

Kasatkinite, $\text{Ba}_2\text{Ca}_8\text{B}_5\text{Si}_8\text{O}_{32}(\text{OH})_3 \cdot 6\text{H}_2\text{O}$, a New Mineral from the Bazhenovskoe Deposit, the Central Urals, Russia¹

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Abstract—A new mineral, kasatkinite, $\text{Ba}_2\text{Ca}_8\text{B}_5\text{Si}_8\text{O}_{32}(\text{OH})_3 \cdot 6\text{H}_2\text{O}$, has been found at the Bazhenovskoe chrysotile asbestos deposit, the Central Urals, Russia in the cavities in rhodinite as a member of two assemblages: (1) on prehnite, with pectolite, calcite, and clinocllore; and (2) on grossular, with diopside and pectolite. Kasatkinite occurs as spherulites or bunches up to 3 mm in size, occasionally combined into crusts. Its individuals are acicular to hair-like, typically split, with a polygonal cross section, up to 0.5 mm (rarely, to 6 mm) in length and to 20 μm in thickness. They consist of numerous misoriented needle-shaped subindividuals up to several dozen μm long and no more than 1 μm thick. Kasatkinite individuals are transparent and colorless; its aggregates are snow white. The luster is vitreous or silky. No cleavage was observed; the fracture is uneven or splintery for aggregates. Individuals are flexible and elastic. The Mohs' hardness is 4–4.5. $D_{\text{meas}} = 2.95(5)$, $D_{\text{calc}} = 2.89 \text{ g/cm}^3$. Kasatkinite is optically biaxial (+), $\alpha = 1.600(5)$, $\beta = 1.603(2)$, $\gamma = 1.626(2)$, $2V_{\text{meas}} = 30(20)^\circ$, $2V_{\text{calc}} = 40^\circ$. The IR spectrum is given. The ¹¹B MAS NMR spectrum shows the presence of BO_4 in the absence of BO_3 groups. The chemical composition of kasatkinite (wt %; electron microprobe, H_2O by gas chromatography) is as follows: 0.23 Na_2O , 0.57 K_2O , 28.94 CaO , 16.79 BaO , 11.57 B_2O_3 , 0.28 Al_2O_3 , 31.63 SiO_2 , 0.05 F , 9.05 H_2O , -0.02 --O=F_2 ; the total is 99.09. The empirical formula (calculated on the basis of $\text{O} + \text{F} = 41$ apfu, taking into account the TGA data) is: $\text{Na}_{0.11}\text{K}_{0.18}\text{Ba}_{1.66}\text{Ca}_{7.84}\text{B}_{5.05}\text{Al}_{0.08}\text{Si}_{8.00}\text{O}_{31.80}(\text{OH})_{3.06}\text{F}_{0.04} \cdot 6.10\text{H}_2\text{O}$. Kasatkinite is monoclinic, space group $P2_1/c$, $P2/c$, or Pc ; the unit-cell dimensions are $a = 5.745(3)$, $b = 7.238(2)$, $c = 20.79(1) \text{ \AA}$, $\beta = 90.82(5)^\circ$, $V = 864(1) \text{ \AA}^3$, $Z = 1$. The strongest reflections ($d \text{ \AA} - [hkl]$) in the X-ray powder diffractions pattern are: $5.89 - 24[012]$, $3.48 - 2.1[006]$, $3.36 - 24[114]$; $3.009 - 100[121, 121, 106]$, $2.925 - 65[106, 122, 122]$, $2.633 - 33[211, 124]$, $2.116 - 29[133, 133, 028]$. Kasatkinite is named in honor of A.V. Kasatkin (b. 1970), a Russian amateur mineralogist and mineral collector who has found this mineral. Type specimen is deposited in the Fersman Mineralogical Museum, Russian Academy of Sciences, Moscow.

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INTRODUCTION

The Bazhenovskoe deposit of chrysotile asbestos hosted in the serpentinized ultramafic rocks in the Central Urals is one of the world's largest deposits of this

type and has been mined over more than 120 years (Zoloev et al., 1985). It is also attractive as a mineralogical object, primarily known by various mineralizations related to the numerous rhodinite bodies. According to Yu. Erokhin, more than 50 mineral species, including some extremely rare, were identified in rhodinites and in products of their low-temperature alteration.

The Bazhenovskoe rhodinites are products of the metasomatic alteration of gabbroic, dioritic and felsic dykes crosscutting serpentinite. Clinopyroxenes (predominantly diopside), ugrandite garnets (predomi-

¹ A new mineral species kasatkinite and its name were recommended by the Commission on New Minerals Russian Mineralogical Society and approved by the Commission on New Minerals, Nomenclature, and Mineral Classification of the International Mineralogical Association on July 14, 2011, IMA No. 2011-045.

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nantly grossular), and Mg-rich chlorite are the major minerals; vesuvianite, clinozoisite, prehnite, serpentine, and amphiboles of the tremolite–actinolite series are usual; pectolite, xonotlite, calcite, zeolites (predominantly calcium and alkali–calcium), and apophyllite-(KOH) are the late minerals filling numerous cavities. Rhodinites of the Bazhenovo deposit have been described in many publications, especially as concerns their mineralogy. The basic publications (*Mineralogy ...*, 1996; Erokhin, 1997; Antonov, 2003; Efimov, 2004) should be noted.

This paper characterizes a new mineral species, kasatkinite, which is a hydrous Ca–Mg borosilicate identified in the hydrothermal assemblage related to rhodinites of the Bazhenovskoe deposit. The mineral was named in honor of Anatoly Vital'evich Kasatkin (born 1970), a Russian amateur mineralogist and collector who has collected, and continues to supplement, one of the largest systematic collections worldwide, including about 4500 mineral species, among which more than 4300 have been reliably determined with analytical techniques. The high degree of comprehension distinguishes it not only among private collections, but also among systematic museum collections. A.V. Kasatkin actively collaborates with professional mineralogists, placing typical and unordinary specimens at their disposal for research, including specimens potentially containing new mineral species. The mineral described in this paper came from the collection of A.V. Kasatkin, who had preliminarily determined it as an unknown Ba–Ca–silicate on the basis of semiquantitative electron microprobe data and kindly placed it at our disposal for further investigation.

The type specimen of kasatkinite was deposited in the Fersman Mineralogical Museum, Russian Academy of Sciences, Moscow, registration number 4129/1.

OCCURRENCE AND GENERAL DESCRIPTION

The specimens with the described mineral were collected in 2005 by E. Novgorodova and A. Loskutov, amateur collectors from the Urals, at the eastern wall of the southern open pit of the Bazhenovskoe deposit, town of Asbest, Sverdlovsk oblast, the Central Urals, Russia.

Kasatkinite was first studied on one promising specimen $2 \times 2 \times 1.5$ cm in size, which is considered a holotype. This specimen is a fragment of a druse cavity in massive prehnite rhodinite. This is a crust of rather well-shaped, weakly split, prismatic crystals of grayish prehnite reaching 0.9 cm in size; the aggregates of kasatkinite cover about half the area of the crust. Pectolite (colorless individuals up to 3 mm in length), calcite (separate colorless fine crystals), and clinocllore (greenish flakes) overgrow prehnite in small amounts.

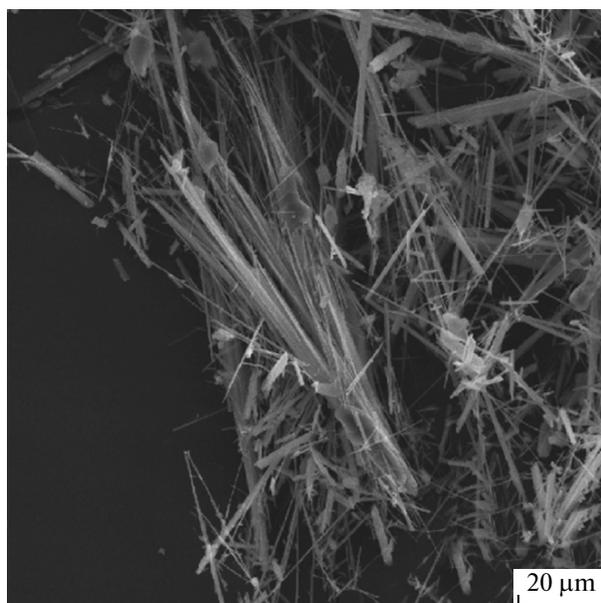


Fig. 1. Individuals and sheaf-like aggregates of kasatkinite. SEM image.

Individuals of kasatkinite are acicular to hair-like, straight or curved, and frequently split. They are polygonal in cross section and slightly flattened (Fig. 1). The crystals are not longer than 0.5 mm, occasionally reaching 6 mm in length with typical thickness up to 5 μm , rarely reaching 20 μm . The individuals of the new mineral are combined into nearly parallel or sheaf-shaped aggregates (Fig. 1); most individuals occur as radial spherulites up to 3 mm in diameter with a dense core and furry surface (Figs. 2a, 2b). These spherulites develop on prehnite separately (Fig. 2a) or are closely intergrown with one another to form crusts of a few cm in area (Fig. 2b). The separate long needles and fibers of the new mineral frequently grow immediately on the surface of the spherulites (Fig. 2a, 2b).

Microscopically, individuals that outwardly resemble single crystals actually consist of numerous misoriented acicular sub-individuals reaching a several dozen μm in length and <1 μm in thickness, which are sporadically curved and intertwined like tightly linked ropes. This feature strongly hampers the single crystal X-ray diffraction study.

Detailed study of other rhodinite specimens with late minerals taken from the same locality showed that kasatkinite also occurs in another mineral assemblage from cavities in diopside–grossular rock. It is associated with fibrous chrysotile, which occurs at the contact of rhodinite with serpentinite, pectolite, and insignificant amounts of tobermorite- and hydrocalcite-type minerals. Kasatkinite forms here two morphological varieties. One of them is similar to that from the holotype specimen; these are acicular to fibrous individuals

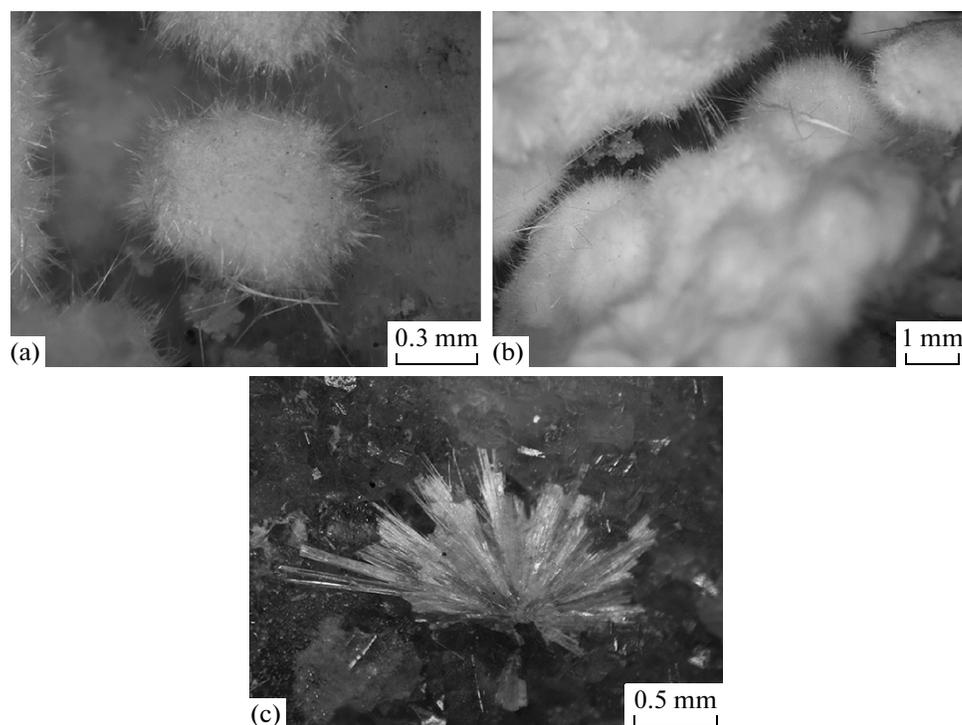


Fig. 2. Morphology of kasatkinite: (a) spherulite on prehnite, (b) spherulitic crust and separate long hair-like individuals on prehnite, (c) rosette-like cluster on grossular. FOV width (mm): (a) 3.3, (b) 8.8, (c) 2.8.

combined into spherulites up to 2 mm in diameter. The second variety is characterized by separate bunches and rosettes consisting of long prisms up to 3×0.1 mm in size (Fig. 2c), which overgrow the druses of light-pink grossular. Microscopically, such prisms are intergrowths of nearly parallel, hair-like individuals, which are easily split by the pressing of a needle. In turn, separate individuals have a microblocky structure similar to that of the holotype specimen of the new mineral.

PHYSICAL PROPERTIES AND OPTICAL DATA

The separate individuals of kasatkinite are transparent and colorless; aggregates of the mineral are snow white, translucent to nearly opaque. The streak is white. The luster in fine-fibrous aggregates is vitreous and silky. The mineral is not fluorescent either in UV light or cathode rays. No cleavage or parting was observed; the fracture is uneven and splintery in aggregates. The individuals of kasatkinite are flexible and elastic (owing to intergrown fine-acicular subindividuals), while dense aggregates are very viscous like nephrite or fibrous wollastonite. The Mohs' hardness is 4–4.5. The density measured by equilibration in heavy liquids (mixed bromoform and iodic methylene) is $2.95(5)$ g/cm³, while the calculated density is 2.89 g/cm³.

Kasatkinite is optically biaxial, positive, $\alpha = 1.600(5)$, $\beta = 1.603(2)$, $\gamma = 1.626(2)$, $2V_{\text{meas}} = 30(20)^\circ$,

$2V_{\text{calc}} = 40^\circ$. No dispersion of optical axes was observed. Microscopically, the mineral is colorless and not pleochroic.

IR SPECTROSCOPY

The infrared absorption spectra of kasatkinite were measured on a Specord 75 IR spectrophotometer. The sample was prepared as KBr pellet. The spectrum of the pure KBr pellet was subtracted during recording. The scale of wavenumbers was calibrated with polystyrene and gaseous ammonia as standards.

The IR spectrum of kasatkinite (Fig. 3) is unique and may be used as a reliable diagnostic tool for the mineral. The wavenumbers of absorption maximums in the IR spectrum (cm⁻¹; s is a strong band, w is a weak band, and sh is a shoulder) and their attribution are as follows: 3345s, 3210, 3160sh (O–H stretching vibrations), 2515w (overtone of B–O stretching mode), 1686, 1630sh (bending vibrations of H₂O molecules), 1293, 1205sh, 1157 (B–O stretching vibrations, presumably of coupled BO₄ tetrahedra), 1050s, 1000sh, 978s, 944s, 910sh, 892s (Si–O stretching vibrations), 820sh, 741w, 723w, 676, 578, 550sh (bending vibrations in SiO₄ and BO₄ tetrahedra and libration vibrations of H₂O molecules), 464s, 430sh, 405sh (combination of Si–O–Si bending and Ca–O stretching vibrations).

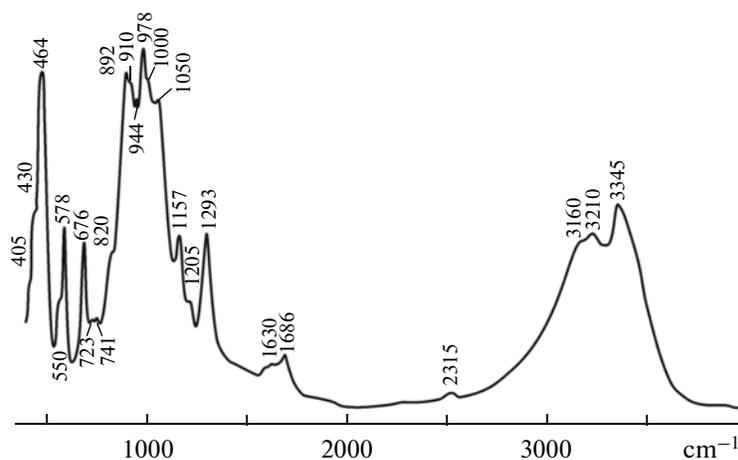


Fig. 3. IR spectrum of kasatkinite.

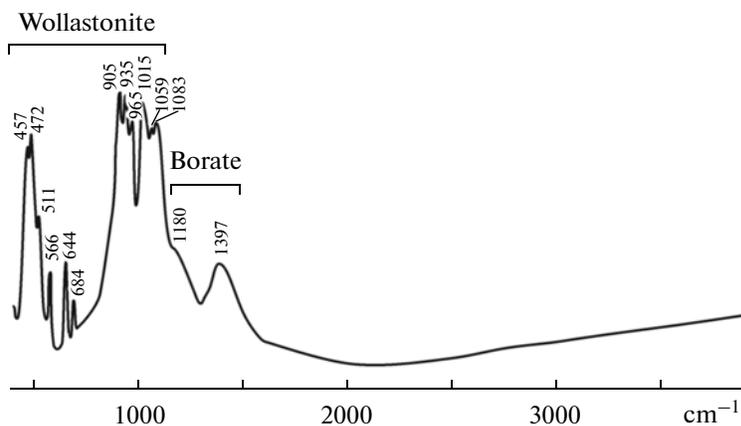


Fig. 4. IR spectrum of products of kasatkinite annealing up to 1100°C.

Bands in the range of 1350 to 1550 cm⁻¹ (to which belong the stretching vibrations of C—O and N—O and bending vibrations of NH₄⁺ groups), as well as typical bands corresponding to the organic groups (hydrocarbon, carboxylate, and carbonyl), are not identified in the IR spectrum of the mineral.

The IR spectrum of the products of kasatkinite annealing up to 1100°C (Fig. 4) corresponds to the mixture of wollastonite and anhydrous vitreous borate (probably, amorphous Ba borate, which gives two broad bands at 1397 and 1180 cm⁻¹).

NMR SPECTROSCOPY

¹¹B MAS NMR (Magic Angle Spinning Nuclear Magnetic Resonance) was used to determine the boron coordination number in kasatkinite. The measurements were performed on a Bruker AVANCE III 850 spectrometer. The spectrometer, operating at a frequency of

272.52 MHz for ¹¹B, has been chosen to reduce the quadrupolar effects arising from the asymmetric coordination of the ¹¹B species, as well as to achieve a high spectral resolution, which is necessary to distinguish signals not only from three- and fourfold coordinated boron species (BO₃/BO₄), but also from nonequivalent states of ¹¹B with similar coordination numbers.

A sample 44 mg in mass was ground and placed into a Kel-F insert assigned for working with minor samples in a standard 4-mm ZrO₂ rotor. Simple single-pulse experiments (128 scans, recycling delay of 10 s, 3988 data points with a spectral width of 100000 Hz, zerofilling to 32768 points without apodization) were performed. To compensate for the residual signal of the sample holder (arising from the boron nitride of the stator), the spectrum of an empty rotor was recorded and subsequently subtracted.

The observed spectrum clearly indicates only the presence of the fourfold coordinated BO₄ species (¹⁴B)

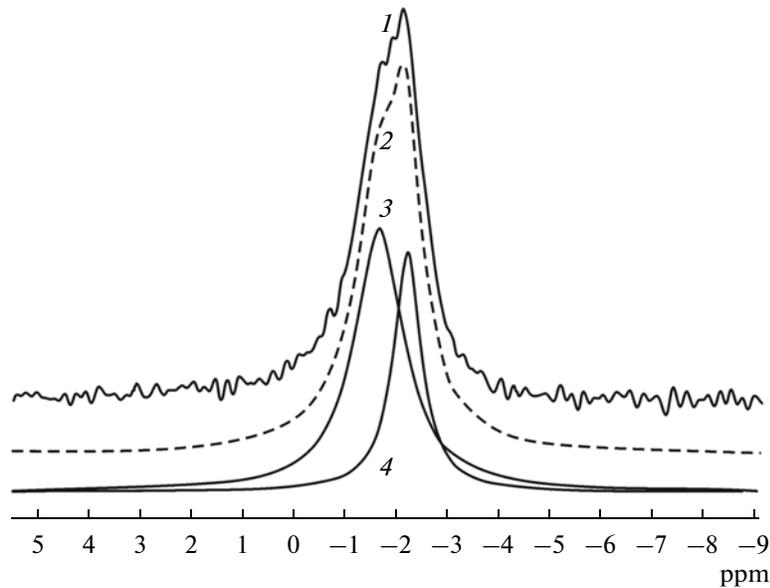


Fig. 5. ^{11}B MAS NMR spectrum of (1) kasatkinite and summary approximating curve (2) with two Gaussian components (3, 4) clearly indicating the occurrence of fourfold coordinated BO_4 species and the absence of threefold coordinated BO_3 species.

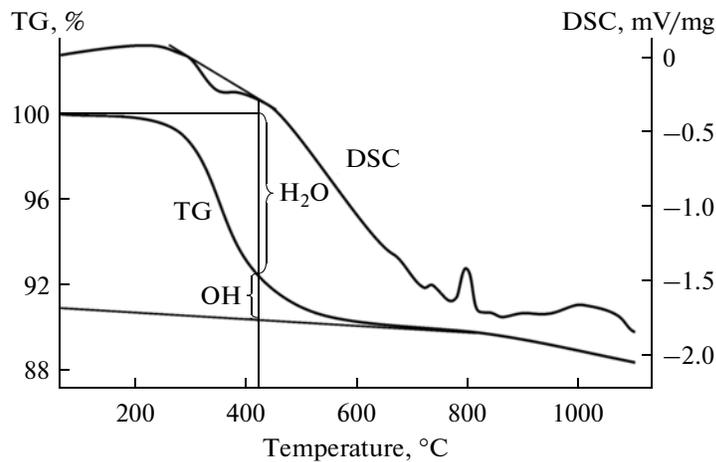


Fig. 6. Thermal (TG and DSC) curves of kasatkinite.

(Fig. 5). Only a broad peak with a chemical shift (0–4 ppm) is observed, corresponding to fourfold coordinated ^{11}B as BO_4 (Fig. 5). However, the asymmetry of the peak indicates at least two different BO_4 species. Deconvolution of the spectrum based on two Gaussian components (Fig. 5) was made using the program Dmfit (Massiot et al. 2002). According to Du and Stebbins (2003a), the two components may be interpreted as $^{41}\text{B}(1\text{B}-\text{O}-\text{B}, 3\text{B}-\text{O}-\text{Si})$ and $^{41}\text{B}(0\text{B}-\text{O}-\text{B}, 4\text{B}-\text{O}-\text{Si})$, respectively. Boron is absent in threefold-coordinated species BO_3 in kasatkinite (a chemical shift for ^{13}B was approximately 15–25 ppm). For more examples of ^{11}B NMR spectra of glasses and minerals with

^{41}B and ^{13}B , see Du and Stebbins (2003b), Du et al. (2004), and Rollion-Bard et al. (2011).

THERMAL DATA

Thermal data for kasatkinite were obtained by means of differential scanning calorimetry (DSC) and thermogravimetry (TG) using a synchronous thermal analyzer STA 409C Luxx produced by the NETZSCH Group. The DSC and TG curves given in Fig. 6 were recorded at a heating rate of 5 K/min in an argon atmosphere.

Total weight loss upon heating to 800°C ($9.1 \pm 0.2\%$) is close to the total H_2O content in the mineral deter-

mined by means of gas chromatography of volatile products of annealing (9.05 wt %).

A distinct endothermic effect with a minimum at 354°C on the DSC curve is accompanied by a weight loss of 7.2–7.5%, which was ascribed to the release of H₂O molecules from kasatkinite. This effect is completed in the temperature range of 420–430°C.

A weight loss of about 1.6–1.9% between 420–430 and 800°C, i.e., after the completion of the above-mentioned endothermic process, is attributed to loss of the rest of the H₂O corresponding to hydroxyl groups. Thus, the ratio H_{OH} : H_{H₂O} in kasatkinite is ~1 : 4. This value was used for the calculation of the OH/H_{H₂O} ratio in its empirical formula.

Exothermal effects at 733 and 795°C are caused by a breakdown of dehydrated mineral into silicate (wollastonite) and borate phases in line with IR spectroscopy data (see above).

CHEMICAL COMPOSITION

The contents of major components, including boron in kasatkinite, were measured on a Camebax SX 100 electron microprobe operating at accelerating voltage 15 kV, beam current 30 nA, and beam diameter 3 μm. The following standards were used: jadeite (Na), orthoclase (K), augite (Ca, Al, Si), BaSO₄ (Ba), BN (B), and MgF₂ (F).

The H₂O content was calculated from the amount of H₂, which was measured by means of gas chromatography of the annealing products of the mineral for CHNS/O using a Vario Micro cube instrument, Elementar GmbH, Germany. The analysis was performed through annealing of the sample at 1150°C in the presence of pure oxygen, followed by the separation of the products in a chromatographic column. The elements were determined from the contents of CO₂, N₂, H₂O, SO₂ in gaseous products; the signal of each oxide was recorded by a heat conductivity detector. The measurement of two mineral samples gave 0.988 and 1.022 wt % H (1.005 wt %, on average).

The chemical composition of kasatkinite (average of 17 point analyses, range of contents in parentheses) is as follows, wt %: 0.23 (0.1–0.4) Na₂O, 0.57 (0.2–0.9) K₂O, 28.94 (27.3–30.8) CaO, 16.79 (15.7–18.3) BaO, 11.57 (9.9–13.8) B₂O₃, 0.28 (0.1–0.6) Al₂O₃, 31.63 (30.1–32.8) SiO₂, 0.05 (0.00–0.25) F, 9.05 H₂O, –0.02 –O = F₂; the total is 99.09. The concentrations of other elements with atomic number above 8 were below the detection limit. The absence of typical bands assigned to the vibrations of C–O, C–H, N–O and N–H in the IR spectrum of kasatkinite indicates that the mineral does not contain carbonate, nitrate, ammonium, or organic groups.

The empirical formula calculated on the basis O + F = 41 apfu is as follows: H_{15.26}Na_{0.11}K_{0.18}Ba_{1.66}Ca_{7.84}B_{5.05}Al_{0.08}Si_{8.00}O_{40.96}F_{0.04}. This normalization procedure was chosen empirically by the lowest integer coefficients of Si and B, which are the major constituents occupying tetrahedral sites B₅(Si,Al)₈. The correctness of this procedure is supported by the calculated density based on this formula (*Z* = 1), which is close to the measured density, and by the extremely low compatibility indices of the composition and properties derived from the Gladstone–Dale equation, which are 0.004 (*superior*) and –0.015 (*superior*) for the measured and calculated density, respectively.

After calculation of the OH/H₂O value on the basis of thermal analysis (see above), the empirical formula looks as Na_{0.11}K_{0.18}Ba_{1.66}Ca_{7.84}B_{5.05}Al_{0.08}Si_{8.00}O_{31.08}[(OH)_{3.06}F_{0.04} · 6.10H₂O]. The simplified formula is Ba₂Ca₈B₅Si₈O₃₂(OH)₃ · 6H₂O with corresponding contents of the following components, wt %: 29.04 CaO, 19.84 BaO, 11.26 B₂O₃, 31.11 SiO₂, 8.75 H₂O; the total is 100.00.

A significant content of boron in kasatkinite is clearly supported by a qualitative color reaction: the solution of quinalizarin in sulfuric acid becomes blue around the mineral grains in less than one minute.

X-RAY AND SYNCHROTRON DIFFRACTION

We failed to obtain single-crystal diffraction data using conventional X-ray radiation because of the low quality of the kasatkinite crystals. A tiny single crystal was studied using synchrotron radiation at the Swiss-Norwegian Beam Lines (SNBL) at the European Synchrotron Radiation Facility (ESRF), Grenoble, France. Diffraction data were collected for a crystal of kasatkinite at room temperature using the MAR345 image plate detector, at wavelength 0.83212 Å. The mineral is monoclinic; the unit-cell dimensions are: *a* = 5.74(2), *b* = 7.234(8), *c* = 20.81 (2) Å, β = 90.70(12)°, *V* = 864(2) Å³. Unfortunately, the low quality of the best single crystal of all tested crystals has prevented the collection a set of reflections applicable to study crystal structure of kasatkinite.

The X-ray powder diffraction pattern of the new mineral (table) was recorded with a Stoe STADI MP diffractometer with CCD detector, monochromatic Cu_{Kα1} radiation. All reflections of the X-ray powder diffraction pattern are well indexed in the monoclinic unit cell obtained with the single-crystal method. Its dimensions refined from the X-ray powder diffraction pattern are: *a* = 5.745(3), *b* = 7.238(2), *c* = 20.79(1) Å, β = 90.82(5)°, *V* = 864(1) Å³, *Z* = 1.

The extinction of reflections in the X-ray powder diffraction pattern (in particular, in the most informative small angle area with *d* > 3 Å) indicates that the

X-ray powder diffraction data for kasatkinite

| I_{meas} | $d_{\text{meas}}, \text{\AA}$ | $d_{\text{calc}}, \text{\AA}$ | hkl |
|-------------------|-------------------------------|--|---|
| 14 | 10.52 | 10.394 | 002 |
| 24 | 5.89 | 5.940 | 012 |
| 19 | 5.68 | 5.744 | 100 |
| 20 | 4.97 | 5.005, 4.998 | 013, 102 |
| 7 | 4.58 | 4.500 | 110 |
| 3 | 4.39 | 4.408, 4.388 | 11 $\bar{1}$, 111 |
| 2 | 4.15 | 4.146 | 11 $\bar{2}$ |
| 8 | 3.83 | 3.827 | 104 |
| 23 | 3.48 | 3.465 | 006 |
| 24 | 3.36 | 3.383 | 114 |
| 2 | 3.18 | 3.208 | 023 |
| 100 | 3.009 | 3.033, 3.026, 2.986 | 12 $\bar{1}$, 121, 10 $\bar{6}$ |
| 65 | 2.925 | 2.948, 2.943, 2.931 | 106, 12 $\bar{2}$, 122 |
| 16 | 2.792 | 2.809, 2.793, 2.779 | 12 $\bar{3}$, 123, 20 $\bar{2}$ |
| 9 | 2.719 | 2.730, 2.730 | 116, 025 |
| 33 | 2.633 | 2.643, 2.629 | 211, 124 |
| 13 | 2.480 | 2.499, 2.491, 2.480, 2.475, 2.466 | 204, 11 $\bar{7}$, 213, 12 $\bar{5}$, 117 |
| 4 | 2.349 | 2.355, 2.350 | 108, 032 |
| 6 | 2.295 | 2.296, 2.286 | 027, 126 |
| 14 | 2.183 | 2, 188, 2.178 | 034, 13 $\bar{2}$ |
| 29 | 2.116 | 2.121, 2.115, 2.111 | 13 $\bar{3}$, 133, 028 |
| 12 | 2.090 | 2.101, 2.087, 2.079 | 216, 035, 0.0.10 |
| 6 | 2.040 | 2.046, 2.041 | 119, 134 |
| 20 | 1.963 | 1.966, 1.964, 1.957 | 135, 1.0.10 $\bar{0}$, 135 |
| 5 | 1.871 | 1.875, 1.873, 1.867 | 21 $\bar{8}$, 037, 136 |
| 4 | 1.849 | 1.851, 1.851, 1.850, 1.847, 1.846 | 310, 12 $\bar{9}$, 218, 230, 31 $\bar{1}$ |
| 10 | 1.805 | 1.809, 1.805, 1.803, 1.803, 1.803 | 040, 30 $\bar{4}$, 20 $\bar{7}$, 041, 0.2.10 |
| 19 | 1.782 | 1.785, 1.784, 1.783, 1.782, 1.781 | 13 $\bar{7}$, 227, 042, 313, 233 |
| 2 | 1.693 | 1.696, 1.695, 1.694, 1.693, 1.692 | 2.0.10 $\bar{0}$, 13 $\bar{8}$, 23 $\bar{5}$, 320, 228 |
| 15 | 1.662 | 1.665, 1.659 | 1.0.12 $\bar{0}$, 045 |
| 4 | 1.596 | 1.598, 1.596, 1.592 | 139, 14 $\bar{5}$, 145 |
| 3 | 1.543 | 1.547, 1.545, 1.542 | 14 $\bar{6}$, 047, 146 |
| 10 | 1.491 | 1.495, 1.495, 1.493, 1.492, 1.489, 1.488, 1.487 | 14 $\bar{7}$, 331, 2.0.12 $\bar{0}$, 243, 147, 0.3.11, 33 $\bar{2}$ |
| 2 | 1.428 | 1.433, 1.433, 1.427, 1.425, 1.424 | 245, 1.0.14, 32 $\bar{8}$, 40 $\bar{2}$, 049 |
| 5 | 1.402 | 1.405, 1.404, 1.404, 1.404, 1.401, 1.400, 1.399 | 1.1.14, 24 $\bar{6}$, 411, 150, 15 $\bar{1}$, 151, 41 $\bar{2}$ |
| 3 | 1.369 | 1.371, 1.370, 1.367 | 336, 1.3.12 $\bar{0}$, 055 |
| 5 | 1.302 | 1.304, 1.303, 1.303, 1.302, 1.301, 1.299, 1.299, 1.299 | 3.2.10, 342, 15 $\bar{6}$, 1.3.13 $\bar{0}$, 057, 156, 0.0.16, 416 |

mineral belongs to one of three space groups $P2_1/c$, $P2/c$, or Pc ; in series $h0l$ and $00l$, only reflections with even l occur. Space group $P2_1/c$ is the most probable, because only reflections with even k are detected in series $0k0$.

DISCUSSION

Data on the natural or synthetic compounds close to kasatkinite with respect to the chemical composition, unit-cell dimensions, X-ray powder diffraction pattern, and IR spectrum were not found in the literature or available databases. In addition to kasatkinite, hyalotekite, (Ba,Pb,K)₄(Ca,Y)₂Si₈(B,Be)₂(Si,B)₂O₂₈F (Christy et al., 1998), is the only mineral that contains Si, B, Ca, and Ba as species-forming components. However, this mineral is anhydrous and markedly differs from kasatkinite in all aforementioned parameters.

The MAS NMR study undoubtedly showed that boron forms only tetrahedral anion groups BO₄⁵⁻ in kasatkinite. Two types of BO₄ positions are assumed: with only B–O–Si oxygen bridges and with both B–O–Si and B–O–B oxygen bridges. Thus, BO₄⁵⁻ and SiO₄⁴⁻ -units probably form a mixed tetrahedral borosilicate motif in kasatkinite. Based on the (Si + B) : O ratio and the IR spectrum, we can conclude that a “normal” BSiO framework (like in danburite, datolite, etc.) is hardly probable. This motif could be an interrupted framework or, more probably, a combined tetrahedral borosilicate chains or layers (layered packets).

Kasatkinite, the first new mineral species discovered at the Bazhenovskoe deposit, is megascopically indistinguishable from fibrous pectolite, tobermorite, and other Ca-silicates, which are abundant here. By this reason, it was missed using visual diagnostics. The collectors who collected the specimens described above took it for pectolite. Somewhat more than 20 specimens have been retained to date; the new mineral has been identified only in five specimens, including the holotype; in other specimens, white fluffy spherulites were pectolite or tobermorite. Nevertheless, judging by the rich clusters of kasatkinite in the studied specimens, some rhodinite bodies were enriched in this mineral.

The appearance at the Bazhenovskoe deposit of a mineral of that composition, even in a substantial amount, is normal. The general boron specialization is typical of this deposit. For example, borate mineralization represented by szaibelyite (Sokolov and Luzin, 1981) is locally abundant in serpentinite; magnesian tourmaline is found in talc–carbonate altered rocks and quartz veins; datolite was occasionally identified in serpentinite and rhodinite as druses of large crystals. Boron mineralization is a product of fluid action of the

adjacent granitic intrusions (Erokhin and Shagalov, 1998).

Barium minerals are few in number and mass. Recently, Erokhin (personal communication) has found cymrite and barite in rhodinite and plagiogranite, respectively. Popov (1995), having published data on the crystal morphology of harmotome from the cavities in the Bazhenovskoe rhodinite, does not adduce any diagnostic data to support that it actually was harmotome rather than abundant phillipsite-K (Antonov, 2003). In 2011, Kasatkin (personal communication) reliably established harmotome in the specimens from the Proletarsky open pit, where it occurs in the cavities of rhodinite as colorless twins up to 4 mm in size with a morphology typical of the phillipsite–harmotome zeolite series. The chemical composition of the mineral (electron microprobe data) corresponds to the following formula calculated on the basis of Si + Al = 16: (Ba_{3.26}Na_{0.96}K_{0.51}Ca_{0.32})_{Σ5.05}(Al_{5.17}Si_{10.83}O_{31.94}) · nH₂O.

Local areas could have been enriched in barium as a result of its release from feldspar (especially potassic) during rhodinitization of intermediate and felsic dikes; both tourmaline of granitic rocks and szaibelyite of serpentinite at the Bazhenovskoe deposit also could be sources of boron for kasatkinite.

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