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Crystal structure of $Ba_2Co(BO_3)_2$

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Single crystals of dibarium cobalt(II) bis(orthoborate), $Ba_2Co(BO_3)_2$, have been obtained from the melt. The crystal structure is composed of two isolated $(BO_3)^{3-}$ triangles linked to Co^{2+} cations. The resulting $[CoO_5]$ square pyramids and the borate anions make up branched rows extending parallel to [010]. The barium cations occupy two sites in the voids of this arrangement and exhibit coordination numbers of nine each. A comparison with the structures of other $A_2M(BO_3)_2$ compounds reveals a unique five-coordination of the small metal M in the title compound instead of four- or six-coordination for the other $A_2M(BO_3)_2$ compounds with M = Cu, Zn, Mg, Ca, or Cd.

1. Chemical context

The crystal chemistry of borates differs from those of silicates, phosphates, sulfates, carbonates or nitrates due to the possibility of forming borate anions with trigonal–planar and tetrahedral configurations (Zhang *et al.*, 2011*a*; Filatov & Bubnova, 2000; Chen *et al.*, 2005; Reshak, 2016). In general, borate compounds are applied in different fields, such as non-linear optical (NLO) materials (Becker, 1998), for photoluminescence (Mergen & Pekgözlü, 2013), for their optical properties (Zhang *et al.*, 2011*b*; Lv *et al.*, 2018), or as ferroelectrics (Dhanasekaran, 2009; Murugan *et al.*, 2001). The borate systems $A_2M(BO_3)_2$, where A = Ba, Sr, Pb and M = Cu, Mg, Cd, Ca, Zn, have been studied previously. For these compounds, several structures types have been reported that depend on the size and nature of the A and M atoms, as shown in Table 1.

In this investigation we have isolated single crystals of $Ba_2Co(BO_3)_2$ from the melt. The new compound crystallizes in the monoclinic system in the same space-group type as some other $A_2M(BO_3)_2$ compounds, but with different cell parameters (Table 1).

2. Structural commentary

In the crystal structure of the title compound, except for the two oxygen atoms O1 and O3 that lie in general positions of the $C2/m$ space group, all atoms are located on a mirror plane (Wyckoff position 4i).

The principal building units in the crystal structure are two trigonal–planar borate anions, one five-coordinate Co^{2+} cation and two nine-coordinate Ba^{2+} cations (Fig. 1). Relevant bond lengths and angles are collated in Table 2. The borate anions are isolated from each other. $(B2O_3)$ anions and $[CoO_5]$

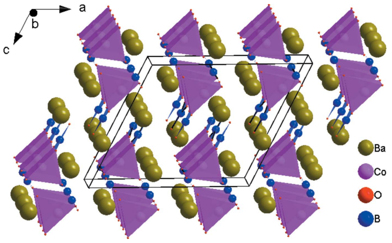

Table 1
Lattice parameters (Å, °), space groups and references for $A_2M(BO_3)_2$ compounds.

Formula	a	b	c	β	Z	Space group	Reference
$Ba_2Ca(BO_3)_2$	9.362 (2)	5.432 (2)	6.635 (2)	119.38 (1)	2	$C2/m$	Akella & Keszler (1995)
$Ba_2Cd(BO_3)_2$	9.6305 (4)	5.3626 (3)	6.5236 (2)	118.079 (3)	2	$C2/m$	Zhang *et al.* (2011*b*)
$Sr_2Mg(BO_3)_2$	9.046 (4)	5.1579 (9)	6.103 (3)	118.691	2	$C2/m$	Chen *et al.* (2007)
$Ba_2Co(BO_3)_2$	11.9784 (4)	5.3256 (2)	10.3220 (3)	117.494 (1)	4	$C2/m$	This work
α-$Sr_2Cu(BO_3)_2$	5.707 (1)	8.796 (2)	6.027 (1)	116.98	2	$P2_1/c$	Smith & Keszler (1989)
$Pb_2Cu(BO_3)_2$	5.6311 (6)	8.7628 (9)	6.2025 (6)	115.706 (1)	2	$P2_1/c$	Pan *et al.* (2006)
$Ba_2Cu(BO_3)_2$	8.023 (1)	11.290 (1)	13.889 (1)		8	$Pnma$	Smith & Keszler (1990)
β-$Sr_2Cu(BO_3)_2$	7.612 (3)	10.854 (7)	13.503 (4)		8	$Pnma$	Smith & Keszler (1989)
$Ba_2Zn(BO_3)_2$	15.068 (2)	8.720 (2)	10.128 (3)		8	$Pca2_1$	Smith & Koliha (1994)
$Ba_2Mg(BO_3)_2$	5.343 (2)	5.343 (2)	16.520 (3)		3	$R\bar{3}m$	Kokh *et al.* (2017)

Table 2
Selected geometric parameters (Å, °).

Ba1—O3	2.7232 (12)	Co1—O2^{iv}	2.0152 (18)
Ba1—O4	2.7266 (4)	Co1—O1	2.0432 (11)
Ba1—O1^{i}	2.7697 (11)	Co1—O3	2.1043 (12)
Ba1—O4^{ii}	2.8215 (19)	B1—O2	1.364 (3)
Ba1—O3^{i}	2.9272 (12)	B1—O1	1.3943 (16)
Ba2—O3	2.7688 (12)	B1—O1^{v}	1.3943 (16)
Ba2—O1^{iii}	2.8064 (11)	B2—O4	1.377 (3)
Ba2—O2^{iv}	2.9009 (8)	B2—O3^{vi}	1.3920 (17)
Ba2—O1^{iv}	2.9668 (12)	B2—O3	1.3920 (17)
Ba2—O4^{ii}	3.1360 (17)		
O2—B1—O1	120.42 (9)	O4—B2—O3^{vi}	122.38 (9)
O2—B1—O1^{v}	120.42 (9)	O4—B2—O3	122.38 (9)
O1—B1—O1^{v}	119.16 (18)	O3^{vi}—B2—O3	115.18 (19)

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+\frac{3}{2}, -y+\frac{1}{2}, -z+1$; (iii) $x+\frac{1}{2}, -y+\frac{1}{2}, z$; (iv) $-x+\frac{3}{2}, -y+\frac{1}{2}, -z+2$; (v) $x, -y, z$; (vi) $x, -y+1, z$.

polyhedra share one edge to form a $\{BCoO_6\}$ group, whereas the $(B1O_3)$ anion is connected through its corners to three different $\{BCoO_6\}$ groups. This arrangement leads to the formation of branched rows extending parallel to [010], as shown in Fig. 2. The rows are linked by pairs of $[BaO_9]$ polyhedra (Fig. 3) into a three-dimensional framework, as shown in Figs. 4 and 5.

The slight deviation of the boron atoms from a planar environment by oxygen atoms is reflected in the maximum deviation of 0.007 (3) Å for B1, compared with 0.019 (3) Å for B2. The average distances B1—O = 1.384 Å and B2—O =

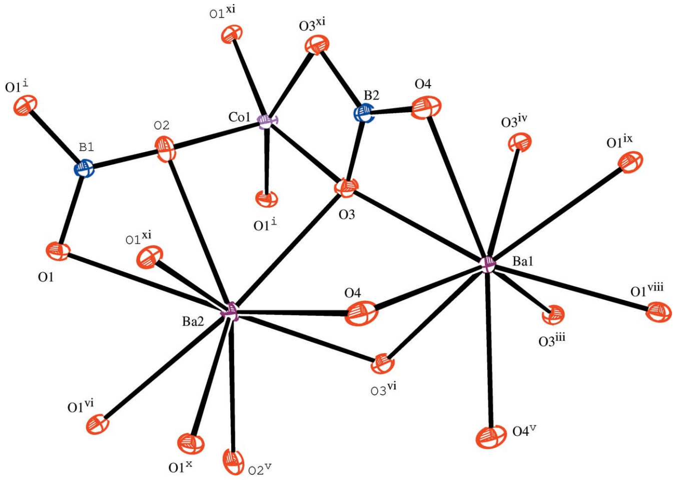

Figure 1
The principal building units in the structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $x, -y, z$; (ii) $x, y-1, z$; (iii) $-x+1, -y, -z+1$; (iv) $-x+1, y, -z+1$; (v) $-x+\frac{3}{2}, -y+\frac{1}{2}, -z+1$; (vi) $x+\frac{1}{2}, -y+\frac{1}{2}, z$; (vii) $x+\frac{1}{2}, y-\frac{1}{2}, z$; (viii) $-x+\frac{3}{2}, -y+\frac{1}{2}, -z+2$; (ix) $-x+\frac{3}{2}, -y-\frac{1}{2}, -z+2$; (x) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+2$; (xi) $x, -y+1, z$.]

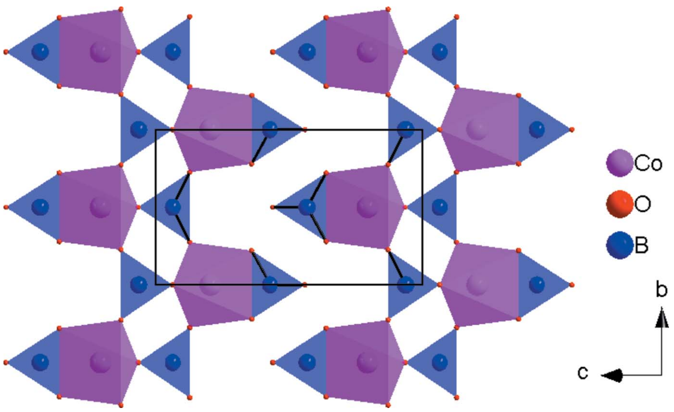

Figure 2
Edge- and corner-sharing $[CoO_5]$ and (BO_3) polyhedra forming branched rows parallel to [010].

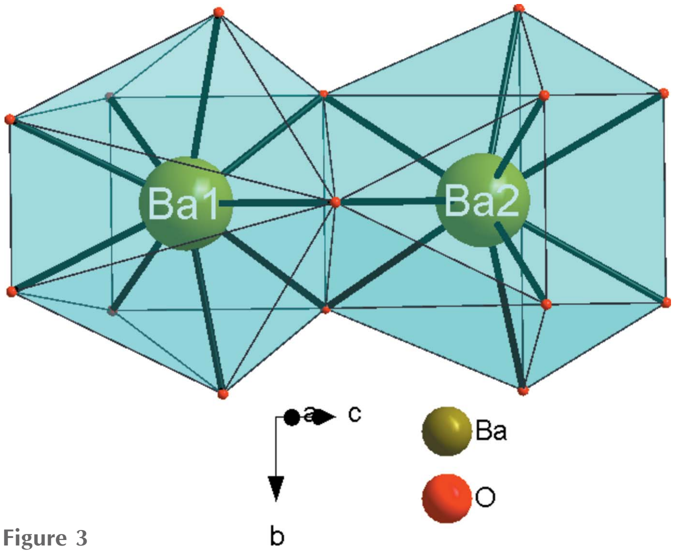

Figure 3
A pair of $[BaO_9]$ polyhedra.

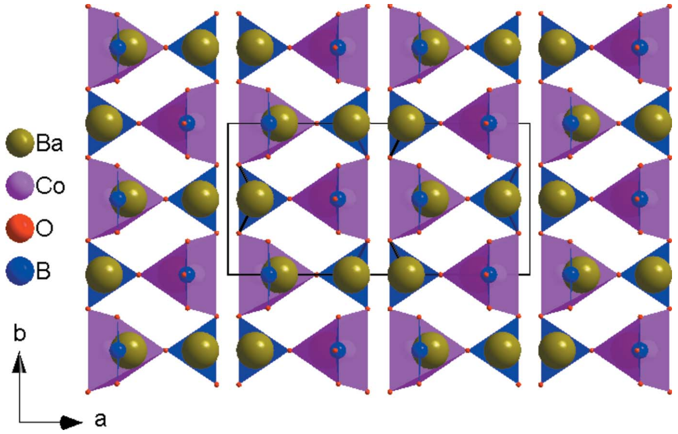

Figure 4
Projection of the crystal structure of $Ba_2Co(BO_3)_2$ along [001].

1.387 Å are similar to those found in other $A_2M(BO_3)_2$ borates where B—O bonds vary between 1.325 and 1.411 Å and are in good agreement with the results of the analysis carried out by Zobetz (1982) on 225 B—O distances belonging to 75 BO_3 groups [1.370 (19) Å]. Addison *et al.* (1984) have proposed the parameter τ_5 to distinguish whether a five-coordinated atom is in a trigonal–bipyramidal or a square-pyramidal environment. With $\tau_5 = -0.01667\alpha + 0.01667\beta = 0$, where $\beta > \alpha$ are the two largest valence angles of the coordination polyhedron, namely α = O1—Co1—O3^i = 157.75° and β = O^i—Co1—O3 = 157.75° [symmetry code: (i) $x, -y + 1, z$], a square-pyramidal environment is realized for the Co^{2+} cation in the structure of the title compound. Each of the two barium cations is surrounded by nine oxygen atoms forming distorted polyhedra with average distances for Ba1—O and Ba2–O of 2.791 and 2.891 Å, respectively.

3. Comparison with related structures

Comparison of the crystal structure of the title compound with those of other orthoborates with formula type $A_2M(BO_3)_2$ listed in Table 1 reveals that the first three compounds crystallize in the monoclinic system with the same space group (*C*2/*m*) but a halved unit-cell volume. α-$Sr_2Cu(BO_3)_2$ and $Pb_2Cu(BO_3)_2$ also crystallize in the monoclinic system but in space group $P2_1/c$. The remaining compounds adopt an orthorhombic structure, except for the last, $Ba_2Mg(BO_3)_2$, which is hexagonal. In the crystal structures of all these borates, the small metal *M* has either a coordination number of four (CuO_4, ZnO_4) or six (CuO_6, MgO_6, CaO_6, CdO_6). Accordingly, it is important to note the originality of the title structure with its five-coordination of the cobalt cation instead of four- or six-coordination for *M* in the other $A_2M(BO_3)_2$ compounds. Moreover, the linkage of $[CoO_5]$ polyhedra and one of the two $(BO_3)^{3-}$ anions by sharing an edge is different from other $A_2M(BO_3)_2$ structures where $[MO_4]$ or $[MO_6]$ polyhedra are linked to the $(BO_3)^{3-}$ anions only through their vertices.

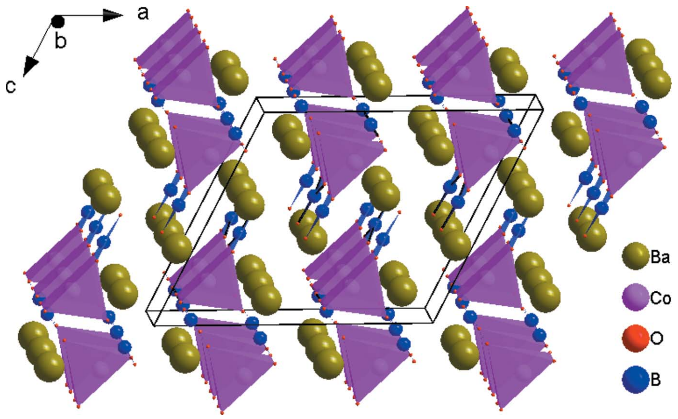

Figure 5
Projection of the crystal structure of $Ba_2Co(BO_3)_2$ approximately along [010], emphasizing the voids between the cobalt borate rows in which the barium cations are located.

Table 3
Experimental details.

Crystal data	
Chemical formula	$Ba_2Co(BO_3)_2$
M_r	451.23
Crystal system, space group	Monoclinic, *C*2/*m*
Temperature (K)	296
a, *b*, *c* (Å)	11.9784 (4), 5.3256 (2), 10.3220 (3)
β (°)	117.494 (1)
V (Å^3)	584.10 (3)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	16.11
Crystal size (mm)	0.36 × 0.27 × 0.20
Data collection	
Diffractometer	Bruker D8 VENTURE Super DUO
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.638, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12996, 1392, 1391
R_{int}	0.032
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.806
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.015, 0.031, 1.41
No. of reflections	1392
No. of parameters	62
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.73, −1.12

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SAINT*, *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2016/6* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), *DIAMOND* (Brandenburg, 2006) and *publCIF* (Westrip, 2010).

4. Synthesis and crystallization

Single crystals of $Ba_2Co(BO_3)_2$ were isolated from the melt, starting from a mixture of $Ba(NO_3)_2$, $Co(NO_3)_2{\cdot}6H_2O$ and H_3BO_3 in a molar ratio of 2:1:2. The mixture was subjected to successive heat treatments at 673 K and at 1073 K. The obtained powder was melted at a temperature of 1433 K, followed by a slow cooling. The resulting product consisted of pink crystals corresponding to the title compound.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The maximum and minimum remaining electron density peaks are at 0.47 Å from Ba1 and 1.08 Å from Co1, respectively.

Acknowledgements

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supporting information

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Crystal structure of $Ba_2Co(BO_3)_2$

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Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT*; program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL2016/6* (Sheldrick, 2015*b*); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012), *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Dibarium cobalt(II) bis(orthoborate)

Crystal data

$Ba_2Co(BO_3)_2$
$M_r = 451.23$
Monoclinic, $C2/m$
$a = 11.9784$ (4) Å
$b = 5.3256$ (2) Å
$c = 10.3220$ (3) Å
$\beta = 117.494$ (1)°
$V = 584.10$ (3) Å^3
$Z = 4$

$F(000) = 788$
$D_x = 5.131$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1392 reflections
$\theta = 3.4$–35.0°
$\mu = 16.11$ mm^{-1}
$T = 296$ K
Block, colourless
0.36 × 0.27 × 0.20 mm

Data collection

Bruker D8 VENTURE Super DUO diffractometer
Radiation source: INCOATEC IμS micro-focus source
HELIOS mirror optics monochromator
Detector resolution: 10.4167 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.638$, $T_{\max} = 0.746$
12996 measured reflections
1392 independent reflections
1391 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.032$
$\theta_{\max} = 35.0$°, $\theta_{\min} = 3.4$°
$h = -19 \rightarrow 18$
$k = -8 \rightarrow 8$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.015$
$wR(F^2) = 0.031$
$S = 1.41$
1392 reflections
62 parameters
0 restraints

$w = 1/[\sigma^2(F_o^2) + (0.004P)^2 + 1.2571P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 1.73$ e Å^{-3}
$\Delta\rho_{\min} = -1.12$ e Å^{-3}
Extinction correction: SHELXL-2016/6 (Sheldrick, 2015*b*), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0101 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ba1	0.59046 (2)	0.000000	0.39992 (2)	0.00733 (4)
Ba2	0.82861 (2)	0.000000	0.84816 (2)	0.00846 (4)
Co1	0.61032 (3)	0.500000	0.79447 (3)	0.00765 (6)
B1	0.5939 (2)	0.000000	0.9373 (2)	0.0065 (3)
B2	0.6356 (2)	0.500000	0.5684 (3)	0.0073 (3)
O1	0.53712 (10)	0.2258 (2)	0.87137 (12)	0.00920 (18)
O3	0.63351 (11)	0.2793 (2)	0.63947 (13)	0.01062 (18)
O2	0.70464 (16)	0.000000	1.0636 (2)	0.0151 (3)
O4	0.64458 (17)	0.500000	0.4400 (2)	0.0120 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.00848 (6)	0.00626 (6)	0.00619 (6)	0.000	0.00250 (4)	0.000
Ba2	0.00697 (6)	0.00742 (6)	0.00910 (6)	0.000	0.00210 (4)	0.000
Co1	0.01018 (11)	0.00530 (11)	0.00871 (12)	0.000	0.00542 (10)	0.000
B1	0.0076 (8)	0.0057 (8)	0.0067 (8)	0.000	0.0038 (7)	0.000
B2	0.0073 (8)	0.0066 (8)	0.0079 (8)	0.000	0.0034 (7)	0.000
O1	0.0105 (4)	0.0064 (4)	0.0101 (4)	0.0006 (3)	0.0043 (4)	0.0018 (3)
O3	0.0151 (5)	0.0069 (4)	0.0094 (4)	−0.0003 (4)	0.0052 (4)	0.0006 (3)
O2	0.0105 (6)	0.0134 (7)	0.0127 (7)	0.000	−0.0020 (6)	0.000
O4	0.0197 (7)	0.0079 (6)	0.0132 (7)	0.000	0.0118 (6)	0.000

Geometric parameters (Å, º)

Ba1—O3	2.7232 (12)	Ba2—O1^{viii}	2.9668 (12)
Ba1—O3^{i}	2.7232 (12)	Ba2—O1^{x}	2.9668 (11)
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Ba1—O3^{iii}	2.9272 (12)	Co1—O3	2.1043 (12)
Ba1—O3^{iv}	2.9272 (12)	B1—O2	1.364 (3)
Ba2—O3^{i}	2.7688 (12)	B1—O1	1.3943 (16)
Ba2—O3	2.7688 (12)	B1—O1^{i}	1.3943 (16)
Ba2—O1^{vi}	2.8064 (11)	B2—O4	1.377 (3)
Ba2—O1^{vii}	2.8064 (11)	B2—O3^{xi}	1.3920 (17)
Ba2—O2^{viii}	2.9009 (8)	B2—O3	1.3920 (17)

Ba2—O2^{ix}	2.9009 (8)

O3—Ba1—O3^{i}	66.22 (5)	O1^{vi}—Ba2—O2^{viii}	75.01 (4)
O3—Ba1—O4^{ii}	117.61 (5)	O1^{vii}—Ba2—O2^{viii}	134.17 (4)
O3^{i}—Ba1—O4^{ii}	52.88 (4)	O3^{i}—Ba2—O2^{ix}	64.04 (4)
O3—Ba1—O4	52.88 (4)	O3—Ba2—O2^{ix}	123.27 (4)
O3^{i}—Ba1—O4	117.61 (5)	O1^{vi}—Ba2—O2^{ix}	134.17 (4)
O4^{ii}—Ba1—O4	155.16 (8)	O1^{vii}—Ba2—O2^{ix}	75.01 (4)
O3—Ba1—O1^{iii}	160.05 (3)	O2^{viii}—Ba2—O2^{ix}	133.25 (7)
O3^{i}—Ba1—O1^{iii}	117.76 (3)	O3^{i}—Ba2—O1^{viii}	154.99 (3)
O4^{ii}—Ba1—O1^{iii}	73.21 (5)	O3—Ba2—O1^{viii}	112.17 (3)
O4—Ba1—O1^{iii}	123.99 (4)	O1^{vi}—Ba2—O1^{viii}	66.44 (4)
O3—Ba1—O1^{iv}	117.76 (3)	O1^{vii}—Ba2—O1^{viii}	96.47 (3)
O3^{i}—Ba1—O1^{iv}	160.05 (3)	O2^{viii}—Ba2—O1^{viii}	48.15 (4)
O4^{ii}—Ba1—O1^{iv}	123.99 (4)	O2^{ix}—Ba2—O1^{viii}	103.68 (4)
O4—Ba1—O1^{iv}	73.21 (5)	O3^{i}—Ba2—O1^{x}	112.17 (3)
O1^{iii}—Ba1—O1^{iv}	51.46 (5)	O3—Ba2—O1^{x}	154.99 (3)
O3—Ba1—O4^{v}	77.18 (4)	O1^{vi}—Ba2—O1^{x}	96.47 (3)
O3^{i}—Ba1—O4^{v}	77.18 (4)	O1^{vii}—Ba2—O1^{x}	66.44 (4)
O4^{ii}—Ba1—O4^{v}	77.69 (4)	O2^{viii}—Ba2—O1^{x}	103.68 (4)
O4—Ba1—O4^{v}	77.69 (4)	O2^{ix}—Ba2—O1^{x}	48.15 (4)
O1^{iii}—Ba1—O4^{v}	122.58 (4)	O1^{viii}—Ba2—O1^{x}	58.98 (4)
O1^{iv}—Ba1—O4^{v}	122.58 (4)	O3^{i}—Ba2—O4^{v}	71.41 (4)
O3—Ba1—O3^{iii}	100.43 (3)	O3—Ba2—O4^{v}	71.41 (4)
O3^{i}—Ba1—O3^{iii}	68.02 (4)	O1^{vi}—Ba2—O4^{v}	66.68 (4)
O4^{ii}—Ba1—O3^{iii}	70.32 (4)	O1^{vii}—Ba2—O4^{v}	66.68 (4)
O4—Ba1—O3^{iii}	130.98 (4)	O2^{viii}—Ba2—O4^{v}	112.77 (4)
O1^{iii}—Ba1—O3^{iii}	66.20 (3)	O2^{ix}—Ba2—O4^{v}	112.77 (4)
O1^{iv}—Ba1—O3^{iii}	92.16 (3)	O1^{viii}—Ba2—O4^{v}	132.76 (3)
O4^{v}—Ba1—O3^{iii}	142.41 (3)	O1^{x}—Ba2—O4^{v}	132.76 (3)
O3—Ba1—O3^{iv}	68.02 (4)	O2^{viii}—Co1—O1^{xi}	104.04 (5)
O3^{i}—Ba1—O3^{iv}	100.43 (3)	O2^{viii}—Co1—O1	104.04 (5)
O4^{ii}—Ba1—O3^{iv}	130.98 (4)	O1^{xi}—Co1—O1	91.26 (6)
O4—Ba1—O3^{iv}	70.32 (4)	O2^{viii}—Co1—O3^{xi}	93.78 (6)
O1^{iii}—Ba1—O3^{iv}	92.16 (3)	O1^{xi}—Co1—O3^{xi}	97.30 (4)
O1^{iv}—Ba1—O3^{iv}	66.20 (3)	O1—Co1—O3^{xi}	157.75 (5)
O4^{v}—Ba1—O3^{iv}	142.41 (3)	O2^{viii}—Co1—O3	93.78 (6)
O3^{iii}—Ba1—O3^{iv}	61.09 (5)	O1^{xi}—Co1—O3	157.75 (5)
O3^{i}—Ba2—O3	64.99 (5)	O1—Co1—O3	97.30 (4)
O3^{i}—Ba2—O1^{vi}	138.10 (4)	O3^{xi}—Co1—O3	67.90 (6)
O3—Ba2—O1^{vi}	100.67 (4)	O2—B1—O1	120.42 (9)
O3^{i}—Ba2—O1^{vii}	100.67 (3)	O2—B1—O1^{i}	120.42 (9)
O3—Ba2—O1^{vii}	138.10 (4)	O1—B1—O1^{i}	119.16 (18)
O1^{vi}—Ba2—O1^{vii}	62.72 (5)	O4—B2—O3^{xi}	122.38 (9)

O3^{i}—Ba2—O2^{viii}	123.27 (4)	O4—B2—O3	122.38 (9)
O3—Ba2—O2^{viii}	64.04 (4)	O3^{xi}—B2—O3	115.18 (19)

Symmetry codes: (i) *x*, −*y*, *z*; (ii) *x*, *y*−1, *z*; (iii) −*x*+1, −*y*, −*z*+1; (iv) −*x*+1, *y*, −*z*+1; (v) −*x*+3/2, −*y*+1/2, −*z*+1; (vi) *x*+1/2, −*y*+1/2, *z*; (vii) *x*+1/2, *y*−1/2, *z*; (viii) −*x*+3/2, −*y*+1/2, −*z*+2; (ix) −*x*+3/2, −*y*−1/2, −*z*+2; (x) −*x*+3/2, *y*−1/2, −*z*+2; (xi) *x*, −*y*+1, *z*.