REVISION 2

Strontiohurlbutite, $SrBe_2(PO_4)_2$, a new mineral from Nanping No. 31 pegmatite, Fujian Province, Southeastern China

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ABSTRACT

Strontiohurlbutite, ideally $SrBe_2(PO_4)_2$, is a new member of hurlbutite group discovered in the Nanping No. 31 pegmatite, Fujian province, southeastern China. Crystals are mainly found in zones I, II and IV; they are platy, subhedral to anhedral, with a length from 5 μm to 1.5 mm. Associated minerals mainly include quartz, muscovite, beryl, hurlbutite, hydroxylherderite, apatite-group minerals, and phenakite. Strontiohurlbutite crystals are light blue, translucent to transparent, and have vitreous luster. The Mohs hardness is about 6, and the tenacity is brittle. Optically, strontiohurlbutite is biaxial (–), $\alpha = 1.563(3)$, $\beta = 1.569(2)$, $\gamma = 1.572(3)$ (white light), $2V_{meas} = 68.5(5)^{o}$, and exhibits weak dispersion, r>v. The optical orientation is X = **b**, Y ≈ **c**. Electron-microprobe and SIMS analyses (average of 16) give SrO 29.30, P_2O_5 51.05, CaO 0.91, BaO 0.64, and BeO 17.71 wt%; total 99.61 wt%. The empirical formula, based on 8 O apfu, is $(Sr_{0.81}Ca_{0.05}Ba_{0.01})_{\Sigma 0.87}Be_{2.02}P_{2.05}O_8$. The stronger eight lines of the measured X-ray powder-diffraction pattern [*d* in Å(*I*)(*hkl*)] are: 3.554(100)(121); 3.355(51)(211); 3.073(38)(022); 2.542(67)(113); 2.230(42) (213); 2.215(87)($32\bar{1}$); 2.046(54)(223); 1.714(32)(143). Strontiohurlbutite is monoclinic, space group $P2_1/c$; unit-cell parameters refined from single-crystal X-ray diffraction data are: $a = 7.997(3)$, $b = 8.979(2)$, $c = 8.420(7)$ Å, $\beta = 90.18(6)°$, $V = 604.7(1)$ Å^3 ($Z = 4$, calculated density = 3.101 g/cm^3). The mineral is isostructural with hurlbutite, $CaBe_2(PO_4)_2$, and with paracelsian, $BaAl_2Si_2O_8$. The formation of strontiohurlbutite is related to the hydrothermal alteration of primary beryl by late Sr- and P-rich fluids.

Keywords: Strontiohurlbutite, $SrBe_2(PO_4)_2$, new mineral, hurlbutite, Nanping No. 31 pegmatite, Fujian province, China

INTRODUCTION

The new mineral strontiohurlbutite, a Sr-dominant analog of hurlbutite, was discovered in the Nanping No. 31 pegmatite, Fujian province, southeastern China. Polarizing microscopy, electron-microprobe analyses, X-ray diffraction measurements, Raman spectroscopy, and Secondary-ion Mass Spectrometry (SIMS), were used to determine its petrographic features, chemical composition and crystal structure. The species and the name have been approved by the International Mineralogical Association, Commission on New Minerals, Nomenclature and Classification (CNMNC) (IMA 2012-032) (Williams et al. 2012). The co-type specimen used for the electron-microprobe analyses, X-ray powder diffraction, XPS, Raman and optical measurements is deposited at the Geological Museum of China, Beijing, China, catalogue number M11803. The co-type sample used for the single-crystal structure measurements is stored at the Laboratory of Mineralogy, University of Liège, catalogue number 20387. This paper presents the occurrence of this new Sr phosphate with the hurlbutite-type structure, and discusses the origin of strontiohurlbutite in the Nanping pegmatite.

OCCURRENCE AND PARAGENESIS

Strontiohurlbutite was found in the Nanping No. 31 pegmatite, Fujian Province, southeastern China, which is located at longitude E 118°06', latitude N 26°40', about 8 km west of the Nanping city. The No. 31 pegmatite is a highly evolved and well-zoned pegmatite

in the Nanping pegmatite district. Five discontinuous mineralogical-textural zones were distinguished from the outermost zone inward (Yang et al. 1987): quartz – albite – muscovite zone (Zone I), saccharoidal albite ± muscovite zone (Zone II); quartz – coarse albite – spodumene zone (Zone III); quartz – spodumene – amblygonite zone (Zone IV); and blocky quartz – K-feldspar zone (Zone V). The petrography and mineral paragenesis of different textural zones in this pegmatite have been well described in previous publications (e.g., Yang et al. 1987; Rao et al. 2009, 2011). Strontiohurlbutite was found in samples from zones I, II and IV.

Strontiohurlbutite from zone I forms subhedral to euhedral crystals up to to 1.5 mm long, mainly in close association with quartz (Fig. 1a). Back-scattered electron (BSE) images show the crystals to be weakly heterogeneous (Fig. 1a), and the brighter areas are slightly richer in Sr than the darker areas. Other associated minerals include muscovite, fluorapatite, and hurlbutite. In zone II, strontiohurlbutite occurs as small aggregates about 5 to 100 μm across. They are closely associated with beryl, hurlbutite, hydroxylherderite, fluorapatite, and phenakite, forming the Be silicate + phosphate mineral associations interstitial to albite crystals (Fig. 1b, Rao et al. 2011: Fig. 4a, the brightest areas). In zones I and IV, strontiohurlbutite also forms aggregates with a size ranging from 2 to 50 μm; it surrounds hurlbutite crystals from zone I, and is distributed along the fractures of Cs-rich beryl from zone IV (Fig. 1c). Other secondary phases observed in this aggregates include beryl, hurlbutite, hydroxylapatite and muscovite.

PHYSICAL AND OPTICAL PROPERTIES

Strontiohurlbutite forms platy, subhedral crystals and anhedral grains. More than 50 grains were found in zones I and II; they are light blue, transparent to translucent, and have vitreous luster. The Mohs hardness is about 6, the tenacity is brittle, and no cleavage was observed. The calculated density, based on the empirical formula and single-crystal unit cell parameters, is 3.101 g/cm^3. Optically, strontiohurlbutite is biaxial negative, with α = 1.563 (2), β = 1.569 (2), γ = 1.572 (3), measured in white light. The 2*V* angle, measured directly by conoscopic observations, is 68.5 (5)°; the calculated 2*V* is 70°. It exhibits weak dispersion, r > v, and it is colorless. The optical orientation is X = **b**, Y ≈ **c**, and pleochroism is absent. Based on the calculated density and the measured indices of refraction, the compatibility index [1 – (K_P/K_C)] is -0.006, and corresponds to the "Superior" category (Mandarino 1981).

RAMAN SPECTROSCOPY

Raman spectra of strontiohurlbutite were collected using a Renishaw RM2000 Laser Raman microprobe in the State Key Laboratory for Mineral Deposits Research at Nanjing University. A 514.5 nm Ar^+ laser with a surface power of 5 mW was used for exciting the radiation. Silicon (520 cm^{-1} Raman shift) was used as a standard. Raman spectra were acquired from 100 to 1000 cm^{-1} and the accumulation time of each spectrum is 60 s. Raman spectra were collected on single crystals of strontiohurlbutite on polished thin section chips. Figure 2 shows the Raman spectrum of strontiohurlbutite, which is remarkably similar to the spectrum of hurlbutite (http://rruff.info/hurlbutite/display=default/R070612), confirming the structural similarity between strontiohurlbutite and hurlbutite. The Raman spectrum contains strong sharp peaks at 1022 cm^{-1}, medium sharp peaks at 587, 575, 550, 442, 343 and 204 cm^{-1},

and weak sharp peaks at 1178, 1135, 492, 421 and 176 cm^{-1}, respectively. The Raman shifts of (PO_4) groups were observed at 1022 (ν_1), 421, 442(ν_2), 1135, 1178 (ν_3) and 550, 575 and 587 cm^{-1} (ν_4). The Be-O vibration modes are probably at 204 and 492 cm^{-1}, and the Raman shifts at 176 and 343 cm^{-1} certainly correspond to Sr-O vibrations.

CHEMICAL COMPOSITION

The chemical composition of strontiohurlbutite (Table 1) was obtained with a JEOL JXA-8100M electron microprobe (WDS mode, 15 kV, 20 nA, beam diameter 1μm) at the State Key Laboratory for Mineral Deposits Research, Nanjing University. The following standards were used: synthetic $Ba_3(PO_4)_2$ (Ba *L*α, P *K*α), synthetic $SrSO_4$ (Sr *L*α), and hornblende (Ca *K*a).

To determine the BeO content of strontiohurlbutite, SIMS measurements were performed with a Cameca IMS-4F ion microprobe installed at CNR-IGG, Pavia (Italy). The experimental conditions are similar to those reported in the literature (Ottolini et al. 1993, 2002; Hatert et al. 2011). We selected a sample of beryllonite (*courtesy* of S. Philippo, Natural History Museum of Luxembourg) as standard for Be. The calibration factor for Be in the standard was obtained through the calculation of the experimental Be ion yield, having chosen P as the inner element for the matrix. We thus derived the IY(Be/P), defined as $(Be^+/P^+)/((Be(at)/P(at))$ where Be^+ and P^+ are the current intensities detected at the electron multiplier and (at) is the elemental atomic concentration. The IY (Be/P) was then used to calculate the Be concentration in the strontiohurlbutite, resulting in 17.71±0.464(1σ) BeO

wt%. Additionally, a few H_2O about 0.066±0.010(1σ) wt% is detected in strontiohurlbutite; lithium is absent.

Representative analyses of strontiohurlbutite (Table 1) lead to the empirical formula $(Sr_{0.81}Ca_{0.05}Ba_{0.01})_{\Sigma 0.87}Be_{2.02}P_{2.05}O_8$, based on 8 O atoms per formula unit. The idealized, end-member formula is $SrBe_2(PO_4)_2$, which requires 35.06 wt% SrO, 16.92 wt% BeO, and 48.02 wt% P_2O_5; total 100.00 wt. %. A careful examination of chemical data (Table 1) indicates significant amounts of Ca and Ba, reaching 3.10 wt% CaO and 0.22 wt% BaO, in strontiohurlbutite from zone IV. This indicates the existence of a possible solid solution between hurlbutite and strontiohurlbutite; such a solid solution is confirmed by the high Sr contents observed in some hurlbutite grains, reaching 10 wt% SrO.

X-RAY POWDER DIFFRACTION

The X-ray powder diffraction pattern of strontiohurlbutite was collected using micro-diffraction data on 5 crystals, with a RIGAKU D/max Rapid IIR micro-diffractometer (CuKα, λ = 1.54056 Å) at the School of Earth Sciences and Info-physics, Central South University, China. The micro-diffractometer was operated under these conditions: 48 kV, 250 mA, 0.05 mm collimator diameter, and 5-hours exposure time. The hurlbutite-based structural model (Huminicki and Hawthorne 2002), in which Ca sites are occupied by Sr atoms, was used to index the powder diffraction data. Table 2 shows the main indexed micro-diffraction data of strontiohurlbutite. The stronger eight lines of the measured X-ray powder-diffraction pattern [*d* in Å(*I*)(*hkl*)] are: 3.554(100)(121); 3.355(51)(211);

3.073(38)(022); 2.542(67)(113); 2.230(42) (213); 2.215(87)(32$\bar{1}$); 2.046(54)(223); 1.714(32)(143). The X-ray powder diffraction studies on the crystals of strontiohurlbutite gave the following unit-cell parameters: a = 8.005 (4), b = 8.998 (5), c =8.426 (5) Å, β = 90.05 (5)°, V = 606.9 (3) Å^3, Z = 4, and space group $P\,2_1/c$.

CRYSTAL STRUCTURE DETERMINATION

The X-ray intensity data, aimed to perform a structure refinement of strontiohurlbutite, were collected on an Agilent Technologies Xcalibur four-circle diffractometer, equipped with an EOS CCD area-detector (University of Liège, Belgium) on a crystal fragment measuring 0.35 × 0.35 × 0.18 mm. A total of 2186 frames with a spatial resolution of 1° were collected by the φ/ω scan technique, with a counting time of 10 s per frame, in the range 6.64° < 2θ < 58.18°. A total of 26214 reflections were extracted from these frames, corresponding to 1566 unique reflections. Unit-cell parameters refined from these reflections are a 7.997(1), b 8.979(1), c 8.420(1) Å, β 90.18(1)°, V 604.7(1)Å^3, space group $P2_1/c$, in good agreement with those refined from the powder-diffraction data. A summary of the crystal data is presented in Table 3. The data were corrected for Lorenz, polarization and absorption effects, the latter with an empirical method using the SCALE3 ABSPACK scaling algorithm included in the CrysAlisRED package (Oxford Diffraction 2007). The structure refinement was performed with anisotropic-displacement parameters for all atoms. The final conventional R_1 factor [$F_0 > 2\sigma(F_0)$] is 0.0197. Atomic coordinates and anisotropic displacement parameters, as well as selected bond distances and angles, are given in Table 4 and Table 5, respectively.

The structure of strontiohurlbutite is based on a tetrahedral framework consisting of corner-sharing BeO_4 and PO_4 tetrahedra (Fig. 3). BeO_4 and PO_4 tetrahedra are assembled in 4- and 8-membered rings, respectively. The 4-membered ring consists of a pair of tetrahedra pointing upwards (U) and a pair of tetrahedra pointing downwards (D), showing the UUDD type rings (Fig. 4a); the 8-membered ring shows the DDUDUUDU pattern (Fig. 4b). Sr atoms are localized in the channels formed by the alignment of the 8-membered rings (Fig. 3). A view perpendicular to the *b* direction shows that BeO_4 and PO_4 tetrahedra connected by corner-sharing form a double crankshaft chain running along *a* (Fig. 4c).

The Sr^{2+} ions are located in 10-coordinated polyhedra, characterized by 7 short bonds [<Sr-O> = 2.596(2) Å] and 3 long bonds [<Sr-O> = 3.227(2) Å]. This polyhedron can be described as a combination of a square pyramid and of a trigonal prism, with one square face in common. Based on the empirical parameters of Brown and Altermatt (1965), the bond-valence sums for strontiohurlbutite were calculated (Table 6). The bond-valence sums for P (5.00-5.04), Be (2.05-2.07), and Sr (2.09) are very close to the theoretical values.

The structure of strontiohurlbutite can be compared to those of hurlbutite (Mrose 1952; Bakakin and Belov 1959; Lindbloom et al. 1974) and paracelsian (Smith 1953; Bakakin and Belov 1960). The replacement of Ca in the structure of hurlbutite (effective ionic radius 1.06 Å; Shannon 1976) by Sr in strontiohurlbutite (effective ionic radius 1.21 Å) leads to an increase of the seven shorter M^{2+}-O bonds from 2.469(6) Å to 2.596(2) Å, respectively. This larger crystallographic site also implies an increase of the unit-cell parameters of strontiohurlbutite, compared to those of hurlbutite (Table 7).

ORIGIN AND SIGNIFICANCE

Strontium is a widespread element in most rocks. Since its crystal-chemistry is similar to that of calcium, Sr commonly substitutes for Ca in minerals, especially in phosphates. Various Sr-bearing phosphate minerals, including stronadelphite (Pekov et al. 2010), palermoite (Mrose 1953; Ni et al. 1993), goedkenite (Moore et al. 1975), and strontiowhitlockite (Britvin et al. 1991), are known to have a Ca-bearing isostructural analogue. The new mineral species described in the present paper, strontiohurlbutite, is the Sr-dominant analogue of hurlbutite, and constitutes a new member of the hurlbutite group (Table 7).

Strontiohurlbutite occurs in close association with hurlbutite, thus indicating that both minerals may crystallize under a comparable range of physicochemical conditions. Their textural relationships suggest that the hurlbutite-group minerals evolved from hurlbutite to strontiohurlbutite. Strontiohurlbutite crystals are enriched in Ba in zones I-II and in Ca in zone IV (Table 1), thus indicating a solid solution with hurlbutite. Consequently, the activity of Sr in the pegmatite fluids seems to be an essential factor controlling the crystallization of strontiohurlbutite.

High Sr activity in late hydrothermal fluids affecting pegmatite systems was documented in the literature (e.g., Moore 1982; Charoy et al. 2003). This high activity induces the replacement of early minerals by secondary Sr-bearing minerals such as palermoite and goyazite (e.g., Ni et al. 1993; Galliski et al. 2012). In the Nanping No. 31 pegmatite, strontiohurlbutite occurs with hurlbutite along fractures of primary beryl (Fig. 1c); this petrographic texture indicates that the primary beryl was affected by a late Sr-, Ca- and P-rich

hydrothermal fluid. Hurlbutite contains high SrO contents, from 5 to 10 wt%, thus indicating that Sr in the late hydrothermal fluids became a trigger for the transition from hurlbutite to strontiohurlbutite. In fact, other secondary Sr-bearing phosphate minerals such as palermoite, goyazite, hydroxylapatite, and bertossaite were found in the Nanping No. 31 pegmatite (Ni et al. 1993; Yang et a. 1994); the source of Sr in the hydrothermal fluids, responsible for the crystallization of these secondary minerals, remains to be determined in the future.

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306

307 **FIGURE CAPTIONS**

308

309 **FIGURE 1.** BSE images showing occurrence and mineral associations of strontiohurlbutite. (a)
310 euhedral strontiohurlbutite crystals in close association with quartz in zone I. (b) Small
311 aggregate of strontiohurlbutite in a Be silicate + phosphate assemblage interstitial to albite
312 crystals in zone II. (c) Strontiohurlbutite associated with secondary phases (beryl, hurlbutite,
313 hydroxylapatite and muscovite) in the fractures of primary beryl from zone IV. Abbr.: Qz -
314 quartz, Srh - strontiohurlbutite, Brl-P - primary beryl, Brl-S - secondary beryl, Phn -
315 phenakite, Ab - albite, Hlb - hurlbutite, Ms - muscovite, Ap - apatite.

316

317 **FIGURE 2.** The Raman spectrum of strontiohurlbutite.

318

319 **FIGURE 3.** The crystal structure of strontiohurlbutite. Note: PO_4 tetrahedra in dark gray; BeO_4
320 tetrahedra in gray; circle for Sr atoms.

321

322 **FIGURE 4.** Chains and rings in the crystal structure of strontiohurlbutite (PO_4 tetrahedra: dark
323 gray; BeO_4 tetrahedra: gray). (a) 4-membered ring with the pattern UUDD; (b) 8-membered
324 ring with the pattern DDUDUUDU; (c) double-crankshaft chain aligned along the *a* axis.

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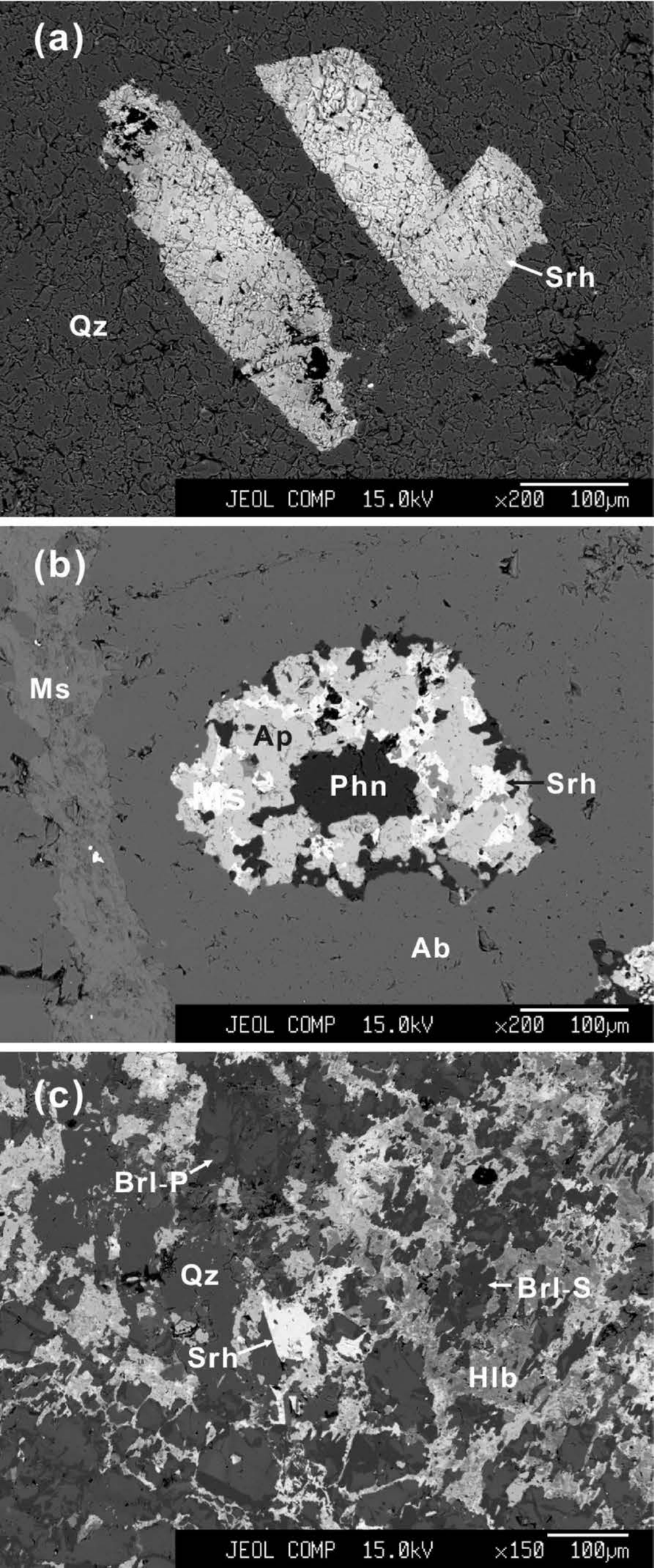
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Qz
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(b)
Ms
Ap
Phn
Srh
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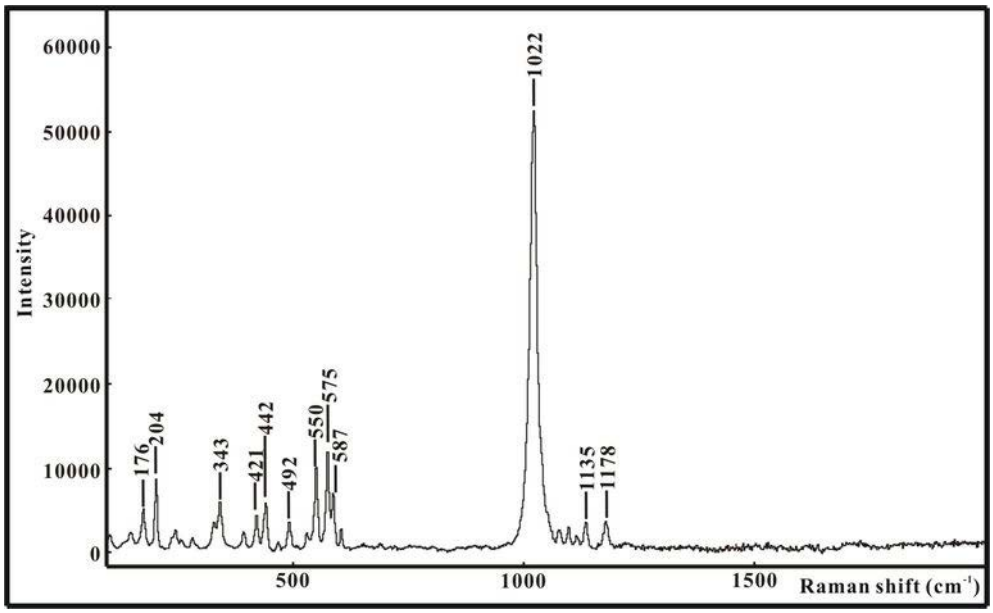
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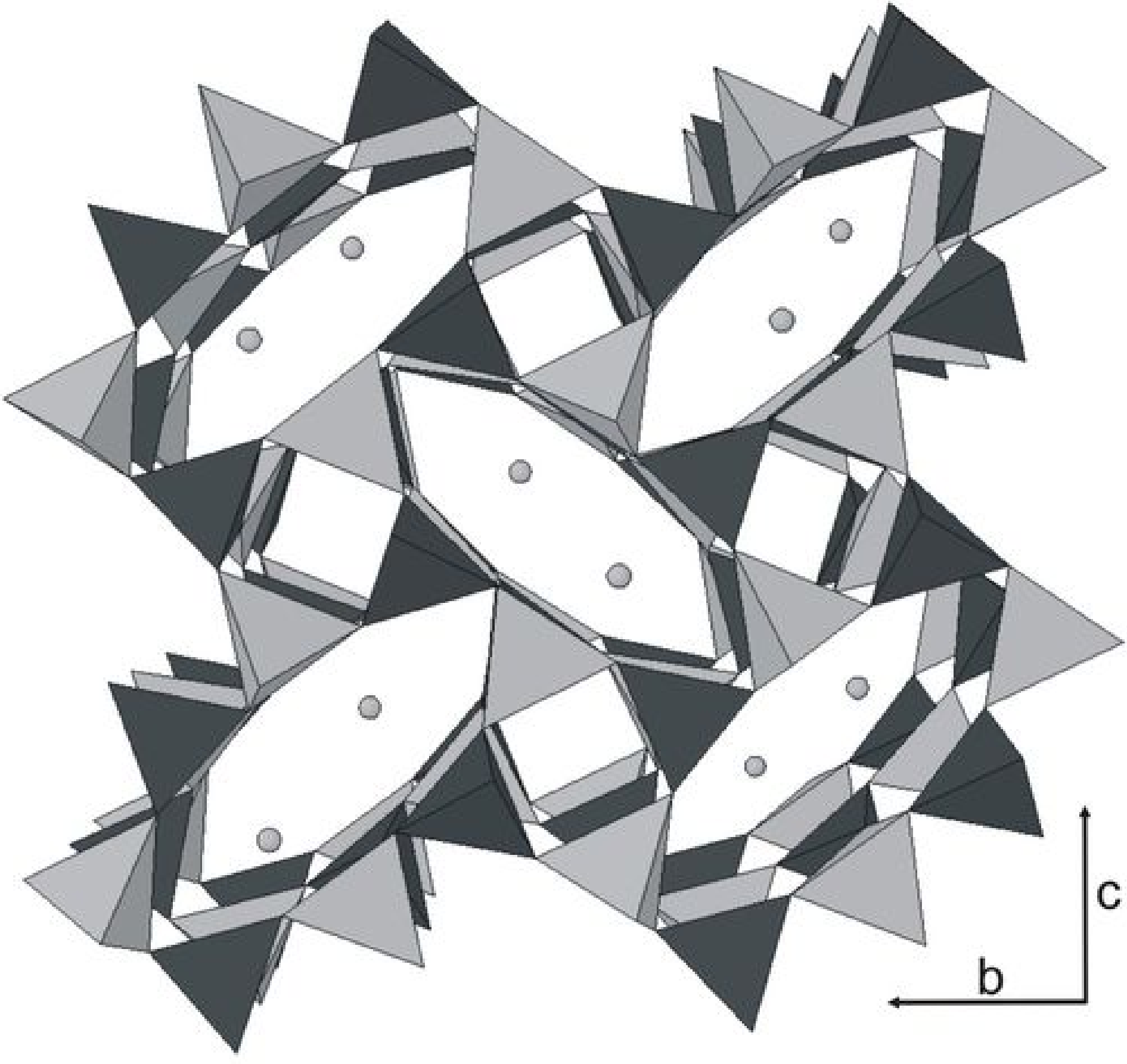
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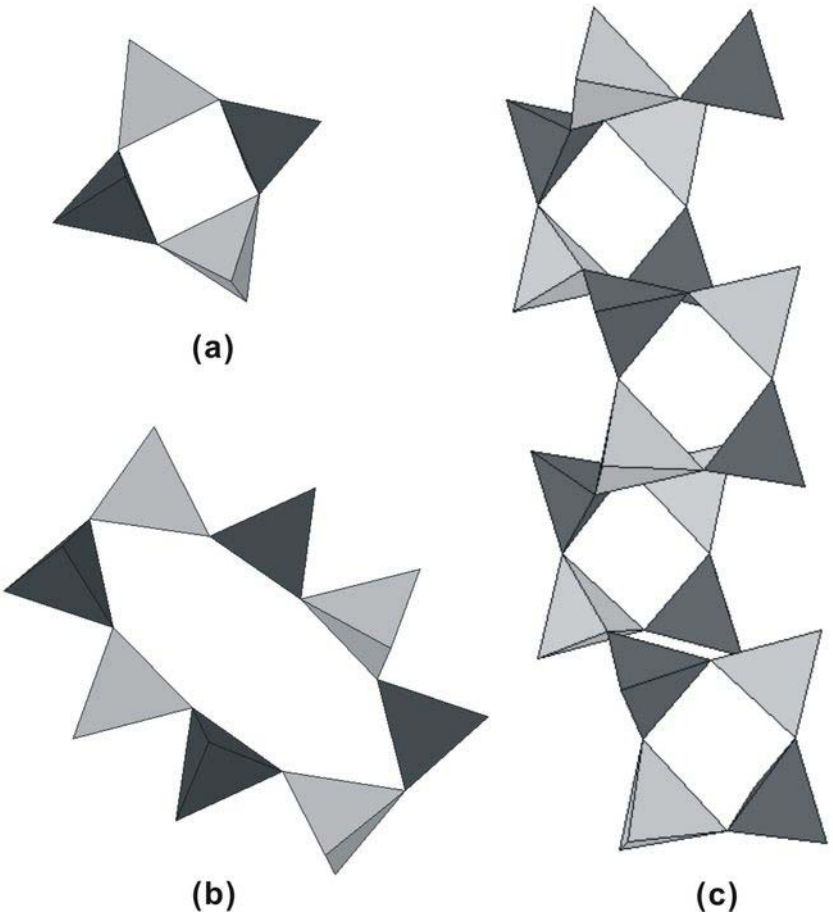
(a)
(b)
(c)

TABLE 1. Representative electron-microprobe results of strontiohurlbutite from the Nanping No. 31 pegmatite dyke

	Strontiohurlbutite from Nanping No. 31 pegmatite						Average	Ideal strontiohurlbutite
	NP-66 (zone I)		NP-14 (zone II)		NP-54 (zone IV)			
P_2O_5 wt.%	50.54	50.54	50.54	52.73	50.75	51.20	51.05	48.02
SrO	29.04	29.67	30.02	28.88	30.61	27.57	29.30	35.06
BeO*	17.71	17.71	17.71	17.71	17.71	17.71	17.71	16.92
CaO	0.07	0.17	0.15	0.18	1.80	3.10	0.91	
BaO	1.21	0.87	1.18	0.18	0.18	0.22	0.64	
Total	98.11	98.55	99.23	99.81	100.98	99.81	99.61	100.00
Structural formulas calculated on the basis of O=8 atoms								
P *apfu*	2.051	2.047	2.043	2.087	2.025	2.036	2.048	2.000
Sr	0.807	0.823	0.831	0.783	0.837	0.751	0.805	1.000
Be	2.039	2.035	2.031	1.989	2.006	1.999	2.016	2.000
Ca	0.004	0.009	0.008	0.009	0.091	0.156	0.046	-
Ba	0.023	0.016	0.022	0.003	0.003	0.004	0.012	-

*: BeO was measured by SIMS.

TABLE 2. Powder X-ray diffraction data for strontiohurlbutite

h	*k*	*l*	d_{meas} (Å)	d_{calc} (Å)	I_{rel}
0	1	1	6.150	6.150	9
1	1	0	5.985	5.981	3
2	1	0	3.653	3.657	5
1	**2**	**1**	**3.554**	**3.555**	**100**
2	**1**	**1**	**3.355**	**3.354**	**51**
0	**2**	**2**	**3.073**	**3.075**	**38**
1	3	0	2.810	2.809	27
0	1	3	2.678	2.681	9
1	**1**	**3**	**2.542**	**2.542**	**67**
0	2	3	2.380	2.383	26
3	2	0	2.294	2.295	1
2	**1**	**3**	**2.230**	**2.227**	**42**
3	**2**	$\bar{1}$	**2.215**	**2.215**	**87**
2	3	$\bar{2}$	2.083	2.086	26
2	**2**	**3**	**2.046**	**2.047**	**54**
3	3	0	1.994	1.994	19
1	1	4	1.986	1.986	13
3	2	3	1.776	1.777	16
2	2	4	1.721	1.722	21
1	**4**	**3**	**1.714**	**1.715**	**32**
0	1	5	1.655	1.656	11
3	$\bar{1}$	$\bar{4}$	1.627	1.627	31
3	1	4	1.623	1.625	6
1	$\bar{2}$	$\bar{5}$	1.549	1.549	10
4	2	3	1.531	1.532	4
5	1	$\bar{3}$	1.376	1.375	6

TABLE 3. Crystal data and refinement parameters for strontiohurlbutite

Crystal size (mm)	0.35 × 0.35 × 0.18
Color	Light blue
Space group	$P2_1/c$
a, b, c (Å)	7.997(1), 8.979(1), 8.420(1)
β (°)	90.18(1)
V (Å^3)	604.7(1)
Z	4
D(calc) (g/cm³)	3.101
$2\theta_{min}$, $2\theta_{max}$	6.64°, 58.18°
Range of indices	$-10 \le h \le 10$, $-12 \le k \le 12$, $-11 \le l \le 11$
Measured intensities	26214
Unique reflections	1566
Independent non-zero [$I > 2\sigma(I)$] reflections	1473
μ (mm^{-1})	9.451
Refined parameters	118
R_1 [$F_0 > 2\sigma(F_0)$]	0.0197
R_1 (all)	0.0234
wR_2 (all)	0.0467
S (goodness of fit)	1.106
Max $\Delta I/\sigma$ in the last l.s. cycle	0.001
Max peak and hole in the final ΔF map (e/Å^3)	+0.44 and –0.42

TABLE 4. Atomic coordinates and displacement parameters ($Å^2$) for strontiohurlbutite

Atom	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{eq}
Sr	0.25553(2)	0.91255(2)	0.10887(2)	0.0093(1)	0.0075(1)	0.0092(1)	-0.00060(7)	-0.00046(7)	0.00024(7)	0.00867(7)
P1	0.56332(7)	0.69579(6)	-0.06627(6)	0.0073(2)	0.0049(2)	0.0049(2)	0.0001(2)	-0.0002(2)	0.0001(2)	0.0057(1)
P2	0.06219(7)	0.58553(6)	0.23174(6)	0.0070(2)	0.0060(2)	0.0046(2)	-0.0003(2)	-0.0004(2)	-0.0002(2)	0.0059(1)
Be1	0.4288(3)	0.9193(3)	-0.2734(3)	0.009(1)	0.008(1)	0.008(1)	0.000(1)	-0.000(1)	0.001(1)	0.0080(5)
Be2	-0.0739(3)	0.6931(3)	-0.0633(3)	0.009(1)	0.009(1)	0.007(1)	0.001(1)	-0.001(1)	-0.000(1)	0.0084(5)
O1	0.4369(2)	0.6818(2)	0.0703(2)	0.0101(7)	0.0093(7)	0.0075(7)	0.0009(6)	0.0014(6)	0.0008(6)	0.0090(3)
O2	0.2404(2)	0.9069(2)	-0.1991(2)	0.0074(7)	0.0162(8)	0.0071(7)	0.0005(6)	0.0000(6)	-0.0004(6)	0.0102(3)
O3	0.5490(2)	0.8580(2)	-0.1277(2)	0.0106(7)	0.0062(7)	0.0082(7)	0.0018(6)	-0.0025(6)	0.0001(6)	0.0083(3)
O4	0.7383(2)	0.6626(2)	-0.0085(2)	0.0082(7)	0.0111(8)	0.0119(7)	0.0029(6)	-0.0001(6)	-0.0003(6)	0.0104(3)
O5	0.4906(2)	1.0885(2)	-0.3003(2)	0.0143(7)	0.0067(7)	0.0074(7)	0.0018(5)	-0.0028(6)	-0.0011(6)	0.0095(3)
O6	-0.0063(2)	0.9273(2)	0.3062(2)	0.0141(8)	0.0062(7)	0.0084(7)	0.0009(5)	0.0023(6)	0.0007(6)	0.0096(3)
O7	0.0564(2)	0.6876(2)	0.0871(2)	0.0102(7)	0.0087(7)	0.0068(7)	0.0015(6)	-0.0020(6)	-0.0014(6)	0.0085(3)
O8	-0.0555(2)	0.8622(2)	-0.1352(2)	0.0090(7)	0.0067(7)	0.0084(7)	0.0017(6)	0.0022(6)	0.0004(6)	0.0080(3

TABLE 5. Selected bond distances (Å) and angles (°) for strontiohurlbutite

P1-O3	1.549(2)	O2-Be1-O3	103.2(2)
P1-O5	1.541(2)	O5-Be1-O2	113.6(2)
P1-O4	1.509(2)	O5-Be1-O3	103.9(2)
P1-O1	1.538(2)	O1-Be1-O2	108.4(2)
Mean	1.535	O1-Be1-O3	113.4(2)
		O1-Be1-O5	113.9(2)
O5-P1-O3	108.92(8)	Mean	109.39
O4-P1-O3	111.16(9)		
O4-P1-O5	111.62(9)	Be2-O8	1.642(3)
O4-P1-O1	110.68(8)	Be2-O7	1.638(3)
O1-P1-O3	106.14(8)	Be2-O4	1.597(3)
O1-P1-O5	108.12(9)	Be2-O6	1.635(3)
Mean	109.44	Mean	1.628
P2-O8	1.539(2)	O7-Be2-O8	104.8(2)
P2-O2	1.540(2)	O7-Be2-O8	110.6(2)
P2-O7	1.525(2)	O7-Be2-O8	111.6(2)
P2-O6	1.523(2)	O7-Be2-O8	113.2(2)
Mean	1.531	O7-Be2-O8	109.5(2)
		O7-Be2-O8	106.8(2)
O8-P2-O2	106.21(8)	Mean	109.40
O7-P2-O8	112.43(9)		
O7-P2-O2	107.53(9)	Sr-O8	2.588(2)
O6-P2-O8	104.89(9)	Sr-O8’	3.253(2)
O6-P2-O2	113.03(9)	Sr-O2	3.295(2)
O6-P2-O7	112.64(9)	Sr-O2’	2.596(2)
Mean	109.45	Sr-O3	2.591(2)
		Sr-O3’	3.122(2)
Be1-O2	1.637(3)	Sr-O5	2.588(2)
Be1-O3	1.651(3)	Sr-O7	2.579(2)
Be1-O5	1.614(3)	Sr-O6	2.680(2)
Be1-O1	1.600(3)	Sr-O1	2.551(2)
Mean	1.627	Mean	2.784

Table 6. Bond valence sums for strontiohurlbutite

	Sr	P1	P2	Be1	Be2	Σ
O1	0.31	1.23		0.55		2.10
O2	0.27 0.04		1.23	0.50		2.05
O3	0.28 0.07	1.20		0.48		2.03
O4		1.33			0.56	1.89
O5	0.28	1.23		0.53		2.04
O6	0.22		1.29		0.50	2.01
O7	0.29		1.28		0.50	2.07
O8	0.28 0.05		123		0.49	2.06
Σ	2.09	5.00	5.04	2.07	2.05	

TABLE 7. Comparison of the physical properties of strontiohurlbutite and hurlbutite

	Strontiohurlbutite	**Hurlbutite (Mrose 1952)**
Color	light blue	colorless to greenish
Structural formula	$SrBe_2(PO_4)_2$	$CaBe_2(PO_4)_2$
Space group	$P2_1/c$	$P2_1/a$
a	7.997 (1) Å	8.29 Å
b	8.979 (1) Å	8.80 Å
c	8.420 (1) Å	7.81 Å
β	90.18 (1)°	90.5°
V	604.7 (1) $Å^3$	570 $Å^3$
Z	4	4
Density	3.101* g/cm^3 (calc)	2.90* g/cm^3 (calc)

* Density calculation based on the empirical formula