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Crystal structure of $Ba_5In_4Sb_6$

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The title compound, pentabarium tetraindium hexaantimony, was synthesized by an indium-flux reaction and its structure features layers composed of edge-sharing In_2Sb_6 units. The voids between the In_4Sb_6 layers are filled by Ba^{2+} cations, which are all surrounded by six Sb atoms and form bicapped octahedral or triangular prismatic coordination geometries. There are five barium ions in the asymmetric unit: one has no imposed crystallographic symmetry, two lie on mirror planes and two have *mm*2 point symmetry. The two In atoms and four Sb atoms in the asymmetric unit all lie on general crystallographic positions.

Keywords: crystal structure; barium; indium; antimony; In—In interconnections.

CCDC reference: 1058152

1. Related literature

For geometrical details of In—In interconnections in other structures, see: Iandelli (1964); Goforth *et al.*, (2008).

2. Experimental

2.1. Crystal data

$Ba_5In_4Sb_6$
$M_r = 1876.48$
Orthorhombic, *Pmmn*
$a = 14.2723$ (13) Å
$b = 18.3578$ (17) Å
$c = 8.2710$ (8) Å
$V = 2167.1$ (4) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 20.39$ mm^{-1}
$T = 120$ K
0.06 × 0.03 × 0.02 mm

2.2. Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.374$, $T_{max} = 0.686$
12962 measured reflections
2676 independent reflections
2098 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$

2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.055$
$S = 1.02$
2676 reflections
79 parameters
$\Delta\rho_{max} = 2.00$ e Å^{-3}
$\Delta\rho_{min} = -1.69$ e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7382).

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Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
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Iandelli, A. (1964). *Z. Anorg. Allg. Chem.* **330**, 221–232.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

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Crystal structure of $Ba_5In_4Sb_6$

Ming-Yan Pan, Sheng-Qing Xia and Xu-Tang Tao

S1. Comment

Single crystal of $Ba_5In_4Sb_6$ was obtained from a high-temperature In-flux reaction and it crystallizes in its own structure type. The layers are constituted by edge-shared In_2Sb_6 units and stack along the crystallographic *b*-axis direction. Each In is four-coordinated which is connected by three Sb and the other In atom. All Ba cations are six-coordinated with the bicapped octahedron or triangular prism geometries formed by Sb anions. The bond lengths of In1—In1 and In2—In2 are 2.9655 (11) and 2.8544 (11) Å, respectively, comparable to In—In interconnections in $EuIn_2As_2$ (2.765 Å) (Goforth *et al.*, 2008) and $CaIn_2$ (2.92 Å) (Iandelli, 1964).

S2. Experimental

The title compound was synthesized through the high temperature In flux reaction. All starting elements were handled inside an Argon-filled glove box with controlled oxygen and moisture levels below 0.1 p.p.m.. The reaction conditions were optimized as follows: Ba, In and Sb in a molar ratio of 3:30:5 were loaded in an alumina crucible, which were subsequently flame-sealed in a fused silica tube. The reactants were heated quickly to 1173 K and allowed to dwell at this temperature for 20 h. After a slow cooling process down to 773 K at a rate of 2 K/h, the molten In was removed by centrifugation.

S3. Refinement

The residual electron densities show a maximum peak of 1.997 e/Å^3 and a minimum hole of -1.689 e/Å^3, which are 0.78 and 1.58 Å to Ba3 and In1, respectively.

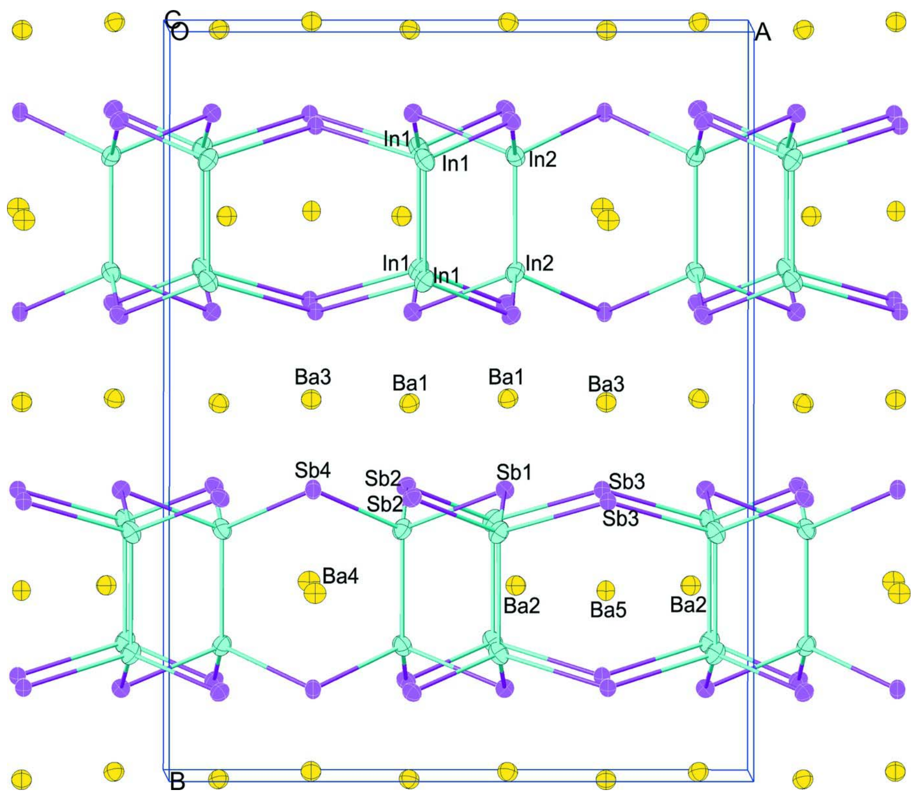

Figure 1

The ellipsoid of Ba5In4Sb6, viewed along the *c*-axis. The barium cations, Indium atoms and antimony anions were plotted as yellow, light blue and purple spheres, respectively. Ellipsoids are drawn at the 80% probability level.

Pentabarium tetraindium hexaantimony

Crystal data

$Ba_5In_4Sb_6$
M_r = 1876.48
Orthorhombic, *Pmmn*
Hall symbol: -P 2ab 2a
a = 14.2723 (13) Å
b = 18.3578 (17) Å
c = 8.2710 (8) Å
V = 2167.1 (4) Å^3
Z = 4
$F(000)$ = 3128
D_x = 5.751 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1832 reflections
θ = 2.9–27.6°
μ = 20.39 mm^{-1}
T = 120 K
Block, black
0.06 × 0.03 × 0.02 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.374, T_{max} = 0.686
12962 measured reflections
2676 independent reflections
2098 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 27.6°, θ_{min} = 1.8°
h = −18→14
k = −23→19
l = −9→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.055$
$S = 1.02$
2676 reflections
79 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0146P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 2.00$ e Å^{-3}
$\Delta\rho_{min} = -1.69$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.000211 (8)

Special details

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

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ba1	0.08681 (3)	0.00085 (2)	0.23996 (5)	0.00924 (11)
Ba2	0.10037 (4)	0.2500	0.26369 (7)	0.00879 (14)
Ba3	0.2500	0.50189 (3)	0.73898 (7)	0.00933 (14)
Ba4	0.2500	0.7500	0.07159 (11)	0.0113 (2)
Ba5	0.2500	0.2500	0.70687 (10)	0.00876 (19)
In1	0.56473 (4)	0.66923 (3)	0.10245 (6)	0.00979 (13)
In2	0.59568 (3)	0.17226 (3)	0.43328 (6)	0.00990 (13)
Sb1	0.07830 (3)	0.11748 (3)	0.57615 (6)	0.00809 (11)
Sb2	0.58565 (3)	0.12044 (3)	0.09457 (6)	0.00865 (12)
Sb3	0.2500	0.12590 (4)	0.05576 (8)	0.00786 (15)
Sb4	0.2500	0.61680 (4)	0.39782 (9)	0.00841 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.0093 (2)	0.0090 (2)	0.0094 (2)	0.00006 (17)	−0.00107 (17)	0.00072 (18)
Ba2	0.0094 (3)	0.0092 (3)	0.0078 (3)	0.000	0.0016 (2)	0.000
Ba3	0.0094 (3)	0.0093 (3)	0.0093 (3)	0.000	0.000	0.0005 (2)
Ba4	0.0116 (5)	0.0101 (5)	0.0122 (5)	0.000	0.000	0.000
Ba5	0.0076 (5)	0.0095 (4)	0.0092 (5)	0.000	0.000	0.000
In1	0.0105 (3)	0.0111 (3)	0.0077 (3)	−0.0025 (2)	−0.0016 (2)	0.0011 (2)
In2	0.0088 (3)	0.0102 (3)	0.0107 (3)	0.0017 (2)	−0.0008 (2)	0.0008 (2)
Sb1	0.0087 (3)	0.0088 (3)	0.0068 (2)	0.0004 (2)	−0.00068 (19)	−0.00060 (18)
Sb2	0.0086 (3)	0.0092 (3)	0.0081 (3)	0.0012 (2)	−0.00116 (19)	−0.00030 (19)
Sb3	0.0068 (4)	0.0081 (4)	0.0087 (4)	0.000	0.000	−0.0002 (3)

Sb4	0.0063 (4)	0.0096 (4)	0.0093 (4)	0.000	0.000	−0.0013 (3)

Geometric parameters (Å, º)

Ba1—Sb4^{i}	3.4343 (7)	Ba5—In1^{xviii}	3.4173 (7)
Ba1—Sb2^{ii}	3.5105 (7)	Ba5—In1^{xix}	3.4173 (7)
Ba1—Sb1	3.5115 (7)	Ba5—In1^{xx}	3.4173 (7)
Ba1—Sb1^{iii}	3.5475 (7)	Ba5—Sb1	3.6184 (6)
Ba1—Sb2^{iv}	3.5516 (7)	Ba5—Sb1^{i}	3.6184 (6)
Ba1—Sb3	3.6077 (7)	Ba5—Sb1^{ix}	3.6184 (6)
Ba1—In1^{i}	3.9649 (7)	Ba5—Sb1^{ii}	3.6184 (6)
Ba1—Ba2	4.5821 (6)	Ba5—Sb3^{xii}	3.6766 (10)
Ba1—Ba1^{ii}	4.6582 (10)	Ba5—Sb3^{xxi}	3.6766 (10)
Ba1—Ba1^{v}	4.6795 (9)	Ba5—Ba2^{i}	4.2423 (10)
Ba1—Ba3^{i}	4.7394 (8)	In1—Sb1^{xxii}	2.8296 (8)
Ba1—Ba3^{vi}	4.7537 (8)	In1—Sb2^{xv}	2.8398 (7)
Ba2—In1^{vii}	3.4100 (8)	In1—In1^{xxiii}	2.9655 (11)
Ba2—In1^{viii}	3.4100 (8)	In1—Sb3^{xxiv}	3.0556 (7)
Ba2—In2^{ii}	3.4400 (8)	In1—Ba2^{xxiv}	3.4100 (8)
Ba2—In2^{i}	3.4400 (8)	In1—Ba5^{xvii}	3.4173 (7)
Ba2—Sb1^{ix}	3.5632 (7)	In1—Ba1^{i}	3.9649 (7)
Ba2—Sb1	3.5632 (7)	In2—Sb4^{xxv}	2.7998 (7)
Ba2—Sb3^{i}	3.5649 (7)	In2—In2^{ix}	2.8544 (11)
Ba2—Sb3	3.5649 (7)	In2—Sb1^{ii}	2.9279 (7)
Ba2—Sb2^{ii}	3.8291 (7)	In2—Sb2	2.9620 (8)
Ba2—Sb2^{i}	3.8291 (7)	In2—Ba2^{i}	3.4400 (8)
Ba2—Ba5	4.2423 (10)	In2—Ba3^{xxv}	4.0820 (8)
Ba2—Ba2^{i}	4.2711 (13)	Sb1—In1^{xx}	2.8296 (8)
Ba3—Sb2^{x}	3.4833 (7)	Sb1—In2^{ii}	2.9279 (7)
Ba3—Sb2^{xi}	3.4833 (7)	Sb1—Ba1^{iii}	3.5475 (7)
Ba3—Sb3^{xii}	3.5169 (9)	Sb1—Ba3^{i}	3.5527 (7)
Ba3—Sb4	3.5230 (9)	Sb2—In1^{xxvi}	2.8398 (7)
Ba3—Sb1^{ix}	3.5527 (7)	Sb2—Ba3^{xxv}	3.4833 (7)
Ba3—Sb1^{i}	3.5527 (7)	Sb2—Ba1^{ii}	3.5105 (7)
Ba3—In2^{x}	4.0820 (8)	Sb2—Ba1^{xxvii}	3.5516 (7)
Ba3—In2^{xi}	4.0820 (8)	Sb2—Ba4^{xiv}	3.6122 (6)
Ba3—Ba5	4.6318 (7)	Sb2—Ba2^{i}	3.8291 (7)
Ba3—Ba1^{ix}	4.7394 (8)	Sb3—In1^{vii}	3.0556 (7)
Ba3—Ba1^{i}	4.7394 (8)	Sb3—In1^{xxvi}	3.0556 (7)
Ba3—Ba1^{xii}	4.7537 (8)	Sb3—Ba3^{vi}	3.5169 (9)
Ba4—Sb2^{xiii}	3.6122 (6)	Sb3—Ba2^{i}	3.5649 (7)
Ba4—Sb2^{xiv}	3.6122 (6)	Sb3—Ba1^{ii}	3.6077 (7)
Ba4—Sb2^{viii}	3.6122 (6)	Sb3—Ba5^{xxviii}	3.6766 (10)
Ba4—Sb2^{xv}	3.6122 (6)	Sb4—In2^{x}	2.7998 (7)
Ba4—Sb4^{xvi}	3.6414 (10)	Sb4—In2^{xi}	2.7998 (7)
Ba4—Sb4	3.6414 (10)	Sb4—Ba1^{ix}	3.4343 (7)
Ba5—In1^{xvii}	3.4173 (7)	Sb4—Ba1^{i}	3.4343 (7)

$Sb4^{i}$—Ba1—$Sb2^{ii}$	177.466 (19)	$Sb2^{xiv}$—Ba4—$Sb2^{viii}$	80.989 (19)
$Sb4^{i}$—Ba1—Sb1	96.078 (18)	$Sb2^{xiii}$—Ba4—$Sb2^{xv}$	80.989 (19)
$Sb2^{ii}$—Ba1—Sb1	82.282 (15)	$Sb2^{xiv}$—Ba4—$Sb2^{xv}$	82.364 (19)
$Sb4^{i}$—Ba1—$Sb1^{iii}$	84.397 (16)	$Sb2^{viii}$—Ba4—$Sb2^{xv}$	135.28 (3)
$Sb2^{ii}$—Ba1—$Sb1^{iii}$	93.674 (16)	$Sb2^{xiii}$—Ba4—$Sb4^{xvi}$	136.392 (16)
Sb1—Ba1—$Sb1^{iii}$	90.625 (16)	$Sb2^{xiv}$—Ba4—$Sb4^{xvi}$	80.779 (13)
$Sb4^{i}$—Ba1—$Sb2^{iv}$	84.553 (18)	$Sb2^{viii}$—Ba4—$Sb4^{xvi}$	80.780 (13)
$Sb2^{ii}$—Ba1—$Sb2^{iv}$	97.002 (15)	$Sb2^{xv}$—Ba4—$Sb4^{xvi}$	136.392 (16)
Sb1—Ba1—$Sb2^{iv}$	177.436 (18)	$Sb2^{xiii}$—Ba4—Sb4	80.780 (13)
$Sb1^{iii}$—Ba1—$Sb2^{iv}$	86.962 (15)	$Sb2^{xiv}$—Ba4—Sb4	136.392 (16)
$Sb4^{i}$—Ba1—Sb3	97.059 (16)	$Sb2^{viii}$—Ba4—Sb4	136.392 (16)
$Sb2^{ii}$—Ba1—Sb3	84.841 (15)	$Sb2^{xv}$—Ba4—Sb4	80.779 (13)
Sb1—Ba1—Sb3	88.211 (17)	$Sb4^{xvi}$—Ba4—Sb4	84.37 (3)
$Sb1^{iii}$—Ba1—Sb3	178.223 (18)	$In1^{xvii}$—Ba5—$In1^{xviii}$	101.39 (2)
$Sb2^{iv}$—Ba1—Sb3	94.182 (17)	$In1^{xvii}$—Ba5—$In1^{xix}$	51.430 (19)
$Sb4^{i}$—Ba1—$In1^{i}$	89.069 (17)	$In1^{xviii}$—Ba5—$In1^{xix}$	125.03 (3)
$Sb2^{ii}$—Ba1—$In1^{i}$	90.672 (16)	$In1^{xvii}$—Ba5—$In1^{xx}$	125.03 (3)
Sb1—Ba1—$In1^{i}$	133.506 (16)	$In1^{xviii}$—Ba5—$In1^{xx}$	51.430 (19)
$Sb1^{iii}$—Ba1—$In1^{i}$	43.815 (13)	$In1^{xix}$—Ba5—$In1^{xx}$	101.39 (2)
$Sb2^{iv}$—Ba1—$In1^{i}$	43.967 (12)	$In1^{xvii}$—Ba5—Sb1	162.493 (19)
Sb3—Ba1—$In1^{i}$	137.062 (18)	$In1^{xviii}$—Ba5—Sb1	84.581 (13)
$Sb4^{i}$—Ba1—Ba2	125.651 (17)	$In1^{xix}$—Ba5—Sb1	111.730 (13)
$Sb2^{ii}$—Ba1—Ba2	54.554 (13)	$In1^{xx}$—Ba5—Sb1	47.322 (13)
Sb1—Ba1—Ba2	50.129 (13)	$In1^{xvii}$—Ba5—$Sb1^{i}$	47.322 (13)
$Sb1^{iii}$—Ba1—Ba2	128.386 (16)	$In1^{xviii}$—Ba5—$Sb1^{i}$	111.730 (13)
$Sb2^{iv}$—Ba1—Ba2	131.250 (16)	$In1^{xix}$—Ba5—$Sb1^{i}$	84.581 (13)
Sb3—Ba1—Ba2	49.885 (14)	$In1^{xx}$—Ba5—$Sb1^{i}$	162.493 (19)
$In1^{i}$—Ba1—Ba2	145.225 (16)	Sb1—Ba5—$Sb1^{i}$	145.23 (3)
$Sb4^{i}$—Ba1—$Ba1^{ii}$	47.298 (11)	$In1^{xvii}$—Ba5—$Sb1^{ix}$	111.730 (13)
$Sb2^{ii}$—Ba1—$Ba1^{ii}$	134.518 (11)	$In1^{xviii}$—Ba5—$Sb1^{ix}$	47.322 (13)
Sb1—Ba1—$Ba1^{ii}$	91.983 (11)	$In1^{xix}$—Ba5—$Sb1^{ix}$	162.493 (19)
$Sb1^{iii}$—Ba1—$Ba1^{ii}$	131.624 (11)	$In1^{xx}$—Ba5—$Sb1^{ix}$	84.581 (13)
$Sb2^{iv}$—Ba1—$Ba1^{ii}$	90.267 (10)	Sb1—Ba5—$Sb1^{ix}$	84.494 (18)
Sb3—Ba1—$Ba1^{ii}$	49.790 (10)	$Sb1^{i}$—Ba5—$Sb1^{ix}$	85.261 (18)
$In1^{i}$—Ba1—$Ba1^{ii}$	123.058 (10)	$In1^{xvii}$—Ba5—$Sb1^{ii}$	84.581 (13)
Ba2—Ba1—$Ba1^{ii}$	87.579 (9)	$In1^{xviii}$—Ba5—$Sb1^{ii}$	162.493 (19)
$Sb4^{i}$—Ba1—$Ba1^{v}$	132.64 (2)	$In1^{xix}$—Ba5—$Sb1^{ii}$	47.322 (13)
$Sb2^{ii}$—Ba1—$Ba1^{v}$	48.878 (11)	$In1^{xx}$—Ba5—$Sb1^{ii}$	111.730 (13)
Sb1—Ba1—$Ba1^{v}$	131.107 (18)	Sb1—Ba5—$Sb1^{ii}$	85.261 (18)
$Sb1^{iii}$—Ba1—$Ba1^{v}$	90.449 (16)	$Sb1^{i}$—Ba5—$Sb1^{ii}$	84.494 (18)
$Sb2^{iv}$—Ba1—$Ba1^{v}$	48.124 (12)	$Sb1^{ix}$—Ba5—$Sb1^{ii}$	145.23 (3)
Sb3—Ba1—$Ba1^{v}$	89.306 (16)	$In1^{xvii}$—Ba5—$Sb3^{xii}$	50.868 (13)
$In1^{i}$—Ba1—$Ba1^{v}$	57.489 (12)	$In1^{xviii}$—Ba5—$Sb3^{xii}$	50.868 (13)
Ba2—Ba1—$Ba1^{v}$	93.748 (14)	$In1^{xix}$—Ba5—$Sb3^{xii}$	84.64 (2)
$Ba1^{ii}$—Ba1—$Ba1^{v}$	121.973 (11)	$In1^{xx}$—Ba5—$Sb3^{xii}$	84.64 (2)
$Sb4^{i}$—Ba1—$Ba3^{i}$	47.852 (14)	Sb1—Ba5—$Sb3^{xii}$	130.627 (17)
$Sb2^{ii}$—Ba1—$Ba3^{i}$	130.506 (15)	$Sb1^{i}$—Ba5—$Sb3^{xii}$	79.508 (13)
Sb1—Ba1—$Ba3^{i}$	48.233 (12)	$Sb1^{ix}$—Ba5—$Sb3^{xii}$	79.508 (13)

Sb1^{iii}—Ba1—Ba3^{i}	86.937 (14)	Sb1^{ii}—Ba5—Sb3^{xii}	130.627 (17)
Sb2^{iv}—Ba1—Ba3^{i}	132.382 (15)	In1^{xvii}—Ba5—Sb3^{xxi}	84.64 (2)
Sb3—Ba1—Ba3^{i}	93.283 (15)	In1^{xviii}—Ba5—Sb3^{xxi}	84.64 (2)
In1^{i}—Ba1—Ba3^{i}	120.632 (14)	In1^{xix}—Ba5—Sb3^{xxi}	50.868 (13)
Ba2—Ba1—Ba3^{i}	87.281 (13)	In1^{xx}—Ba5—Sb3^{xxi}	50.868 (13)
Ba1^{ii}—Ba1—Ba3^{i}	60.565 (7)	Sb1—Ba5—Sb3^{xxi}	79.508 (13)
Ba1^{v}—Ba1—Ba3^{i}	177.275 (17)	Sb1^{i}—Ba5—Sb3^{xxi}	130.627 (17)
Sb4^{i}—Ba1—Ba3^{vi}	89.567 (16)	Sb1^{ix}—Ba5—Sb3^{xxi}	130.627 (17)
Sb2^{ii}—Ba1—Ba3^{vi}	92.956 (14)	Sb1^{ii}—Ba5—Sb3^{xxi}	79.508 (13)
Sb1—Ba1—Ba3^{vi}	135.534 (16)	Sb3^{xii}—Ba5—Sb3^{xxi}	76.58 (3)
Sb1^{iii}—Ba1—Ba3^{vi}	133.841 (15)	In1^{xvii}—Ba5—Ba2	142.027 (19)
Sb2^{iv}—Ba1—Ba3^{vi}	46.886 (12)	In1^{xviii}—Ba5—Ba2	90.531 (15)
Sb3—Ba1—Ba3^{vi}	47.337 (14)	In1^{xix}—Ba5—Ba2	142.027 (19)
In1^{i}—Ba1—Ba3^{vi}	90.508 (13)	In1^{xx}—Ba5—Ba2	90.531 (15)
Ba2—Ba1—Ba3^{vi}	91.559 (13)	Sb1—Ba5—Ba2	53.194 (13)
Ba1^{ii}—Ba1—Ba3^{vi}	60.662 (7)	Sb1^{i}—Ba5—Ba2	94.75 (2)
Ba1^{v}—Ba1—Ba3^{vi}	61.312 (12)	Sb1^{ix}—Ba5—Ba2	53.194 (13)
Ba3^{i}—Ba1—Ba3^{vi}	121.212 (11)	Sb1^{ii}—Ba5—Ba2	94.75 (2)
In1^{vii}—Ba2—In1^{viii}	51.55 (2)	Sb3^{xii}—Ba5—Ba2	132.701 (10)
In1^{vii}—Ba2—In2^{ii}	93.462 (18)	Sb3^{xxi}—Ba5—Ba2	132.701 (10)
In1^{viii}—Ba2—In2^{ii}	114.91 (2)	In1^{xvii}—Ba5—Ba2^{i}	90.531 (15)
In1^{vii}—Ba2—In2^{i}	114.91 (2)	In1^{xviii}—Ba5—Ba2^{i}	142.027 (19)
In1^{viii}—Ba2—In2^{i}	93.462 (18)	In1^{xix}—Ba5—Ba2^{i}	90.531 (15)
In2^{ii}—Ba2—In2^{i}	49.02 (2)	In1^{xx}—Ba5—Ba2^{i}	142.027 (19)
In1^{vii}—Ba2—Sb1^{ix}	158.09 (2)	Sb1—Ba5—Ba2^{i}	94.75 (2)
In1^{viii}—Ba2—Sb1^{ix}	109.515 (14)	Sb1^{i}—Ba5—Ba2^{i}	53.194 (13)
In2^{ii}—Ba2—Sb1^{ix}	85.158 (18)	Sb1^{ix}—Ba5—Ba2^{i}	94.75 (2)
In2^{i}—Ba2—Sb1^{ix}	49.389 (14)	Sb1^{ii}—Ba5—Ba2^{i}	53.194 (13)
In1^{vii}—Ba2—Sb1	109.515 (14)	Sb3^{xii}—Ba5—Ba2^{i}	132.701 (10)
In1^{viii}—Ba2—Sb1	158.09 (2)	Sb3^{xxi}—Ba5—Ba2^{i}	132.701 (10)
In2^{ii}—Ba2—Sb1	49.389 (14)	Ba2—Ba5—Ba2^{i}	60.45 (2)
In2^{i}—Ba2—Sb1	85.158 (18)	Sb1^{xxii}—In1—Sb2^{xv}	119.01 (2)
Sb1^{ix}—Ba2—Sb1	86.12 (2)	Sb1^{xxii}—In1—In1^{xxiii}	109.617 (14)
In1^{vii}—Ba2—Sb3^{i}	86.49 (2)	Sb2^{xv}—In1—In1^{xxiii}	108.387 (14)
In1^{viii}—Ba2—Sb3^{i}	51.906 (14)	Sb1^{xxii}—In1—Sb3^{xxiv}	104.82 (2)
In2^{ii}—Ba2—Sb3^{i}	161.643 (18)	Sb2^{xv}—In1—Sb3^{xxiv}	109.04 (2)
In2^{i}—Ba2—Sb3^{i}	114.761 (14)	In1^{xxiii}—In1—Sb3^{xxiv}	105.090 (16)
Sb1^{ix}—Ba2—Sb3^{i}	88.083 (16)	Sb1^{xxii}—In1—Ba2^{xxiv}	165.95 (2)
Sb1—Ba2—Sb3^{i}	147.05 (2)	Sb2^{xv}—In1—Ba2^{xxiv}	74.947 (19)
In1^{vii}—Ba2—Sb3	51.906 (14)	In1^{xxiii}—In1—Ba2^{xxiv}	64.226 (10)
In1^{viii}—Ba2—Sb3	86.49 (2)	Sb3^{xxiv}—In1—Ba2^{xxiv}	66.660 (19)
In2^{ii}—Ba2—Sb3	114.761 (14)	Sb1^{xxii}—In1—Ba5^{xvii}	70.071 (19)
In2^{i}—Ba2—Sb3	161.643 (18)	Sb2^{xv}—In1—Ba5^{xvii}	170.58 (2)
Sb1^{ix}—Ba2—Sb3	147.05 (2)	In1^{xxiii}—In1—Ba5^{xvii}	64.285 (10)
Sb1—Ba2—Sb3	88.083 (16)	Sb3^{xxiv}—In1—Ba5^{xvii}	68.962 (19)
Sb3^{i}—Ba2—Sb3	79.45 (2)	Ba2^{xxiv}—In1—Ba5^{xvii}	96.07 (2)
In1^{vii}—Ba2—Sb2^{ii}	45.739 (13)	Sb1^{xxii}—In1—Ba1^{i}	60.226 (15)
In1^{viii}—Ba2—Sb2^{ii}	80.925 (18)	Sb2^{xv}—In1—Ba1^{i}	60.260 (15)

In2^{ii}—Ba2—Sb2^{ii}	47.723 (14)
In2^{i}—Ba2—Sb2^{ii}	80.950 (18)
Sb1^{ix}—Ba2—Sb2^{ii}	128.88 (2)
Sb1—Ba2—Sb2^{ii}	77.265 (13)
Sb3^{i}—Ba2—Sb2^{ii}	129.50 (2)
Sb3—Ba2—Sb2^{ii}	80.918 (14)
In1^{vii}—Ba2—Sb2^{i}	80.925 (18)
In1^{viii}—Ba2—Sb2^{i}	45.739 (13)
In2^{ii}—Ba2—Sb2^{i}	80.950 (18)
In2^{i}—Ba2—Sb2^{i}	47.723 (14)
Sb1^{ix}—Ba2—Sb2^{i}	77.265 (13)
Sb1—Ba2—Sb2^{i}	128.88 (2)
Sb3^{i}—Ba2—Sb2^{i}	80.918 (14)
Sb3—Ba2—Sb2^{i}	129.50 (2)
Sb2^{ii}—Ba2—Sb2^{i}	76.80 (2)
In1^{vii}—Ba2—Ba5	147.398 (15)
In1^{viii}—Ba2—Ba5	147.398 (15)
In2^{ii}—Ba2—Ba5	93.275 (18)
In2^{i}—Ba2—Ba5	93.275 (18)
Sb1^{ix}—Ba2—Ba5	54.396 (13)
Sb1—Ba2—Ba5	54.396 (13)
Sb3^{i}—Ba2—Ba5	96.619 (17)
Sb3—Ba2—Ba5	96.619 (17)
Sb2^{ii}—Ba2—Ba5	131.656 (13)
Sb2^{i}—Ba2—Ba5	131.656 (13)
In1^{vii}—Ba2—Ba2^{i}	98.579 (14)
In1^{viii}—Ba2—Ba2^{i}	98.579 (14)
In2^{ii}—Ba2—Ba2^{i}	144.428 (13)
In2^{i}—Ba2—Ba2^{i}	144.428 (13)
Sb1^{ix}—Ba2—Ba2^{i}	95.073 (13)
Sb1—Ba2—Ba2^{i}	95.073 (13)
Sb3^{i}—Ba2—Ba2^{i}	53.198 (11)
Sb3—Ba2—Ba2^{i}	53.198 (11)
Sb2^{ii}—Ba2—Ba2^{i}	133.895 (11)
Sb2^{i}—Ba2—Ba2^{i}	133.895 (11)
Ba5—Ba2—Ba2^{i}	59.775 (11)
Sb2^{x}—Ba3—Sb2^{xi}	84.66 (2)
Sb2^{x}—Ba3—Sb3^{xii}	97.024 (18)
Sb2^{xi}—Ba3—Sb3^{xii}	97.024 (18)
Sb2^{x}—Ba3—Sb4	86.702 (17)
Sb2^{xi}—Ba3—Sb4	86.702 (17)
Sb3^{xii}—Ba3—Sb4	174.94 (2)
Sb2^{x}—Ba3—Sb1^{ix}	178.605 (18)
Sb2^{xi}—Ba3—Sb1^{ix}	94.053 (13)
Sb3^{xii}—Ba3—Sb1^{ix}	82.585 (17)
Sb4—Ba3—Sb1^{ix}	93.769 (17)
Sb2^{x}—Ba3—Sb1^{i}	94.053 (13)
Sb2^{xi}—Ba3—Sb1^{i}	178.605 (18)
In1^{xxiii}—In1—Ba1^{i}	141.952 (10)
Sb3^{xxiv}—In1—Ba1^{i}	112.95 (2)
Ba2^{xxiv}—In1—Ba1^{i}	132.730 (18)
Ba5^{xvii}—In1—Ba1^{i}	129.15 (2)
Sb4^{xxv}—In2—In2^{ix}	111.322 (17)
Sb4^{xxv}—In2—Sb1^{ii}	109.93 (2)
In2^{ix}—In2—Sb1^{ii}	110.086 (14)
Sb4^{xxv}—In2—Sb2	113.15 (2)
In2^{ix}—In2—Sb2	108.733 (14)
Sb1^{ii}—In2—Sb2	103.32 (2)
Sb4^{xxv}—In2—Ba2^{i}	173.81 (3)
In2^{ix}—In2—Ba2^{i}	65.488 (10)
Sb1^{ii}—In2—Ba2^{i}	67.497 (17)
Sb2—In2—Ba2^{i}	73.039 (18)
Sb4^{xxv}—In2—Ba3^{xxv}	58.068 (19)
In2^{ix}—In2—Ba3^{xxv}	140.012 (10)
Sb1^{ii}—In2—Ba3^{xxv}	109.592 (19)
Sb2—In2—Ba3^{xxv}	56.626 (15)
Ba2^{i}—In2—Ba3^{xxv}	127.911 (18)
In1^{xx}—Sb1—In2^{ii}	101.88 (2)
In1^{xx}—Sb1—Ba1	161.99 (2)
In2^{ii}—Sb1—Ba1	85.363 (18)
In1^{xx}—Sb1—Ba1^{iii}	75.959 (17)
In2^{ii}—Sb1—Ba1^{iii}	79.632 (17)
Ba1—Sb1—Ba1^{iii}	89.375 (16)
In1^{xx}—Sb1—Ba3^{i}	84.155 (19)
In2^{ii}—Sb1—Ba3^{i}	161.77 (2)
Ba1—Sb1—Ba3^{i}	84.272 (16)
Ba1^{iii}—Sb1—Ba3^{i}	85.293 (16)
In1^{xx}—Sb1—Ba2	117.27 (2)
In2^{ii}—Sb1—Ba2	63.114 (17)
Ba1—Sb1—Ba2	80.729 (16)
Ba1^{iii}—Sb1—Ba2	141.977 (19)
Ba3^{i}—Sb1—Ba2	129.426 (19)
In1^{xx}—Sb1—Ba5	62.606 (19)
In2^{ii}—Sb1—Ba5	117.648 (19)
Ba1—Sb1—Ba5	128.543 (19)
Ba1^{iii}—Sb1—Ba5	137.18 (2)
Ba3^{i}—Sb1—Ba5	80.461 (15)
Ba2—Sb1—Ba5	72.411 (18)
In1^{xxvi}—Sb2—In2	118.55 (2)
In1^{xxvi}—Sb2—Ba3^{xxv}	158.88 (2)
In2—Sb2—Ba3^{xxv}	78.130 (18)
In1^{xxvi}—Sb2—Ba1^{ii}	82.178 (18)
In2—Sb2—Ba1^{ii}	84.879 (18)
Ba3^{xxv}—Sb2—Ba1^{ii}	86.909 (16)
In1^{xxvi}—Sb2—Ba1^{xxvii}	75.772 (18)
In2—Sb2—Ba1^{xxvii}	159.71 (2)

Sb3^{xii}—Ba3—Sb1^{i}	82.585 (17)
Sb4—Ba3—Sb1^{i}	93.769 (17)
Sb1^{ix}—Ba3—Sb1^{i}	87.23 (2)
Sb2^{x}—Ba3—In2^{x}	45.244 (13)
Sb2^{xi}—Ba3—In2^{x}	91.297 (18)
Sb3^{xii}—Ba3—In2^{x}	140.454 (14)
Sb4—Ba3—In2^{x}	42.412 (12)
Sb1^{ix}—Ba3—In2^{x}	135.44 (2)
Sb1^{i}—Ba3—In2^{x}	88.172 (14)
Sb2^{x}—Ba3—In2^{xi}	91.297 (18)
Sb2^{xi}—Ba3—In2^{xi}	45.244 (13)
Sb3^{xii}—Ba3—In2^{xi}	140.454 (14)
Sb4—Ba3—In2^{xi}	42.412 (12)
Sb1^{ix}—Ba3—In2^{xi}	88.172 (14)
Sb1^{i}—Ba3—In2^{xi}	135.44 (2)
In2^{x}—Ba3—In2^{xi}	65.310 (18)
Sb2^{x}—Ba3—Ba5	130.270 (14)
Sb2^{xi}—Ba3—Ba5	130.270 (14)
Sb3^{xii}—Ba3—Ba5	51.447 (18)
Sb4—Ba3—Ba5	123.49 (2)
Sb1^{ix}—Ba3—Ba5	50.390 (12)
Sb1^{i}—Ba3—Ba5	50.390 (12)
In2^{x}—Ba3—Ba5	138.151 (14)
In2^{xi}—Ba3—Ba5	138.151 (14)
Sb2^{x}—Ba3—Ba1^{ix}	132.982 (18)
Sb2^{xi}—Ba3—Ba1^{ix}	91.140 (13)
Sb3^{xii}—Ba3—Ba1^{ix}	129.919 (16)
Sb4—Ba3—Ba1^{ix}	46.281 (12)
Sb1^{ix}—Ba3—Ba1^{ix}	47.495 (11)
Sb1^{i}—Ba3—Ba1^{ix}	90.133 (16)
In2^{x}—Ba3—Ba1^{ix}	88.244 (15)
In2^{xi}—Ba3—Ba1^{ix}	55.877 (11)
Ba5—Ba3—Ba1^{ix}	86.529 (14)
Sb2^{x}—Ba3—Ba1^{i}	91.140 (13)
Sb2^{xi}—Ba3—Ba1^{i}	132.982 (18)
Sb3^{xii}—Ba3—Ba1^{i}	129.919 (16)
Sb4—Ba3—Ba1^{i}	46.281 (12)
Sb1^{ix}—Ba3—Ba1^{i}	90.133 (16)
Sb1^{i}—Ba3—Ba1^{i}	47.495 (11)
In2^{x}—Ba3—Ba1^{i}	55.877 (11)
In2^{xi}—Ba3—Ba1^{i}	88.244 (15)
Ba5—Ba3—Ba1^{i}	86.529 (14)
Ba1^{ix}—Ba3—Ba1^{i}	58.870 (14)
Sb2^{x}—Ba3—Ba1^{xii}	48.100 (12)
Sb2^{xi}—Ba3—Ba1^{xii}	89.545 (17)
Sb3^{xii}—Ba3—Ba1^{xii}	48.968 (13)
Sb4—Ba3—Ba1^{xii}	134.789 (16)
Sb1^{ix}—Ba3—Ba1^{xii}	131.442 (18)
Ba3^{xxv}—Sb2—Ba1^{xxvii}	85.014 (17)
Ba1^{ii}—Sb2—Ba1^{xxvii}	82.998 (15)
In1^{xxvi}—Sb2—Ba4^{xiv}	93.71 (2)
In2—Sb2—Ba4^{xiv}	96.72 (2)
Ba3^{xxv}—Sb2—Ba4^{xiv}	97.149 (16)
Ba1^{ii}—Sb2—Ba4^{xiv}	175.863 (18)
Ba1^{xxvii}—Sb2—Ba4^{xiv}	96.509 (19)
In1^{xxvi}—Sb2—Ba2^{i}	59.314 (17)
In2—Sb2—Ba2^{i}	59.238 (16)
Ba3^{xxv}—Sb2—Ba2^{i}	135.28 (2)
Ba1^{ii}—Sb2—Ba2^{i}	77.125 (15)
Ba1^{xxvii}—Sb2—Ba2^{i}	132.629 (18)
Ba4^{xiv}—Sb2—Ba2^{i}	100.382 (15)
In1^{vii}—Sb3—In1^{xxvi}	119.85 (3)
In1^{vii}—Sb3—Ba3^{vi}	81.640 (18)
In1^{xxvi}—Sb3—Ba3^{vi}	81.641 (18)
In1^{vii}—Sb3—Ba2^{i}	123.96 (2)
In1^{xxvi}—Sb3—Ba2^{i}	61.434 (16)
Ba3^{vi}—Sb3—Ba2^{i}	141.785 (14)
In1^{vii}—Sb3—Ba2	61.434 (16)
In1^{xxvi}—Sb3—Ba2	123.96 (2)
Ba3^{vi}—Sb3—Ba2	141.785 (14)
Ba2^{i}—Sb3—Ba2	73.60 (2)
In1^{vii}—Sb3—Ba1	77.750 (14)
In1^{xxvi}—Sb3—Ba1	154.85 (2)
Ba3^{vi}—Sb3—Ba1	83.695 (17)
Ba2^{i}—Sb3—Ba1	126.13 (2)
Ba2—Sb3—Ba1	79.407 (14)
In1^{vii}—Sb3—Ba1^{ii}	154.85 (2)
In1^{xxvi}—Sb3—Ba1^{ii}	77.750 (14)
Ba3^{vi}—Sb3—Ba1^{ii}	83.695 (17)
Ba2^{i}—Sb3—Ba1^{ii}	79.407 (14)
Ba2—Sb3—Ba1^{ii}	126.13 (2)
Ba1—Sb3—Ba1^{ii}	80.42 (2)
In1^{vii}—Sb3—Ba5^{xxviii}	60.170 (15)
In1^{xxvi}—Sb3—Ba5^{xxviii}	60.170 (15)
Ba3^{vi}—Sb3—Ba5^{xxviii}	80.13 (2)
Ba2^{i}—Sb3—Ba5^{xxviii}	89.005 (18)
Ba2—Sb3—Ba5^{xxviii}	89.005 (18)
Ba1—Sb3—Ba5^{xxviii}	136.530 (13)
Ba1^{ii}—Sb3—Ba5^{xxviii}	136.530 (13)
In2^{x}—Sb4—In2^{xi}	103.75 (3)
In2^{x}—Sb4—Ba1^{ix}	162.15 (3)
In2^{xi}—Sb4—Ba1^{ix}	83.388 (15)
In2^{x}—Sb4—Ba1^{i}	83.388 (15)
In2^{xi}—Sb4—Ba1^{i}	162.15 (3)
Ba1^{ix}—Sb4—Ba1^{i}	85.40 (2)
In2^{x}—Sb4—Ba3	79.52 (2)

$Sb1^{i}$—Ba3—$Ba1^{xii}$	89.193 (13)	$In2^{xi}$—Sb4—Ba3	79.52 (2)
$In2^{x}$—Ba3—$Ba1^{xii}$	92.751 (13)	$Ba1^{ix}$—Sb4—Ba3	85.867 (17)
$In2^{xi}$—Ba3—$Ba1^{xii}$	125.221 (17)	$Ba1^{i}$—Sb4—Ba3	85.867 (17)
Ba5—Ba3—$Ba1^{xii}$	92.258 (15)	$In2^{x}$—Sb4—Ba4	97.21 (2)
$Ba1^{ix}$—Ba3—$Ba1^{xii}$	178.779 (18)	$In2^{xi}$—Sb4—Ba4	97.21 (2)
$Ba1^{i}$—Ba3—$Ba1^{xii}$	121.212 (11)	$Ba1^{ix}$—Sb4—Ba4	98.083 (19)
$Sb2^{xiii}$—Ba4—$Sb2^{xiv}$	135.28 (3)	$Ba1^{i}$—Sb4—Ba4	98.083 (19)
$Sb2^{xiii}$—Ba4—$Sb2^{viii}$	82.364 (19)	Ba3—Sb4—Ba4	174.60 (3)

Symmetry codes: (i) −*x*+1/2, −*y*+1/2, *z*; (ii) −*x*+1/2, *y*, *z*; (iii) −*x*, −*y*, −*z*+1; (iv) *x*−1/2, −*y*, −*z*; (v) −*x*, −*y*, −*z*; (vi) −*x*+1/2, −*y*+1/2, *z*−1; (vii) *x*−1/2, *y*−1/2, −*z*; (viii) *x*−1/2, −*y*+1, −*z*; (ix) *x*, −*y*+1/2, *z*; (x) −*x*+1, *y*+1/2, −*z*+1; (xi) *x*−1/2, *y*+1/2, −*z*+1; (xii) −*x*+1/2, −*y*+1/2, *z*+1; (xiii) *x*−1/2, *y*+1/2, −*z*; (xiv) −*x*+1, −*y*+1, −*z*; (xv) −*x*+1, *y*+1/2, −*z*; (xvi) −*x*+1/2, −*y*+3/2, *z*; (xvii) −*x*+1, −*y*+1, −*z*+1; (xviii) *x*−1/2, −*y*+1, −*z*+1; (xix) −*x*+1, *y*−1/2, −*z*+1; (xx) *x*−1/2, *y*−1/2, −*z*+1; (xxi) *x*, *y*, *z*+1; (xxii) *x*+1/2, *y*+1/2, −*z*+1; (xxiii) *x*, −*y*+3/2, *z*; (xxiv) *x*+1/2, *y*+1/2, −*z*; (xxv) *x*+1/2, *y*−1/2, −*z*+1; (xxvi) −*x*+1, *y*−1/2, −*z*; (xxvii) *x*+1/2, −*y*, −*z*; (xxviii) *x*, *y*, *z*−1.