Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Terbium (lithium zinc) distannide, $TbLi_{1-x}Zn_xSn_2$ ($x = 0.2$)

Andrij Stetskiv,[a] Ivan Tarasiuk,[b]* Beata Rozdzynska-Kielbik,[c] Igor Oshchapovsky[b] and Volodymyr Pavlyuk[b,c]

[a]Ivano-Frankivsk National Medical University, Department of Chemistry, Galytska str. 2, 76018 Ivano-Frankivsk, Ukraine, [b]Department of Inorganic Chemistry, Ivan Franko Lviv National University, Kyryla and Mefodiya str. 6, 79005 Lviv, Ukraine, and [c]Institute of Chemistry, Environment Protection and Biotechnology, Jan Dlugosz University, al. Armii Krajowej 13/15, 42-200 Czestochowa, Poland
Correspondence e-mail: tarasiuk.i@gmail.com

Received 17 November 2011; accepted 17 January 2012

Key indicators: single-crystal X-ray study; $T = 293$ K; mean σ(Sn–Sn) = 0.001 Å; disorder in main residue; R factor = 0.027; wR factor = 0.066; data-to-parameter ratio = 13.1.

The new terbium (lithium zinc) distannide, $TbLi_{1-x}Zn_xSn_2$ ($x = 0.2$) crystallizes in the orthorhombic $CeNiSi_2$ structure type with space group *Cmcm* and Pearson symbol *oS*16. Of the four independent 4*c* atom positions (*m*2*m* site symmetry), three are fully occupied by individual atoms (two by Sn and one by Tb atoms) and the fourth is occupied by Li and Zn atoms with a statistical distribution. The Tb coordination polyhedron is a 21-vertex pseudo-Frank–Kasper polyhedron. One Sn atom is enclosed in a tricapped trigonal prism, the second Sn atom is in a cuboctahedron and the statistically distributed (Li,Zn) site is in a tetragonal antiprism with one added atom. Electronic structure calculations were used for the elucidation of reasons for and the ability of mutual substitution of lithium and transition metals. Positive charge density was observed around the rare earth atom and the Li and Zn atoms, the negative charge density in the proximity of the Sn atoms.

Related literature

For general background, see: Andersen *et al.* (1986); Pavlyuk *et al.* (2009). For related structures, see: Pavlyuk & Bodak (1992*a*,*b*); Pavlyuk *et al.* (1991, 1993). For isotypic structures, see: Pavlyuk *et al.* (1989).

Experimental

Crystal data

$TbLi_{0.8}Zn_{0.2}Sn_2$
$M_r = 414.85$
Orthorhombic, *Cmcm*
$a = 4.4495$ (7) Å
$b = 17.699$ (3) Å
$c = 4.3978$ (7) Å
$V = 346.33$ (9) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 35.55$ mm^{-1}
$T = 293$ K
$0.08 \times 0.04 \times 0.02$ mm

Data collection

Oxford Diffraction Xcalibur3 CCD diffractometer
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2008)
$T_{min} = 0.344$, $T_{max} = 0.658$
1198 measured reflections
261 independent reflections
190 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.066$
$S = 1.19$
261 reflections
20 parameters
$\Delta\rho_{max} = 2.15$ e Å^{-3}
$\Delta\rho_{min} = -2.64$ e Å^{-3}

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2008); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

Financial support from the Ministry of Education and Science, Youth and Sport of Ukraine (No. 0111U001089) is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2120).

References

Andersen, K., Povlovska, Z. & Jepsen, O. (1986). *Phys. Rev. B*, **34**, 51–53.
Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Oxford Diffraction (2008). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, England.
Pavlyuk, V. & Bodak, O. (1992*a*). *Inorg. Mater.* **28**, 877–879.
Pavlyuk, V. & Bodak, O. (1992*b*). *Akad. Nauk SSSR Izvest. Metally*. **6**, 207-210.
Pavlyuk, V., Bodak, O. & Bruskov, V. (1991). *Dopov. Akad. Nauk Ukr.*, **1**, 112–114.
Pavlyuk, V., Bodak, O. & Kevorkov, D. (1993). *Dopov. Akad. Nauk Ukr.*, **9**, 84–87.
Pavlyuk, V., Bodak, O., Pecharskii, V., Skolozdra, R. & Gladyshevskii, E. (1989). *Inorg. Mater.* **25**, 962–965.
Pavlyuk, V., Oshchapovsky, I. & Marciniak, B. (2009). *J. Alloys Compd*, **477**, 145–148.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2012). E**68**, i16 [**doi:10.1107/S1600536812002103**]

Terbium (lithium zinc) distannide, $TbLi_{1-x}Zn_xSn_2$ ($x = 0.2$)

A. Stetskiv, I. Tarasiuk, B. Rozdzynska-Kielbik, I. Oshchapovsky and **V. Pavlyuk**

Comment

During the systematic investigation of alloys of the Tb–Li–Sn and Tb–Zn–Sn ternary systems the ternary compounds with the corresponding compositions $TbLiSn_2$ (Pavlyuk *et al.*, 1989) and $TbZnSn_2$ (Pavlyuk *et al.*, 2009) were found. According to the X-ray data, $TbLiSn_2$ crystallizes with orthorhombic symmetry (space group *Cmcm*, $CeNiSi_2$ structure type) and the $TbZnSn_2$ with tetragonal symmetry (space group *P*4/*nmm*, $HfCuSi_2$ structure type). Structural studies of the four-component alloys from $TbLiSn_2$–$TbZnSn_2$ sections indicate the existence of $TbLi_{1-x}Zn_xSn_2$ ($x = 0 - 1/5$) limited solid solution. In the ternary $TbLiSn_2$ compound lithium atoms occupy the same crystallographic position that the atoms of transition metal in the original $CeNiSi_2$ structure type. The same was observed previously when we studied RELiGe with the ZrNiAl type (Pavlyuk *et al.*, 1991 and Pavlyuk *et al.*, 1992*a*) and $RE_3Li_2Ge_3$ with $Hf_3Ni_2Si_3$ type (Pavlyuk & Bodak, 1992*b*). X-ray single-crystal study showed that the $TbLi_{1-x}Zn_xSn_2$ solid solution formed by the partial substitution of lithium atoms by zinc atoms in 4*c* site. The ability of lithium atoms to substitute the atoms of transition metals we observed previously studying solid solutions $RELi_xCu_{2-x}Si_2$ and $RELi_xCu_{2-x}Ge_2$ (Pavlyuk *et al.*, 1993).

The projection of the unit cell and coordination polyhedra of the atoms are shown in Fig. 1. The coordination polyhedra of atoms are: Tb1 – 21-vertex pseudo Frank-Kasper polyhedron $[Tb(Zn,Li)_5Sn_{10}Tb_6]$, Sn1 – 9-vertex tricapped trigonal prism $[Sn1(Li,Zn)Sn_2Tb_6]$, Sn2 – 12-vertex cuboctahedron $[Sn2(Li,Zn)_4Sn_4Tb_4]$ and statistical mixture (Li,Zn) – 9-vertex tetragonal antiprism with one added atom $[(Li,Zn)Sn_5Tb_4]$.

Formation of the same $RELi_{1-x}Zn_xSn_2$ solid solutions were observed with other rare earth metals, such as Gd, Dy, Ho and Y.

The electronic structure calculations using TB-LMTO-ASA (Andersen *et al.*, 1986) program package were performed for the elucidation of reasons of the formation of solid solutions and the ability to mutual substitution of lithium and transition metals. The ordered model of $RELiSn_2$ ternary phase and hypothetical $REZnSn_2$ with $CeNiSi_2$ structure type were analyzed. Among the rare earth metals was taken yttrium, which has less number of electrons than majority of other rare earth metals.

According to the results of calculations in the both models the rare earth atoms donate their electrons to tin atoms. The lithium atoms (Fig. 2a) and zinc atoms (Fig. 2 b) also loses their electrons. So positive charge density in various scale can be observed around rare earth, lithium and zinc atoms and negative charge density is around tin atoms. Taking into account these data and also the closeness of the effective radius of zinc and lithium atoms in intermetallic compounds it can be concluded that nothing prevents their mutual substitution.

Experimental

Terbium, lithium, zinc and tin, all with a nominal purity more than 99.9 wt. %, were used as starting elements. First, the pieces of the pure metals with a stoichiometry $Tb_{25}Li_{20}Zn_5Sn_{50}$ were pressed into pellets, enclosed in a tantalum crucible and placed in a resistance furnace with a thermocouple controller. The sample was heated to 670 K at a rate of 5 K/min, maintained over a period of 48 h and then temperature was increased to 1070 K over a period of 10 h. The alloy was annealed at 670 K for 120 h and cooled slowly to room temperature. Small, good-quality single-crystals of the title compound were isolated from an alloy by mechanical fragmentation.

Refinement

The Li position (Wyckoff sites 4*c*) showed displacement parameters considerably smaller than it should be for the lithium, suggesting that this position is partially occupied by the heavier Zn atom. The refinement of the occupancy of this statistically mixed position showed, that it contains 80% of Li and 20% of Zn atoms.

Figures

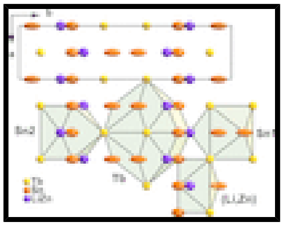

Fig. 1. Unit cell projection and coordination polyhedra of atoms in the $TbLi_{1-x}Zn_xSn_2$ compound. Thermal ellipsoids are drawn at a 95% probability level.

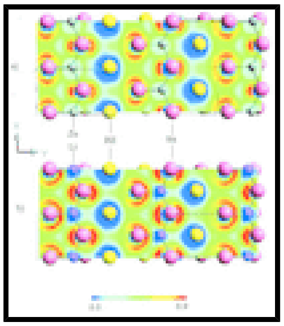

Fig. 2. The results of electron localization function calculations for ordered structure models of $REZnSn_2$ (*a*) and $RELiSn_2$ (*b*). ELF map drawn at *z* = 0.

terbium (lithium zinc) distannide

Crystal data

$TbLi_{0.8}Zn_{0.2}Sn_2$	$F(000) = 693.6$
$M_r = 414.85$	$D_x = 7.956$ Mg m^{-3}
Orthorhombic, *Cmcm*	Mo *Kα* radiation, λ = 0.71073 Å
Hall symbol: -C 2c 2	Cell parameters from 261 reflections
a = 4.4495 (7) Å	θ = 4.6–28.0°
b = 17.699 (3) Å	μ = 35.55 mm^{-1}
c = 4.3978 (7) Å	*T* = 293 K
V = 346.33 (9) Å^3	Prism, metallic dark grey
Z = 4	0.08 × 0.04 × 0.02 mm

Data collection

Oxford Diffraction Xcalibur3 CCD diffractometer	261 independent reflections

Radiation source: fine-focus sealed tube

graphite

Detector resolution: 0 pixels mm^{-1}

ω scans

Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2008)

$T_{min} = 0.344$, $T_{max} = 0.658$

1198 measured reflections

190 reflections with $I > 2\sigma(I)$

$R_{int} = 0.041$

$\theta_{max} = 28.0°$, $\theta_{min} = 4.6°$

$h = -5 \rightarrow 5$

$k = -17 \rightarrow 23$

$l = -5 \rightarrow 5$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.066$

$S = 1.19$

261 reflections

20 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$w = 1/[\sigma^2(F_o^2) + (0.0272P)^2 + 2.6711P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 2.15$ e Å^{-3}

$\Delta\rho_{min} = -2.64$ e Å^{-3}

Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0039 (4)

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Tb1	0.0000	0.39911 (5)	0.2500	0.0156 (4)	
Sn1	0.0000	0.06101 (10)	0.2500	0.0296 (6)	
Sn2	0.0000	0.75076 (8)	0.2500	0.0274 (6)	
Zn	0.0000	0.1960 (5)	0.2500	0.022 (3)	0.198 (11)
Li	0.0000	0.1960 (5)	0.2500	0.022 (3)	0.80

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

Tb1	0.0152 (5)	0.0167 (5)	0.0149 (6)	0.000	0.000	0.000
Sn1	0.0132 (8)	0.0638 (16)	0.0119 (9)	0.000	0.000	0.000
Sn2	0.0180 (8)	0.0423 (14)	0.0220 (10)	0.000	0.000	0.000
Zn	0.019 (5)	0.024 (5)	0.022 (6)	0.000	0.000	0.000
Li	0.019 (5)	0.024 (5)	0.022 (6)	0.000	0.000	0.000

Geometric parameters (Å, °)

Tb1—Sn1^{i}	3.2067 (6)	Sn2—Li^{viii}	2.392 (4)
Tb1—Sn1^{ii}	3.2067 (6)	Sn2—Zn^{viii}	2.392 (4)
Tb1—Sn1^{iii}	3.2067 (6)	Sn2—Li^{vii}	2.392 (4)
Tb1—Sn1^{iv}	3.2067 (6)	Sn2—Zn^{vii}	2.392 (4)
Tb1—Sn2^{v}	3.4414 (13)	Sn2—Li^{xi}	2.427 (4)
Tb1—Sn2^{vi}	3.4414 (13)	Sn2—Zn^{xi}	2.427 (4)
Tb1—Sn2^{vii}	3.4454 (14)	Sn2—Li^{xii}	2.427 (4)
Tb1—Sn2^{viii}	3.4454 (14)	Sn2—Zn^{xii}	2.427 (4)
Tb1—Li^{ii}	3.552 (4)	Sn2—Sn2^{xiii}	3.1282 (4)
Tb1—Zn^{ii}	3.552 (4)	Sn2—Sn2^{xiv}	3.1282 (4)
Tb1—Li^{i}	3.552 (4)	Sn2—Sn2^{xv}	3.1282 (4)
Tb1—Zn^{i}	3.552 (4)	Sn2—Sn2^{xvi}	3.1282 (4)
Sn1—Zn	2.389 (9)	Zn—Sn2^{viii}	2.392 (4)
Sn1—Sn1^{ix}	3.082 (3)	Zn—Sn2^{vii}	2.392 (4)
Sn1—Sn1^{x}	3.082 (3)	Zn—Sn2^{vi}	2.427 (4)
Sn1—Tb1^{i}	3.2067 (6)	Zn—Sn2^{v}	2.427 (4)
Sn1—Tb1^{ii}	3.2067 (6)	Zn—Tb1^{ii}	3.552 (4)
Sn1—Tb1^{iv}	3.2067 (6)	Zn—Tb1^{i}	3.552 (4)
Sn1—Tb1^{iii}	3.2067 (6)	Zn—Tb1^{iii}	3.552 (4)
Sn1—Tb1^{v}	3.6277 (15)	Zn—Tb1^{iv}	3.552 (4)
Sn1—Tb1^{vi}	3.6277 (15)		
Sn1^{i}—Tb1—Sn1^{ii}	154.57 (8)	Li^{viii}—Sn2—Zn^{viii}	0.0
Sn1^{i}—Tb1—Sn1^{iii}	87.86 (2)	Li^{viii}—Sn2—Li^{vii}	133.6 (4)
Sn1^{ii}—Tb1—Sn1^{iii}	86.59 (2)	Zn^{viii}—Sn2—Li^{vii}	133.6 (4)
Sn1^{i}—Tb1—Sn1^{iv}	86.59 (2)	Li^{viii}—Sn2—Zn^{vii}	133.6 (4)
Sn1^{ii}—Tb1—Sn1^{iv}	87.86 (2)	Zn^{viii}—Sn2—Zn^{vii}	133.6 (4)
Sn1^{iii}—Tb1—Sn1^{iv}	154.57 (8)	Li^{vii}—Sn2—Zn^{vii}	0.0 (4)
Sn1^{i}—Tb1—Sn2^{v}	128.06 (4)	Li^{viii}—Sn2—Li^{xi}	99.05 (15)
Sn1^{ii}—Tb1—Sn2^{v}	73.71 (3)	Zn^{viii}—Sn2—Li^{xi}	99.05 (15)
Sn1^{iii}—Tb1—Sn2^{v}	73.71 (3)	Li^{vii}—Sn2—Li^{xi}	99.05 (15)
Sn1^{iv}—Tb1—Sn2^{v}	128.06 (4)	Zn^{vii}—Sn2—Li^{xi}	99.05 (15)
Sn1^{i}—Tb1—Sn2^{vi}	73.71 (3)	Li^{viii}—Sn2—Zn^{xi}	99.05 (15)
Sn1^{ii}—Tb1—Sn2^{vi}	128.06 (4)	Zn^{viii}—Sn2—Zn^{xi}	99.05 (15)
Sn1^{iii}—Tb1—Sn2^{vi}	128.06 (4)	Li^{vii}—Sn2—Zn^{xi}	99.05 (15)

Sn1^{iv}—Tb1—Sn2^{vi}	73.71 (3)	Zn^{vii}—Sn2—Zn^{xi}	99.05 (15)
Sn2^{v}—Tb1—Sn2^{vi}	80.55 (4)	Li^{xi}—Sn2—Zn^{xi}	0.0
Sn1^{i}—Tb1—Sn2^{vii}	127.38 (4)	Li^{viii}—Sn2—Li^{xii}	99.05 (15)
Sn1^{ii}—Tb1—Sn2^{vii}	74.44 (3)	Zn^{viii}—Sn2—Li^{xii}	99.05 (15)
Sn1^{iii}—Tb1—Sn2^{vii}	127.38 (4)	Li^{vii}—Sn2—Li^{xii}	99.05 (15)
Sn1^{iv}—Tb1—Sn2^{vii}	74.44 (3)	Zn^{vii}—Sn2—Li^{xii}	99.05 (15)
Sn2^{v}—Tb1—Sn2^{vii}	54.030 (13)	Li^{xi}—Sn2—Li^{xii}	132.9 (4)
Sn2^{vi}—Tb1—Sn2^{vii}	54.030 (13)	Zn^{xi}—Sn2—Li^{xii}	132.9 (4)
Sn1^{i}—Tb1—Sn2^{viii}	74.44 (3)	Li^{viii}—Sn2—Zn^{xii}	99.05 (15)
Sn1^{ii}—Tb1—Sn2^{viii}	127.38 (4)	Zn^{viii}—Sn2—Zn^{xii}	99.05 (15)
Sn1^{iii}—Tb1—Sn2^{viii}	74.44 (3)	Li^{vii}—Sn2—Zn^{xii}	99.05 (15)
Sn1^{iv}—Tb1—Sn2^{viii}	127.38 (4)	Zn^{vii}—Sn2—Zn^{xii}	99.05 (15)
Sn2^{v}—Tb1—Sn2^{viii}	54.030 (13)	Li^{xi}—Sn2—Zn^{xii}	132.9 (4)
Sn2^{vi}—Tb1—Sn2^{viii}	54.030 (13)	Zn^{xi}—Sn2—Zn^{xii}	132.9 (4)
Sn2^{vii}—Tb1—Sn2^{viii}	79.32 (4)	Li^{xii}—Sn2—Zn^{xii}	0.0 (4)
Sn1^{i}—Tb1—Li^{ii}	164.43 (14)	Li^{viii}—Sn2—Sn2^{xiii}	130.50 (8)
Sn1^{ii}—Tb1—Li^{ii}	41.00 (13)	Zn^{viii}—Sn2—Sn2^{xiii}	130.50 (8)
Sn1^{iii}—Tb1—Li^{ii}	95.41 (3)	Li^{vii}—Sn2—Sn2^{xiii}	50.01 (8)
Sn1^{iv}—Tb1—Li^{ii}	96.57 (3)	Zn^{vii}—Sn2—Sn2^{xiii}	50.01 (8)
Sn2^{v}—Tb1—Li^{ii}	39.97 (9)	Li^{xi}—Sn2—Sn2^{xiii}	49.05 (7)
Sn2^{vi}—Tb1—Li^{ii}	92.49 (12)	Zn^{xi}—Sn2—Sn2^{xiii}	49.05 (7)
Sn2^{vii}—Tb1—Li^{ii}	40.55 (9)	Li^{xii}—Sn2—Sn2^{xiii}	130.43 (9)
Sn2^{viii}—Tb1—Li^{ii}	91.74 (12)	Zn^{xii}—Sn2—Sn2^{xiii}	130.43 (9)
Sn1^{i}—Tb1—Zn^{ii}	164.43 (14)	Li^{viii}—Sn2—Sn2^{xiv}	50.01 (8)
Sn1^{ii}—Tb1—Zn^{ii}	41.00 (13)	Zn^{viii}—Sn2—Sn2^{xiv}	50.01 (8)
Sn1^{iii}—Tb1—Zn^{ii}	95.41 (3)	Li^{vii}—Sn2—Sn2^{xiv}	130.50 (8)
Sn1^{iv}—Tb1—Zn^{ii}	96.57 (3)	Zn^{vii}—Sn2—Sn2^{xiv}	130.50 (8)
Sn2^{v}—Tb1—Zn^{ii}	39.97 (9)	Li^{xi}—Sn2—Sn2^{xiv}	130.43 (9)
Sn2^{vi}—Tb1—Zn^{ii}	92.49 (12)	Zn^{xi}—Sn2—Sn2^{xiv}	130.43 (9)
Sn2^{vii}—Tb1—Zn^{ii}	40.55 (9)	Li^{xii}—Sn2—Sn2^{xiv}	49.05 (7)
Sn2^{viii}—Tb1—Zn^{ii}	91.74 (12)	Zn^{xii}—Sn2—Sn2^{xiv}	49.05 (7)
Li^{ii}—Tb1—Zn^{ii}	0.0 (3)	Sn2^{xiii}—Sn2—Sn2^{xiv}	179.01 (11)
Sn1^{i}—Tb1—Li^{i}	41.00 (13)	Li^{viii}—Sn2—Sn2^{xv}	50.01 (8)
Sn1^{ii}—Tb1—Li^{i}	164.43 (14)	Zn^{viii}—Sn2—Sn2^{xv}	50.01 (8)
Sn1^{iii}—Tb1—Li^{i}	96.57 (3)	Li^{vii}—Sn2—Sn2^{xv}	130.50 (8)
Sn1^{iv}—Tb1—Li^{i}	95.41 (3)	Zn^{vii}—Sn2—Sn2^{xv}	130.50 (8)
Sn2^{v}—Tb1—Li^{i}	92.49 (12)	Li^{xi}—Sn2—Sn2^{xv}	49.05 (7)
Sn2^{vi}—Tb1—Li^{i}	39.97 (9)	Zn^{xi}—Sn2—Sn2^{xv}	49.05 (7)
Sn2^{vii}—Tb1—Li^{i}	91.74 (12)	Li^{xii}—Sn2—Sn2^{xv}	130.43 (9)
Sn2^{viii}—Tb1—Li^{i}	40.55 (9)	Zn^{xii}—Sn2—Sn2^{xv}	130.43 (9)
Li^{ii}—Tb1—Li^{i}	123.4 (3)	Sn2^{xiii}—Sn2—Sn2^{xv}	89.326 (13)

Zn^{ii}—Tb1—Li^{i}	123.4 (3)	Sn2^{xiv}—Sn2—Sn2^{xv}	90.665 (13)
Sn1^{i}—Tb1—Zn^{i}	41.00 (13)	Li^{viii}—Sn2—Sn2^{xvi}	130.50 (8)
Sn1^{ii}—Tb1—Zn^{i}	164.43 (14)	Zn^{viii}—Sn2—Sn2^{xvi}	130.50 (8)
Sn1^{iii}—Tb1—Zn^{i}	96.57 (3)	Li^{vii}—Sn2—Sn2^{xvi}	50.01 (8)
Sn1^{iv}—Tb1—Zn^{i}	95.41 (3)	Zn^{vii}—Sn2—Sn2^{xvi}	50.01 (8)
Sn2^{v}—Tb1—Zn^{i}	92.49 (12)	Li^{xi}—Sn2—Sn2^{xvi}	130.43 (9)
Sn2^{vi}—Tb1—Zn^{i}	39.97 (9)	Zn^{xi}—Sn2—Sn2^{xvi}	130.43 (9)
Sn2^{vii}—Tb1—Zn^{i}	91.74 (12)	Li^{xii}—Sn2—Sn2^{xvi}	49.05 (7)
Sn2^{viii}—Tb1—Zn^{i}	40.55 (9)	Zn^{xii}—Sn2—Sn2^{xvi}	49.05 (7)
Li^{ii}—Tb1—Zn^{i}	123.4 (3)	Sn2^{xiii}—Sn2—Sn2^{xvi}	90.665 (13)
Zn^{ii}—Tb1—Zn^{i}	123.4 (3)	Sn2^{xiv}—Sn2—Sn2^{xvi}	89.326 (13)
Li^{i}—Tb1—Zn^{i}	0.0 (3)	Sn2^{xv}—Sn2—Sn2^{xvi}	179.01 (11)
Zn—Sn1—Sn1^{ix}	134.48 (5)	Sn1—Zn—Sn2^{viii}	113.2 (2)
Zn—Sn1—Sn1^{x}	134.48 (5)	Sn1—Zn—Sn2^{vii}	113.2 (2)
Sn1^{ix}—Sn1—Sn1^{x}	91.03 (10)	Sn2^{viii}—Zn—Sn2^{vii}	133.6 (4)
Zn—Sn1—Tb1^{i}	77.28 (4)	Sn1—Zn—Sn2^{vi}	113.5 (2)
Sn1^{ix}—Sn1—Tb1^{i}	130.05 (5)	Sn2^{viii}—Zn—Sn2^{vi}	80.95 (15)
Sn1^{x}—Sn1—Tb1^{i}	70.427 (15)	Sn2^{vii}—Zn—Sn2^{vi}	80.95 (15)
Zn—Sn1—Tb1^{ii}	77.28 (4)	Sn1—Zn—Sn2^{v}	113.5 (2)
Sn1^{ix}—Sn1—Tb1^{ii}	70.427 (15)	Sn2^{viii}—Zn—Sn2^{v}	80.95 (15)
Sn1^{x}—Sn1—Tb1^{ii}	130.05 (5)	Sn2^{vii}—Zn—Sn2^{v}	80.95 (15)
Tb1^{i}—Sn1—Tb1^{ii}	154.57 (8)	Sn2^{vi}—Zn—Sn2^{v}	132.9 (4)
Zn—Sn1—Tb1^{iv}	77.28 (4)	Sn1—Zn—Tb1^{ii}	61.72 (13)
Sn1^{ix}—Sn1—Tb1^{iv}	70.427 (15)	Sn2^{viii}—Zn—Tb1^{ii}	139.08 (5)
Sn1^{x}—Sn1—Tb1^{iv}	130.05 (5)	Sn2^{vii}—Zn—Tb1^{ii}	67.52 (6)
Tb1^{i}—Sn1—Tb1^{iv}	86.59 (2)	Sn2^{vi}—Zn—Tb1^{ii}	139.77 (5)
Tb1^{ii}—Sn1—Tb1^{iv}	87.86 (2)	Sn2^{v}—Zn—Tb1^{ii}	67.36 (6)
Zn—Sn1—Tb1^{iii}	77.28 (4)	Sn1—Zn—Tb1^{i}	61.72 (13)
Sn1^{ix}—Sn1—Tb1^{iii}	130.05 (5)	Sn2^{viii}—Zn—Tb1^{i}	67.52 (6)
Sn1^{x}—Sn1—Tb1^{iii}	70.427 (15)	Sn2^{vii}—Zn—Tb1^{i}	139.08 (5)
Tb1^{i}—Sn1—Tb1^{iii}	87.86 (2)	Sn2^{vi}—Zn—Tb1^{i}	67.36 (6)
Tb1^{ii}—Sn1—Tb1^{iii}	86.59 (2)	Sn2^{v}—Zn—Tb1^{i}	139.77 (5)
Tb1^{iv}—Sn1—Tb1^{iii}	154.57 (8)	Tb1^{ii}—Zn—Tb1^{i}	123.4 (3)
Zn—Sn1—Tb1^{v}	142.173 (19)	Sn1—Zn—Tb1^{iii}	61.72 (13)
Sn1^{ix}—Sn1—Tb1^{v}	56.40 (4)	Sn2^{viii}—Zn—Tb1^{iii}	67.52 (6)
Sn1^{x}—Sn1—Tb1^{v}	56.40 (4)	Sn2^{vii}—Zn—Tb1^{iii}	139.08 (5)
Tb1^{i}—Sn1—Tb1^{v}	126.82 (4)	Sn2^{vi}—Zn—Tb1^{iii}	139.77 (5)
Tb1^{ii}—Sn1—Tb1^{v}	75.43 (3)	Sn2^{v}—Zn—Tb1^{iii}	67.36 (6)
Tb1^{iv}—Sn1—Tb1^{v}	126.82 (4)	Tb1^{ii}—Zn—Tb1^{iii}	76.49 (11)
Tb1^{iii}—Sn1—Tb1^{v}	75.43 (3)	Tb1^{i}—Zn—Tb1^{iii}	77.56 (11)
Zn—Sn1—Tb1^{vi}	142.173 (19)	Sn1—Zn—Tb1^{iv}	61.72 (13)

Sn1$^{\mathrm{ix}}$—Sn1—Tb1$^{\mathrm{vi}}$	56.40 (4)	Sn2$^{\mathrm{viii}}$—Zn—Tb1$^{\mathrm{iv}}$	139.08 (5)
Sn1$^{\mathrm{x}}$—Sn1—Tb1$^{\mathrm{vi}}$	56.40 (4)	Sn2$^{\mathrm{vii}}$—Zn—Tb1$^{\mathrm{iv}}$	67.52 (6)
Tb1$^{\mathrm{i}}$—Sn1—Tb1$^{\mathrm{vi}}$	75.43 (3)	Sn2$^{\mathrm{vi}}$—Zn—Tb1$^{\mathrm{iv}}$	67.36 (6)
Tb1$^{\mathrm{ii}}$—Sn1—Tb1$^{\mathrm{vi}}$	126.82 (4)	Sn2$^{\mathrm{v}}$—Zn—Tb1$^{\mathrm{iv}}$	139.77 (5)
Tb1$^{\mathrm{iv}}$—Sn1—Tb1$^{\mathrm{vi}}$	75.43 (3)	Tb1$^{\mathrm{ii}}$—Zn—Tb1$^{\mathrm{iv}}$	77.56 (11)
Tb1$^{\mathrm{iii}}$—Sn1—Tb1$^{\mathrm{vi}}$	126.82 (4)	Tb1$^{\mathrm{i}}$—Zn—Tb1$^{\mathrm{iv}}$	76.49 (11)
Tb1$^{\mathrm{v}}$—Sn1—Tb1$^{\mathrm{vi}}$	75.65 (4)	Tb1$^{\mathrm{iii}}$—Zn—Tb1$^{\mathrm{iv}}$	123.4 (3)

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

Fig. 1

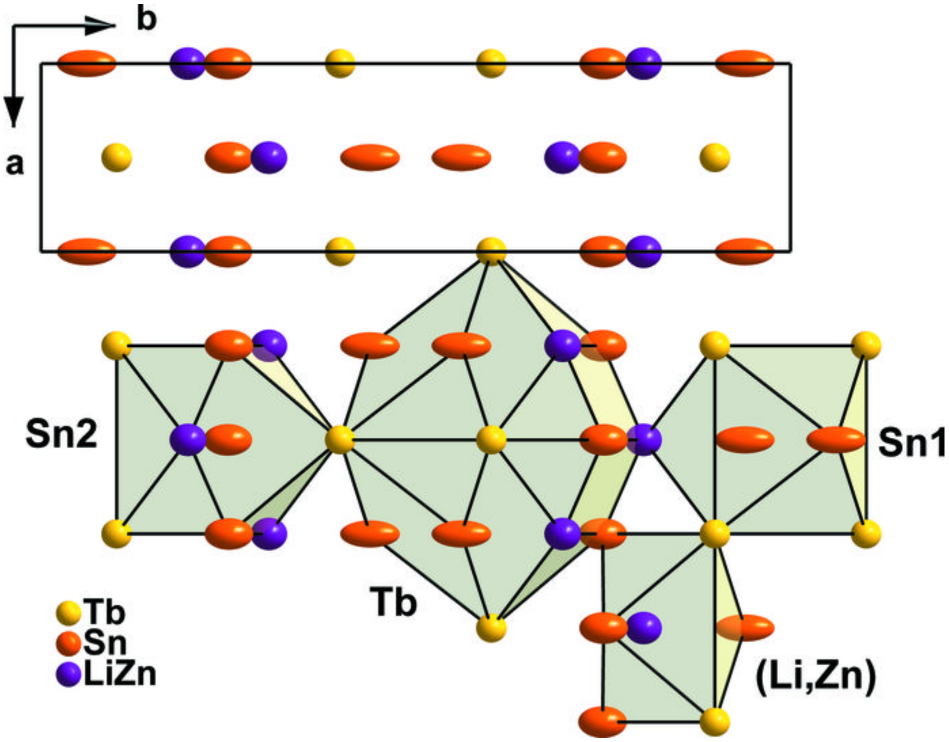

Fig. 2