Mineralogical Magazine (2024), **88**, 585–593
doi:10.1180/mgm.2024.58

Article

Strontioborite: revalidation as a mineral species and new data

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Abstract

Strontioborite, which was first described in 1960 and later discredited by the then named Commission on New Minerals and Mineral Names of the International Mineralogical Association (IMA CNMMN), has been re-investigated (electron microprobe, single-crystal and powder X-ray diffraction, crystal structure determination and IR spectroscopy) on two specimens, including the holotype, and revalidated by the IMA Commission on New Minerals, Nomenclature and Classification (CNMNC). Strontioborite is known only at the Chelkar salt dome (North Caspian Region, Western Kazakhstan), in halite rocks with bischofite, magnesite, anhydrite, halurgite, boracite, ginorite and celestine. It forms colourless lamellar, scaly or tabular crystals up to 2 mm across. The chemical composition (wt.%, H_2O is calculated for $(OH)_4 = 4$ H apfu, according to structural data; holotype/neotype) is: CaO 1.42/0.27, SrO 23.10/23.79, B_2O_3 67.37/67.57, H_2O 8.73/8.72, total 100.62/100.37. The empirical formulae [calculated based on 15 O apfu = $O_{11}(OH)_4$ pfu] of the holotype and neotype specimens are $Sr_{0.92}Ca_{0.10}B_{7.98}O_{11}(OH)_4$ and $Sr_{0.95}Ca_{0.02}B_{8.02}O_{11}(OH)_4$, respectively. The idealised formula is $Sr[B_8O_{11}(OH)_4]$. Strontioborite is monoclinic, space group $P2_1$, $a = 7.6192(3)$, $b = 8.1867(2)$, $c = 9.9164(3)$ Å, $\beta = 108.357(4)°$, $V = 587.07(3)$ Å^3 and $Z = 2$. The strongest reflections of the powder X-ray diffraction pattern [d,Å(I)(hkl)] are: 7.22(100)(100), 5.409(61)(110), 4.090(64)(020), 3.300(48)(210), 2.121(30)($\bar{1}24$) and 2.043(37)(040, 024, $\bar{2}24$). The crystal structure, solved from single-crystal X-ray diffraction data ($R = 0.0372$), is based upon the (100) layers of polymerised B–O–OH polyanions $[B_8O_{11}(OH)_4]^{2-}$ and Sr-centred nine-fold polyhedra $SrO_6(OH)_3$. The B–O–OH polyanion is the cluster of three tetrahedra and three triangles; these clusters are decorated by the $[B_2O_2(OH)_3]$ pyro-group consisting of two triangles. The layers are linked *via* vertices of Sr-centred polyhedra, which share seven vertices with B-centred polyhedra of one layer and two vertices with B-centred polyhedra of the adjacent layer, and by the system of H bonds. The crystal chemistry of strontioborite is discussed in comparison with other natural and synthetic borates.

Keywords: strontioborite; borate mineral; strontium borate; crystal structure; evaporite deposit; Chelkar salt dome; Western Kazakhstan

(Received 11 May 2024; accepted 13 August 2024)

Introduction

This paper reports the revalidation of strontioborite, a borate mineral which was discovered in 1960, and named without approval of the Commission on New Minerals and Mineral Names of the International Mineralogical Association (IMA CNMMN). This occurred only a year after the foundation of the IMA CNMMN (1959) and the IMA rule to submit any proposal for a new mineral species to the Commission for its approval before publication was not yet in wide practice. In 1962, the published data on strontioborite were critically considered by the IMA CNMMN and the name strontioborite was rejected. On the basis of this IMA Commission decision, strontioborite was listed with the status D (discredited) in *The IMA/CNMNC List of Mineral Names* compiled by Nickel and Nichols (2004) and subsequently the later *The official IMA-CNMNC List of Mineral Names* issued by the IMA Commission on New Minerals, Nomenclature and Classification (CNMNC), http://cnmnc.units.it/ (Pasero, 2024).

Regardless of data obtained in the period of 1964–1975 which demonstrated its chemical and structural individuality, strontioborite was not added to the 'official' IMA status of a valid mineral species for almost sixty years because of a formality: these new data had not been submitted to the IMA CNMMN/CNMNC. In addition, the data from this period were incomplete. The missing data e.g. correct quantitative chemical data for this mineral, definitely obtained on pure material, are first reported in the present paper.

We carried out a revision study of strontioborite using type material and submitted a proposal to revalidate this mineral to the IMA CNMNC. In particular, we proposed to keep the name *strontioborite* given by the pioneer discoverer, Lobanova (1960) to the mineral because it is a strontium borate. Our proposal (IMA2020–017) was approved (Pekov *et al.*, 2020) and, thus, since 2020 strontioborite has the status of valid mineral species (symbol Srbo, Warr, 2021). Type specimens are deposited in the collections of the Fersman Mineralogical Museum of the Russian Academy of Sciences, Moscow, Russia with the catalogue numbers 69851 (holotype) and ST-7069 (neotype).

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Associate Editor: Sergey V Krivovichev

Cite this article: Pekov I.V., Zubkova N.V., Chukanov N.V., Yapaskurt V.O., Britvin S.N., Ksenofontov D.A., Pushcharovsky D.Y. (2024) Strontioborite: revalidation as a mineral species and new data. *Mineralogical Magazine* **88**, 585–593. https://doi.org/10.1180/mgm.2024.58

History of previous studies

Strontioborite was discovered by Lobanova (1960) in samples from cores of several boreholes drilled in boron-bearing evaporitic rocks of the Chelkar (another spelling: Shalkar) salt dome in the North Caspian Region, Western Kazakhstan. Note that the geographic information in the cited paper was limited by the term 'Caspian Region' due to the secrecy of materials on boron deposits in the Soviet Union. Pekov (1998) was the first to publish a full geographic account of the strontioborite locality. The first description of strontioborite contains information on the occurrence and associated minerals, its general appearance and some physical properties, as well as a wet chemical analysis [CaO 4.15, SrO 21.66, MgO 5.75, B_2O_3 57.85, H_2O 11.52, total 100.93 wt.%] and powder X-ray diffraction (XRD) data (Table 1). The formula $4(Sr,Ca)O·2MgO·12B_2O_3·9H_2O$ with Sr:Ca = 3:1 was suggested for the mineral (Lobanova, 1960). In his abstract of Lobanova (1960) for New Mineral Names, M. Fleischer in 1961 concluded that strontioborite '*requires verification*' and that '*some of the data could be construed as indicating a mixture of strontioginorite, boracite, and anhydrite*' (Fleischer, 1961; Hey, 1961). Probably, the doubts concerning the correctness of the chemical composition together with the absence of unit-cell data caused the rather negative voting in the IMA CNMMN: strontioborite ended up in the category of mineral names "*rejected by 60% or more of the Commission*" (IMA, 1962) and, as a result, was subsequently discredited.

The first single-crystal XRD data for strontioborite were reported by Kondrat'eva (1964), who studied several crystals of the mineral separated from the type material (received from the discoverer, V.V. Lobanova) and obtained reproducible results. It was found that strontioborite is monoclinic, with a unique unit cell and space group either $P21$ or $P21/m$. The presence of a piezoelectric effect confirmed the non-centrosymmetric space group $P21$. The improved powder XRD pattern of strontioborite (Table 1) was also reported (Kondrat'eva, 1964; English abstract: Fleischer, 1965). Kondrat'eva (1969) also mentioned that the simplified formula $3SrO·CaO·2MgO·11B_2O_3·8.5H_2O$ better corresponds to the original chemical analysis than $4(Sr,Ca)O·2MgO·12B_2O_3·9H_2O$. However, in general, both formulae were considered as doubtful in the light of the obtained unit-cell data: the calculated Z values were not whole-number ones (Kondrat'eva, 1964, 1969).

In the same period, strontioborite was found independently in drillcores of other boreholes at the Chelkar salt dome by I.I. Khalturina (Avrova *et al.*, 1968). On the single crystal separated from this material, Brovkin *et al.* (1975) solved the crystal structure of the mineral ($R = 0.11$), which turned out to be unique. The structure obtained by Brovkin *et al.* (1975) confirmed both the space group and unit-cell parameters reported by Kondrat'eva (1964) for strontioborite and made it possible to radically revise its formula (Table 1). Based on the crystal structure refinement, even despite the absence of new quantitative chemical data, Brovkin *et al.* (1975) suggested for strontioborite the idealised formula $Sr[B_8O_{11}(OH)_4]$ and described a novel borate polyanion in this mineral. This idealised formula of strontioborite entered into the reference books of Malinko *et al.* (1991), Pekov (1998), Anthony *et al.* (2003) and Chukanov (2014).

Material used for our studies

Samples from cores of several boreholes drilled at the Chelkar salt dome in 1950s – 1960s remain the only source of strontioborite to date. The type specimen of strontioborite collected by V.V. Lobanova in 1950s was given by her in 1960s (catalogued in 1967) to the Fersman Mineralogical Museum of the Russian Academy of Sciences (in that period, the Academy of Sciences of the Soviet Union), Moscow, Russia and is deposited in the systematic collection of the Museum with the catalogue no. 69851 (Pekov, 1998). The strontioborite specimen collected by I.I. Khalturina, is preserved in the collection of the outstanding Russian mineralogist and mineral collector V.I. Stepanov. He donated his collection to the Fersman Mineralogical Museum in the 1980s (Pekov *et al.*, 2015) and this specimen of strontioborite, received by V.I. Stepanov directly from I.I. Khalturina in 1968, is now deposited in the Museum with the catalogue no. ST-7069.

Table 1. Formula and crystal data on strontioborite: historical overview.

Source	Lobanova (1960)	Kondrat'eva (1964, 1969)	Brovkin *et al.* (1975)	Our work
Formula	$4(Sr,Ca)O·2MgO·12B_2O_3·9H_2O$	$3SrO·CaO·2MgO·11B_2O_3·8.5H_2O$ (?)*	$Sr[B_8O_{11}(OH)_4]$	$Sr[B_8O_{11}(OH)_4]$
Crystal system	Monoclinic (?)	Monoclinic	Monoclinic	Monoclinic
Space group	Unknown	$P2_1$**	$P2_1$**	$P2_1$
Unit-cell parameters				
a (Å)	Unknown	7.55(2)	7.623(1)	7.6192(3)
b (Å)		8.22(2)	8.130(10)	8.1867(2)
c (Å)		9.83(3)	9.909(5)	9.9164(3)
β (°)		107.77(17)	108.4(2)	108.357(4)
V (Å^3)		581	583	587.1
Z		Unknown	2	2
Crystal structure: R_1	Unknown	Unknown	0.11	0.0372
Strong reflections of the measured powder X-ray diffraction pattern (d, Å – I)	7.33–100	7.2–100	Not reported	7.22–100
	5.46–40	5.40–70		5.409–61
	4.09–80	4.09–90		4.090–64
	3.50–70	3.52–70		3.508–23
	3.32–70	3.29–80		3.300–48
	3.06–60	3.07–70		3.082–28
	2.298–40	2.61–70		2.926–25
	2.167–40	2.17–70		2.121–30
	2.033–60	2.038–70		2.043–37
	1.997–40			1.998–25

*The formula was first reported in the paper by Kondrat'eva (1969). **In papers by Kondrat'eva (1964, 1969) and Brovkin *et al.* (1975), the unit cell of strontioborite was reported in the setting with the a and c parameters reversed compared to that given here.

Both samples are glass vials with white, loose water-insoluble residues remaining after dissolution of rock salt in water. After examination the residues turned out to be mixtures of small crystals of strontioborite and the associated water-insoluble minerals listed below.

We studied both these specimens and detected in them the same mineral, strontioborite, with identical XRD characteristics and physical properties and only a slight difference in the amount of minor Ca (Table 2). In specimen ST-7069, we found single crystals of strontioborite larger and more perfect than in the specimen 69851. A single crystal separated from the specimen ST-7069 was used by us for the crystal structure determination; note, the first study of the strontioborite structure was carried out by Brovkin *et al.* (1975) also on the crystal separated from the material collected by I.I. Khalturina (see above). Thus, the material originally studied by Lobanova (1960) and represented in the Fersman Mineralogical Museum by specimen no. 69851 retains its status as the holotype for strontioborite, whereas specimen ST-7069 is now considered as the neotype of this mineral.

Occurrence and general appearance

Strontioborite occurs in rocks mainly consisting of halite. It is associated with bischofite, magnesite, anhydrite, halurgite, boracite, ginorite and celestine. Strontioborite occurs embedded in halite as crude crystals that are flattened on {100}. They are lamellar, scaly or, rarely, tabular. The major crystal form is the pinacoid {100}, other faces are not indexed. Some scales show a hexagonal outline, however, strontioborite crystals are commonly polygonal, irregular in shape, some of them are divergent or blocky (Fig. 1). Crystals are typically 0.1–0.2 mm, rarely up to 2 mm across. Aggregates (up to 1 cm in size) of strontioborite intimately intergrown with halurgite, boracite, ginorite and/or magnesite were observed (Lobanova, 1960; Avrova *et al.*, 1968; our data).

Strontioborite is a sedimentary mineral or was formed as a result of the diagenesis processes in boron-bearing evaporitic rocks.

Physical properties and optical data

Strontioborite is transparent, colourless, with white streak and vitreous lustre. Some crystals are white and semi-transparent due to abundant micro-inclusions of other minerals. Strontioborite is non-fluorescent under ultraviolet light or an electron beam. The mineral is brittle. Its Mohs' hardness is *ca* 2½. Perfect, mica-like cleavage on {100} is observed. The fracture is stepped or laminated. The density measured by flotation in heavy liquids (bromoform + ethanol) is 2.40(2) g cm^{-3}. The density calculated for the holotype using the empirical formula and unit-cell volume obtained from the single-crystal XRD data is 2.35 g cm^{-3} (Lobanova, 1960; our data).

Strontioborite is optically biaxial (+), $\alpha = 1.470(2)$, $\beta = 1.510(2)$, $\gamma = 1.579(2)$ (589 nm), $2V_{meas.} = 85(5)°$ and $2V_{calc.} = 77.5°$. Dispersion of optical axes was not observed. Elongation is positive or negative (for different crystals), inclined. Under the microscope the mineral is colourless and non-pleochroic (Lobanova, 1960).

Infrared spectroscopy

In order to obtain an infrared (IR) absorption spectrum, a powdered sample of strontioborite was mixed with anhydrous KBr, pelletised, and analysed using an ALPHA FTIR spectrometer (Bruker Optics) at a resolution of 4 cm^{-1}. 16 scans were collected in the wavenumber range from 360 to 3800 cm^{-1}. The IR spectrum of an analogous pellet of pure KBr was used as a reference.

In the IR spectrum of strontioborite (Fig. 2), four bands of O–H stretching vibrations of OH groups are observed in the range from 3000 to 3500 cm^{-1}. This is in agreement with structural data (Tables 6, 7). According to the equation $\nu\ (cm^{-1}) = 3592{-}304\cdot10^9\cdot\exp[-d(O\cdots O)/0.1321]$ for hydrogen bonds (Libowitzky, 1999), the O–H stretching bands with the absorption maxima at 3013, 3161, 3355 and 3401 cm^{-1} correspond to the O···O distances of 2.65, 2.69, 2.77 and 2.80 Å, respectively. These values are rather close to the $D\cdots A$ distances of 2.620, 2.698, 2.852 and 2.919 Å determined from the crystal structure refinement (Table 5). Some discrepancies for the long $d(O\cdots O)$ distances are due to a high inaccuracy of the above-mentioned correlation as applied to weak hydrogen bonds.

Two groups of strong bands observed in the ranges 1300–1500 and 900–1230 cm^{-1} correspond to $^{[3]}$B–O and $^{[4]}$B–O stretching vibrations, respectively. The bands in the range 590–900 cm^{-1} are mainly due to O–B–O bending vibrations. Weak bands observed below 550 cm^{-1} correspond to mixed lattice modes. Weak bands in the range 2000–2800 cm^{-1} are overtones and combination modes.

The IR spectrum of strontioborite is unique and can be used as a reliable diagnostic tool.

It should be noted that two IR spectra of samples labelled as 'strontioborite' in the book by Chukanov (2014) were obtained, as is now clear, on the material significantly contaminated by halurgite and boracite. Thus, the first correct IR spectrum of strontioborite is reported in the present paper (Fig. 2).

Chemistry

The chemical composition of both above-described samples of strontioborite was studied using a JEOL JSM-6480LV scanning

Table 2. Chemical composition of strontioborite (wt.%, two samples from the collections of the Fersman Mineralogical Museum of the Russian Academy of Sciences – FMM: see text).

	Holotype: FMM 69851			Neotype: FMM ST-7069				
Constituent	Average	Range	S.D.	Average	Range	S.D.	Probe standard	$Sr[B_8O_{11}(OH)_4]$, calculated
CaO	1.42	0.89–2.04	0.48	0.27	0.18–0.33	0.07	diopside	
SrO	23.10	23.61–22.33	0.58	23.79	23.69–23.85	0.07	$SrSO_4$	24.78
B_2O_3	67.37	66.87–68.28	0.65	67.59	66.64–68.62	0.83	BN	66.60
$H_2O_{calc.}$*	8.73			8.72				8.62
Total	100.62			100.37				100.00

*Calculated for $(OH)_4 = 4$ H atoms per formula unit, according to structural data. S.D. – standard deviation.

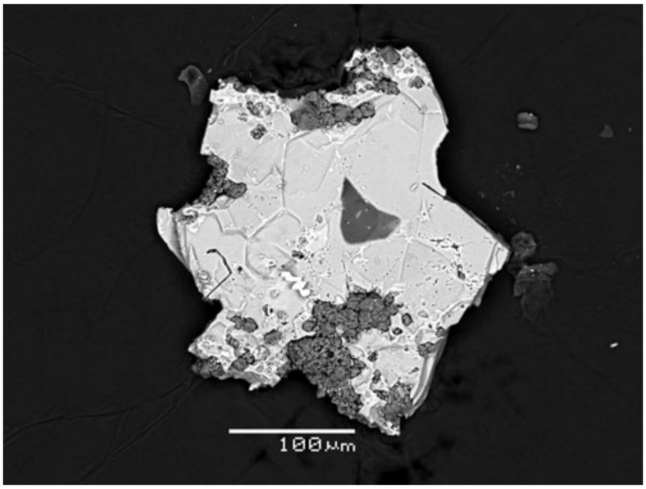

Figure 1. Blocky lamellar crystal of strontioborite enclosing aggregates of small crystals of magnesite (grey) and minor celestine (bright white). SEM (BSE) image, neotype ST-7069.

electron microscope equipped with an INCA-Wave 500 wavelength-dispersive spectrometer (Laboratory of Analytical Techniques of High Spatial Resolution, Dept. of Petrology, Moscow State University). The WDS mode was used (with an acceleration voltage of 20 kV and a beam current of 10 nA; electron beam was rastered to the 5 × 5 µm area) and gave detectable contents of Ca, Sr and B. The contents of other elements with atomic numbers > 4, except oxygen, are below detection limits. Analytical data (in wt.%, average of four spot analyses for each sample) and standards used are given in Table 2. H_2O was not determined because of the paucity of pure material. H_2O content was calculated from the structure data (see below) that showed a good agreement with electron microprobe data (Table 2). CO_2 was not analysed because the structure data show the absence of this constituent. The absence of gas release in hydrochloric acid also indicates that strontioborite does not contain carbonate groups.

The empirical formulae calculated on the basis of 15 O atoms per formula unit (apfu) = $O_{11}(OH)_4$ pfu, taking into account the structure data (see below), are: $Sr_{0.92}Ca_{0.10}B_{7.98}O_{11}(OH)_4$ for sample FMM 69851; and $Sr_{0.95}Ca_{0.02}B_{8.02}O_{11}(OH)_4$ for sample FMM ST-7069. They clearly correspond to the structure-confirmed idealised formula $SrB_8O_{11}(OH)_4$.

The values of the Gladstone–Dale compatibility index $1 - (K_p/K_c)$ (Mandarino, 1981) for the holotype calculated with $D_{meas.}$ and $D_{calc.}$ are −0.033 (excellent) and −0.055 (good), respectively. Strontioborite is insoluble in water and easily dissolves in cold

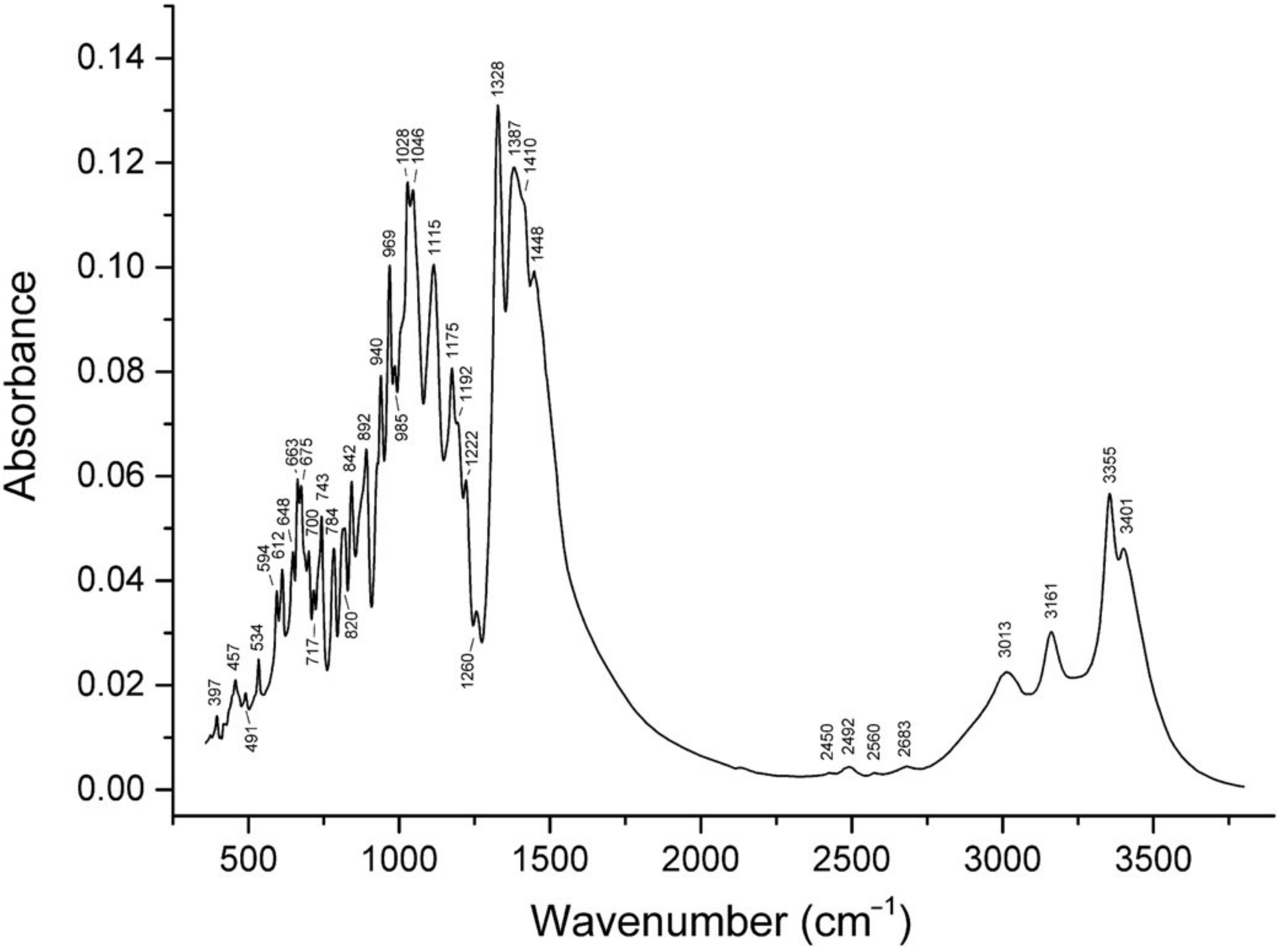

Figure 2. Powder infrared absorption spectrum of strontioborite.

Table 3. Powder X-ray diffraction data (*d* in Å) of strontioborite.

I_{obs}	d_{obs}	I_{calc}*	d_{calc}**	*h k l*	I_{obs}	d_{obs}	I_{calc}*	d_{calc}**	*h k l*
12	9.40	9	9.411	001	22	2.179	17	2.178	230
100	**7.22**	100	7.231	100			3	2.176	301
5	6.87	4	6.875	$\bar{1}01$	8	2.156	3	2.155	$\bar{3}21$
21	6.17	15	6.177	011			3	2.146	132
61	**5.409**	40	5.420	110	**30**	**2.121**	1	2.125	$\bar{3}22$
7	5.019	4	5.021	101			20	2.120	$\bar{1}24$
17	4.690	7	4.706	002	9	2.105	6	2.103	311
		7	4.674	$\bar{1}02$	**37**	**2.043**	9	2.047	040
6	4.281	4	4.280	111			12	2.040	024
64	**4.090**	73	4.093	020			13	2.030	$\bar{2}24$
		4	4.080	012	**25**	**1.998**	2	2.000	041
15	3.792	13	3.799	$\bar{2}01$			3	2.000	$\bar{3}23$
12	3.756	5	3.754	021			11	1.993	114
10	3.614	9	3.616	200	16	1.973	9	1.974	$\bar{3}14$
12	3.560	12	3.562	120			2	1.973	$\bar{2}33$
23	**3.508**	12	3.517	$\bar{1}21$			5	1.969	140
8	3.431	3	3.446	$\bar{2}11$	3	1.924	2	1.925	$\bar{1}15$
48	**3.300**	30	3.308	210			1	1.922	321
12	3.177	2	3.199	112	8	1.883	2	1.886	$\bar{2}15$
		5	3.173	121			1	1.882	005
		2	3.169	$\bar{2}12$			2	1.881	133
28	**3.082**	12	3.088	022			2	1.877	042
		14	3.079	$\bar{1}22$	8	1.843	2	1.848	232
		7	3.067	201			1	1.846	223
9	3.047	6	3.045	$\bar{1}13$			4	1.841	$\bar{4}11$
25	**2.926**	18	2.930	013			2	1.838	$\bar{3}32$
12	2.857	8	2.856	$\bar{2}03$	9	1.807	1	1.808	400
6	2.786	6	2.785	$\bar{2}21$			8	1.807	330
19	2.699	7	2.697	$\bar{2}13$	4	1.780	1	1.782	034
19	2.620	18	2.621	031			1	1.781	240
7	2.595	7	2.595	103			2	1.780	$\bar{3}05$
6	2.535	1	2.536	$\bar{1}31$	2	1.753	1	1.755	$\bar{3}33$
		6	2.535	$\bar{3}01$	4	1.712	1	1.715	$\bar{4}21$
4	2.511	3	2.511	202			2	1.710	025
12	2.484	2	2.487	$\bar{3}02$	6	1.701	1	1.702	241
		2	2.479	$\bar{1}04$			1	1.701	331
9	2.398	4	2.400	212			3	1.700	214
		2	2.398	131	6	1.683	4	1.682	$\bar{4}14$
8	2.382	5	3.379	$\bar{3}12$	2	1.661	1	1.661	115
11	2.343	7	2.342	$\bar{2}23$	5	1.650	2	1.654	420
		3	2.337	$\bar{2}04$			1	1.649	233
15	2.314	15	2.312	310	8	1.641	1	1.644	$\bar{1}06$
5	2.252	1	2.261	014			3	1.642	134
		2	2.247	$\bar{2}14$			1	1.640	$\bar{2}06$
13	2.192	9	2.192	123			1	1.640	313
9	1.633	4	1.633	$\bar{3}25$	4	1.479	1	1.481	$\bar{5}13$
		3	1.631	$\bar{3}34$			1	1.481	152
5	1.606	2	1.607	143			1	1.478	$\bar{2}52$
		1	1.603	$\bar{1}35$	4	1.466	1	1.470	$\bar{4}25$
4	1.578	1	1.580	$\bar{2}35$			1	1.466	234
		2	1.578	$\bar{1}44$			1	1.465	$\bar{1}53$
3	1.569	1	1.567	332			1	1.465	215
		1	1.567	125	3	1.453	2	1.454	$\bar{4}34$
5	1.554	1	1.554	421			1	1.452	053
		3	1.553	$\bar{4}31$	3	1.428	2	1.431	431
3	1.538	1	1.540	$\bar{2}44$			1	1.428	$\bar{5}22$
		1	1.534	402			1	1.427	333
5	1.525	1	1.526	$\bar{3}43$	2	1.421	1	1.421	$\bar{2}53$
		1	1.526	$\bar{1}26$			1	1.420	116
		1	1.524	$\bar{4}33$	1	1.408	1	1.407	$\bar{4}16$
		1	1.522	$\bar{2}26$	2	1.398	1	1.399	225
1	1.504	1	1.504	$\bar{2}51$			1	1.398	342
3	1.492	2	1.492	250	3	1.369	2	1.369	413
		1	1.491	341			1	1.368	$\bar{3}52$

*For the calculated pattern, only reflections with intensities ≥1 are given; **for the unit-cell parameters obtained from single-crystal data. The strongest reflections are highlighted in bold.

dilute HCl aqueous solution without effervescence. The solution obtained shows characteristic colour reaction with quinalizarin clearly indicating the presence of boron.

X-ray crystallography and crystal structure determination details

Powder XRD data for both samples were collected with a Rigaku R-AXIS Rapid II single-crystal diffractometer equipped with cylindrical image plate detector (radius 127.4 mm) using Debye-Scherrer geometry, Co$K\alpha$ radiation (rotating anode with VariMAX microfocus optics), 40 kV, 15 mA and 15 minutes exposure. Angular resolution of the detector is 0.045 2θ (pixel size 0.1 mm). The data were integrated using the software package *Osc2Tab* (Britvin *et al.*, 2017). Powder XRD data for the neotype sample FMM ST-7069 are reported in Table 3. The strongest reflections of the powder X-ray diffraction pattern [d,Å(I)(hkl)] are: 7.22(100)(100); 5.409(61)(110); 4.090(64)(020); 3.300(48)(210); 2.121(30)($\bar{1}24$) and 2.043(37)(040, 024, $\bar{2}24$). The powder XRD pattern for the holotype sample FMM 69851 is very close. The monoclinic unit cell parameters refined from the powder data for the holotype are: $a = 7.622(3)$, $b = 8.183(2)$, $c = 9.919(4)$ Å, $\beta = 108.36(3)°$ and $V = 587.2(5)$ Å^3.

Single-crystal XRD studies of neotype strontioborite were carried out using an Xcalibur S diffractometer equipped with a CCD detector. A full sphere of three-dimensional data was collected. Data reduction was performed using *CrysAlisPro* Version 1.171.39.46 (Rigaku Oxford Diffraction, 2018). The data were corrected for Lorentz, polarisation and absorption effects. The structure was solved by direct methods and refined using the *SHELX* software package (Sheldrick, 2015) to $R = 0.0372$ for 2751 unique reflections with $I > 2\sigma(I)$. H atoms were located in a difference-Fourier map and refined with O–H distances restrained to 0.90(1) Å and U_{iso} (H) = 1.2 U_{eq} (O). Minor Ca was taken into account in the Sr site. The crystal data, data collection information and structure refinement details are given in Table 4, atom coordinates, equivalent and anisotropic displacement parameters in Table 5, selected interatomic distances and H-bonding scheme in Tables 6 and 7 and bond-valence calculations in Table 8. The crystallographic information file has been deposited with the Principal Editor of *Mineralogical Magazine* and is available as Supplementary material (see below).

Discussion

Crystal structure and comparative crystal chemistry of strontioborite and related borates

Our results confirmed the correctness of the structure data obtained for strontioborite by Brovkin *et al.* (1975). The crystal structure of this mineral (Fig. 3a) is based upon the (100) layers of polymerised B–O–OH polyanions $[B_8O_{11}(OH)_4]^{2-}$ and Sr-centred nine-fold polyhedra $SrO_6(OH)_3$. The layers are linked *via* vertices of Sr-centred polyhedra, which share seven vertices with B-centred polyhedra of one adjacent layer and two vertices with B-centred polyhedra of the other adjacent layer, and by the system of H bonds. According to the classification of fundamental building blocks (FBB) in borates (Grice *et al.*, 1999), the FBB in strontioborite (Fig. 3b) could be presented as 5Δ3□:[ϕ]<Δ2□> | <Δ2□> | <Δ2□> | 2Δ. This means that three <Δ2□> rings containing two B-centred tetrahedra and one B-centred triangle are linked sharing tetrahedra, each ring

Table 4. Crystal data, data collection information and structure refinement details for strontioborite.

Crystal data	
Crystal system, space group, *Z*	Monoclinic, $P2_1$, 2
Unit-cell dimensions (Å / °)	$a = 7.6192(3)$
	$b = 8.1867(2)$
	$c = 9.9164(3)$
	$\beta = 108.357(4)$
V (Å^3)	587.07(3)
Absorption coefficient μ (mm^{-1})	4.154
F_{000}	399
Crystal size (mm)	0.08 × 0.31 × 0.44
Collection information	
Diffractometer	Xcalibur S CCD
Temperature (K)	293(2)
Radiation and wavelength (Å)	Mo*K*α; 0.71073
Absorption correction	Gaussian
θ range for data collection (°)	2.817–28.282
Index ranges	$-10 \leq h \leq 10$
	$-10 \leq k \leq 10$
	$-13 \leq l \leq 13$
Refinement	
Reflections collected	9897
Independent reflections	2893 ($R_{int} = 0.0542$)
Independent reflections with $I > 2\sigma(I)$	2751
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Number of refined parameters	230
Final *R* indices [$I > 2\sigma(I)$]	$R1 = 0.0372$, $wR2 = 0.0795$
R indices (all data)	$R1 = 0.0406$, $wR2 = 0.0812$
GoF	1.061
Largest diff. peak and hole, e^-/Å^3	0.49 and −0.48

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

Sr–O4	2.560(4)	B4–O8	1.450(8)
Sr–O2	2.586(3)	B4–O4	1.456(7)
Sr–O1	2.595(3)	B4–O5	1.465(7)
Sr–O13	2.653(5)	B4–O3	1.522(8)
Sr–O15	2.672(4)	<B4–O>	1.473
Sr–O6	2.679(4)		
Sr–O9	2.684(4)	B5–O5	1.359(7)
Sr–O5	2.689(4)	B5–O1	1.361(9)
Sr–O7	2.754(4)	B5–O6	1.364(7)
<Sr–O>	2.652	<B5–O>	1.361
B1–O1	1.444(7)	B6–O8	1.357(6)
B1–O6	1.453(7)	B6–O13	1.367(8)
B1–O11	1.468(7)	B6–O12	1.374(6)
B1–O3	1.513(7)	<B6–O>	1.366
<B1–O>	1.470		
		B7–O14	1.350(8)
B2–O2	1.449(7)	B7–O11	1.363(7)
B2–O10	1.458(7)	B7–O10	1.371(7)
B2–O9	1.461(7)	<B7–O>	1.361
B2–O3	1.517(7)		
<B2–O>	1.471	B8–O15	1.355(7)
		B8–O12	1.371(6)
B3–O2	1.361(8)	B8–O7	1.377(7)
B3–O9	1.368(7)	<B8–O>	1.368
B3–O4	1.369(7)		
<B3–O>	1.366		

sharing one tetrahedron with two adjacent rings. Thus, three tetrahedra share common vertices and the hexaborate group with three tetrahedra and three triangles is formed. These hexaborate groups are decorated by the $[B_2O_2(OH)_3]$ pyro-group 2Δ consisting of two triangles.

In terms of crystal structure, strontioborite is unique among minerals but has the isostructural synthetic analogue with Ca instead of Sr, $Ca[B_8O_{11}(OH)_4]$ (Zayakina and Brovkin, 1978; Yamnova *et al.*, 2005; Wiggin and Weller, 2005). Topologically the same FBB was reported in the structures of some other

Table 5. Atom coordinates, equivalent and anisotropic displacement parameters (in Å^2) for strontioborite.

Site	*x*	*y*	*Z*	U_{eq}	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Sr = $Sr_{0.899(8)}Ca_{0.134(8)}$	0.11526(6)	0.39385(6)	0.28043(4)	0.01120(15)	0.0159(2)	0.0137(2)	0.0048(2)	0.0000(3)	0.00439(16)	0.0001(3)
B1	0.1040(9)	0.4888(8)	0.9079(6)	0.0135(12)	0.019(3)	0.016(3)	0.006(3)	−0.001(2)	0.005(2)	−0.003(2)
B2	0.1087(9)	0.4893(7)	0.6486(6)	0.0119(12)	0.016(3)	0.014(3)	0.006(3)	−0.001(2)	0.002(2)	−0.001(2)
B3	−0.0094(9)	0.2308(8)	0.5156(6)	0.0115(12)	0.016(3)	0.013(3)	0.006(3)	−0.001(2)	0.005(2)	−0.001(2)
B4	0.1177(9)	0.7878(8)	0.2818(6)	0.0131(12)	0.015(3)	0.020(3)	0.006(3)	0.002(2)	0.006(2)	0.001(2)
B5	−0.0337(9)	0.2394(8)	−0.0224(6)	0.0118(12)	0.016(3)	0.015(3)	0.006(3)	−0.001(2)	0.006(2)	0.001(2)
B6	0.3928(8)	0.8972(15)	0.4740(6)	0.0210(12)	0.017(3)	0.035(3)	0.011(2)	0.002(5)	0.006(2)	0.001(5)
B7	0.4004(9)	0.4919(8)	0.8536(6)	0.0168(13)	0.022(3)	0.020(3)	0.009(3)	0.000(2)	0.005(3)	0.000(3)
B8	0.6134(8)	0.3981(18)	0.2759(6)	0.0207(12)	0.019(3)	0.033(3)	0.011(2)	0.003(4)	0.006(2)	0.002(4)
O1	0.0481(5)	0.3886(8)	0.0072(3)	0.0163(8)	0.0277(19)	0.0144(17)	0.0087(15)	−0.003(3)	0.0084(14)	−0.007(3)
O2	0.0818(5)	0.3760(7)	0.5316(3)	0.0138(9)	0.0245(19)	0.011(2)	0.0088(15)	−0.0013(17)	0.0087(14)	−0.0057(19)
O3	0.0349(5)	0.4157(6)	0.7604(3)	0.0115(9)	0.0179(17)	0.012(2)	0.0066(15)	0.0000(15)	0.0061(13)	−0.0016(18)
O4	0.0824(6)	0.6746(5)	0.3835(4)	0.0127(8)	0.018(2)	0.014(2)	0.0075(19)	0.0012(14)	0.0067(17)	0.0016(16)
O5	0.1123(6)	0.6875(5)	0.1582(4)	0.0132(9)	0.019(2)	0.016(2)	0.0057(19)	0.0002(14)	0.0060(16)	0.0034(15)
O6	−0.0310(6)	0.1533(5)	0.0961(4)	0.0153(9)	0.025(2)	0.0140(19)	0.0087(18)	0.0013(15)	0.0078(17)	−0.0012(17)
O7	0.7373(6)	0.4304(6)	0.2038(4)	0.0259(13)	0.024(2)	0.045(4)	0.0076(17)	0.0033(18)	0.0028(16)	0.002(2)
H7	0.684(8)	0.427(9)	0.1087(18)	0.031*						
O8	0.2950(5)	0.8694(6)	0.3359(4)	0.0172(11)	0.0162(18)	0.027(3)	0.0078(16)	0.0007(18)	0.0028(14)	−0.0026(18)
O9	−0.0114(6)	0.1431(5)	0.3977(4)	0.0140(8)	0.023(2)	0.014(2)	0.0072(18)	−0.0025(15)	0.0073(17)	−0.0019(17)
O10	0.3073(5)	0.5139(5)	0.7121(4)	0.0157(9)	0.016(2)	0.025(2)	0.0066(18)	0.0015(16)	0.0036(15)	0.0007(17)
O11	0.3068(5)	0.4888(5)	−0.0497(4)	0.0183(9)	0.018(2)	0.030(2)	0.0073(19)	−0.0017(16)	0.0049(16)	−0.0004(18)
O12	0.3118(5)	0.8851(9)	0.5794(3)	0.0232(9)	0.0171(18)	0.043(2)	0.0103(16)	−0.004(3)	0.0051(14)	−0.009(3)
O13	0.4274(6)	0.4479(8)	0.4893(4)	0.0396(17)	0.019(2)	0.090(5)	0.010(2)	0.001(2)	0.0050(17)	0.019(2)
H13	0.411(11)	0.468(10)	0.574(4)	0.048*						
O14	0.5852(6)	0.4700(7)	0.9036(4)	0.0329(13)	0.020(2)	0.068(3)	0.011(2)	0.004(2)	0.0058(18)	0.005(2)
H14	0.645(9)	0.469(9)	0.838(6)	0.039*						
O15	0.4283(5)	0.3841(10)	0.2132(4)	0.0309(11)	0.0202(19)	0.062(3)	0.0097(16)	0.006(3)	0.0039(15)	0.001(3)
H15	0.392(9)	0.413(10)	0.122(3)	0.037*						

*U_{iso}.

Table 7. H-bonding scheme (Å,°) in the structure of strontioborite.

D–H···*A*	*D*–H	H···*A*	*D*···*A*	∠(*D*–H···*A*)
O7–H7···O14	0.902(14)	1.97(2)	2.852(6)	167(7)
O13–H13···O10	0.900(15)	1.82(3)	2.698(5)	163(7)
O14–H14···O8	0.899(15)	2.09(4)	2.919(6)	153(7)
O15–H15···O11	0.894(14)	1.731(18)	2.620(6)	173(8)

D – donor; A – Acceptor

synthetic borates, namely $PbB_8O_{11}(OH)_4$ (Belokoneva *et al.*, 1999; Wang *et al.*, 2006), $BaB_8O_{11}(OH)_4$ (Sun *et al.*, 2010), apparently, $BaB_8O_{11}(OH)_4{\cdot}3H_2O$ (Wang and Liang, 2019) and $SnB_8O_{11}(OH)_4$ (Schönegger *et al.*, 2018). The difference between the compounds $AB_8O_{11}(OH)_4$ with A = Ca, Sr *vs.* A = Pb, Ba, Sn is in the configuration of the layer and in the arrangement of the neighbouring layers (Yamnova *et al.*, 2005; Schönegger *et al.*, 2018).

Among minerals, FBB 5Δ3□:[ϕ]<Δ2□> | <Δ2□> | <Δ2□> | 2Δ is known only in strontioborite. At the same time, FBB 3Δ3□:[ϕ]<Δ2□> | <Δ2□> | <Δ2□> | representing a part of the FBB in strontioborite (i.e. the cluster of three tetrahedra and three triangles formed by three rings consisting of two tetrahedra and one triangle with three tetrahedra share common vertex) is rather common (Grice *et al.*, 1999). As an isolated cluster it occurs in the structures of mcallisterite $Mg_2[B_6O_7(OH)_6]_2{\cdot}9H_2O$ (dal Negro *et al.*, 1969), aksaite $Mg[B_6O_7(OH)_6]{\cdot}2H_2O$ (dal Negro *et al.*, 1971) and rivadavite $Na_6Mg[B_6O_7(OH)_6]_4{\cdot}10H_2O$ (dal Negro *et al.*, 1973). In polymerised forms this FBB can be detected in chains in aristarainite $Na_2Mg[B_6O_8(OH)_4]_2{\cdot}4H_2O$ (Ghose and Wan, 1977) and in sheets in tunellite $Sr[B_6O_9(OH)_2]{\cdot}3H_2O$ (Clark, 1964; Burns and Hawthorne, 1994) and nobleite $Ca[B_6O_9(OH)_2]{\cdot}3H_2O$ (Karanović *et al.*, 2004). In the structures of ginorite $Ca_2B_{14}O_{20}(OH)_6{\cdot}5H_2O$ (Pankova *et al.*, 2018) and strontioginorite $SrCaB_{14}O_{20}(OH)_6{\cdot}5H_2O$ (Konnert *et al.*, 1970; Grice, 2005), the strontioborite-type FBB is a part of a more complex FBB 8Δ6□:[ϕ]<Δ2□> | <Δ2□> | <Δ2□> | - [ϕ]<Δ2□> | <Δ2□> | <Δ2□> | 2Δ (Grice *et al.*, 1999).

Two borates with Sr as the only species-defining metal cation are known as valid mineral species to date, namely veatchite $Sr_2B_{11}O_{16}(OH)_5{\cdot}H_2O$ (represented by three polytypes: −1*M*, −2*M* and −1*A*, Grice and Pring, 2012) and tunellite $SrB_6O_9(OH)_2{\cdot}3H_2O$ (Erd *et al.*, 1961; Clark, 1964; Burns and Hawthorne, 1994). Veatchite and strontioborite are quite different in terms of crystal structure, whereas tunellite demonstrates similarity with strontioborite in unit-cell parameters [tunellite: a = 14.415(3), b = 8.213(1), c = 9.951(2) Å, β = 114.05(1)°, V = 1075.8 Å^3 and Z = 4, Burns and Hawthorne, 1994] and some structural features (Fig. 4). Heteropolyhedral layers formed by Sr-centred ten-fold polyhedral in tunellite and the hexaborate FBBs 3Δ3□:[ϕ]<Δ2□> | <Δ2□> | <Δ2□> are topologically related to those formed in strontioborite even though Sr in the latter is nine-fold coordinated and FBBs forming the layer are decorated by additional $[B_2O_2(OH)_3]$ pyro-groups. The kinds of linkage of the layers in these minerals are different: in tunellite, Sr-centred polyhedra of adjacent layers share a vertex occupied by an H_2O molecule (Burns and Hawthorne, 1994) whereas in strontioborite Sr-centred polyhedra of one layer share two vertices with B-centred polyhedra of the adjacent layer. The powder XRD patterns of these minerals are markedly different.

Correspondence between earlier published data on strontioborite and our results

The results of our studies of strontioborite clearly confirm the correctness of crystallographic and crystal-structure data reported by Kondrat'eva (1964) and Brovkin *et al.* (1975). The powder XRD data of the mineral published by Lobanova (1960) and Kondrat'eva (1964, 1969) are in agreement with both our measured and calculated powder XRD patterns (Tables 1 and 3). We used optical data of strontioborite reported by Lobanova (1960) for the calculation of the Gladstone–Dale compatibility index (Mandarino, 1981) and obtained the values corresponding to *excellent* / *good* rates for D_{meas} / D_{calc}, respectively. Thus, the samples studied by Lobanova (1960), Avrova *et al.* (1968), Kondrat'eva (1964, 1969), Brovkin *et al.* (1975), and our team (this work) undoubtedly belong to the same mineral species, strontioborite. Its idealised formula is $Sr[B_8O_{11}(OH)_4]$ and, thus, we confirmed the assumptions by Fleischer (1965), Kondrat'eva (1964, 1969) and Brovkin *et al.* (1975) that the original chemical analysis of strontioborite reported by Lobanova

Table 8. Bond valence calculations for strontioborite.

Site	Sr*	B1	B2	B3	B4	B5	B6	B7	B8	Σ	H-bonding	Σ
O1	0.25	0.82				1.03				2.10		2.10
O2	0.26		0.81	1.03						2.10		2.10
O3		0.67	0.67		0.66					2.00		2.00
O4	0.28			1.01	0.79					2.08		2.08
O5	0.21				0.77	1.04				2.02		2.02
O6	0.21	0.80				1.02				2.03		2.03
O7=OH	0.18								0.99	1.17	−0.17(O14)	1.00
O8					0.80		1.04			1.84	+0.15(O14)	1.99
O9	0.21		0.78	1.01						2.00		2.00
O10			0.79					1.00		1.79	+0.23(O13)	2.02
O11		0.76						1.03		1.79		2.06
O12							0.99		1.00	1.99		1.99
O13=OH	0.22						1.01			1.23	−0.23(O10)	1.00
O14=OH								1.06		1.06	+0.17(O7) −0.15(O8)	1.08
O15=OH	0.22								1.05	1.27	−0.27(O11)	1.00
Σ	2.04	3.05	3.05	3.05	3.02	3.09	3.04	3.09	3.04			

Bond-valence parameters were taken from Gagné and Hawthorne (2015) and from Ferraris and Ivaldi (1988) for H-bonding.
*The occupancy of Sr site of $Sr_{0.866(8)}Ca_{0.134(8)}$ was taken into account.

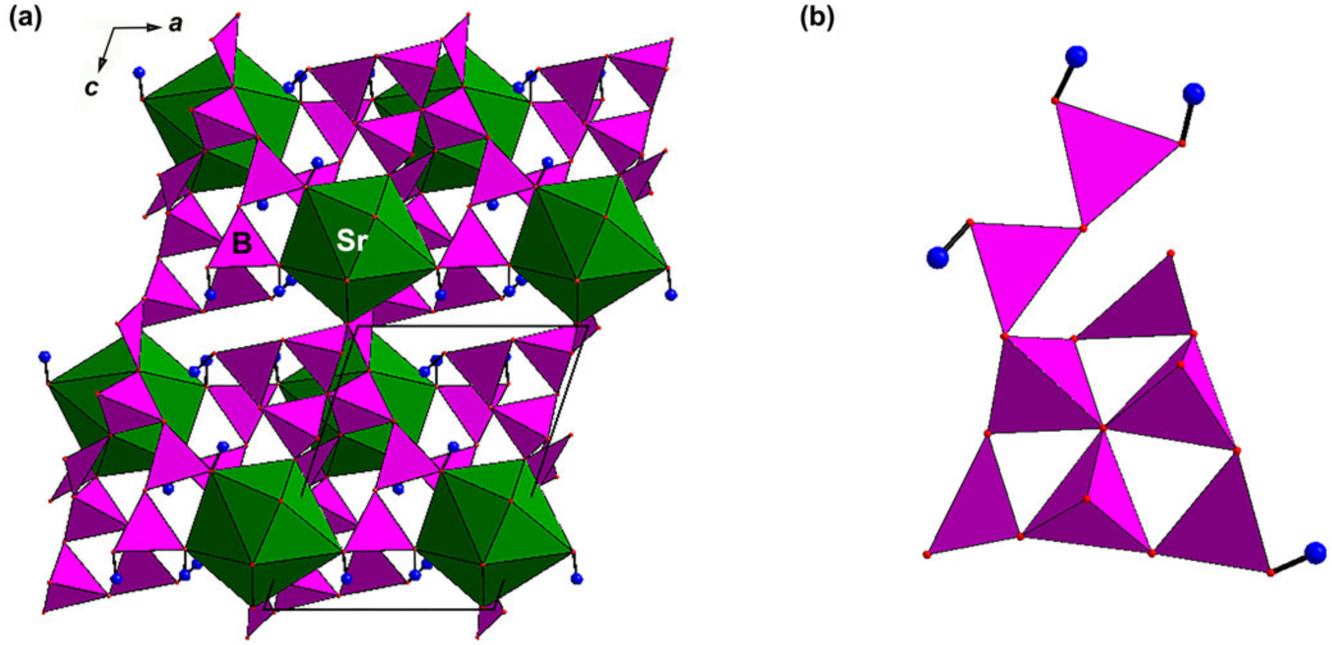

Figure 3. The crystal structure of strontioborite projected along the *b* axis (a) and the FBB in the structure of strontioborite (b). H atoms of OH groups are shown as blue spheres. The unit cell is outlined. Drawn using *Diamond*, Version 3.2k (Crystal Impact, 2024).

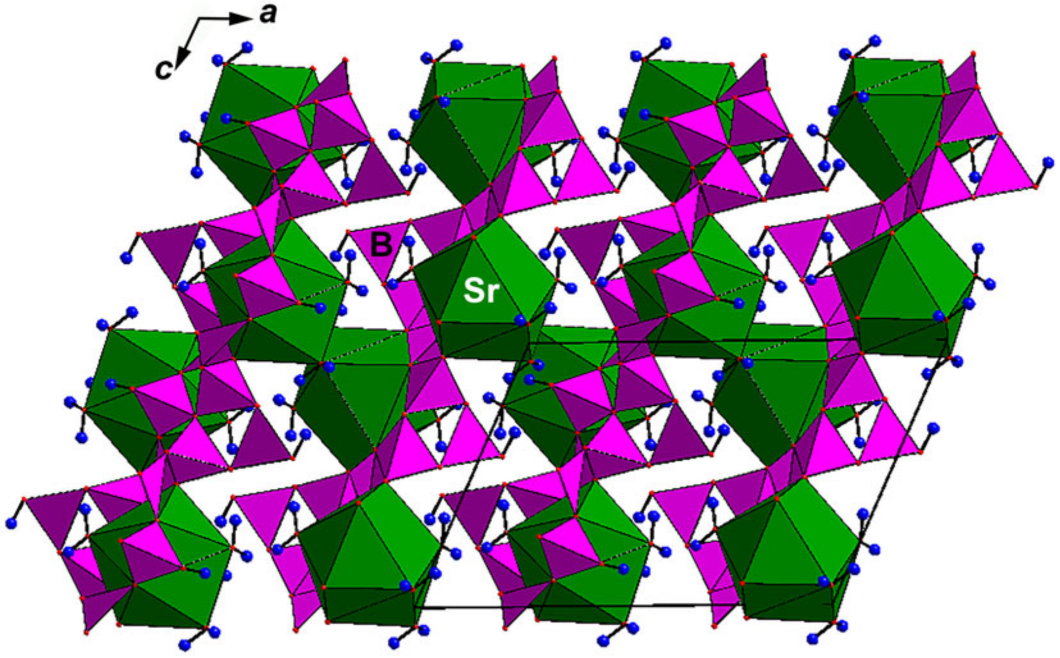

Figure 4. Crystal structure of tunellite $SrB_6O_9(OH)_2·3H_2O$ projected along the *b* axis (drawn after Burns and Hawthorne, 1994). H atoms of OH groups and H_2O molecules are shown as blue spheres. The unit cell is outlined.

(1960) is wrong, having been carried out on a mixture of minerals. Based on the IR spectra published in the book (Chukanov, 2014) – see above, we assume that the original sample could have been contaminated by halurgite $Mg_4[B_8O_{13}(OH)_2]_2·7H_2O$ and/or boracite $Mg_3B_7O_{13}Cl$, which can be a source of Mg impurity. Another source of Mg could be admixed magnesite (see Fig. 1). It is not excluded that a source of Ca impurity could be ginorite $Ca(Ca,Sr)B_{14}O_{20}(OH)_6·5H_2O$. Halurgite, ginorite and magnesite, all intimately associated with strontioborite, form colourless lamellae visually resembling strontioborite individuals.

Supplementary material. The supplementary material for this article can be found at https://doi.org/10.1180/mgm.2024.58.

Acknowledgements. We thank Edward Grew and anonymous referee for their valuable comments. The works were performed in accordance with the State Tasks of the Russian Federation: mineralogical and crystal chemical studies – no. 121061600049-4, IR spectroscopy – no. 124013100858-3, powder XRD study – no. AAAA-A19-119091190094.

Competing interests. The authors declare none.

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