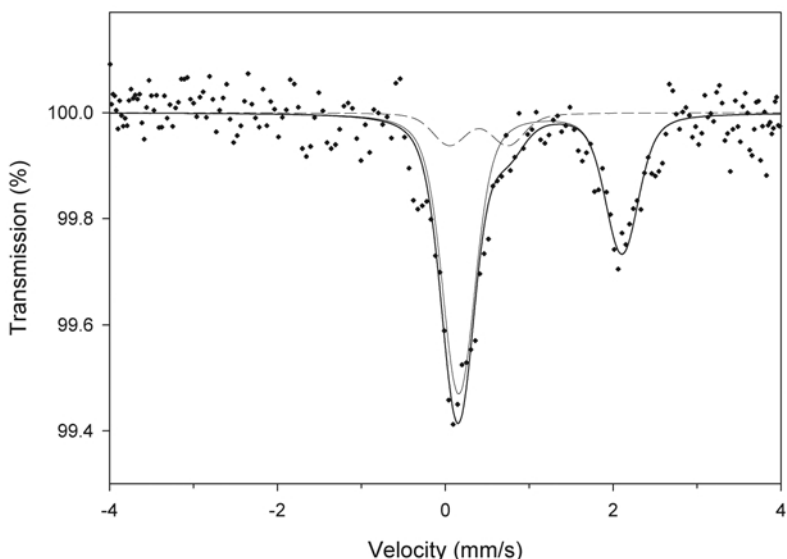


FIG. 4. The Mössbauer spectrum of cámaraita recorded on a single crystal with a point γ -ray source.

TABLE 2. Powder-diffraction pattern for cámaraité.

<i>I</i>	<i>d</i> _{meas.} (Å)	<i>d</i> _{calc.} (Å)	<i>h</i>	<i>k</i>	<i>l</i>
<10	4.23 ¹				
<10	4.00	4.001	2	$\bar{2}$	2
		4.000	2	2	1
30	3.83	3.831	$\bar{2}$	0	4
		3.821	$\bar{2}$	$\bar{2}$	3
		3.820	$\bar{2}$	2	2
10	3.53	3.516	0	0	6
50	3.39	3.402	2	$\bar{2}$	4
		3.400	2	2	3
20	3.26	3.268	0	4	3
		3.267	0	4	1
		3.244	2	0	5
50	3.18	3.187	$\bar{2}$	$\bar{2}$	5
		3.186	$\bar{2}$	2	4
40	2.87	2.878	0	4	3
		2.871	$\bar{2}$	$\bar{4}$	2
		2.871	$\bar{2}$	4	0
90	2.79	2.803	$\bar{2}$	$\bar{4}$	3
		2.802	$\bar{2}$	4	1
		2.791	2	$\bar{2}$	6
		2.790	2	2	5
10	2.68	2.701	$\bar{2}$	$\bar{4}$	4 ²
100	2.63	2.632	4	0	1
10	2.259	2.258	$\bar{2}$	$\bar{4}$	7
		2.257	$\bar{2}$	4	5
20	2.212	2.213	4	0	5
<10	2.161	2.162	4	$\bar{2}$	5
		2.161	4	2	4
50	2.101	2.103	4	$\bar{4}$	2
		2.103	$\bar{4}$	4	0
30	2.012	2.012	4	$\bar{2}$	7
		2.012	4	2	6
70	1.721	1.723	$\bar{2}$	$\bar{4}$	11
		1.722	$\bar{2}$	4	9
		1.718	0	$\bar{8}$	2
50d ³	1.578	1.579	$\bar{6}$	$\bar{4}$	1
		1.579	$\bar{6}$	$\bar{4}$	2
		1.579	6	$\bar{4}$	1
		1.579	$\bar{6}$	4	0
30d	1.440	1.439	4	$\bar{8}$	3
		1.439	4	$\bar{8}$	1
20d	1.331	1.330	$\bar{8}$	0	2

¹ This reflection is due to admixture of bafertisite, of which it is the (210) reflection; other strong lines of bafertisite overlap, e.g., (120), *I* = 100, *d* = 3.25 Å.

² not included in cell-parameter refinement.

³ d = diffuse reflection.

The space group $C\bar{1}$

Cámaraité is triclinic, space group $C\bar{1}$, *Z* = 4. The non-conventional space group $C\bar{1}$ was used rather than the conventional choice of $P\bar{1}$. Cámaraité, Ba₃NaTi₄(Fe²⁺, Mn)₈(Si₂O₇)₄O₄(OH, F)₇, is a Ti-di-orthosilicate mineral with a TS (Titanium Silicate) block. It is closely related to jinshajiangite, ideally Ba₂Na₂Ti₄Fe₈²⁺(Si₂O₇)₄O₄(OH)₄F₂, and bafertisite, ideally Ba₂Ti₂Fe₄²⁺(Si₂O₇)₂O₂(OH)₄. Cámaraité, jinshajiangite (Sokolova *et al.*, 2009) and bafertisite (Guan *et al.*, 1963) have a TS block of the same topology [Fe²⁺-dominant Group-II minerals in the terminology of Sokolova (2006)]. The TS block consists of a central trioctahedral (O) sheet and two adjacent heteropolyhedral (H) sheets of [5]- and [6]-coordinated polyhedra and (Si₂O₇) groups. The TS block is characterized by a planar cell based on translation vectors, **t**₁ and **t**₂, with *t*₁ ~ 5.5 and *t*₂ ~ 7 Å and **t**₁ ^ **t**₂ close to 90°. For cámaraité, we chose the unconventional space group $C\bar{1}$ and corresponding unit-cell parameters *a* = 10.6965 (2 *t*₁) and *b* = 13.7861 (2 *t*₂) for better comparison with the related Group-II structures of bafertisite, jinshajiangite, hejtmanite, perraultite and surkhobite (Table 3) and 22 other minerals with the TS block, detailed structural descriptions of which can be found in Sokolova (2006), Cámarita and Sokolova (2007), Sokolova and Hawthorne (2008) and Sokolova *et al.* (2009). Here, we also report the (Niggli) reduced unit cell: *a* = 8.724(2) Å, *b* = 8.725(1) Å, *c* = 21.478(4) Å, α = 81.20(3)°, β = 84.06(3)°, γ = 75.62(3)°, *V* = 1561.3(6) Å³, space group $P\bar{1}$, *Z* = 2. The $P\bar{1}$ cell can be derived from the $C\bar{1}$ cell *via* the transformation matrix [−½ ½ 0 / ½ ½ 0 / 0 0 −1]. The crystal structure of cámaraité will be discussed in a separate paper with regard to the crystal chemistry of 27 minerals possessing the TS block.

Acknowledgements

We thank Dmitriy Belakovskii, Fersman Mineralogical Museum (RAS, Moscow, Russia), for lending us the sample used for this work. We acknowledge the comments of two anonymous reviewers, Giovanni Ferraris, Associate Editor Sergey Krivovichev and Principal Editor Mark Welch. This work was supported by the Program of Fundamental Research of the Ministry of Education and Science of the Republic of Kazakhstan 2006–2008 (Geology) to AVS, GKB

TABLE 3. Comparison of cámaraité, bafertisite, jinshajiangite, hejtmánite, perraultite and surkhobite.

Mineral	Fe ²⁺ -dominant minerals		Mn ²⁺ -dominant minerals		Surkhobite
	Cámaraité	Bafertisite	Jinshajiangite	Perraultite	
Simplified formula ¹	Ba ₃ NaTi ₄ (Fe ²⁺ ,Mn) ₈ (Si ₂ O ₇) ₄ O ₄ (OH,F) ⁷	Ba ₂ Ti ₂ (Fe ²⁺ ,Mn) ₄ (Si ₂ O ₇) ₂ O ₂ (OH,F) ₄	Ba ₂ Na ₂ Ti ₄ (Fe ²⁺ ,Mn) ₈ (Si ₂ O ₇) ₄ O ₄ (OH,F) ₆	Ba ₂ Na ₂ Ti ₄ (Mn,Fe ²⁺) ₈ (Si ₂ O ₇) ₄ O ₄ (OH,F) ₆	(Ba,K) ₂ CaNaTi ₄ (Mn,Fe ²⁺ ,Fe ³⁺) ₈ (Si ₂ O ₇) ₄ O ₄ (F,OH,O) ₆
Reference ²	This work	(1)	(2)	(4)	(5)
Space group	C $\bar{1}$	Cm	C2/m	P2 ₁ /m	C2
a (Å)	10.6965(7)	10.60	10.6785	5.361	10.723
b (Å)	13.7861(9)	13.64	13.786	6.906	13.826
c (Å)	21.4778(15)	12.47	20.700	12.556	20.791
$\alpha(^{\circ})$	99.345(1)	119.5	94.937	119.8	95.00
$\beta(^{\circ})$	92.315(2)	4	4	1	4
$\gamma(^{\circ})$	89.993(2)	4	4	4	4
Z	4	4	4	4	4
Reference	This work	(6)	(2)	(7)	(8, 9)
D _{calc.} (g cm ⁻³)	4.018	3.8	3.767	4.29	3.98
D _{meas.} (g cm ⁻³)	3.871	3.96–4.25	3.61	4.02	3.84
Strongest lines in the X-ray powder-diffraction pattern, d/n (Å) (I)	2.63 (100)	2.65 (100)	3.44 (100)	2.726 (100)	3.454 (100)
	2.79 (90)	2.11 (40)	3.15 (80)	5.472 (32)	2.592 (70)
	1.721 (70)	1.72 (40)	2.630 (80)	3.241 (21)	2.074 (40)
	3.39 (50)	2.52 (30)	2.570 (80)	3.215 (21)	10.39 (20)
	3.18 (50)	2.23 (30)	10.2 (70)	3.455 (17)	2.084 (15)
	2.101 (50)	2.07 (30)	1.715 (50 broad)	2.180 (16)	2.867 (13)
	1.578 (50)	1.75 (30)	2.202 (40)	2.535 (14)	1.728 (15)
Optical class (sign)	biaxial (+)	biaxial (-)	biaxial (+)	biaxial (-)	biaxial (-)
α (589.3 nm)	>1.80	1.805	1.792	1.814	1.790 (calc. from 2V)
β	—	1.835	1.801	1.846	1.86
γ	—	1.862	1.852	1.867	1.89
2V _{meas.} ($^{\circ}$)	93(1)	86	72	76.4	65(5)
2V _{calc.}	—	—	—	—	—
Reference	This work	(1,10-optics)	(11, 2)	(8)	(5)

¹ except for surkhobite

² each reference applies to the information given above in the column: (1) Anthony *et al.* (1995); (2) Sokolova *et al.* (2009); (3) Vrána *et al.* (1992); (4) Sokolova (2006); (5) Rastsvetaeva *et al.* (2008); (6) Guan *et al.* (1963); (7) Rastsvetaeva *et al.* (1991); (8) Chao (1991); (9) Yamnova *et al.* (1998); (10) Yakovlevskaya and Mineev (1965); (11) Hong and Fu (1982); (12) Pekov *et al.* (1999).

and PEK and a Canada Research Chair in Crystallography and Mineralogy and by Natural Sciences and Engineering Research Council of Canada Discovery, Equipment and Major Installation grants of the Natural Sciences and Engineering Research Council of Canada, and by Innovation grants from the Canada Foundation for Innovation to FCH.

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