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The crystal structure of quaternary (Sn,Pb,Bi)Pt

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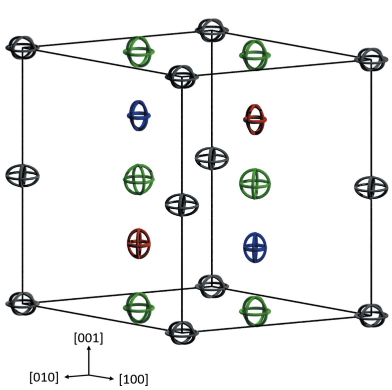
Quaternary (Sn,Pb,Bi)Pt was synthesized by melting of the elements in an evacuated silica glass ampoule. The crystal structure was established by single-crystal X-ray diffraction and adopts an atomic arrangement of the NiAs type with additional occupation of the voids. Decisive for the refinement was the composition of the crystals as determined by energy dispersive X-ray spectroscopy (EDXS), resulting in a formula of $(Sn_{0.15}Pb_{0.54}Bi_{0.31})Pt$.



1. Chemical context

Platinum-based intermetallic compounds possess promising properties as electrocatalysts and provide necessary stability for the harsh application conditions in acidic electrolytes (Rössner & Armbrüster, 2019). SnPt, PbPt and BiPt are interesting electrocatalysts for the oxidation of small organic molecules and have the NiAs type of crystal structure (Oftedal, 1928; Nowotny *et al.*, 1946; Zhuravlev *et al.*, 1962). So far, the existence of a substitutional solid solution between PtPb and PtBi was confirmed by powder X-ray diffraction, with the site occupancy deduced from the nominal composition (Zhuravlev *et al.*, 1962), which also holds for all three binary end members. To obtain material for electrocatalytic investigations, the synthesis of single-phase (Sn,Pb,Bi)Pt was attempted. Large hexagonal crystals were found on the top of an otherwise microgranular ingot. Preliminary EDXS analysis indicated the presence of all four elements in the crystal. Further structural investigations besides the original structure reports for PtSn (Harris *et al.*, 1968; Shelton *et al.*, 1981; Durussel *et al.*, 1994), PtPb (Zhuravlev *et al.* 1962; Sidorov *et al.*, 2021) and PtBi (Zhuravlev & Stepanova, 1962*a*,*b*) provide no full structural characterization by means of single-crystal X-ray diffraction. Thus, structural data for binary, ternary or quaternary samples in the (Sn,Pb,Bi)Pt system are incomplete. To provide such data, one of the obtained crystals was studied by means of single-crystal X-ray diffraction.

2. Structural commentary

As a result of the very similar scattering power of three of the four atoms (Bi, Pb and Pt), the direct assignment of the atomic positions to the respective elements was not possible. Atoms were distributed based on crystal-chemical considerations as well as by achieving an agreement between the refined composition and the result of the EDXS analysis (Fig. 1). The 2*a* site was assigned to Pt in agreement with structural studies of binary endmembers. A mixed occupancy of Sn, Pb and Bi

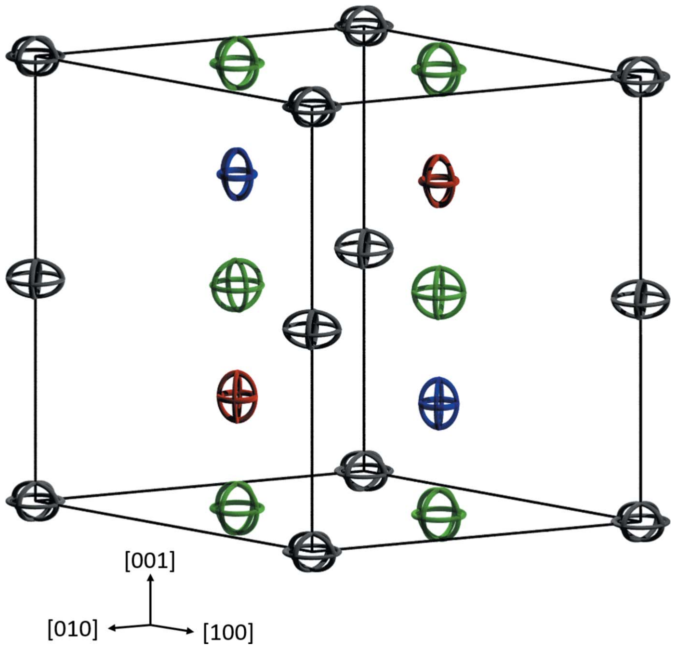


Figure 1
Representation of the unit cell of quaternary (Sn,Pb,Bi)Pt. Color code: Grey – Pt1; red – Sn1, Pb1, Bi1; blue – Sn2; green – Sn3. Displacement ellipsoids are drawn at the 95% probability level..

Table 1
Experimental details.

Crystal data	
Chemical formula	(Sn·Pb·Bi)Pt
M_r	389.32
Crystal system, space group	Hexagonal, $P6_3/mmc$
Temperature (K)	293
a, c (Å)	4.228 (1), 5.481 (2)
V (Å^3)	84.84 (5)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	169.4
Crystal size (mm)	0.04 × 0.03 × 0.02
Data collection	
Diffractometer	Rigaku AFC7 four-circle
Absorption correction	Multi-scan (Blessing, 1995)
T_{min}, T_{max}	0.037, 0.081
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	1549, 123, 120
R_{int}	0.043
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.900
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.025, 0.041, 1.51
No. of reflections	123
No. of parameters	13
No. of restraints	1
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	2.08, −1.43

Computer programs: *CrystalClear* (Rigaku, 2008), *SIR-2014* (Burla *et al.*, 2015), *SHELXL* (Sheldrick, 2015) and *DIAMOND* (Brandenburg & Putz, 2018).

was assumed for the 2c position. The statistical distribution of these elements at the same atomic site is based on the full miscibility of the elements in the molten state and on the missing site preference in the only known binary phase $Pb_{0.7}Bi_{0.3}$ (Mg type of crystal structure; Kurnakov & Ageeva, 1937). Additional electron density was detected on the 2c ($\overline{6}m2$) and 4f (3m.) sites, for which two possible scenarios can be considered. Either those positions are occupied by the smaller Sn atoms as a result of the enlarged unit-cell volume of 84.84 Å^3, which is 7.2% higher compared to 79.14 Å^3 for SnPt (Oftedal, 1928), or the presence of stacking faults. Neither can be proven here.

As a result of the potential partial occupation of 2c ($\overline{6}m2$) and 4f (3m.) in the hexagonal lattice of the quaternary sample, we assign the crystal structure to the NiAs type. The refined composition of 7.5%$_{at}$ Sn, 27.0%$_{at}$ Pb, 15.5%$_{at}$ Bi and 50%$_{at}$ Pt is in broad agreement with the results of EDXS measurements (12.35%$_{at}$ Sn, 25.87%$_{at}$ Pb, 9.49%$_{at}$ Bi and 52.29%$_{at}$ Pt) considering the error of this method, which to our experience is up to 5%$_{at}$ for standardless quantifications of non-ideal samples, *i.e.* mirror-finished surfaces.

3. Synthesis and crystallization

Elements were weighed in an Ar-filled glove-box (O_2 and H_2O content < 0.1 ppm) according to the nominal composition of 20.83%$_{at}$ Sn (99.999%, granules, ChemPUR), 20.83%$_{at}$ Pb (99.999%, granules, AlutervFKI), 8.33%$_{at}$ Bi (99.997%, granules, AlfaAesar) and 50.00%$_{at}$ Pt (99.95%, foil, Goodfellow), then sealed in an evacuated silica glass ampoule. The ampoule was placed into a furnace at 1473 K for 24 h, then cooled down from 1473 K to 873 K at a rate of 0.2 K min^{-1}. The temperature of 873 K was held for seven days and subsequently the ampoule was quenched in cold water. Single crystals with a hexagonal shape were selected from the top of an otherwise microgranular sample, which was composed of phases with the Cu_3Au and NiAs type of crystal structure, based on powder X-ray diffraction data. As a result of the high X-ray absorption of the investigated material, hexagonal-shaped specimens were too large for single crystal X-ray data collection. For this experiment, a relatively small piece was mechanically separated from a hexagonally shaped block. The composition of the investigated single crystal was determined by EDXS (Quantax, Bruker).

4. Refinement

Crystallographic data, data collection and structure refinement details are summarized in Table 1.

To decrease the number of parameters, the Pt site was constrained to full occupation at the 2a ($\overline{3}m$.) site. Even though the standardless quantification by means of EDXS data is 52.3%$_{at}$ Pt, recent results of bulk samples from the quasi-ternary cut of the quaternary Sn–Pb–Bi–Pt system indicate a strict upper compositional limit of 50%$_{at}$ Pt (Rössner *et al.*, 2023). An initial refinement was done for Pb and Bi, using EDXS values as a starting point, then the additional electron density was considered by adding Sn. After multiple cycles, it was decided that a compromise had to be made between excellent refinement results and compositions close to the ones from EDXS results. The final model is presented here.

Furthermore, it has to be noted that Sn3 was refined with isotropic displacement parameters, as the minor site occupancy (2.7%), does not justify to add additional parameters to enable a refinement with anisotropic displacement parameters. It has to be stressed that the ratio of 13 parameters for 123 independent reflections is already at the recommended upper limit (ratio parameters:reflections < 1:10).

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Computing details

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear* (Rigaku, 2008); data reduction: *CrystalClear* (Rigaku, 2008); program(s) used to solve structure: *SIR-2014* (Burla *et al.*, 2015); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2018); software used to prepare material for publication: *SHELXL* (Sheldrick, 2015).

(Tin, lead, bismuth) platinum

Crystal data

(Sn·Pb·Bi)Pt
M_r = 389.32
Hexagonal, $P6_3/mmc$
a = 4.228 (1) Å
c = 5.481 (2) Å
V = 84.84 (5) Å^3
Z = 2
F(000) = 311
D_x = 15.23 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.710730 Å
Cell parameters from 924 reflections
θ = 9.3–43.0°
μ = 169.4 mm^{-1}
T = 293 K
Irregular shaped, grey
0.04 × 0.03 × 0.02 mm

Data collection

Rigaku AFC7 four-circle diffractometer
Radiation source: Sealed Tube
Graphite Monochromator monochromator
Detector resolution: 28.5714 pixels mm^{-1}
profile data from φ–scans
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.037, T_{max} = 0.081
1549 measured reflections
123 independent reflections
120 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 39.8°, θ_{min} = 5.6°
h = −7→5
k = −6→7
l = −5→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.041
S = 1.51
123 reflections
13 parameters
1 restraint
$w = 1/[\sigma^2(F_o^2) + (0.012P)^2 + 0.2655P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.013
$\Delta\rho_{max}$ = 2.08 e Å^{-3}
$\Delta\rho_{min}$ = −1.43 e Å^{-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}	Occ. (<1)
Pt1	0	0	0	0.0110 (2)	
Bi1	0.3333	0.6667	0.2500	0.0077 (3)	0.31 (5)
Pb1	0.3333	0.6667	0.2500	0.0077	0.54 (5)
Sn1	0.3333	0.6667	0.2500	0.0077	0.03 (4)
Sn2	0.3333	0.6667	0.7500	0.0077	0.064 (6)
Sn3	0.3333	0.6667	0.501 (5)	0.012 (7)*	0.027 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.0133 (3)	0.0133	0.0063 (3)	0.00667 (13)	0	0
Bi1	0.0061 (3)	0.0061	0.0108 (4)	0.00307 (14)	0	0
Pb1	0.0061	0.0061	0.0108	0.00307	0	0
Sn1	0.0061	0.0061	0.0108	0.00307	0	0
Sn2	0.0061	0.0061	0.0108	0.00307	0	0

Geometric parameters (Å, º)

Pt1—Sn3^{i}	2.4410 (6)	Pb1—Sn3^{x}	2.797 (13)
Pt1—Sn3^{ii}	2.4410 (6)	Pb1—Sn3^{xiii}	2.797 (13)
Pt1—Sn3^{iii}	2.4410 (6)	Sn1—Sn3	1.37 (3)
Pt1—Sn3^{iv}	2.4410 (6)	Sn1—Sn3^{i}	1.37 (3)
Pt1—Sn3^{v}	2.4411 (6)	Sn1—Sn2^{ix}	2.4410 (6)
Pt1—Sn3^{vi}	2.4411 (6)	Sn1—Sn2^{x}	2.4410 (6)
Pt1—Pt1^{vii}	2.7402 (9)	Sn1—Sn2^{xi}	2.4410 (6)
Pt1—Pt1^{ii}	2.7402 (9)	Sn1—Sn2	2.7403 (8)
Pt1—Bi1^{viii}	2.7993 (5)	Sn1—Sn2^{xii}	2.7402 (9)
Pt1—Sn1^{viii}	2.7993 (5)	Sn1—Sn3^{iv}	2.797 (13)
Pt1—Pb1^{viii}	2.7993 (5)	Sn1—Sn3^{ix}	2.797 (13)
Pt1—Sn2^{ix}	2.7993 (5)	Sn1—Sn3^{vi}	2.797 (13)
Bi1—Sn3	1.37 (3)	Sn1—Sn3^{x}	2.797 (13)
Bi1—Sn3^{i}	1.37 (3)	Sn1—Sn3^{xiii}	2.797 (13)
Bi1—Sn2^{ix}	2.4410 (6)	Sn2—Sn3^{xiv}	1.37 (3)
Bi1—Sn2^{x}	2.4410 (6)	Sn2—Sn3	1.37 (3)
Bi1—Sn2^{xi}	2.4410 (6)	Sn2—Sn1^{ix}	2.4410 (6)
Bi1—Sn2	2.7403 (8)	Sn2—Pb1^{ix}	2.4410 (6)
Bi1—Sn2^{xii}	2.7402 (9)	Sn2—Bi1^{ix}	2.4410 (6)
Bi1—Sn3^{iv}	2.797 (13)	Sn2—Sn1^{x}	2.4410 (6)
Bi1—Sn3^{ix}	2.797 (13)	Sn2—Sn1^{xi}	2.4410 (6)

Bi1—Sn3^{vi}	2.797 (13)
Bi1—Sn3^{x}	2.797 (13)
Bi1—Sn3^{xiii}	2.797 (13)
Pb1—Sn3	1.37 (3)
Pb1—Sn3^{i}	1.37 (3)
Pb1—Sn2^{ix}	2.4410 (6)
Pb1—Sn2^{x}	2.4410 (6)
Pb1—Sn2^{xi}	2.4410 (6)
Pb1—Sn2	2.7403 (8)
Pb1—Sn2^{xii}	2.7402 (9)
Pb1—Sn3^{iv}	2.797 (13)
Pb1—Sn3^{ix}	2.797 (13)
Pb1—Sn3^{vi}	2.797 (13)
Sn2—Pb1^{x}	2.4410 (6)
Sn2—Pb1^{xi}	2.4410 (6)
Sn2—Bi1^{x}	2.4410 (6)
Sn2—Bi1^{xi}	2.4410 (6)
Sn3—Sn3^{ix}	2.4410 (6)
Sn3—Pt1^{xv}	2.4410 (6)
Sn3—Pt1^{xvi}	2.4410 (6)
Sn3—Pt1^{vii}	2.4410 (6)
Sn3—Sn3^{x}	2.4411 (6)
Sn3—Sn3^{xi}	2.4411 (7)
Sn3—Sn3^{xiv}	2.73 (5)
Sn3—Sn3^{i}	2.75 (5)

Sn3^{i}—Pt1—Sn3^{ii}	180.0
Sn3^{iii}—Pt1—Sn3^{iv}	180.0
Sn3^{i}—Pt1—Sn3^{v}	119.999 (5)
Sn3^{iii}—Pt1—Sn3^{v}	119.999 (4)
Sn3^{ii}—Pt1—Sn3^{vi}	119.999 (5)
Sn3^{iv}—Pt1—Sn3^{vi}	119.999 (4)
Sn3^{v}—Pt1—Sn3^{vi}	180.0
Sn3^{i}—Pt1—Pt1^{vii}	90.1 (6)
Sn3^{ii}—Pt1—Pt1^{vii}	89.9 (6)
Sn3^{iii}—Pt1—Pt1^{vii}	90.1 (6)
Sn3^{iv}—Pt1—Pt1^{vii}	89.9 (6)
Sn3^{v}—Pt1—Pt1^{vii}	90.1 (6)
Sn3^{vi}—Pt1—Pt1^{vii}	89.9 (6)
Sn3^{i}—Pt1—Pt1^{ii}	89.9 (6)
Sn3^{ii}—Pt1—Pt1^{ii}	90.1 (6)
Sn3^{iii}—Pt1—Pt1^{ii}	89.9 (6)
Sn3^{iv}—Pt1—Pt1^{ii}	90.1 (6)
Sn3^{v}—Pt1—Pt1^{ii}	89.9 (6)
Sn3^{vi}—Pt1—Pt1^{ii}	90.1 (6)
Pt1^{vii}—Pt1—Pt1^{ii}	180.0
Sn3^{i}—Pt1—Bi1^{viii}	150.6 (6)
Sn3^{ii}—Pt1—Bi1^{viii}	29.4 (6)
Sn3^{iii}—Pt1—Bi1^{viii}	64.1 (3)
Sn3^{iv}—Pt1—Bi1^{viii}	115.9 (3)
Sn3^{v}—Pt1—Bi1^{viii}	64.1 (3)
Sn3^{vi}—Pt1—Bi1^{viii}	115.9 (3)
Pt1^{vii}—Pt1—Bi1^{viii}	119.305 (9)
Pt1^{ii}—Pt1—Bi1^{viii}	60.695 (9)
Sn3^{i}—Pt1—Sn1^{viii}	150.6 (6)
Sn3^{ii}—Pt1—Sn1^{viii}	29.4 (6)
Sn3^{iii}—Pt1—Sn1^{viii}	64.1 (3)
Sn3^{iv}—Pt1—Sn1^{viii}	115.9 (3)
Sn3^{v}—Pt1—Sn1^{viii}	64.1 (3)
Sn3^{vi}—Pt1—Sn1^{viii}	115.9 (3)
Sn3^{i}—Sn1—Sn2^{x}	90.000 (4)
Sn2^{ix}—Sn1—Sn2^{x}	120.0
Sn3—Sn1—Sn2^{xi}	90.000 (5)
Sn3^{i}—Sn1—Sn2^{xi}	90.000 (4)
Sn2^{ix}—Sn1—Sn2^{xi}	120.0
Sn2^{x}—Sn1—Sn2^{xi}	120.0
Sn3—Sn1—Sn2	0.000 (6)
Sn3^{i}—Sn1—Sn2	180.0
Sn2^{ix}—Sn1—Sn2	90.0
Sn2^{x}—Sn1—Sn2	90.0
Sn2^{xi}—Sn1—Sn2	90.0
Sn3—Sn1—Sn2^{xii}	180.0
Sn3^{i}—Sn1—Sn2^{xii}	0.000 (1)
Sn2^{ix}—Sn1—Sn2^{xii}	90.0
Sn2^{x}—Sn1—Sn2^{xii}	90.0
Sn2^{xi}—Sn1—Sn2^{xii}	90.0
Sn2—Sn1—Sn2^{xii}	180.0
Sn3—Sn1—Sn3^{iv}	119.2 (5)
Sn3^{i}—Sn1—Sn3^{iv}	60.8 (5)
Sn2^{ix}—Sn1—Sn3^{iv}	29.2 (5)
Sn2^{x}—Sn1—Sn3^{iv}	115.87 (13)
Sn2^{xi}—Sn1—Sn3^{iv}	115.87 (13)
Sn2—Sn1—Sn3^{iv}	119.2 (5)
Sn2^{xii}—Sn1—Sn3^{iv}	60.8 (5)
Sn3—Sn1—Sn3^{ix}	60.8 (5)
Sn3^{i}—Sn1—Sn3^{ix}	119.2 (5)
Sn2^{ix}—Sn1—Sn3^{ix}	29.2 (5)
Sn2^{x}—Sn1—Sn3^{ix}	115.87 (13)
Sn2^{xi}—Sn1—Sn3^{ix}	115.87 (13)
Sn2—Sn1—Sn3^{ix}	60.8 (5)
Sn2^{xii}—Sn1—Sn3^{ix}	119.2 (5)
Sn3^{iv}—Sn1—Sn3^{ix}	58.5 (10)
Sn3—Sn1—Sn3^{vi}	119.2 (5)
Sn3^{i}—Sn1—Sn3^{vi}	60.8 (5)

$Pt1^{vii}$—Pt1—$Sn1^{viii}$	119.305 (9)	$Sn2^{ix}$—Sn1—$Sn3^{vi}$	115.87 (13)
$Pt1^{ii}$—Pt1—$Sn1^{viii}$	60.695 (9)	$Sn2^{x}$—Sn1—$Sn3^{vi}$	115.87 (13)
$Bi1^{viii}$—Pt1—$Sn1^{viii}$	0.0	$Sn2^{xi}$—Sn1—$Sn3^{vi}$	29.2 (5)
$Sn3^{i}$—Pt1—$Pb1^{viii}$	150.6 (6)	Sn2—Sn1—$Sn3^{vi}$	119.2 (5)
$Sn3^{ii}$—Pt1—$Pb1^{viii}$	29.4 (6)	$Sn2^{xii}$—Sn1—$Sn3^{vi}$	60.8 (5)
$Sn3^{iii}$—Pt1—$Pb1^{viii}$	64.1 (3)	$Sn3^{iv}$—Sn1—$Sn3^{vi}$	98.2 (6)
$Sn3^{iv}$—Pt1—$Pb1^{viii}$	115.9 (3)	$Sn3^{ix}$—Sn1—$Sn3^{vi}$	128.3 (3)
$Sn3^{v}$—Pt1—$Pb1^{viii}$	64.1 (3)	Sn3—Sn1—$Sn3^{x}$	60.8 (5)
$Sn3^{vi}$—Pt1—$Pb1^{viii}$	115.9 (3)	$Sn3^{i}$—Sn1—$Sn3^{x}$	119.2 (5)
$Pt1^{vii}$—Pt1—$Pb1^{viii}$	119.305 (9)	$Sn2^{ix}$—Sn1—$Sn3^{x}$	115.87 (13)
$Pt1^{ii}$—Pt1—$Pb1^{viii}$	60.695 (9)	$Sn2^{x}$—Sn1—$Sn3^{x}$	29.2 (5)
$Bi1^{viii}$—Pt1—$Pb1^{viii}$	0.0	$Sn2^{xi}$—Sn1—$Sn3^{x}$	115.87 (13)
$Sn1^{viii}$—Pt1—$Pb1^{viii}$	0.0	Sn2—Sn1—$Sn3^{x}$	60.8 (5)
$Sn3^{i}$—Pt1—$Sn2^{ix}$	64.2 (3)	$Sn2^{xii}$—Sn1—$Sn3^{x}$	119.2 (5)
$Sn3^{ii}$—Pt1—$Sn2^{ix}$	115.8 (3)	$Sn3^{iv}$—Sn1—$Sn3^{x}$	128.3 (3)
$Sn3^{iii}$—Pt1—$Sn2^{ix}$	150.8 (6)	$Sn3^{ix}$—Sn1—$Sn3^{x}$	98.2 (6)
$Sn3^{iv}$—Pt1—$Sn2^{ix}$	29.2 (6)	$Sn3^{vi}$—Sn1—$Sn3^{x}$	128.3 (3)
$Sn3^{v}$—Pt1—$Sn2^{ix}$	64.2 (3)	Sn3—Sn1—$Sn3^{xiii}$	119.2 (5)
$Sn3^{vi}$—Pt1—$Sn2^{ix}$	115.8 (3)	$Sn3^{i}$—Sn1—$Sn3^{xiii}$	60.8 (5)
$Pt1^{vii}$—Pt1—$Sn2^{ix}$	60.695 (9)	$Sn2^{ix}$—Sn1—$Sn3^{xiii}$	115.87 (13)
$Pt1^{ii}$—Pt1—$Sn2^{ix}$	119.305 (10)	$Sn2^{x}$—Sn1—$Sn3^{xiii}$	29.2 (5)
Sn3—Bi1—$Sn3^{i}$	180.0	$Sn2^{xi}$—Sn1—$Sn3^{xiii}$	115.87 (13)
Sn3—Bi1—$Sn2^{ix}$	90.000 (1)	Sn2—Sn1—$Sn3^{xiii}$	119.2 (5)
$Sn3^{i}$—Bi1—$Sn2^{ix}$	89.999 (1)	$Sn2^{xii}$—Sn1—$Sn3^{xiii}$	60.8 (5)
Sn3—Bi1—$Sn2^{x}$	90.000 (4)	$Sn3^{iv}$—Sn1—$Sn3^{xiii}$	98.2 (6)
$Sn3^{i}$—Bi1—$Sn2^{x}$	90.000 (4)	$Sn3^{ix}$—Sn1—$Sn3^{xiii}$	128.3 (3)
$Sn2^{ix}$—Bi1—$Sn2^{x}$	120.0	$Sn3^{vi}$—Sn1—$Sn3^{xiii}$	98.2 (6)
Sn3—Bi1—$Sn2^{xi}$	90.000 (5)	$Sn3^{x}$—Sn1—$Sn3^{xiii}$	58.5 (10)
$Sn3^{i}$—Bi1—$Sn2^{xi}$	90.000 (4)	$Sn3^{xiv}$—Sn2—Sn3	180.0
$Sn2^{ix}$—Bi1—$Sn2^{xi}$	120.0	$Sn3^{xiv}$—Sn2—$Sn1^{ix}$	89.999 (1)
$Sn2^{x}$—Bi1—$Sn2^{xi}$	120.0	Sn3—Sn2—$Sn1^{ix}$	90.000 (1)
Sn3—Bi1—Sn2	0.000 (6)	$Sn3^{xiv}$—Sn2—$Pb1^{ix}$	89.999 (1)
$Sn3^{i}$—Bi1—Sn2	180.0	Sn3—Sn2—$Pb1^{ix}$	90.000 (1)
$Sn2^{ix}$—Bi1—Sn2	90.0	$Sn1^{ix}$—Sn2—$Pb1^{ix}$	0.0
$Sn2^{x}$—Bi1—Sn2	90.0	$Sn3^{xiv}$—Sn2—$Bi1^{ix}$	89.999 (1)
$Sn2^{xi}$—Bi1—Sn2	90.0	Sn3—Sn2—$Bi1^{ix}$	90.000 (1)
Sn3—Bi1—$Sn2^{xii}$	180.0	$Sn1^{ix}$—Sn2—$Bi1^{ix}$	0.0
$Sn3^{i}$—Bi1—$Sn2^{xii}$	0.000 (1)	$Pb1^{ix}$—Sn2—$Bi1^{ix}$	0.0
$Sn2^{ix}$—Bi1—$Sn2^{xii}$	90.0	$Sn3^{xiv}$—Sn2—$Sn1^{x}$	90.000 (6)
$Sn2^{x}$—Bi1—$Sn2^{xii}$	90.0	Sn3—Sn2—$Sn1^{x}$	90.000 (6)
$Sn2^{xi}$—Bi1—$Sn2^{xii}$	90.0	$Sn1^{ix}$—Sn2—$Sn1^{x}$	120.0
Sn2—Bi1—$Sn2^{xii}$	180.0	$Pb1^{ix}$—Sn2—$Sn1^{x}$	120.0
Sn3—Bi1—$Sn3^{iv}$	119.2 (5)	$Bi1^{ix}$—Sn2—$Sn1^{x}$	120.0
$Sn3^{i}$—Bi1—$Sn3^{iv}$	60.8 (5)	$Sn3^{xiv}$—Sn2—$Sn1^{xi}$	90.000 (7)
$Sn2^{ix}$—Bi1—$Sn3^{iv}$	29.2 (5)	Sn3—Sn2—$Sn1^{xi}$	90.000 (7)
$Sn2^{x}$—Bi1—$Sn3^{iv}$	115.87 (13)	$Sn1^{ix}$—Sn2—$Sn1^{xi}$	120.0
$Sn2^{xi}$—Bi1—$Sn3^{iv}$	115.87 (13)	$Pb1^{ix}$—Sn2—$Sn1^{xi}$	120.0
Sn2—Bi1—$Sn3^{iv}$	119.2 (5)	$Bi1^{ix}$—Sn2—$Sn1^{xi}$	120.0

Sn2^{xii}—Bi1—Sn3^{iv}	60.8 (5)	Sn1^{x}—Sn2—Sn1^{xi}	120.0
Sn3—Bi1—Sn3^{ix}	60.8 (5)	Sn3^{xiv}—Sn2—Pb1^{x}	90.000 (6)
Sn3^{i}—Bi1—Sn3^{ix}	119.2 (5)	Sn3—Sn2—Pb1^{x}	90.000 (6)
Sn2^{ix}—Bi1—Sn3^{ix}	29.2 (5)	Sn1^{ix}—Sn2—Pb1^{x}	120.0
Sn2^{x}—Bi1—Sn3^{ix}	115.87 (13)	Pb1^{ix}—Sn2—Pb1^{x}	120.0
Sn2^{xi}—Bi1—Sn3^{ix}	115.87 (13)	Bi1^{ix}—Sn2—Pb1^{x}	120.0
Sn2—Bi1—Sn3^{ix}	60.8 (5)	Sn1^{x}—Sn2—Pb1^{x}	0.0
Sn2^{xii}—Bi1—Sn3^{ix}	119.2 (5)	Sn1^{xi}—Sn2—Pb1^{x}	120.0
Sn3^{iv}—Bi1—Sn3^{ix}	58.5 (10)	Sn3^{xiv}—Sn2—Pb1^{xi}	90.000 (7)
Sn3—Bi1—Sn3^{vi}	119.2 (5)	Sn3—Sn2—Pb1^{xi}	90.000 (7)
Sn3^{i}—Bi1—Sn3^{vi}	60.8 (5)	Sn1^{ix}—Sn2—Pb1^{xi}	120.0
Sn2^{ix}—Bi1—Sn3^{vi}	115.87 (13)	Pb1^{ix}—Sn2—Pb1^{xi}	120.0
Sn2^{x}—Bi1—Sn3^{vi}	115.87 (13)	Bi1^{ix}—Sn2—Pb1^{xi}	120.0
Sn2^{xi}—Bi1—Sn3^{vi}	29.2 (5)	Sn1^{x}—Sn2—Pb1^{xi}	120.0
Sn2—Bi1—Sn3^{vi}	119.2 (5)	Sn1^{xi}—Sn2—Pb1^{xi}	0.0
Sn2^{xii}—Bi1—Sn3^{vi}	60.8 (5)	Pb1^{x}—Sn2—Pb1^{xi}	120.0
Sn3^{iv}—Bi1—Sn3^{vi}	98.2 (6)	Sn3^{xiv}—Sn2—Bi1^{x}	90.000 (6)
Sn3^{ix}—Bi1—Sn3^{vi}	128.3 (3)	Sn3—Sn2—Bi1^{x}	90.000 (6)
Sn3—Bi1—Sn3^{x}	60.8 (5)	Sn1^{ix}—Sn2—Bi1^{x}	120.0
Sn3^{i}—Bi1—Sn3^{x}	119.2 (5)	Pb1^{ix}—Sn2—Bi1^{x}	120.0
Sn2^{ix}—Bi1—Sn3^{x}	115.87 (13)	Bi1^{ix}—Sn2—Bi1^{x}	120.0
Sn2^{x}—Bi1—Sn3^{x}	29.2 (5)	Sn1^{x}—Sn2—Bi1^{x}	0.0
Sn2^{xi}—Bi1—Sn3^{x}	115.87 (13)	Sn1^{xi}—Sn2—Bi1^{x}	120.0
Sn2—Bi1—Sn3^{x}	60.8 (5)	Pb1^{x}—Sn2—Bi1^{x}	0.0
Sn2^{xii}—Bi1—Sn3^{x}	119.2 (5)	Pb1^{xi}—Sn2—Bi1^{x}	120.0
Sn3^{iv}—Bi1—Sn3^{x}	128.3 (3)	Sn3^{xiv}—Sn2—Bi1^{xi}	90.000 (7)
Sn3^{ix}—Bi1—Sn3^{x}	98.2 (6)	Sn3—Sn2—Bi1^{xi}	90.000 (7)
Sn3^{vi}—Bi1—Sn3^{x}	128.3 (3)	Sn1^{ix}—Sn2—Bi1^{xi}	120.0
Sn3—Bi1—Sn3^{xiii}	119.2 (5)	Pb1^{ix}—Sn2—Bi1^{xi}	120.0
Sn3^{i}—Bi1—Sn3^{xiii}	60.8 (5)	Bi1^{ix}—Sn2—Bi1^{xi}	120.0
Sn2^{ix}—Bi1—Sn3^{xiii}	115.87 (13)	Sn1^{x}—Sn2—Bi1^{xi}	120.0
Sn2^{x}—Bi1—Sn3^{xiii}	29.2 (5)	Sn1^{xi}—Sn2—Bi1^{xi}	0.0
Sn2^{xi}—Bi1—Sn3^{xiii}	115.87 (13)	Pb1^{x}—Sn2—Bi1^{xi}	120.0
Sn2—Bi1—Sn3^{xiii}	119.2 (5)	Pb1^{xi}—Sn2—Bi1^{xi}	0.0
Sn2^{xii}—Bi1—Sn3^{xiii}	60.8 (5)	Bi1^{x}—Sn2—Bi1^{xi}	120.0
Sn3^{iv}—Bi1—Sn3^{xiii}	98.2 (6)	Sn3^{xiv}—Sn2—Bi1	180.0
Sn3^{ix}—Bi1—Sn3^{xiii}	128.3 (3)	Sn3—Sn2—Bi1	0.000 (6)
Sn3^{vi}—Bi1—Sn3^{xiii}	98.2 (6)	Sn1^{ix}—Sn2—Bi1	90.0
Sn3^{x}—Bi1—Sn3^{xiii}	58.5 (10)	Pb1^{ix}—Sn2—Bi1	90.0
Sn3—Pb1—Sn3^{i}	180.0	Bi1^{ix}—Sn2—Bi1	90.0
Sn3—Pb1—Sn2^{ix}	90.000 (1)	Sn1^{x}—Sn2—Bi1	90.0
Sn3^{i}—Pb1—Sn2^{ix}	89.999 (1)	Sn1^{xi}—Sn2—Bi1	90.0
Sn3—Pb1—Sn2^{x}	90.000 (4)	Pb1^{x}—Sn2—Bi1	90.0
Sn3^{i}—Pb1—Sn2^{x}	90.000 (4)	Pb1^{xi}—Sn2—Bi1	90.0
Sn2^{ix}—Pb1—Sn2^{x}	120.0	Bi1^{x}—Sn2—Bi1	90.0
Sn3—Pb1—Sn2^{xi}	90.000 (5)	Bi1^{xi}—Sn2—Bi1	90.0
Sn3^{i}—Pb1—Sn2^{xi}	90.000 (4)	Sn2—Sn3—Bi1	180.0
Sn2^{ix}—Pb1—Sn2^{xi}	120.0	Sn2—Sn3—Pb1	180.0

$Sn2^{x}$—Pb1—$Sn2^{xi}$	120.0	Bi1—Sn3—Pb1	0.0
Sn3—Pb1—Sn2	0.000 (6)	Sn2—Sn3—Sn1	180.0
$Sn3^{i}$—Pb1—Sn2	180.0	Bi1—Sn3—Sn1	0.0
$Sn2^{ix}$—Pb1—Sn2	90.0	Pb1—Sn3—Sn1	0.0
$Sn2^{x}$—Pb1—Sn2	90.0	Sn2—Sn3—$Sn3^{ix}$	90.2 (13)
$Sn2^{xi}$—Pb1—Sn2	90.0	Bi1—Sn3—$Sn3^{ix}$	89.8 (13)
Sn3—Pb1—$Sn2^{xii}$	180.0	Pb1—Sn3—$Sn3^{ix}$	89.8 (13)
$Sn3^{i}$—Pb1—$Sn2^{xii}$	0.000 (1)	Sn1—Sn3—$Sn3^{ix}$	89.8 (13)
$Sn2^{ix}$—Pb1—$Sn2^{xii}$	90.0	Sn2—Sn3—$Pt1^{xv}$	90.1 (6)
$Sn2^{x}$—Pb1—$Sn2^{xii}$	90.0	Bi1—Sn3—$Pt1^{xv}$	89.9 (6)
$Sn2^{xi}$—Pb1—$Sn2^{xii}$	90.0	Pb1—Sn3—$Pt1^{xv}$	89.9 (6)
Sn2—Pb1—$Sn2^{xii}$	180.0	Sn1—Sn3—$Pt1^{xv}$	89.9 (6)
Sn3—Pb1—$Sn3^{iv}$	119.2 (5)	$Sn3^{ix}$—Sn3—$Pt1^{xv}$	179.7 (19)
$Sn3^{i}$—Pb1—$Sn3^{iv}$	60.8 (5)	Sn2—Sn3—$Pt1^{xvi}$	90.1 (6)
$Sn2^{ix}$—Pb1—$Sn3^{iv}$	29.2 (5)	Bi1—Sn3—$Pt1^{xvi}$	89.9 (6)
$Sn2^{x}$—Pb1—$Sn3^{iv}$	115.87 (13)	Pb1—Sn3—$Pt1^{xvi}$	89.9 (6)
$Sn2^{xi}$—Pb1—$Sn3^{iv}$	115.87 (13)	Sn1—Sn3—$Pt1^{xvi}$	89.9 (6)
Sn2—Pb1—$Sn3^{iv}$	119.2 (5)	$Sn3^{ix}$—Sn3—$Pt1^{xvi}$	60.000 (1)
$Sn2^{xii}$—Pb1—$Sn3^{iv}$	60.8 (5)	$Pt1^{xv}$—Sn3—$Pt1^{xvi}$	120.000 (4)
Sn3—Pb1—$Sn3^{ix}$	60.8 (5)	Sn2—Sn3—$Pt1^{vii}$	90.1 (6)
$Sn3^{i}$—Pb1—$Sn3^{ix}$	119.2 (5)	Bi1—Sn3—$Pt1^{vii}$	89.9 (6)
$Sn2^{ix}$—Pb1—$Sn3^{ix}$	29.2 (5)	Pb1—Sn3—$Pt1^{vii}$	89.9 (6)
$Sn2^{x}$—Pb1—$Sn3^{ix}$	115.87 (13)	Sn1—Sn3—$Pt1^{vii}$	89.9 (6)
$Sn2^{xi}$—Pb1—$Sn3^{ix}$	115.87 (13)	$Sn3^{ix}$—Sn3—$Pt1^{vii}$	60.000 (5)
Sn2—Pb1—$Sn3^{ix}$	60.8 (5)	$Pt1^{xv}$—Sn3—$Pt1^{vii}$	120.000 (4)
$Sn2^{xii}$—Pb1—$Sn3^{ix}$	119.2 (5)	$Pt1^{xvi}$—Sn3—$Pt1^{vii}$	120.000 (4)
$Sn3^{iv}$—Pb1—$Sn3^{ix}$	58.5 (10)	Sn2—Sn3—$Sn3^{x}$	90.2 (13)
Sn3—Pb1—$Sn3^{vi}$	119.2 (5)	Bi1—Sn3—$Sn3^{x}$	89.8 (13)
$Sn3^{i}$—Pb1—$Sn3^{vi}$	60.8 (5)	Pb1—Sn3—$Sn3^{x}$	89.8 (13)
$Sn2^{ix}$—Pb1—$Sn3^{vi}$	115.87 (13)	Sn1—Sn3—$Sn3^{x}$	89.8 (13)
$Sn2^{x}$—Pb1—$Sn3^{vi}$	115.87 (13)	$Pt1^{xv}$—Sn3—$Sn3^{x}$	60.0
$Sn2^{xi}$—Pb1—$Sn3^{vi}$	29.2 (5)	$Pt1^{xvi}$—Sn3—$Sn3^{x}$	60.000 (1)
Sn2—Pb1—$Sn3^{vi}$	119.2 (5)	$Pt1^{vii}$—Sn3—$Sn3^{x}$	179.7 (19)
$Sn2^{xii}$—Pb1—$Sn3^{vi}$	60.8 (5)	Sn2—Sn3—$Sn3^{xi}$	90.2 (13)
$Sn3^{iv}$—Pb1—$Sn3^{vi}$	98.2 (6)	Bi1—Sn3—$Sn3^{xi}$	89.8 (13)
$Sn3^{ix}$—Pb1—$Sn3^{vi}$	128.3 (3)	Pb1—Sn3—$Sn3^{xi}$	89.8 (13)
Sn3—Pb1—$Sn3^{x}$	60.8 (5)	Sn1—Sn3—$Sn3^{xi}$	89.8 (13)
$Sn3^{i}$—Pb1—$Sn3^{x}$	119.2 (5)	$Pt1^{xv}$—Sn3—$Sn3^{xi}$	59.999 (4)
$Sn2^{ix}$—Pb1—$Sn3^{x}$	115.87 (13)	$Pt1^{xvi}$—Sn3—$Sn3^{xi}$	179.7 (19)
$Sn2^{x}$—Pb1—$Sn3^{x}$	29.2 (5)	$Pt1^{vii}$—Sn3—$Sn3^{xi}$	60.000 (6)
$Sn2^{xi}$—Pb1—$Sn3^{x}$	115.87 (13)	Sn2—Sn3—$Sn3^{xiv}$	0.0
Sn2—Pb1—$Sn3^{x}$	60.8 (5)	Bi1—Sn3—$Sn3^{xiv}$	180.0
$Sn2^{xii}$—Pb1—$Sn3^{x}$	119.2 (5)	Pb1—Sn3—$Sn3^{xiv}$	180.0
$Sn3^{iv}$—Pb1—$Sn3^{x}$	128.3 (3)	Sn1—Sn3—$Sn3^{xiv}$	180.0
$Sn3^{ix}$—Pb1—$Sn3^{x}$	98.2 (6)	$Sn3^{ix}$—Sn3—$Sn3^{xiv}$	90.2 (13)
$Sn3^{vi}$—Pb1—$Sn3^{x}$	128.3 (3)	$Pt1^{xv}$—Sn3—$Sn3^{xiv}$	90.1 (6)
Sn3—Pb1—$Sn3^{xiii}$	119.2 (5)	$Pt1^{xvi}$—Sn3—$Sn3^{xiv}$	90.1 (6)
$Sn3^{i}$—Pb1—$Sn3^{xiii}$	60.8 (5)	$Pt1^{vii}$—Sn3—$Sn3^{xiv}$	90.1 (6)

$Sn2^{ix}—Pb1—Sn3^{xiii}$	115.87 (13)	$Sn3^{x}—Sn3—Sn3^{xiv}$	90.2 (13)
$Sn2^{x}—Pb1—Sn3^{xiii}$	29.2 (5)	$Sn3^{xi}—Sn3—Sn3^{xiv}$	90.2 (13)
$Sn2^{xi}—Pb1—Sn3^{xiii}$	115.87 (13)	Sn2—Sn3—$Sn3^{i}$	180.0
Sn2—Pb1—$Sn3^{xiii}$	119.2 (5)	Bi1—Sn3—$Sn3^{i}$	0.0
$Sn2^{xii}—Pb1—Sn3^{xiii}$	60.8 (5)	Pb1—Sn3—$Sn3^{i}$	0.0
$Sn3^{iv}—Pb1—Sn3^{xiii}$	98.2 (6)	Sn1—Sn3—$Sn3^{i}$	0.0
$Sn3^{ix}—Pb1—Sn3^{xiii}$	128.3 (3)	$Sn3^{ix}—Sn3—Sn3^{i}$	89.8 (13)
$Sn3^{vi}—Pb1—Sn3^{xiii}$	98.2 (6)	$Pt1^{xv}—Sn3—Sn3^{i}$	89.9 (6)
$Sn3^{x}—Pb1—Sn3^{xiii}$	58.5 (10)	$Pt1^{xvi}—Sn3—Sn3^{i}$	89.9 (6)
Sn3—Sn1—$Sn3^{i}$	180.0	$Pt1^{vii}—Sn3—Sn3^{i}$	89.9 (6)
Sn3—Sn1—$Sn2^{ix}$	90.000 (1)	$Sn3^{x}—Sn3—Sn3^{i}$	89.8 (13)
$Sn3^{i}—Sn1—Sn2^{ix}$	89.999 (1)	$Sn3^{xi}—Sn3—Sn3^{i}$	89.8 (13)
Sn3—Sn1—$Sn2^{x}$	90.000 (4)	$Sn3^{xiv}—Sn3—Sn3^{i}$	180.0

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