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Sphaerobertrandite, $Be_3SiO_4(OH)_2$: new data, crystal structure and genesis

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Abstract: The insufficiently studied beryllium silicate sphaerobertrandite has been known since 1957. The present work presents new findings, verifies that the mineral is a valid species with a unique structure. The original name sphaerobertrandite has been kept in spite of its unjustifiable connection to bertrandite. The mineral is named after the typical spherulitic morphology of its aggregates, and its similarity to bertrandite in the main chemical constituents. Sphaerobertrandite was recently found in alkaline pegmatites at Sengischorr Mountain, Lovozero massif, Kola peninsula, Russia, inside epididymite segregations, coexisting with eudidymite, aegirine, mangan-neptunite, *etc*., and in Tuften quarry, Tvedalen, South Norway, coexisting with hambergite, analcime, chiavennite, *etc*. The mineral forms spherulites up to 2 mm, as well as fibrous crusts. Sphaerobertrandite from Sengischorr Mountain occurs as thin tabular, prismatic crystals up to 0.5 x 0.2 x 0.05 mm in aggregates overgrowing epididymite. The main crystal form is {001}, small faces {012}, {102} and {10-2} are present. Transparent to translucent; colourless, white, yellow, brownish, greyish, beige. Streak white. Lustre vitreous. Mohs' hardness 5. Brittle. Cleavage perfect on (001). D (meas.) is 2.46 – 2.54, D (calc.) is 2.52 g/cm^3. Biaxial, negative, $\alpha = 1.597(3)$, $\beta = 1.607(4)$, $\gamma = 1.616(3)$, 2V (meas) is 70(±20)° Orientation: Z = *c*. IR spectrum is unique; frequencies of absorption bands are (cm^{-1}; sh – shoulder, w – weak; the most intensive bands are underlined): 3605, 3540, 3505, 3370sh, 3250sh, 3060w, 1620sh, 1400sh, 1150, 1115, 1090sh, 995sh, $\underline{933}$, $\underline{900}$, $\underline{835}$, $\underline{768}$, $\underline{721}$, 680sh, 639, 612, 573w, 555w, 491, 424, 410sh. Chemical composition of the sample from Sengischorr Mountain is: BeO 45.88, SiO_2 38.46, H_2O+ 12.54, total 96.88 wt. %, corresponding to $Be_{2.97}Si_{1.03}O_{4.06}(OH)_{1.94} \bullet 0.155H_2O$. Monoclinic, $P2_1/c$, with $a = 5.081(3)$, $b = 4.639(1)$, $c = 17.664(9)$ Å, $\beta = 106.09(5)°$, V = 400.0 Å^3, with a strongly pseudo-orthorhombic cell, which is the likely reason for the samples being invariably twinned by pseudo-merohedry. The strongest lines in the X-ray powder pattern are (d in Å -I[hkl]): 4.885-90[100]; 4.236-62[004]; 3.161-100[111, 11-3]; 2.836-70[104]; 2.538-55[20-2]; 2.318-90[020]; 2.174-55[10-8]. The crystal structure has been refined to R = 0.090. Better refinement could not be achieved because of twinning by pseudo-merohedry with low obliquity, which produces partial overlapping of reflections. The structure consists of mixed framework formed by Be- and Si-tetrahedra which comprises 6- and 4-membered rings. All vertices of SiO_4 tetrahedra are shared with 2 BeO_4 tetrahedra. The OH anions are shared only between two Be tetrahedra. The structure contains $Be(3)O_3$ chains screwed around 2_1 axis and reinforced by SiO_4 tetrahedra. These (Be,Si,O) chains are linked by the dimers $Be(2)_2O_6$ and by $Be(1)O_4$ tetrahedra.

Key-words: sphaerobertrandite, beryllium silicate, crystal structure, alkaline rocks, Lovozero, Kola peninsula, Tvedalen, Norway.

Introduction

Until recently, only two hydrous beryllium silicates were considered as valid mineral species: bertrandite, $Be_4Si_2O_7(OH)_2$, and beryllite, an insufficiently studied mineral with alleged formula $Be_3SiO_4(OH)_2 \bullet H_2O$. For almost half a century, another natural hydrous beryllium silicate has been known. This mineral was described by Semenov (1957) and named sphaerobertrandite. Its status has been somewhat dubious because the mineral was poorly studied. Fleischer (1958) did not accept the mineral as a valid species due to the apparent similarity in the original data between sphaerobertrandite and bertrandite. Guillemin & Permingeat (1959) stated that the individuality of sphaerobertrandite

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had not been demonstrated, while Beus (1966) suggested that the mineral was most probably akin to bertrandite. Sphaerobertrandite (some authors used the spelling spherobertrandite) was mentioned as a variety of bertrandite by Clark (1993), Gaines *et al.* (1997), de Fourestier (1999) and, before this study, Pekov (2000).

In the year 2000, Russian (IVP and NVC) and Norwegian (AOL) authors independently initiated studies of sphaerobertrandite, based on new occurrences of the mineral from Sengischorr Mountain, Lovozero massif, Kola peninsula, Russia, and Tuften quarry, Tvedalen, Larvik, Norway, respectively. It was decided, however, to make a cooperative study. The holotype specimen of Semenov's sphaerobertrandite from Mannepakhk Mountain, Lovozero massif (deposited at Fersman Mineralogical Museum of Russian Academy of Sciences, Moscow, catalogue no. 61069), was revised too. All obtained data undoubtedly show that sphaerobertrandite is an individual mineral species, and represents a previously unknown structural type. The proposal for the confirmation of its status as a mineral species was submitted to the Commission on New Minerals and Mineral Names of the IMA. Based on the new data, the Commission on the 3rd of December 2001 decided that it must be considered as a valid species with the status of G ("grandfather") mineral, and recommended the use of name sphaerobertrandite as the correct spelling. We suggest that the new material from Sengischorr Mountain, Lovozero, and Tuften quarry, Tvedalen, is a neotype specimens.

History of research

Sphaerobertrandite was first described by Semenov (1957) who found the mineral in some pegmatites in Lovozero and Khibiny alkaline massifs, both on the Kola peninsula. It is interesting to quote some short fragments of the original paper by Semenov (1957) from where sphaerobertrandite was described as a new mineral:

> *...Sphaerobertrandite is a mineral close to bertrandite, distinguished from it by X-ray powder diagram and chemical composition. ...Sphaerobertrandite is so-called because of its characteristic spherulitic morphology. ...Sphaerobertrandite has been found in pegmatites at Mountains Mannepakhk, Kuftnyun, Sengischorr (Lovozero) and Yukspor (Khibiny). In all these pegmatites, sphaerobertrandite occurs as spherulites in cavities of epididymite druses...*

Semenov (1957) gave the complete chemical composition of sphaerobertrandite from Mannepakhk Mountain. X-ray powder data, optical data, TGA data, density (2.5 g/cm^3), and Mohs' hardness (5) were reported. From the chemical data, the formula $Be_5Si_2O_7(OH)_4$ was proposed for sphaerobertrandite, and it was supposed that Be/Si ratio can vary in bertrandite-like minerals. The absence of single-crystal X-ray data and/or structural analogies with known phases did not allow the determination of the symmetry or the unit cell dimensions of sphaerobertrandite. Not even approximate values were proposed. Fleischer (1958) concluded that the mineral could not be accepted as a valid species without further study. These events took place before the foundation of the Commission on New Minerals and Mineral Names of the IMA in 1959. Sphaerobertrandite was therefore not included in the system of valid mineral species. On the other hand, the mineral has never been formally discredited.

Bukin (1967, 1969) published data on hydrothermal synthesis of sphaerobertrandite in different hydrothermal systems together with bertrandite, epididymite, phenakite, etc. Semenov (1969) briefly described sphaerobertrandite from a pegmatite at the Ilimaussaq alkaline complex, South Greenland. Semenov (1972) described one more occurrence of sphaerobertrandite at Lovozero, at Lepkhe-Nelm ("Nepkha") Mountain, and gave new chemical analysis of sphaerobertrandite from Kuftnyun Mountain, Lovozero. Sphaerobertrandite has been discovered in the hydrothermal-metasomatic beryllium deposit Hsianghualing, China (Huang *et al.*, 1988).

Occurrences

Lovozero massif, Kola peninsula, Russia. At Mannepakhk Mountain, sphaerobertrandite was found in a large, schlieren-like pegmatite occurring in eudialyte lujavrite near the margin of poikilitic nepheline-sodalite syenites. The pegmatite consists of microcline, eudialyte, nepheline, sodalite, lorenzenite, lamprophyllite, murmanite and arfvedsonite. Later assemblage includes green aegirine, analcime, natrolite, albite, mangan-neptunite, fluorite, thorite, altered serandite and epididymite. Sphaerobertrandite and beryllite occur in cavities in aggregates of the latter minerals. Sphaerobertrandite has been found together with epididymite in pseudomorphs after chkalovite in pegmatite at Lepkhe-Nelm Mountain (Semenov, 1957, 1972).

In 2000 – 2001, two of the authors (VGG and IVP) collected sphaerobertrandite from several pegmatites related to naujaite and tawite at upper Tavaiok river, Sengischorr Mountain. These lenticular pegmatites, up to 20 – 30 m long and up to 1 m thick, consist mainly of microcline, nepheline, sodalite, arfvedsonite, aegirine and eudialyte, whereas murmanite, lamprophyllite, lorenzenite and sphalerite occur in smaller amounts. Sporadically, almost monomineral roundish segregations of fibrous, green aegirine, fine-scale, pale-brown polylithionite (up to 40 cm across), and coarsely crystalline, tabular, colourless epididymite (up to 30 cm and 13 kg!) are observed. Late-stage minerals like natrolite, analcime, albite, aegirine, mangan-neptunite, fluorapatite, kuzmenkoite-Mn, organovaite-Mn, vinogradovite, thorite, chabazite-Ca, monazite-(Ce) and rhabdophane-(Ce) occur in cavities of these pegmatites. Sphaerobertrandite together with eudidymite was only found in epididymite aggregates. It forms spherulites among epididymite crystals and also in small cavities. Sphaerobertrandite has been observed overgrowing epididymite and vice versa, as well as cases of simultaneous crystallisation of both minerals.

Khibiny massif, Kola peninsula, Russia. Sphaerobertrandite was mentioned in a single large specimen consisting of monomineral epididymite found in eluvium at Yukspor Mountain (Semenov, 1957).

Ilimaussaq complex, South Greenland. Sphaerobertrandite has been found as small spherulites together with

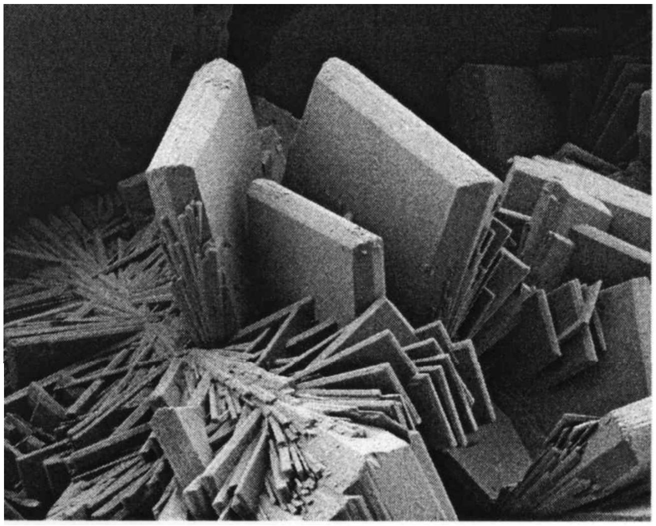

Fig. 1. Sphaerobertrandite crystals from Sengischorr Mountain, Lovozero massif. SEM photo.

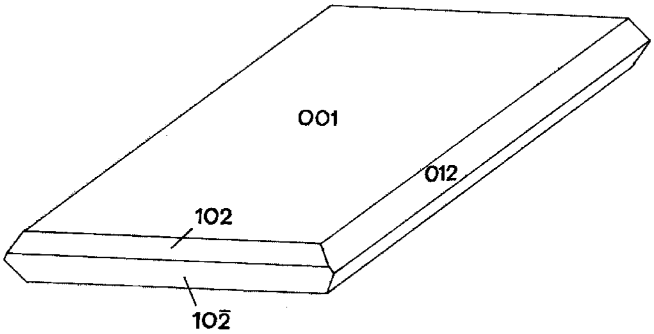

Fig. 2. Drawing of an idealized crystal of sphaerobertrandite from Sengischorr Mountain, Lovozero.

epididymite inside pseudomorphs after chkalovite in pegmatites at Qeqertaussaq, northern coast of Kangerluarsuk fjord (Semenov, 1969).

Tvedalen, Larvik, South Norway. In 1990, two private collectors, S.A. Berge and F. Andersen, found an unknown mineral in one of many pegmatite dikes in the western Tuften larvikite quarry, Tvedalen. The mineral was subsequently identified as an OH-bearing Be-silicate by one of the authors (AOL), and provisionally named *unknown species UK-10* by Andersen *et al.* (1996). Further study showed that it was identical to sphaerobertrandite. The mineral occurs as a white, greyish to beige, finely fibrous crust, partly developed as spherulites up to 0.5 mm across, on the surface of large hambergite crystals where these crystals protruded into open vugs in coarsely crystalline analcime. Calcite, chiavennite and montmorillonite also occur in the vugs, and these minerals were crystallized later than sphaerobertrandite. Tiny amounts of sphaerobertrandite were also observed on small hambergite crystals at Mørje II larvikite quarry, 2 km NNW of Tuften quarry.

Hsianghualing, Hunan Province, China. Sphaerobertrandite was reported among the products of hydrothermal alteration of greisen-like metasomatite developed after high-magnesia rocks. In a vein consisting mainly of hsianghualite, sphaerobertrandite replaces bromellite as white coatings and also occurs in interstices (Huang *et al.*, 1988). This is the only find of sphaerobertrandite not related to alkaline rocks.

Morphology, physical and optical properties

In Lovozero, Khibiny and Ilimaussaq massifs, sphaerobertrandite occurs mainly as compact spherulites and aggregates. In Tvedalen, the mineral also forms finely crystalline crusts and spherulites, which consist of densely packed, thin prismatic to lamellar individuals. The diameter of the spherulites are usually not larger than 0.5 mm across. At Mannepakhk and Sengischorr Mountains (Lovozero), spherulites up to 2 mm across, spherulite clusters up to 7 mm and garlands to 10 mm long are observed. At Sengischorr Mountain, we also found disc-shaped spherulites. Flattened, prismatic crystals up to 0.5 x 0.2 x 0.05 mm in aggregates overgrowing epididymite are rarely observed (Fig. 1). Indices were found by measuring interfacial angles from oriented crystals on SEM photomicrographs. The main crystal form of sphaerobertrandite from Sengischorr Mountain is a pinacoid {001}. A prism {012} is small, and the crystals are terminated by the pinacoids {102} and {10-2} (Fig. 2).

Sphaerobertrandite is transparent to translucent. Usually, the mineral is colourless, yellow, brownish (Lovozero, Khibiny, Ilimaussaq), sometimes white, greyish, beige (Tvedalen). The typical feature is concentric zonation of spherulites with interchange of differently coloured zones: colourless and yellowish (Lovozero) or white and pale brown (Tvedalen). Streak white. Lustre vitreous. Sphaerobertrandite is non-fluorescent in ultraviolet light. Mohs' hardness is 5. Brittle. Perfect cleavage on (001). A cleavage plane parallel [001] with angle ~45° to (010) has been observed under the microscope. Fracture uneven. The density of sphaerobertrandite from Sengischorr Mountain, measured using heavy liquids, is 2.46(2) g/cm^3, calculated density from structural data is 2.52 g/cm^3. Measured density of the mineral from Tvedalen is 2.54(1) g/cm^3. The compatibility index, using the measured density 2.46 g/cm^3, is 0.027, which is in the "excellent" category of Mandarino (1981).

Sphaerobertrandite is optically biaxial, negative. Our data for the mineral from Sengischorr Mountain are (wavelength 589 nm): $\alpha = 1.597(3)$, $\beta = 1.607(4)$, $\gamma = 1.616(3)$, $2V_{meas} = -70(\pm 20)°$, $2V_{calc} = -86.5°$ (for the mineral from Tvedalen: $2V_{meas} = -40$ to $-50°$). The extinction angle was ~10° to the direction of elongation of the crystal. Dispersion of the optical axes was not observed. Optical orientation: Z = *c*. Usually colourless, non-pleochroic. Semenov (1957) gave the following optical data: $\alpha = 1.595$, $\gamma = 1.612$, $2V_{meas} = -70°$, and mentioned weak pleochroism for yellow sphaerobertrandite: from yellowish (X) to colourless (Z), absorption scheme: X > Z.

IR spectroscopy

The IR spectra of all studied samples of sphaerobertrandite, including the holotype, are practically identical. The IR spectrum of this mineral is unique and can be considered as a diagnostic tool. It differs clearly from spectra of bertrandite and beryllite (Fig. 3). Sphaerobertrandite from Sengischorr Mountain was mixed with anhydrous KBr, pelletized, and analysed in a Specord 75 IR spectrometer, while sphaerobertrandite from Tvedalen was analysed by a Perkin Elmer S-2000 FTIR spectrometer. Frequencies of absorption bands in the IR spectrum are (cm^{-1}; sh – shoulder, w – weak; the most intensive bands are underlined): 3605, 3540, 3505, 3370sh, 3250sh, 3060w, 1620sh, 1400sh, 1150, 1115, 1090sh, 995sh, 933, 900, 835, 768, 721, 680sh, 639, 612, 573w, 555w, 491, 424, 410sh. Bands in the area 850 – 600 cm^{-1} correspond to stretching vibrations of BeO-tetrahedra. Bands in the area 3620 – 3500 cm^{-1} (in the spectrum of sphaerobertrandite from Tvedalen, their frequencies are: 3613, 3548, 3506 cm^{-1}) correspond to (OH) groups vibrations. Splitting of the bands indicate that (OH) groups occupy different sites in the structure. Low intensity bands at 3370 and 1620 cm^{-1} in the spectra of sphaerobertrandite both from Lovozero and Tvedalen probably correspond to vibrations of molecular water. The presence of bands corresponding to molecular water confirms the excess of water (in comparison with the theoretical value) in sphaerobertrandite as shown by the thermogravimetric analysis. The relative intensity of these bands correlates with the redundancy (see Table 1).

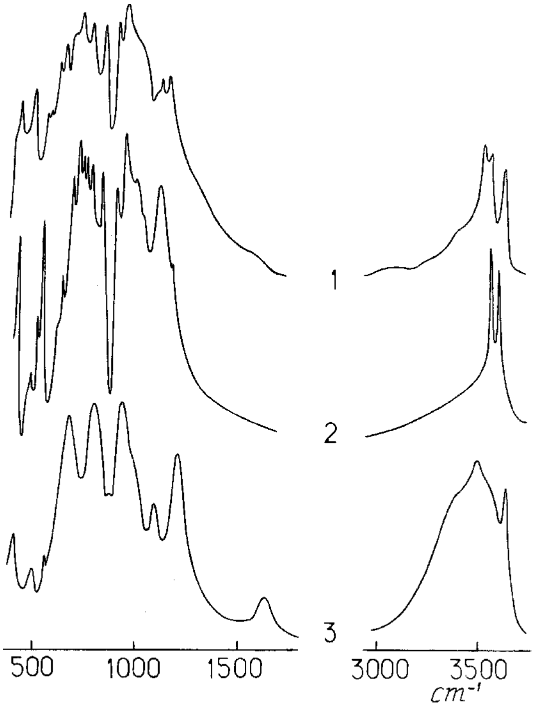

Fig. 3. IR spectra of sphaerobertrandite from Sengischorr Mountain, Lovozero (1), bertrandite from Karaoba, Central Kazakhstan (2), and beryllite from Karnasurt Mountain, Lovozero (3).

Table 1. Chemical composition of sphaerobertrandite, wt.%.

Sample	# 1	# 2	# 3	# 4	# 5
BeO	45.20	44.58	45.88	42.8	49.00
Al_2O_3	1.40	0.93	bdl	bdl	-
Fe_2O_3	0.07	0.02	bdl	1.0	-
SiO_2	41.03	39.78	38.46	43.3	39.23
H_2O+	11.70	14.02	12.54	14.7	11.77
Others	0.30*	0.95*	bdl	0.3*	-
Total	99.70	100.28	96.88	102.1	100.00

1 – Mannepakhk Mountain, Lovozero (Semenov, 1957),
* H_2O- 0.30;
# 2 – Kuftnyun Mountain, Lovozero (Semenov, 1972),
* Na_2O 0.57, CaO 0.10, MgO 0.28;
# 3 – Sengischorr Mountain, Lovozero;
# 4 – Tuften quarry, Tvedalen, * MnO 0.3;
# 5 – ideal formula requires for $Be_3SiO_4(OH)_2$;
bdl – below detection limit.

Chemical composition and thermal data

So far, two chemical analyses of sphaerobertrandite have been published: from Mannepakhk Mountain (Semenov, 1957) and Kuftnyun Mountain (Semenov, 1972), both from the Lovozero massif.

We determined the chemical composition of samples from Sengischorr Mountain, Lovozero, and from Tvedalen. For the former sample, Be was determined by wet chemical method (phosphate precipitation) from 9.302 mg, while Si was measured by a Camebax electron microprobe, using PAP calculation with corrections for the presence of Be and H_2O. For the sample from Tvedalen (1.275 mg), the elements were analysed by using atomic absorption spectrometry after microwave assisted decomposition with HF and H_2SO_4 in a closed vessel. The results are shown in Table 1.

In the first analyses of sphaerobertrandite (Semenov, 1957, 1972), subordinate amounts of Al, Fe, Mg, Na, Ca were reported. In the sample from Sengischorr Mountain, the contents of these and all other elements with atomic number higher than oxygen (except Si) are below the detection limits of the electron microprobe method (<0.05–0.1 wt.%). In sphaerobertrandite from Tvedalen, minor amounts of Fe and Mn were detected, and the brownish colour of this mineral is probably a consequence of this peculiarity.

A thermogravimetric study showed that weight loss for sphaerobertrandite from Sengischorr Mountain, (12.54 wt.%, from 22.504 mg) took place in a single step in the temperature interval 550–800°C gradually, without additional effects. The thermogravimetric curve for sphaerobertrandite from Tvedalen (1.1060 mg) showed a weight loss of 3.2 % between room temperature and 110°C due to absorbed water. There was a gradual loss of water between 110°C and about 500°C. Above 500°C the loss of water was more rapid until constant weight was reached at about 800°C. The total loss of weight between 110°C and 1000°C was 14.7 wt.%. The progress of dehydroxylation of sphaerobertrandite indicates that the water is present mainly in the

Table 2. X-ray powder diffraction data for sphaerobertrandite.

# 1		# 2		# 3		# 4		# 5		*hkl*
I_{meas}	d_{meas}	I_{meas}	d_{meas}	I_{meas}	d_{meas}	I_{meas}	d_{meas}	I_{calc}	d_{calc}	
				12	8.46	5	8.472	2	8.486	002
9	4.89	6	4.86	90	4.885	52	4.873	90	4.882	100
4	4.61	4	4.42	40	4.471	19	4.464	42	4.475	011
4	4.20	4	4.20	62	4.236	100	4.239	56	4.243	004
				7	4.060	7	4.063	12	4.071	012
8	3.80	6	3.75	48	3.781	29	3.795	44	3.801	102
								14	3.760	10-4
				6	3.600			1	3.587	013
		1	3.42			8	3.417	12	3.426	11-1
3	3.39	1	3.30	7	3.339	9	3.346	12	3.353	11-2
10	3.15	10	3.15	100	3.161	58	3.162	14	3.185	111
								100	3.169	11-3
				2	3.129	17	3.126	11	3.134	014
		1	2.93			13	2.916	15	2.921	11-4
9	2.84	9	2.84	70	2.836	67	2.834	82	2.839	104
8	2.73	7	2.73	35	2.741	33	2.736	51	2.739	015
		1	2.65	13	2.668	5	2.670	4	2.675	113
9	2.53	9	2.53	55	2.538	34	2.536	46	2.540	20-2
						7	2.437	6	2.441	200
								8	2.426	20-4
9	2.39	8	2.39	47	2.402	25	2.399	35	2.402	11-6
10	2.32	9	2.31	90	2.318	42	2.314	86	2.320	020
				20	2.223	10	2.224	16	2.228	21-2
						24	2.186	17	2.190	202
								10	2.189	115
10	2.17	9	2.17	55	2.174	30	2.176	23	2.179	10-8
						31	2.171	18	2.173	11-7
						7	2.147	2	2.149	017
						8	2.063	10	2.050	121
6	2.04	6	2.05	27	2.046	8	2.046	5	2.046	12-3
7	1.970	3	1.97	33	1.971	12	1.961	16	1.965	21-6
4	1.937	2	1.93	14	1.929	9	1.927	9	1.929	018
		1	1.85	6	1.887			2	1.893	123
								1.5	1.886	12-5
								2	1.880	20-8
1.5	1.807	1	1.80	20	1.796	5	1.792	9	1.796	124
				3	1.774	7	1.773	7	1.774	108
1.5	1.757	1	1.75	7	1.747	5	1.746	4	1.747	019
				20	1.704	5	1.709	2	1.703	22-3
4	1.688	1	1.67	12	1.683	4	1.684	6	1.688	12-7
6	1.628	2	1.63	18	1.628	6	1.625	13	1.627	300
6	1.587	3	1.580	16	1.588	5	1.586	7	1.592	222
								3	1.591	31-3
								5	1.588	12-8
								4	1.585	31-2
1	1.558					2	1.558	5	1.561	31-5
7	1.525	3	1.515	15	1.526	11	1.524	16	1.525	119
						8	1.520	8	1.522	302
				2	1.493			1	1.495	311
								1	1.493	12-9
1	1.474			2	1.472			5	1.473	13-2
1	1.454			7	1.454	1	1.451	4	1.453	034
5	1.431	2	1.430	13	1.432	4	1.430	7	1.433	2.1.-11
								4	1.432	132
								6	1.430	13-4
7	1.411	2	1.410	10	1.415	17	1.414	14	1.414	0.0.12
1	1.381			7	1.380			7	1.381	3.0.-10
8	1.352	8	1.345	32	1.356	6	1.352	21	1.355	13-6
		1	1.330	7	1.334			5	1.332	320
5	1.317	1	1.315	18	1.319	3	1.318	12	1.321	23-2

1 – Mannepakhk Mountain, Lovozero: Debye-Scherrer camera, diameter is 57.3 mm (Semenov, 1957);

2 – Hsianghualing, China: Debye-Scherrer camera, diameter not reported (Huang *et al.*, 1988);

3 – Sengischorr Mountain, Lovozero: diffractometer DRON UM-1, Fe-filtered Co$K\alpha$-radiation;

4 – Tuften quarry, Tvedalen: diffractometer Philips X'pert, graphite monochromated Cu$K\alpha_1$-radiation;

5 – Theoretical X-ray powder diagram calculated using the program LAZY PULVERIX (Yvon *et al.*, 1977).

form of (OH) groups, in accordance with the IR spectroscopic data.

Calculation of the empirical formulae of sphaerobertrandite was based on the sum of cations = 4, and taking into account the structural data. Anion ratios were calculated from charge balance with two schemes: 1) total H_2O+ corresponding to (OH) groups; 2) $(O,OH)_{\Sigma 6} \bullet nH_2O$. The latter takes into consideration the thermal data and IR spectra. All empirical formulae given below (numbers correspond to those in Table 1) are close to the idealized formula, $Be_3SiO_4(OH)_2$, obtained for sphaerobertrandite from structural data:

1. Mannepakhk Mountain, Lovozero (Semenov, 1957):
$Be_{2.87}Al_{0.04}Si_{1.08}O_{4.06}(OH)_{2.06}$, or
$Be_{2.87}Al_{0.04}Si_{1.08}O_{4.18}(OH)_{1.82} \bullet 0.12H_2O$;

2. Kuftnyun Mountain, Lovozero (Semenov, 1972):
$Be_{2.89}Al_{0.03}Si_{1.08}O_{3.83}(OH)_{2.53}$, or
$Be_{2.89}Al_{0.03}Si_{1.08}O_{4.19}(OH)_{1.81} \bullet 0.36H_2O$;

3. Sengischorr Mountain, Lovozero, this work:
$Be_{2.97}Si_{1.03}O_{3.905}(OH)_{2.25}$, or
$Be_{2.97}Si_{1.03}O_{4.06}(OH)_{1.94} \bullet 0.155H_2O$;

4. Tuften quarry, Tvedalen, this work:
$Be_{2.80}Fe_{0.02}Mn_{0.01}Si_{1.18}O_{3.86}(OH)_{2.67}$, or
$Be_{2.80}Fe_{0.02}Mn_{0.01}Si_{1.18}O_{4.40}(OH)_{1.60} \bullet 0.535H_2O$.

X-ray crystallography

The X-ray powder diffraction pattern of sphaerobertrandite (Table 2) is unique. All authors who described this mineral used X-ray powder data as their main diagnostic tool (Semenov, 1957, 1972; Bukin, 1967, 1969; Huang *et al.*, 1988). As shown in Table 3, sphaerobertrandite clearly differs from bertrandite and beryllite. X-ray powder diffractogram of sphaerobertrandite from different localities (including the holotype) and of its synthetic analogue (Bukin, 1969) are also very close to that calculated from structural data (Yvon *et al.*, 1977), despite some discrepancies between I_{obs} and I_{calc} (Table 2). This can be explained by the preferred orientation of plate-like grains resulting in variations of I_{obs} specifically for the 00*l* reflections.

The unit cell dimensions of sphaerobertrandite, refined from X-ray powder data, are:
Sengischorr Mountain, Lovozero: a = 5.081(3), b = 4.639(1), c = 17.664(9) Å, β= 106.09(5)°, V = 400.0 Å^3;
Tuften quarry, Tvedalen: a = 5.0716(6), b = 4.6289(5), c = 17.647(2) Å, β= 106.04(1)°, V = 398.15 Å^3.

The sphaerobertrandite sample from Tvedalen and the holotype mineral from Mannepakhk Mountain, Lovozero, were examined in a JEOL 200 keV transmission electron microscope. The mineral showed no signs of degradation in the electron beam. Both samples were, within the accuracy of the electron diffraction data, crystallographically identical.

The crystal structure of sphaerobertrandite was studied on a crystal from Sengischorr Mountain, Lovozero. Details of the single crystal X-ray data collection and structure refinement of sphaerobertrandite are given in Table 4.

Table 3. Comparative characteristics of natural hydrous beryllium silicates.

Mineral	Sphaerobertrandite	Bertrandite	Beryllite
Formula	$Be_3SiO_4(OH)_2$	$Be_4Si_2O_7(OH)_2$	$Be_3SiO_4(OH)_2 \cdot H_2O$?
Crystal system	Monoclinic	Orthorhombic	Orthorhombic
Space group	$P2_1/c$	$Cmc2_1$	or monoclinic ?
Unit cell dimensions			
a (Å)	5.08	8.71	
b (Å)	4.64	15.27	Unknown
c (Å)	17.66	4.57	
β (°)	106.1	90	
V (Å^3)	400	608	
Z	4	4	
Density meas. (g/cm^3)	2.46 – 2.54	2.59 – 2.60	2.20 – 2.25
Chemical composition (major constituents in wt.%)			
BeO	42.8 – 45.9	40.7 – 42.0	38.0 – 40.0
SiO_2	38.5 – 43.3	49.3 – 51.0	30.7 – 34.1
H_2O	11.7 – 14.7	6.9 – 8.9	19.0 – 22.7
Strongest lines of the X-ray powder pattern (d in Å – I)	4.885 – 90	7.56 – 10	6.43 – 5
	4.471 – 40	4.385 – 55	4.01 – 10
	4.236 – 62	4.350 – 35	3.64 – 9
	3.161 – 100	3.914 – 20	3.39 – 7
	2.836 – 70	3.807 – 100	2.34 – 10
	2.741 – 35	3.161 – 45	2.12 – 7
	2.538 – 55	2.543 – 75	2.03 – 7
	2.402 – 47	2.521 – 40	1.937 – 7
	2.318 – 90	2.283 – 20	1.807 – 5
	2.174 – 55	2.222 – 14	1.703 – 6
Optical properties			
α	1.597	1.583 – 1.592	1.50 – 1.54
β	1.607	1.598 – 1.606	1.51(?) – 1.55
γ	1.616	1.608 – 1.614	1.52 – 1.56
optical sign, 2V	(-) 70°	(-) 70-81°	(-) <45°
References	Semenov, 1957; this work	Chukhrov, 1972; Anthony *et al.*, 1995	Kuzmenko, 1954; Andersen, 1967

A single crystal with dimensions 0.2 x 0.2 x 0.04 mm was initially tested by optical microscopy. The same crystal was used for the structure determination at room temperature. The unit cell dimensions a = 5.082(2), b = 4.640(2), c = 17.696(8) Å and β = 106.13(3)° were obtained by least square refinement of 40 reflections in the range $8 \leq 2\theta \leq 27°$. The crystal structure was solved by direct methods and refined in the space group $P2_1/c$ using the SHELX-97 package (Sheldrick, 1997). The refinement, carried out with isotropic displacement parameters for all atoms (Table 4), converged to $R(F) = 0.20$ for 583 reflections with $F > 4\sigma(F)$. In spite of the high value of residual R-factor, the structural model obtained at this stage seemed to be very reasonable and led us to look for possible twinning. In fact through the transformation matrix [100/010/101] a new setting with cell parameters a = 5.082, b = 4.640, c = 17.000 Å, β = 89.44° is obtained, presenting a nearly orthorhombic metric in the

Table 4. Crystal data, structure solution and refinement for sphaerobertrandite.

Chemical formula	$Be_3SiO_4(OH)_2$
Molecular weight	152.13
Temperature	293 (2) K
Radiation and wavelength	Mo $K\alpha$, 0.71069 Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions (from single-crystal data)	a = 5.082 (2) Å b = 4.640 (2) Å c = 17.696 (8) Å β = 106.13 (3)°
Volume	400.85 (4) $Å^3$
Z	4
Density (calculated)	2.52 g/cm^3
Absorption coefficient μ	0.52 mm^{-1}
F(000)	300.0
Crystal size	0.2 x 0.2 x 0.04 mm
Data collection method	Single crystal diffractometer Siemens P4
θ range for data collection	3.00° to 25.00°
Index ranges	$-6 \le h \le 1$, $-1 \le k \le 5$, $-20 \le l \le 21$
Reflections collected	1319
Unique reflections	702 (R_{int} = 0.049)
Reflections with F>4σ(F)	583
Absorption correction	ψ-scan
Structure solution	Direct methods
Refinement method	Full-matrix least-squares refinement on F^2
Number of refined parameters	48
$R(F)_{obs}$ [F>4σ(F)]	0.090
$Rw(F^2)$ [F>4σ(F)]	0.237
GooF = S	1.095
R indices (all data)	R(F) = 0.118, $Rw(F^2)$ = 0.310, S = 1.324
Largest diff. peak and hole	0.97 and -0.82 $e/Å^3$

Table 5. Fractional atom coordinates and displacement parameters U (in $Å^2$) for sphaerobertrandite.

Atom	x	y	z	U
Si	0.0274(6)	0.4195(4)	0.3755(1)	0.0073(8)*
Be(1)	0.290(2)	0.416(2)	0.1198(6)	0.006(2)
Be(2)	0.629(3)	0.089(2)	0.9604(6)	0.007(2)
Be(3)	0.110(2)	0.917(2)	0.2924(6)	0.006(2)
O(1)	0.023(1)	0.574(1)	0.1430(3)	0.008(1)
O(2)	0.045(1)	0.571(1)	0.2933(4)	0.008(2)
O(3)	0.228(1)	0.069(1)	0.0990(3)	0.001(1)
O(4)	0.697(1)	0.974(1)	0.0540(4)	0.008(1)
O(5)	0.307(1)	0.575(1)	0.0413(4)	0.011(2)
O(6)	0.557(2)	0.465(1)	0.1939(4)	0.013(2)

*The equivalent isotropic displacement for Si atom was converted from the anisotropic parameters

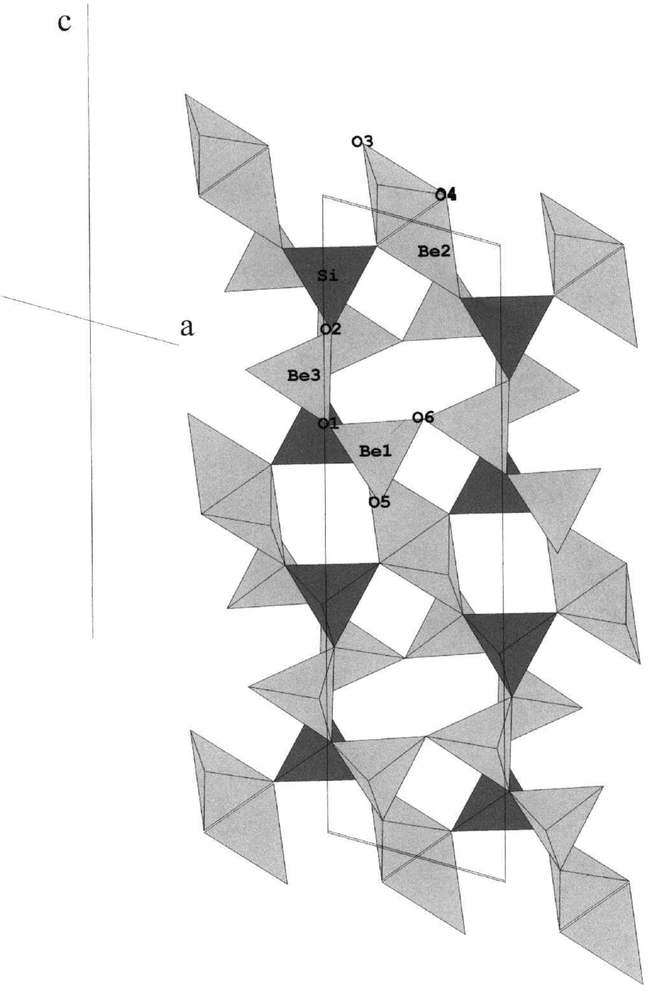

Fig. 4. The crystal structure of sphaerobertrandite; view along [010].

space group $P2_1/n$. Assuming a pseudo-merohedric twin (Nespolo & Ferraris, 2000) with twin plane (001), the refinement converged to R = 0.108 and indicated a volume ratio of the two individuals 0.3:0.7. Through Weissenberg photographs, collected with b as rotation axis, the twinning and the twin law were confirmed. As indicated by the β angle of 89.44° in the pseudo-orthorhombic cell, the obliquity of the twin is 0.56°; consequently there is neither a perfect superposition, nor a neat separation of the diffractions from the two individuals.

We carried on the refinement with the TWIN option in SHELX97, which would be fully justified only with obliquity zero. The incomplete accounting for the twinning explains the relatively high R = 0.09 value obtained at the end of the refinement process, carried on with anisotropic displacement parameters for silicon atom and isotropic displacement parameters for all the other atoms, after omitting a total of 14 reflections for which the imperfect twin treatment resulted in relatively marked disagreement between observed and calculated structure amplitudes.

A difference Fourier map showed very low residual peaks close to O(5) and O(6), *i.e.* in expected positions for hydroxyl groups. However, hydrogen atoms were not eventually included in the refinement. The final difference Fourier map was featureless: $\delta\rho$ maximum and minimum were 0.97 $e/Å^3$ and -0.82 $e/Å^3$. The atomic coordinates, thermal displacement parameters, selected interatomic distances are shown in Tables 5 and 6. The crystal structure, drawn by the program ATOMS (Dowty, 1995), is shown in Fig. 4.

Table 6. Selected interatomic distances in the structure of sphaerobertrandite (in Å).

Si-O(4)	1.617(7)	Be(1)-O(5)	1.60(1)	Be(2)-O(5)	1.59(1)	Be(3)-O(2)	1.64(1)
Si-O(2)	1.640(7)	Be(1)-O(6)	1.62(1)	Be(2)-O(3)	1.61(1)	Be(3)-O(1)	1.65(1)
Si-O(1)	1.641(6)	Be(1)-O(3)	1.66(1)	Be(2)-O(4)	1.63(1)	Be(3)-O(6)	1.66(1)
Si-O(3)	1.644(7)	Be(1)-O(1)	1.69(1)	Be(2)-O(4)’	1.68(1)	Be(3)-O(2)’	1.66(1)
<Si-O>		<Be(1)-O>		<Be(2)-O>		<Be(3)-O>	
O(1)-O(2)	2.631(8)	O(1)-O(3)	2.763(8)	O(3)-O(4)	2.747(10)	O(1)-O(2)	2.656(9)
O(1)-O(3)	2.726(9)	O(1)-O(5)	2.602(9)	O(3)-O(4)’	2.843(10)	O(1)-O(2’)	2.631(8)
O(1)-O(4)	2.688(9)	O(1)-O(6)	2.661(10)	O(3)-O(5)	2.588(9)	O(1)-O(6)	2.803(10)
O(2)-O(3)	2.653(9)	O(3)-O(5)	2.632(8)	O(4)-O(4)’	2.363(14)	O(2)-O(2)’	2.748(7)
O(2)-O(4)	2.693(9)	O(3)-O(6)	2.725(9)	O(4)-O(5)	2.677(9)	O(2)-O(6)	2.689(10)
O(3)-O(4)	2.632(10)	O(5)-O(6)	2.695(9)	O(4)’-O(5)	2.684(9)	O(2)’-O(6)	2.658(10)

The crystal structure: description and discussion

Sphaerobertrandite, $Be_3SiO_4(OH)_2$, has a unique crystal structure with no analogues among minerals or synthetic compounds. The structure consists of a mixed framework formed by Be- and Si-tetrahedra (Fig. 4). This is similar to two other beryllosilicates, phenakite (Be_2SiO_4) and bertrandite ($Be_4Si_2O_7(OH)_2$), which comprises 6- and 4-membered rings (Hazen & Au, 1986). All vertices of [SiO_4] tetrahedra in sphaerobertrandite are shared with 2 [BeO_4] tetrahedra. The OH anions (O5 and O6) are shared only between two Be tetrahedra. The sharing coefficient of the tetrahedral framework is 2.67 (Zoltai, 1960). The structure of sphaerobertrandite contains [BeO_3] chains with two tetrahedra in the repeat unit, in common with euclase (Hazen *et al.*, 1986). In the present structure these chains are formed by [Be(3)O_4] tetrahedra and screwed around 2_1 axis. In common with euclase, the contacts between [Be(3)O_4] tetrahedra within these chains are reinforced by [SiO_4] tetrahedra. Consequently, in both structures the unit cell parameters parallel to 2_1 axis are essentially the same: 4.64 Å in sphaerobertrandite and 4.78 Å in euclase. It is worth noting that in sphaerobertrandite, in common with many other structures which contain the complex chains formed by chemically different tetrahedra (for example euclase, väyrynenite, stillwellite, hellandite *etc.*), the tetrahedra of cations with lower valence (Be) make up the core of the chains, whereas tetrahedra of higher valence cations (Si) can be considered as its “branches”. However, the interconnection of these fragments in euclase and in sphaerobertrandite is different. In euclase there are Al-octahedron, whereas in sphaerobertrandite (Be,Si,O) chains are linked by the dimers [Be_2O_6], formed by two [Be(2)O_4] tetrahedra with shared edges, and by additional [Be(1)O_4] tetrahedron. The tetrahedral dimers [Be_2O_6] were earlier reported in the structures of epididymite (Robinson & Fang, 1970), eudidymite (Fang *et al.*, 1972), sorensenite (Metcalf-Johansen & Hazell, 1976) and in several synthetic beryllosilicates, namely $K_2Be_2Si_3O_9$ (Bu *et al.*, 1996), $Na_2Be_2Si_3O_9$ (Ginderow *et al.*, 1982) and $K_2Zn_2Be_2(SiO_4)(Si_2O_7)$ (Balko *et al.*, 1979). The common feature of the dimers [Be_2O_6] in all these structures is the short O-O distance, which corresponds to the shared edge between [BeO_4] tetrahedra; 2.36 Å in $Na_2Be_2Si_3O_9$ and in the studied structure, 2.38 in sorensenite, 2.40 in $K_2Zn_2Be_2(SiO_4)(Si_2O_7)$, 2.42 in epididymite and eudidymite, 2.43 in $K_2Be_2Si_3O_9$. Consequently, Be-O bonds have considerable covalent character, whereas these values are close to the sum of the ionic radii Be + O. As stated above, O(5) and O(6) belong to hydroxyl groups. The bond-valence balance calculations, computed following Brese & O’Keeffe (1991) (Table 7) and the O…O bond distances led us to depict the following hydrogen bond scheme: O(5) is linked to an hydrogen atom pointing toward O(1) [O(5)…O(1) 3.299(8) Å], whereas O(6) is linked to an hydrogen atom pointing toward an equivalent O(6) [O(6)…O(6) 3.209(10) Å]. The incorporation in the bond-valence sums of the contribution of the hydrogen bonds for both donor and acceptor oxygen atoms, computed following Ferraris & Ivaldi (1988), led to a very good match with the ideal values for O^{2-} and $(OH)^-$ anions. The role of donor and acceptor O(6) oxygen atoms could be interchanged: O(6) atoms involved in the hydrogen bonds are shifted each other by *b*/2, being symmetry-related through the 2_1 screw axes. Each oxygen could have its hydrogen either upward- or downward-pointing. Therefore within each channel the hydrogen bonds are ordered (namely, all upward- or downward-pointing), but long-scale correlation might not occur between neighbour channels. This could explain the major difficulties in finding the hydrogen atom linked to O(6) in the difference Fourier map, whereas the other hydrogen, linked to O(5), was more easily detected.

Table 7. Bond-valence balance calculations for sphaerobertrandite. Parameters taken from Brese & O’Keeffe (1991) and Ferraris & Ivaldi (1988).

	Si	Be(1)	Be(2)	Be(3)	H-bonds	$\Sigma_v a$
O(1)	0.955	0.434		0.485	+0.092	1.966
O(2)	0.958			0.498 + 0.465		1.921
O(3)	0.947	0.468	0.539			1.954
O(4)	1.019		0.509 + 0.443			1.971
O(5)*		0.559	0.562		-0.092	1.029
O(6)*		0.524		0.472	-0.100 + 0.100	0.996
$\Sigma_v c$	3.879	1.985	2.053	1.920		

* – (OH) groups

The comparison of Be-silicate sphaerobertrandite with Mn,Zn-silicate hodgkinsonite, $MnZn_2SiO_4(OH)_2$, can be used as an illustration of the functional substitution of polyhedra. Both structures contain the layer fragments formed by euclase-like mixed tetrahedral chains linked by additional tetrahedra. In sphaerobertrandite these tetrahedral sheets are linked by the dimers Be_2O_6 whereas in hodgkinsonite they are linked by the layers formed by $[MnO_6]$ octahedra. Both minerals complement the structural similarity between Be-silicates and Zn-silicates, earlier demonstrated in the pairs zincite – bromellite, willemite – phenakite, clinohedrite – euclase.

It is worth noting that sphaerobertrandite exhibits orthorhombic pseudosymmetry. The pseudosymmetry is rather typical for beryllosilicates and related compounds. Bertrandite and beryllonite are pseudohexagonal whereas barylite and synthetic Rb-fluoroberyllate, Rb_2BeF_4, possess pseudo-inversion centres. According to Belov (1976), this peculiarity of Be-minerals is due to the low number of electrons (4) at Be atoms which obviously interferes with their spheric symmetry and leads to the general lowering of the symmetry of Be-containing crystals.

Genesis

Sphaerobertrandite is a relatively common beryllium mineral of pegmatites related to alkaline rocks. The paragenesis of sphaerobertrandite, $Be_3SiO_4(OH)_2$, with epididymite, $NaBeSi_3O_7(OH)$, frequently with this order of crystallisation, and both minerals as pseudomorphs after chkalovite, $Na_2BeSi_2O_6$, undoubtedly shows that sphaerobertrandite is formed under decreasing alkalinity and temperature during hydrothermal stages of the evolution of the pegmatite system. Later, under further decrease of the temperature, more water-enriched alkali-free beryllium minerals appear in these pegmatites: beryllite, $Be_3SiO_4(OH)_2{\cdot}{\bullet}H_2O$(?), moraesite, $Be_2PO_4(OH){\bullet}4H_2O$ (Semenov, 1972; Pekov, 2000), and “gelbertrandite”, $Be_4Si_2O_7(OH)_2{\bullet}nH_2O$(?). The latter mineral is an insufficiently described phase, which has an X-ray powder pattern very similar to bertrandite but with broad and weak lines (Semenov, 1957). It is probably a poorly crystalline, hydrated variety of bertrandite.

Experimental data obtained by Bukin (1967, 1969) indicate some physical and chemical conditions of the hydrothermal fluids from which sphaerobertrandite has been formed. The charge is $Be(OH)_2 + 3SiO_2 + NaCl$ and water solution, and contains NaCl (20 %) + NaOH (10^{-5}–10^{-4} N). It was found that during the intervals 300–500°C and pH 9.1–10.2, epididymite as the major phase, plus sphaerobertrandite and phenakite, have been crystallized. The same was observed with a charge of $Be(OH)_2 + 3SiO_2 + NaF$ and an aqueous solution of NaF (20%) + NaOH (10^{-4} N) below 400°C and pH 10.4. After the increase of pH in the above-mentioned chloride system to 11.3 (NaOH 10^{-3} N) below 400°C, chkalovite with smaller amounts of epididymite were crystallized. On further increasing the pH, chkalovite becomes the only crystallized phase. In the system $Be(OH)_2 + 3SiO_2 + NaF$ with 20 % NaF aqueous solution (pH 8.7, 400°C), sphaerobertrandite becomes a major phase, whereas phenakite and epididymite are present only in subordinate amounts (Bukin, 1969).

In the system with the charge $1Be(OH)_2 + 1SiO_2$ and an aqueous solution of NaCl (20 %) + NaOH (10^{-5}N) below 300°C and pH 9.4, sphaerobertrandite (major phase), bertrandite, phenakite, quartz and “phase A” crystallized. Based on its optical properties, “phase A” can probably be identified as beryllite. In the same system, but below 500°C, phenakite dominates, whereas sphaerobertrandite, bertrandite and “phase A” appear in smaller amounts. Bukin (1967) claimed that crystallization of sphaerobertrandite depends directly on the value of pH. In the interval pH 4.8 – 8.3, only bertrandite has been crystallized, while sphaerobertrandite appears with increasing alkalinity. It was also mentioned that bertrandite and sphaerobertrandite crystallize more readily under lower temperatures, 270–400°C rather than 500°C (Bukin, 1967).

From these results, it can be concluded that alkalinity is the main factor determining the appearance of beryllium minerals in hydrothermalites, and it explains why the majority of the occurrences of sphaerobertrandite, an alkali-free mineral, have been reported from alkaline complexes. The data also correlates very well with observations on the evolution of beryllium mineralization in the Lovozero pegmatites. It is worth noting that sphaerobertrandite and beryllite (Si:Be = 1:3) are formed in pegmatites related to nepheline syenites, while bertrandite (Si:Be = 1:2) is a typical mineral of Si-enriched formations such as granite pegmatites, greisens, etc. Taking into account the occurrence of sphaerobertrandite in Hsianghualing, it can be assumed that the hydrothermal solutions which influenced the beryllium ores of this deposit had high alkalinity during one of its stages of activity.

Conclusion

All previous and new data show that sphaerobertrandite is an individual mineral species, unique both in chemical composition and crystal structure. Forty-five years after its discovery and first description, the mineral is now confirmed and takes its valid place in the mineralogical nomenclature. We have kept the original name sphaerobertrandite given by the discoverer, E.I. Semenov, in spite of its unjustified relationship to bertrandite. This relationship proves to be not so close as previously assumed. Other examples of usage of a similar name for significantly different minerals are also known: cobaltite – sphaerocobaltite, beryl – chrysoberyl, boracite – hydroboracite, etc. This practice can be justified also in the present case. The mineral is named due to the typical spherulitic morphology of aggregates, and the similarity to bertrandite in its main chemical constituents.

Neotype specimen of sphaerobertrandite from Sengischorr Mountain, Lovozero, has been deposited at Fersman Mineralogical Museum of Russian Academy of Sciences, Moscow, while neotype specimen from Tuften quarry, Tvedalen, has been deposited at Mineralogisk-Geologisk Museum, Oslo.

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