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R-Ferrite-type barium cobalt stannate, $BaCo_2Sn_4O_{11}$

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ(Co–O) = 0.004 Å; disorder in main residue; R factor = 0.018; wR factor = 0.041; data-to-parameter ratio = 8.2.

$BaCo_2Sn_4O_{11}$ is isotypic with *R*-ferrite, $BaTi_2Fe_4O_{11}$. The Co atoms fully occupy trigonal–bipyramidal sites ($\bar{6}m2$) and are disordered with Sn atoms in octahedral sites (.2/*m* symmetry), as represented in the formula $BaCoSn_2(Co_{0.34}Sn_{0.66})_4O_{11}$. Ba atoms are situated in a 12-fold coordinated site ($\bar{6}m2$ symmetry).

Related literature

For reports on *R*-ferrite structures, $BaTi_2Fe_4O_{11}$, see: Haberey & Velicescu (1974); Obradors *et al.* (1983); Cadée & Ijdo (1984); Sosnowska *et al.* (1996). For reports on R-ferrite structure with other compositions, see: Cadée & Ijdo (1984); Kanke *et al.* (1992); Martínez *et al.* (1993); Foo *et al.* (2006). Sosnowska *et al.* (1996). For $Ba_3SnCo_{10}O_{20}$, another phase in the Ba–Co–Sn–O system, see: Sonne & Müller-Buschbaum (1993).

Experimental

Crystal data

$BaCo_2Sn_4O_{11}$
M_r = 905.96
Hexagonal, $P6_3/mmc$
a = 6.0880 (2) Å
c = 14.1049 (6) Å
V = 452.74 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 18.76 mm^{-1}
T = 293 (2) K
0.06 × 0.04 × 0.03 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: numerical (*NUMABS*; Higashi, 1999)
T_{min} = 0.524, T_{max} = 0.801
3945 measured reflections
230 independent reflections
215 reflections with $I > 2\sigma(I)$
R_{int} = 0.072

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.041
S = 1.13
230 reflections
28 parameters
1 restraint
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −1.81 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ba1—O1	2.918 (3)	Sn2—O2	2.127 (3)
Ba1—O2	3.051 (6)	Co2—O2	1.969 (4)
Sn1—O3	2.068 (3)	Co2—O3	2.437 (6)
Sn2—O1	2.040 (3)		
O3—Sn1—O3^{iv}	180	O1—Sn2—O2	89.07 (8)
O3—Sn1—O1^{v}	94.67 (11)	O2^{v}—Co2—O2^{iii}	120
O3^{iv}—Sn1—O1^{v}	85.33 (11)	O2^{v}—Co2—O3	90
O1^{ii}—Sn2—O1	101.38 (11)	O3—Co2—O3^{i}	180
O1^{ii}—Sn2—O2	163.32 (12)		

Symmetry codes: (i) $x, y, -z+\frac{1}{2}$; (ii) $-y, x-y, z$; (iii) $-x+y+1, -x+1, z$; (iv) $-x+1, -y, -z$; (v) $-y+1, x-y, z$.

Data collection: *PROCESS-AUTO* (Rigaku/MSC, 2005); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *VESTA* (Momma & Izumi, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MG2057).

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supplementary materials

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R-Ferrite-type barium cobalt stannate, $BaCo_2Sn_4O_{11}$

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Comment

$BaTi_2Fe_4O_{11}$ crystallizes in a six-layer hexagonal structure (*R*-type, space group $P6_3/mmc$) (Haberey & Velicescu, 1974; Obradors *et al.*, 1983; Cadée & Ijdo, 1984; Sosnowska *et al.*, 1996) that is adopted by many multinary iron oxides and transition metal oxides exhibiting complex magnetic behavior (Cadée & Ijdo, 1984; Kanke *et al.*, 1992; Martínez *et al.*, 1993; Foo *et al.*, 2006). $BaCo_2Sn_4O_{11}$ has been indicated to be the end member in a solid solution series $BaFe_{4-2x}Sn_{2+x}Co_xO_{11}$, where the distribution of Fe, Co, and Sn cations was determined by combined powder X-ray and neutron diffraction (Martínez *et al.*, 1993). However, no crystallographic information (cell parameters and atomic positions) was reported except for the Co and Sn site occupancies in $BaCo_2Sn_4O_{11}$. The present paper reports the detailed structure of $BaCo_2Sn_4O_{11}$ determined by single-crystal X-ray diffraction.

The structure of $BaCo_2Sn_4O_{11}$ can be described in terms of cation-centered oxygen polyhedra (Fig. 1). The disorder within the octahedral 6*g* site (occupancies of 0.664 (7) Sn1 and 0.336 (7) Co1) agrees with results reported by Martínez *et al.* (1993) (0.7 Sn1 and 0.3 Co1). These Sn1/Co1-centered octahedra share edges to form layers perpendicular to the *c* axis. Located between these layers are pillars of two face-sharing Sn2-centered octahedra stacked along the *c* axis. The trigonal bipyramidal 2*d* site is occupied exclusively by Co2 atoms and exhibits a displacement ellipsoid elongated along the *c* direction (Fig. 2). Ba atoms are situated in a 12-fold coordination site (2*c*).

Experimental

A mixture of $BaCO_3$ (99.99%, Wako Pure Chemical Ind.), Co_3O_4 (99.95%, Kanto Chemical Co. Inc.), and SnO_2 (99.9%, Rare Metallic Co. Ltd.) powders in a molar ratio of Ba:Co:Sn = 1:2:4 was ground together and pressed into a pellet. The pellet was placed on a platinum plate and heated in air for 1 h at 1473 K or 1823 K in an electric furnace. The pellet was melted at 1823 K and green transparent single crystals of $BaCo_2Sn_4O_{11}$ were obtained. The chemical analysis of the polycrystalline single phase $BaCo_2Sn_4O_{11}$ prepared at 1473 K was carried out by inductively coupled plasma (ICP) emission spectrometry for Ba, Co and Sn, and by the He carrier melting-infrared absorption method (TC-436, LECO) for O. The results of the chemical analysis (Ba 14.9 (5), Co 13.8 (5), Sn 52.9 (8), and O 19.1 (8) wt%) agreed with the ideal contents (Ba 15.2, Co 13.4, Sn 51.9, O 19.5 wt%).

The magnetic susceptibility of $BaCo_2Sn_4O_{11}$ was measured with a superconducting quantum interference device (SQUID) magnetometer (Quantum Design, MPMS XL) from 5 to 400 K under a magnetic field of 5 kOe. The polycrystalline sample followed the Curie–Weiss law above the Neel temperature (T_N). The T_N of 7 K, the Weiss temperature (Θ) of -42 K, and the magnetic moment (μ_{eff}) of 4.7 μ_B per Co measured for the sample were consistent with the values reported by Martínez *et al.* (1993) (T_N = 9 K, Θ = -44 K, μ_{eff} = 4.4 μ_B).

Refinement

In the structure analysis using powder X-ray and neutron diffraction data for $BaTi_2Fe_4O_{11}$ and $BaSn_2Fe_4O_{11}$ (Obradors *et al.*, 1983; Cadée & Ijdo,1984; Martínez *et al.*, 1993), the 2*d* site of Fe atoms was statistically split into two site (4*f*). We applied this split site model and refined the positional parameter of *z* for the Co2 site, but it converged into 0.250 within an estimated deviation. Thus, we fixed the position at 2*d* site for the final refinement.

Figures

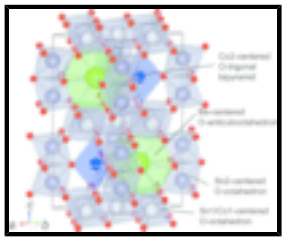


Fig. 1. Structure of $BaCo_2Sn_4O_{11}$ in terms of cation-centered oxygen polyhedra.

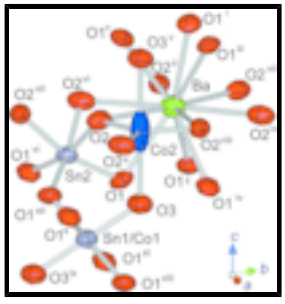


Fig. 2. The O-atom coordination around the cation sites of $BaCo_2Sn_4O_{11}$ (symmetry codes as in Table 1). Displacement ellipsoids are drawn at the 99% probability level.

barium cobalt stannate

Crystal data

$BaCo_2Sn_4O_{11}$	$Z = 2$
$M_r = 905.96$	$F_{000} = 796$
Hexagonal, $P6_3/mmc$	$D_x = 6.646$ Mg m^{-3}
Hall symbol: -P 6c 2c	Mo $K\alpha$ radiation $\lambda = 0.71075$ Å
$a = 6.0880$ (2) Å	Cell parameters from 3536 reflections
$b = 6.0880$ (2) Å	$\theta = 7.7$–54.7º
$c = 14.1049$ (6) Å	$\mu = 18.76$ mm^{-1}
$\alpha = 90$º	$T = 293$ (2) K
$\beta = 90$º	Block, green
$\gamma = 120$º	0.06 × 0.04 × 0.03 mm
$V = 452.74$ (3) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	230 independent reflections

Radiation source: fine-focus sealed tube	215 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.072$
Detector resolution: 10.00 pixels mm^{-1}	$\theta_{max} = 27.4°$
$T = 293(2)$ K	$\theta_{min} = 3.9°$
ω scans	$h = -7 \rightarrow 7$
Absorption correction: numerical (NUMABS; Higashi, 1999)	$k = -7 \rightarrow 7$
$T_{min} = 0.524$, $T_{max} = 0.801$	$l = -18 \rightarrow 18$
3945 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.018$	$w = 1/[\sigma^2(F_o^2) + 0.8941P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.041$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.13$	$\Delta\rho_{max} = 0.73$ e Å^{-3}
230 reflections	$\Delta\rho_{min} = -1.81$ e Å^{-3}
28 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
1 restraint	Extinction coefficient: 0.0041 (4)

Special details

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ba1	0.3333	0.6667	0.2500	0.0147 (2)	
Sn1	0.5000	0.0000	0.0000	0.0112 (3)	0.664 (7)
Co1	0.5000	0.0000	0.0000	0.0112 (3)	0.336 (7)
Sn2	0.0000	0.0000	0.14643 (4)	0.0096 (2)	
Co2	0.6667	0.3333	0.2500	0.0203 (4)	
O1	0.1728 (3)	0.3456 (5)	0.0815 (2)	0.0118 (7)	
O2	0.2933 (8)	0.1466 (4)	0.2500	0.0129 (10)	
O3	0.6667	0.3333	0.0772 (4)	0.0136 (12)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.0169 (3)	0.0169 (3)	0.0103 (4)	0.00844 (15)	0.000	0.000

Sn1	0.0139 (4)	0.0110 (4)	0.0076 (4)	0.0055 (2)	0.00013 (10)	0.0003 (2)
Co1	0.0139 (4)	0.0110 (4)	0.0076 (4)	0.0055 (2)	0.00013 (10)	0.0003 (2)
Sn2	0.0113 (3)	0.0113 (3)	0.0062 (3)	0.00563 (14)	0.000	0.000
Co2	0.0086 (5)	0.0086 (5)	0.0436 (13)	0.0043 (3)	0.000	0.000
O1	0.0139 (12)	0.0132 (17)	0.0080 (17)	0.0066 (8)	0.0015 (6)	0.0030 (13)
O2	0.010 (2)	0.0174 (18)	0.009 (2)	0.0051 (11)	0.000	0.000
O3	0.0159 (18)	0.0159 (18)	0.009 (3)	0.0080 (9)	0.000	0.000

Geometric parameters (Å, °)

Ba1—O1^{i}	2.918 (3)	Sn2—O2^{xii}	2.127 (3)
Ba1—O1^{ii}	2.918 (3)	Sn2—Sn2^{v}	2.9217 (11)
Ba1—O1^{iii}	2.918 (3)	Sn2—O3^{xvi}	3.6479 (15)
Ba1—O1	2.918 (3)	Sn2—O3^{xvii}	3.6479 (15)
Ba1—O1^{iv}	2.918 (3)	Sn2—O3	3.6479 (15)
Ba1—O1^{v}	2.918 (3)	Sn2—Ba1^{xviii}	3.8064 (2)
Ba1—O2^{ii}	3.051 (6)	Sn2—Co2^{xvi}	3.8064 (2)
Ba1—O2^{vi}	3.051 (6)	Co2—O2^{x}	1.969 (4)
Ba1—O2^{vii}	3.051 (6)	Co2—O2^{viii}	1.969 (4)
Ba1—O2^{iv}	3.051 (6)	Co2—O2	1.969 (4)
Ba1—O2	3.051 (6)	Co2—O3	2.437 (6)
Ba1—O2^{viii}	3.051 (6)	Co2—O3^{v}	2.437 (6)
Sn1—O3	2.068 (3)	Co2—Ba1^{xix}	3.51492 (11)
Sn1—O3^{ix}	2.068 (3)	O1—Co1^{viii}	2.074 (2)
Sn1—O1^{x}	2.074 (2)	O1—Sn1^{viii}	2.074 (2)
Sn1—O1^{xi}	2.074 (2)	O1—Co1^{vi}	2.074 (2)
Sn1—O1^{xii}	2.074 (2)	O1—Sn1^{vi}	2.074 (2)
Sn1—O1^{xiii}	2.074 (2)	O1—O3^{xx}	2.806 (5)
Sn1—Sn1^{x}	3.04401 (10)	O1—O3	3.045 (2)
Sn1—Sn1^{xiv}	3.04401 (10)	O1—O3^{xvi}	3.045 (2)
Sn1—Co1^{x}	3.04401 (10)	O1—Co2^{xvi}	3.8627 (19)
Sn1—Co1^{xiv}	3.04401 (10)	O2—Sn2^{v}	2.127 (3)
Sn1—Sn1^{xv}	3.04401 (10)	O2—Ba1^{xviii}	3.052 (3)
Sn1—Co1^{xv}	3.04401 (10)	O2—O3^{v}	3.133 (5)
Sn2—O1^{vi}	2.040 (3)	O2—O3	3.133 (5)
Sn2—O1	2.040 (3)	O3—Co1^{x}	2.068 (3)
Sn2—O1^{xii}	2.040 (3)	O3—Sn1^{x}	2.068 (3)
Sn2—O2	2.127 (3)	O3—Co1^{viii}	2.068 (3)
Sn2—O2^{vi}	2.127 (3)	O3—Sn1^{viii}	2.068 (3)
O1^{i}—Ba1—O1^{ii}	109.09 (11)	O2—Sn2—Sn2^{v}	46.63 (8)
O1^{i}—Ba1—O1^{iii}	60.31 (9)	O2^{vi}—Sn2—Sn2^{v}	46.63 (8)
O1^{ii}—Ba1—O1^{iii}	146.28 (5)	O2^{xii}—Sn2—Sn2^{v}	46.63 (8)

O1^{i}—Ba1—O1	146.28 (5)	O1^{vi}—Sn2—O3^{xvi}	56.59 (3)
O1^{ii}—Ba1—O1	60.31 (9)	O1—Sn2—O3^{xvi}	56.59 (3)
O1^{iii}—Ba1—O1	146.28 (5)	O1^{xii}—Sn2—O3^{xvi}	137.79 (12)
O1^{i}—Ba1—O1^{iv}	146.28 (5)	O2—Sn2—O3^{xvi}	122.27 (6)
O1^{ii}—Ba1—O1^{iv}	60.31 (9)	O2^{vi}—Sn2—O3^{xvi}	58.89 (11)
O1^{iii}—Ba1—O1^{iv}	109.09 (12)	O2^{xii}—Sn2—O3^{xvi}	122.27 (6)
O1—Ba1—O1^{iv}	60.31 (9)	Sn2^{v}—Sn2—O3^{xvi}	105.52 (8)
O1^{i}—Ba1—O1^{v}	60.31 (9)	O1^{vi}—Sn2—O3^{xvii}	56.59 (3)
O1^{ii}—Ba1—O1^{v}	146.28 (5)	O1—Sn2—O3^{xvii}	137.79 (12)
O1^{iii}—Ba1—O1^{v}	60.31 (9)	O1^{xii}—Sn2—O3^{xvii}	56.59 (3)
O1—Ba1—O1^{v}	109.09 (11)	O2—Sn2—O3^{xvii}	122.27 (6)
O1^{iv}—Ba1—O1^{v}	146.28 (5)	O2^{vi}—Sn2—O3^{xvii}	122.27 (6)
O1^{i}—Ba1—O2^{ii}	58.59 (5)	O2^{xii}—Sn2—O3^{xvii}	58.89 (11)
O1^{ii}—Ba1—O2^{ii}	58.59 (5)	Sn2^{v}—Sn2—O3^{xvii}	105.52 (8)
O1^{iii}—Ba1—O2^{ii}	118.76 (5)	O3^{xvi}—Sn2—O3^{xvii}	113.12 (7)
O1—Ba1—O2^{ii}	92.30 (4)	O1^{vi}—Sn2—O3	137.79 (12)
O1^{iv}—Ba1—O2^{ii}	118.76 (5)	O1—Sn2—O3	56.59 (3)
O1^{v}—Ba1—O2^{ii}	92.30 (5)	O1^{xii}—Sn2—O3	56.59 (3)
O1^{i}—Ba1—O2^{vi}	92.30 (4)	O2—Sn2—O3	58.89 (11)
O1^{ii}—Ba1—O2^{vi}	92.30 (4)	O2^{vi}—Sn2—O3	122.27 (6)
O1^{iii}—Ba1—O2^{vi}	118.76 (5)	O2^{xii}—Sn2—O3	122.27 (6)
O1—Ba1—O2^{vi}	58.59 (5)	Sn2^{v}—Sn2—O3	105.52 (8)
O1^{iv}—Ba1—O2^{vi}	118.76 (5)	O3^{xvi}—Sn2—O3	113.12 (7)
O1^{v}—Ba1—O2^{vi}	58.59 (5)	O3^{xvii}—Sn2—O3	113.12 (7)
O2^{ii}—Ba1—O2^{vi}	67.94 (15)	O1^{vi}—Sn2—Ba1^{xviii}	125.796 (15)
O1^{i}—Ba1—O2^{vii}	58.59 (5)	O1—Sn2—Ba1^{xviii}	125.796 (15)
O1^{ii}—Ba1—O2^{vii}	58.59 (5)	O1^{xii}—Sn2—Ba1^{xviii}	49.26 (9)
O1^{iii}—Ba1—O2^{vii}	92.30 (4)	O2—Sn2—Ba1^{xviii}	53.189 (6)
O1—Ba1—O2^{vii}	118.76 (5)	O2^{vi}—Sn2—Ba1^{xviii}	114.06 (8)
O1^{iv}—Ba1—O2^{vii}	92.30 (4)	O2^{xii}—Sn2—Ba1^{xviii}	53.189 (6)
O1^{v}—Ba1—O2^{vii}	118.76 (5)	Sn2^{v}—Sn2—Ba1^{xviii}	67.432 (8)
O2^{ii}—Ba1—O2^{vii}	52.06 (15)	O3^{xvi}—Sn2—Ba1^{xviii}	172.95 (8)
O2^{vi}—Ba1—O2^{vii}	120.000 (1)	O3^{xvii}—Sn2—Ba1^{xviii}	69.99 (4)
O1^{i}—Ba1—O2^{iv}	92.30 (4)	O3—Sn2—Ba1^{xviii}	69.99 (4)
O1^{ii}—Ba1—O2^{iv}	92.30 (4)	O1^{vi}—Sn2—Co2^{xvi}	76.11 (5)
O1^{iii}—Ba1—O2^{iv}	58.59 (5)	O1—Sn2—Co2^{xvi}	76.11 (5)
O1—Ba1—O2^{iv}	118.76 (5)	O1^{xii}—Sn2—Co2^{xvi}	175.88 (9)
O1^{iv}—Ba1—O2^{iv}	58.59 (5)	O2—Sn2—Co2^{xvi}	94.13 (5)
O1^{v}—Ba1—O2^{iv}	118.76 (5)	O2^{vi}—Sn2—Co2^{xvi}	20.80 (8)
O2^{ii}—Ba1—O2^{iv}	120.0	O2^{xii}—Sn2—Co2^{xvi}	94.13 (5)
O2^{vi}—Ba1—O2^{iv}	172.06 (15)	Sn2^{v}—Sn2—Co2^{xvi}	67.432 (8)

$O2^{vii}$—Ba1—$O2^{iv}$	67.94 (15)	$O3^{xvi}$—Sn2—$Co2^{xvi}$	38.09 (8)
$O1^{i}$—Ba1—O2	118.76 (5)	$O3^{xvii}$—Sn2—$Co2^{xvi}$	123.20 (2)
$O1^{ii}$—Ba1—O2	118.76 (5)	O3—Sn2—$Co2^{xvi}$	123.20 (2)
$O1^{iii}$—Ba1—O2	92.30 (4)	$Ba1^{xviii}$—Sn2—$Co2^{xvi}$	134.863 (15)
O1—Ba1—O2	58.59 (5)	$O2^{x}$—Co2—$O2^{viii}$	120.000 (1)
$O1^{iv}$—Ba1—O2	92.30 (4)	$O2^{x}$—Co2—O2	120.0
$O1^{v}$—Ba1—O2	58.59 (5)	$O2^{viii}$—Co2—O2	120.0
$O2^{ii}$—Ba1—O2	120.0	$O2^{x}$—Co2—O3	90.0
$O2^{vi}$—Ba1—O2	52.06 (15)	$O2^{viii}$—Co2—O3	90.000 (1)
$O2^{vii}$—Ba1—O2	172.06 (15)	O2—Co2—O3	90.0
$O2^{iv}$—Ba1—O2	120.0	$O2^{x}$—Co2—$O3^{v}$	90.0
$O1^{i}$—Ba1—$O2^{viii}$	118.76 (5)	$O2^{viii}$—Co2—$O3^{v}$	90.0
$O1^{ii}$—Ba1—$O2^{viii}$	118.76 (5)	O2—Co2—$O3^{v}$	90.0
$O1^{iii}$—Ba1—$O2^{viii}$	58.59 (5)	O3—Co2—$O3^{v}$	180.0
O1—Ba1—$O2^{viii}$	92.30 (4)	$O2^{x}$—Co2—$Ba1^{xix}$	60.0
$O1^{iv}$—Ba1—$O2^{viii}$	58.59 (5)	$O2^{viii}$—Co2—$Ba1^{xix}$	60.0
$O1^{v}$—Ba1—$O2^{viii}$	92.30 (4)	O2—Co2—$Ba1^{xix}$	180.0
$O2^{ii}$—Ba1—$O2^{viii}$	172.06 (15)	O3—Co2—$Ba1^{xix}$	90.0
$O2^{vi}$—Ba1—$O2^{viii}$	120.0	$O3^{v}$—Co2—$Ba1^{xix}$	90.0
$O2^{vii}$—Ba1—$O2^{viii}$	120.0	Sn2—O1—$Co1^{viii}$	126.84 (8)
$O2^{iv}$—Ba1—$O2^{viii}$	52.06 (15)	Sn2—O1—$Sn1^{viii}$	126.84 (8)
O2—Ba1—$O2^{viii}$	67.94 (15)	$Co1^{viii}$—O1—$Sn1^{viii}$	0.0
O3—Sn1—$O3^{ix}$	180.0 (3)	Sn2—O1—$Co1^{vi}$	126.84 (8)
O3—Sn1—$O1^{x}$	94.67 (11)	$Co1^{viii}$—O1—$Co1^{vi}$	94.45 (12)
$O3^{ix}$—Sn1—$O1^{x}$	85.33 (11)	$Sn1^{viii}$—O1—$Co1^{vi}$	94.45 (12)
O3—Sn1—$O1^{xi}$	85.33 (11)	Sn2—O1—$Sn1^{vi}$	126.84 (8)
$O3^{ix}$—Sn1—$O1^{xi}$	94.67 (11)	$Co1^{viii}$—O1—$Sn1^{vi}$	94.45 (12)
$O1^{x}$—Sn1—$O1^{xi}$	180.00 (14)	$Sn1^{viii}$—O1—$Sn1^{vi}$	94.45 (12)
O3—Sn1—$O1^{xii}$	94.67 (11)	$Co1^{vi}$—O1—$Sn1^{vi}$	0.0
$O3^{ix}$—Sn1—$O1^{xii}$	85.33 (11)	Sn2—O1—$O3^{xx}$	153.78 (16)
$O1^{x}$—Sn1—$O1^{xii}$	89.97 (16)	$Co1^{viii}$—O1—$O3^{xx}$	47.25 (6)
$O1^{xi}$—Sn1—$O1^{xii}$	90.03 (16)	$Sn1^{viii}$—O1—$O3^{xx}$	47.25 (6)
O3—Sn1—$O1^{xiii}$	85.33 (11)	$Co1^{vi}$—O1—$O3^{xx}$	47.25 (6)
$O3^{ix}$—Sn1—$O1^{xiii}$	94.67 (11)	$Sn1^{vi}$—O1—$O3^{xx}$	47.25 (6)
$O1^{x}$—Sn1—$O1^{xiii}$	90.03 (16)	Sn2—O1—Ba1	98.77 (12)
$O1^{xi}$—Sn1—$O1^{xiii}$	89.97 (16)	$Co1^{viii}$—O1—Ba1	102.93 (9)
$O1^{xii}$—Sn1—$O1^{xiii}$	180.00 (14)	$Sn1^{viii}$—O1—Ba1	102.93 (9)
O3—Sn1—$Sn1^{x}$	42.60 (9)	$Co1^{vi}$—O1—Ba1	102.93 (9)
$O3^{ix}$—Sn1—$Sn1^{x}$	137.40 (9)	$Sn1^{vi}$—O1—Ba1	102.93 (9)
$O1^{x}$—Sn1—$Sn1^{x}$	91.55 (7)	$O3^{xx}$—O1—Ba1	107.45 (11)
$O1^{xi}$—Sn1—$Sn1^{x}$	88.45 (7)	Sn2—O1—O3	89.42 (7)

O1^{xii}—Sn1—Sn1^{x}	137.22 (6)	Co1^{viii}—O1—O3	42.59 (8)
O1^{xiii}—Sn1—Sn1^{x}	42.78 (6)	Sn1^{viii}—O1—O3	42.59 (8)
O3—Sn1—Sn1^{xiv}	137.40 (9)	Co1^{vi}—O1—O3	136.98 (15)
O3^{ix}—Sn1—Sn1^{xiv}	42.60 (9)	Sn1^{vi}—O1—O3	136.98 (15)
O1^{x}—Sn1—Sn1^{xiv}	88.45 (7)	O3^{xx}—O1—O3	89.84 (10)
O1^{xi}—Sn1—Sn1^{xiv}	91.55 (7)	Ba1—O1—O3	91.63 (10)
O1^{xii}—Sn1—Sn1^{xiv}	42.78 (6)	Sn2—O1—O3^{xvi}	89.42 (7)
O1^{xiii}—Sn1—Sn1^{xiv}	137.22 (6)	Co1^{viii}—O1—O3^{xvi}	136.98 (15)
Sn1^{x}—Sn1—Sn1^{xiv}	180.0	Sn1^{viii}—O1—O3^{xvi}	136.98 (15)
O3—Sn1—Co1^{x}	42.60 (9)	Co1^{vi}—O1—O3^{xvi}	42.59 (8)
O3^{ix}—Sn1—Co1^{x}	137.40 (9)	Sn1^{vi}—O1—O3^{xvi}	42.59 (8)
O1^{x}—Sn1—Co1^{x}	91.55 (7)	O3^{xx}—O1—O3^{xvi}	89.84 (10)
O1^{xi}—Sn1—Co1^{x}	88.45 (7)	Ba1—O1—O3^{xvi}	91.63 (10)
O1^{xii}—Sn1—Co1^{x}	137.22 (6)	O3—O1—O3^{xvi}	176.68 (18)
O1^{xiii}—Sn1—Co1^{x}	42.78 (6)	Sn2—O1—Co2	73.06 (6)
Sn1^{x}—Sn1—Co1^{x}	0.0	Co1^{viii}—O1—Co2	76.66 (3)
Sn1^{xiv}—Sn1—Co1^{x}	180.0	Sn1^{viii}—O1—Co2	76.66 (3)
O3—Sn1—Co1^{xiv}	137.40 (9)	Co1^{vi}—O1—Co2	157.83 (12)
O3^{ix}—Sn1—Co1^{xiv}	42.60 (9)	Sn1^{vi}—O1—Co2	157.83 (12)
O1^{x}—Sn1—Co1^{xiv}	88.45 (7)	O3^{xx}—O1—Co2	120.06 (6)
O1^{xi}—Sn1—Co1^{xiv}	91.55 (7)	Ba1—O1—Co2	60.56 (4)
O1^{xii}—Sn1—Co1^{xiv}	42.78 (6)	O3—O1—Co2	39.11 (11)
O1^{xiii}—Sn1—Co1^{xiv}	137.22 (6)	O3^{xvi}—O1—Co2	143.08 (14)
Sn1^{x}—Sn1—Co1^{xiv}	180.0	Sn2—O1—Co2^{xvi}	73.06 (6)
Sn1^{xiv}—Sn1—Co1^{xiv}	0.0	Co1^{viii}—O1—Co2^{xvi}	157.83 (12)
Co1^{x}—Sn1—Co1^{xiv}	180.0	Sn1^{viii}—O1—Co2^{xvi}	157.83 (12)
O3—Sn1—Sn1^{xv}	137.40 (9)	Co1^{vi}—O1—Co2^{xvi}	76.66 (3)
O3^{ix}—Sn1—Sn1^{xv}	42.60 (9)	Sn1^{vi}—O1—Co2^{xvi}	76.66 (3)
O1^{x}—Sn1—Sn1^{xv}	42.78 (6)	O3^{xx}—O1—Co2^{xvi}	120.06 (6)
O1^{xi}—Sn1—Sn1^{xv}	137.22 (6)	Ba1—O1—Co2^{xvi}	60.56 (4)
O1^{xii}—Sn1—Sn1^{xv}	88.45 (7)	O3—O1—Co2^{xvi}	143.08 (14)
O1^{xiii}—Sn1—Sn1^{xv}	91.55 (7)	O3^{xvi}—O1—Co2^{xvi}	39.11 (11)
Sn1^{x}—Sn1—Sn1^{xv}	120.0	Co2—O1—Co2^{xvi}	104.01 (7)
Sn1^{xiv}—Sn1—Sn1^{xv}	60.0	Co2—O2—Sn2	136.63 (8)
Co1^{x}—Sn1—Sn1^{xv}	120.0	Co2—O2—Sn2^{v}	136.63 (8)
Co1^{xiv}—Sn1—Sn1^{xv}	60.0	Sn2—O2—Sn2^{v}	86.75 (15)
O3—Sn1—Co1^{xv}	137.40 (9)	Co2—O2—Ba1^{xviii}	86.03 (8)
O3^{ix}—Sn1—Co1^{xv}	42.60 (9)	Sn2—O2—Ba1^{xviii}	92.88 (5)
O1^{x}—Sn1—Co1^{xv}	42.78 (6)	Sn2^{v}—O2—Ba1^{xviii}	92.88 (5)
O1^{xi}—Sn1—Co1^{xv}	137.22 (6)	Co2—O2—Ba1	86.03 (8)
O1^{xii}—Sn1—Co1^{xv}	88.45 (7)	Sn2—O2—Ba1	92.88 (5)

O1^{xiii}—Sn1—Co1^{xv}	91.55 (7)	Sn2^{v}—O2—Ba1	92.88 (5)
Sn1^{x}—Sn1—Co1^{xv}	120.0	Ba1^{xviii}—O2—Ba1	172.06 (15)
Sn1^{xiv}—Sn1—Co1^{xv}	60.0	Co2—O2—O3^{v}	51.07 (9)
Co1^{x}—Sn1—Co1^{xv}	120.0	Sn2—O2—O3^{v}	172.31 (15)
Co1^{xiv}—Sn1—Co1^{xv}	60.0	Sn2^{v}—O2—O3^{v}	85.56 (7)
Sn1^{xv}—Sn1—Co1^{xv}	0.0	Ba1^{xviii}—O2—O3^{v}	87.51 (5)
O1^{vi}—Sn2—O1	101.38 (11)	Ba1—O2—O3^{v}	87.51 (5)
O1^{vi}—Sn2—O1^{xii}	101.38 (11)	Co2—O2—O3	51.07 (9)
O1—Sn2—O1^{xii}	101.38 (11)	Sn2—O2—O3	85.56 (7)
O1^{vi}—Sn2—O2	163.32 (12)	Sn2^{v}—O2—O3	172.31 (15)
O1—Sn2—O2	89.07 (8)	Ba1^{xviii}—O2—O3	87.51 (5)
O1^{xii}—Sn2—O2	89.07 (8)	Ba1—O2—O3	87.51 (5)
O1^{vi}—Sn2—O2^{vi}	89.07 (8)	O3^{v}—O2—O3	102.13 (17)
O1—Sn2—O2^{vi}	89.07 (8)	Sn1—O3—Co1^{x}	94.80 (17)
O1^{xii}—Sn2—O2^{vi}	163.32 (12)	Sn1—O3—Sn1^{x}	94.80 (17)
O2—Sn2—O2^{vi}	78.03 (12)	Co1^{x}—O3—Sn1^{x}	0.0
O1^{vi}—Sn2—O2^{xii}	89.07 (8)	Sn1—O3—Co1^{viii}	94.80 (17)
O1—Sn2—O2^{xii}	163.32 (12)	Co1^{x}—O3—Co1^{viii}	94.80 (17)
O1^{xii}—Sn2—O2^{xii}	89.07 (8)	Sn1^{x}—O3—Co1^{viii}	94.80 (17)
O2—Sn2—O2^{xii}	78.03 (12)	Sn1—O3—Sn1^{viii}	94.80 (17)
O2^{vi}—Sn2—O2^{xii}	78.03 (12)	Co1^{x}—O3—Sn1^{viii}	94.80 (17)
O1^{vi}—Sn2—Sn2^{v}	116.69 (9)	Sn1^{x}—O3—Sn1^{viii}	94.80 (17)
O1—Sn2—Sn2^{v}	116.69 (9)	Co1^{viii}—O3—Sn1^{viii}	0.0
O1^{xii}—Sn2—Sn2^{v}	116.69 (9)		

Symmetry codes: (i) −*x*+*y*, −*x*+1, −*z*+1/2; (ii) −*x*+*y*, −*x*+1, *z*; (iii) −*y*+1, *x*−*y*+1, −*z*+1/2; (iv) −*y*+1, *x*−*y*+1, *z*; (v) *x*, *y*, −*z*+1/2; (vi) −*y*, *x*−*y*, *z*; (vii) *x*, *y*+1, *z*; (viii) −*x*+*y*+1, −*x*+1, *z*; (ix) −*x*+1, −*y*, −*z*; (x) −*y*+1, *x*−*y*, *z*; (xi) *y*, −*x*+*y*, −*z*; (xii) −*x*+*y*, −*x*, *z*; (xiii) *x*−*y*+1, *x*, −*z*; (xiv) −*y*, *x*−*y*−1, *z*; (xv) −*x*+*y*+1, −*x*, *z*; (xvi) *x*−1, *y*, *z*; (xvii) *x*−1, *y*−1, *z*; (xviii) *x*, *y*−1, *z*; (xix) *x*+1, *y*, *z*; (xx) −*x*+1, −*y*+1, −*z*.

Fig. 1

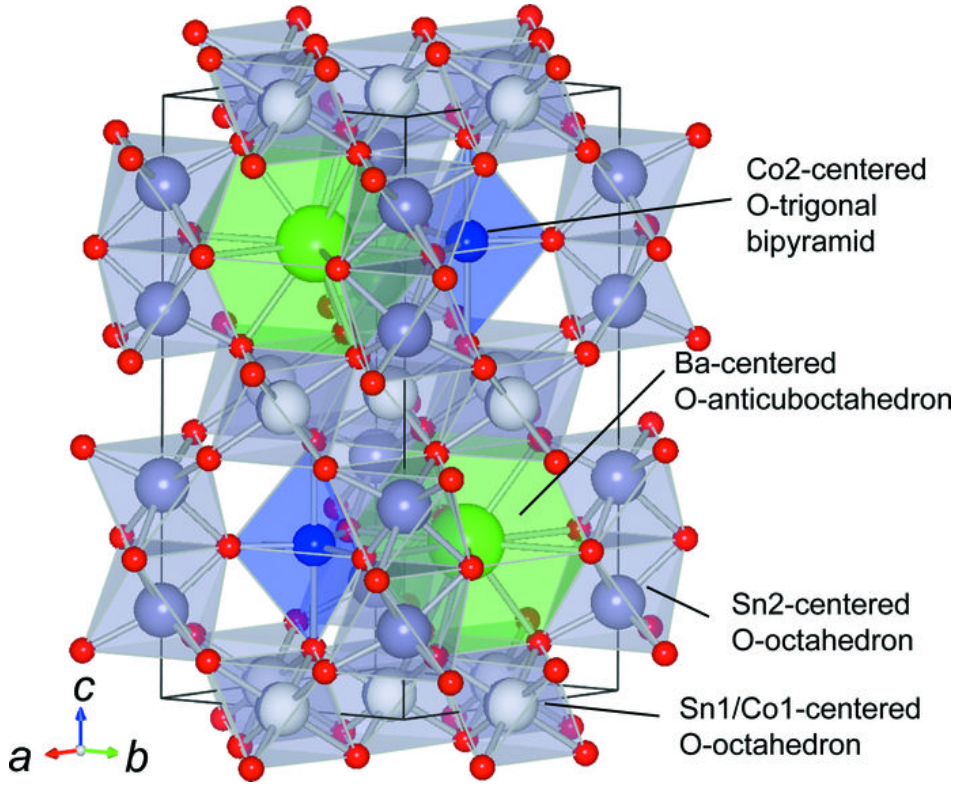
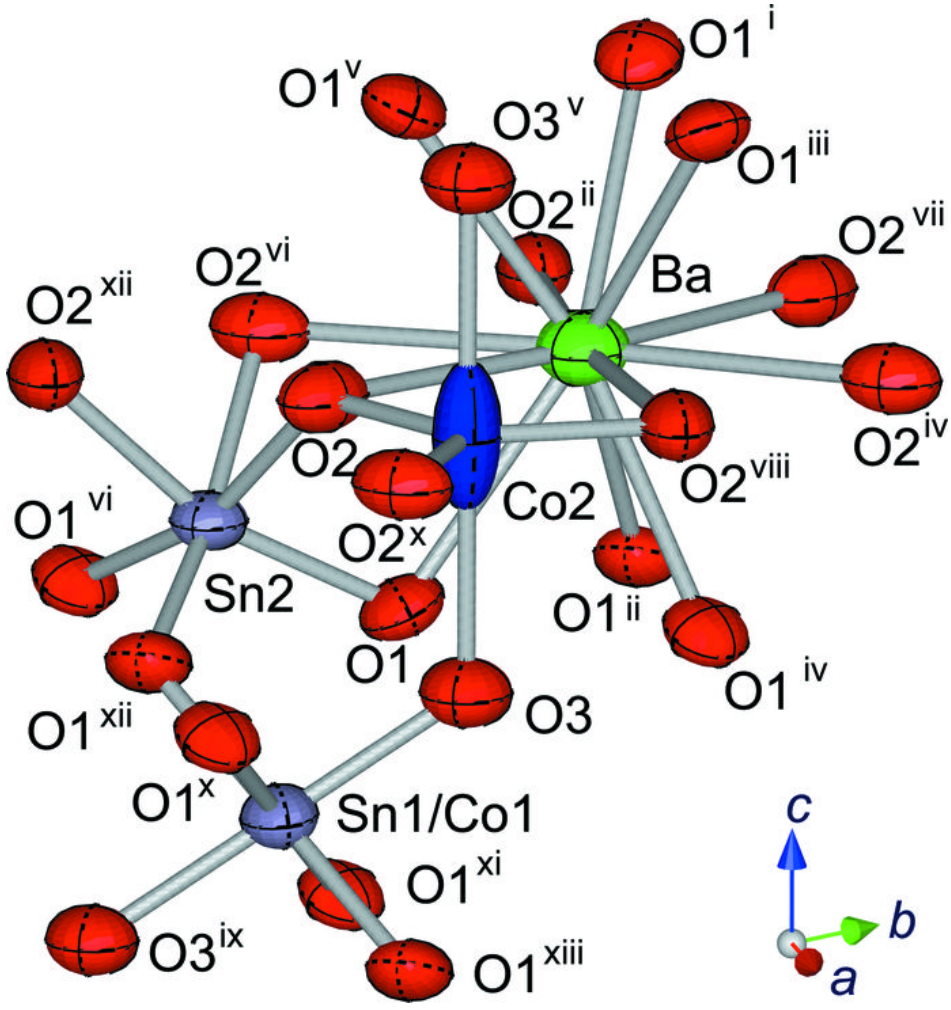

Co2-centered
O-trigonal
bipyramid
Ba-centered
O-anticuboctahedron
Sn2-centered
O-octahedron
Sn1/Co1-centered
O-octahedron
c
a
b

Fig. 2


O1 i
O1 v
O3 v
O1 iii
O2 ii
O2 vii
O2 vi
Ba
O2 xii
O2 iv
O2
O2 viii
Co2
O1 vi
O2 x
Sn2
O1 ii
O1
O1 iv
O3
O1 xii
O1 x
Sn1/Co1
O1 xi
O3 ix
O1 xiii
c
b
a