

TbNb₆Sn₆: the first ternary compound from the rare earth–niobium–tin system

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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{Sn–Sn}) = 0.002$ Å; R factor = 0.017; wR factor = 0.038; data-to-parameter ratio = 13.9.

The title compound, terbium hexaniobium hexastannide, TbNb₆Sn₆, is the first ternary compound from the rare earth–niobium–tin system. It has the HfFe₆Ge₆ structure type, which can be analysed as an intergrowth of the Zr₄Al₃ and CaCu₅ structures. All the atoms lie on special positions; their coordination geometries and site symmetries are: Tb (dodecahedron) $6/mmm$; Nb (distorted icosahedron) $2mm$; Sn (Frank–Caspar polyhedron, CN = 14–15) $6mm$ and $\bar{6}m2$; Sn (distorted icosahedron) $\bar{6}m2$. The structure contains a graphite-type Sn network, Kagome nets of Nb atoms, and Tb atoms alternating with Sn₂ dumbbells in the channels.

Related literature

For background to niobium alloys, see: Ateev & Shamrai (1966). For related structures and background to intermetallics, see: Nowotny (1942); Raeuchle & Rundle (1952); Schobinger-Papamantellos *et al.* (1998); Wilson *et al.* (1960). A statistical test of the distribution of the E values using the program *E-STATS* from *WinGX* system (Farrugia, 1999) suggested that the structure is centrosymmetric. For MgCo₆Ge₆, see: Gieck *et al.* (2006).

Experimental

Crystal data

TbNb ₆ Sn ₆	$Z = 1$
$M_r = 1428.52$	Mo $K\alpha$ radiation
Hexagonal, $P6/mmm$	$\mu = 25.66$ mm ⁻¹
$a = 5.7650$ (1) Å	$T = 293$ K
$c = 9.5387$ (4) Å	$0.050 \times 0.020 \times 0.004$ mm
$V = 274.55$ (1) Å ³	

Data collection

Oxford Diffraction Xcalibur3 diffractometer with CCD detector	Diffraction, 2008)
Absorption correction: multi-scan (<i>CrysAlis RED</i> ; Oxford)	$T_{\min} = 0.592$, $T_{\max} = 1.000$
	2493 measured reflections
	208 independent reflections
	181 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.017$	15 parameters
$wR(F^2) = 0.038$	$\Delta\rho_{\text{max}} = 1.68$ e Å ⁻³
$S = 1.29$	$\Delta\rho_{\text{min}} = -2.35$ e Å ⁻³
208 reflections	

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: *pubCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5709).

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Comment

Niobium compounds have very useful properties for superconductive materials: high critical fields and plasticity which gives an opportunity to make superconductive windings. The main disadvantage of these compounds is the low critical temperature (Ateev & Shamrai, 1966). Superconductive Nb₃Sn with T_c=18.2 K is a high performance superconductor and the gold standard of the world's superconductor industry.

So far, no ternary compounds in the RE–Nb–Sn (RE - rare-earth metals) systems are known. TbNb₆Sn₆ is the first ternary Rare earth – Niobium – Tin compound. According to the X-ray single-crystal data the TbNb₆Sn₆ compound crystallizes with hexagonal symmetry (space group *P6/mmm*, HfFe₆Ge₆ structure type). In TbNb₆Sn₆ planar graphite-type layers of Sn atoms and Kagome nets of Nb atoms alternate along the *c* axis, similar to the recently reported MgCo₆Ge₆ compound (Gieck *et al.*, 2006). The resulting columns of vertex-sharing trigonal bipyramids form a three-dimensional Nb–Sn network with hexagonal tunnels (Figure 1). These tunnels are alternately centered by Tb atoms and Sn₂ dumbbells (with Sn–Sn distances of 3.24 Å). The coordination polyhedra of the atoms are: Tb1 — 20-vertex polyhedron (CN=20), Sn2 — Frank-Casper polyhedron (CN=15), Sn3 — distorted icosahedron (CN=12), Sn4 — Frank-Casper polyhedron (CN=14) and Nb5 — distorted icosahedron (CN=12).

The HfFe₆Ge₆ structure type (Schobinger-Papamantellos *et al.*, 1998), also referred to MgFe₆Ge₆ or LiCo₆Ge₆, can be described as an intergrowth of the Zr₄Al₃ (Wilson *et al.*, 1960) and CaCu₅ (Nowotny, 1942) structure types (see Fig.2). Another possibility to describe the HfFe₆Ge₆ structure is a transformation of the CaCu₅ structure via multiple substitution and ordering of atoms. The first step is the doubling of the CaCu₅ unit cell along the *c* axis. The substitution of every second Ca atom (R) along the *c* axis by a pair of atoms (2X) transforms this structure into the hexagonal modification of TiBe₁₂ (Raeuchle & Rundle, 1952). As a result, the *c/a* ratio increases to 1.733. Further ordering of X atoms in the TiBe₁₂ leads to the HfFe₆Ge₆ structure. Perhaps the presence of atoms of different radii leads to closer packing of the layers in the ternary HfFe₆Ge₆ compared to the binary TiBe₁₂. Therefore, the *c/a* ratio of 1.591 for ternary HfFe₆Ge₆ is much closer to the ideal value of 1.596 (*c/a* = 1.6546 for TbNb₆Sn₆).

Experimental

Single crystals of the title compound were first found in a sample with the composition 2Tb:3Zn:5Sn, which was synthesized by induction heating of the pure elements in a niobium crucible. The sample was heated at 1100° C in an induction furnace (Hüttinger Elektronik, Freiburg, Type TIG 2.5/300) under continuous argon flow for 1 h followed by cooling to 700° C at a rate of 10 degrees/min. Finally it was quenched by switching off the furnace. A reaction between the sample and the Nb container was observed. Good-quality hexagonal plate-like crystals were selected from annealed sample by mechanical fragmentation. Single-crystal intensity data of TbNb₆Sn₆ were collected at room temperature on an Oxford-Xcalibur3 CCD area detector diffractometer. After the measurement, the single crystal was analyzed with a JEOL SEM 5900LV scanning

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electron microscope. No impurity elements heavier than sodium were observed. The EDX analysis of well-shaped single crystal reveals the composition (in atomic percentages) Tb 8(3), Nb 45 (6), and Sn 47 (7), which is in good agreement with the compositions resulting from XRD data refinement. Further, a sample with the composition of Tb:6Nb:6Sn was prepared by arc melting and examined by powder X-ray diffraction. As-cast sample does not contain TbNb₆Sn₆ phase. However, after grinding, pressing and annealing it at 900°C for 12 h a significant amount of the TbNb₆Sn₆ phase was observed. Magnetic measurements of the annealed sample were performed using a MPMS XL5 SQUID magnetometer (Quantum Design). Cooling the sample without magnetic field and rising the temperature in the presence of a field of 15 Oe from 1.8 K to 50 K revealed at approximately 18 K only the superconducting behavior of the Nb₃Sn impurity.

Refinement

A statistical test of the distribution of the E values using the program E-STATS from *WinGX* system (Farrugia, 1999) suggested that the structure is centrosymmetric. The analysis of systematic extinctions yielded the space group *P6/mmm*, and it was confirmed by the following structure refinement. The structure was solved by the direct methods.

Figures

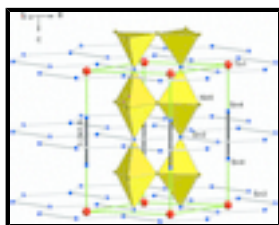


Fig. 1. View of the TbNb₆Sn₆ structure. The graphite-type Sn layers, Ge₂ dumbbells and condensed Nb₃Sn₂ bipyramids are emphasized.

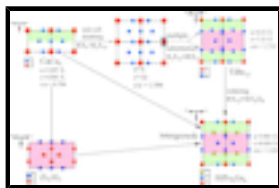


Fig. 2. Relationships between the HfFe₆Ge₆, Zr₄Al₃ and CaCu₅ structures.

terbium hexaniobium hexatin

Crystal data

TbNb₆Sn₆

$M_r = 1428.52$

Hexagonal, *P6/mmm*

Hall symbol: -P 6 2

$a = 5.7650 (1) \text{ \AA}$

$c = 9.5387 (4) \text{ \AA}$

$V = 274.55 (1) \text{ \AA}^3$

$Z = 1$

$F(000) = 611$

$D_x = 8.640 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 181 reflections

$\theta = 4.1\text{--}30.0^\circ$

$\mu = 25.66 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Hexagonal plate, metallic gray

$0.05 \times 0.02 \times 0.004 \text{ mm}$

Data collection

Oxford Diffraction Xcalibur3 diffractometer with CCD detector	208 independent reflections
Radiation source: Enhance (Mo) X-ray Source graphite	181 reflections with $I > 2\sigma(I)$
Detector resolution: 16.0238 pixels mm^{-1}	$R_{\text{int}} = 0.027$
ω and π scans	$\theta_{\text{max}} = 30.0^\circ$, $\theta_{\text{min}} = 4.1^\circ$
Absorption correction: multi-scan (Crys.Alis RED, Oxford Diffraction, 2008)	$h = -8 \rightarrow 7$
$T_{\text{min}} = 0.592$, $T_{\text{max}} = 1.000$	$k = -5 \rightarrow 8$
2493 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.017$	$w = 1/[\sigma^2(F_o^2) + (0.0113P)^2 + 2.3749P]$
$wR(F^2) = 0.038$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.29$	$(\Delta/\sigma)_{\text{max}} < 0.001$
208 reflections	$\Delta\rho_{\text{max}} = 1.68 \text{ e } \text{\AA}^{-3}$
15 parameters	$\Delta\rho_{\text{min}} = -2.35 \text{ e } \text{\AA}^{-3}$
0 restraints	Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.0333 (12)

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Tb1	0.0000	0.0000	0.0000	0.0101 (3)
Sn2	0.3333	0.6667	0.5000	0.0074 (2)
Sn3	0.3333	0.6667	0.0000	0.0066 (2)
Sn4	0.0000	0.0000	0.33003 (11)	0.0091 (2)
Nb5	0.0000	0.5000	0.24932 (6)	0.0053 (2)

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Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Tb1	0.0082 (3)	0.0082 (3)	0.0140 (5)	0.00408 (16)	0.000	0.000
Sn2	0.0084 (3)	0.0084 (3)	0.0054 (4)	0.00421 (14)	0.000	0.000
Sn3	0.0070 (3)	0.0070 (3)	0.0058 (4)	0.00349 (14)	0.000	0.000
Sn4	0.0063 (3)	0.0063 (3)	0.0148 (5)	0.00314 (15)	0.000	0.000
Nb5	0.0047 (3)	0.0050 (3)	0.0060 (3)	0.00235 (17)	0.000	0.000

Geometric parameters (\AA , $^\circ$)

Tb1—Sn4	3.1481 (10)	Sn3—Nb5 ^{ix}	2.9027 (5)
Tb1—Sn4 ⁱ	3.1481 (10)	Sn3—Nb5	2.9027 (5)
Tb1—Sn3 ⁱⁱ	3.3284	Sn3—Tb1 ^{xiii}	3.3284
Tb1—Sn3 ⁱⁱⁱ	3.3284	Sn3—Tb1 ^{xiv}	3.3284
Tb1—Sn3 ⁱ	3.3284	Sn4—Nb5	2.9835 (3)
Tb1—Sn3	3.3284	Sn4—Nb5 ^{xv}	2.9835 (3)
Tb1—Sn3 ^{iv}	3.3285	Sn4—Nb5 ^{ix}	2.9835 (3)
Tb1—Sn3 ^v	3.3285	Sn4—Nb5 ^{xvi}	2.9835 (3)
Sn2—Nb5	2.9133 (5)	Sn4—Nb5 ^v	2.9835 (3)
Sn2—Nb5 ^{vi}	2.9133 (5)	Sn4—Nb5 ^{xvii}	2.9835 (3)
Sn2—Nb5 ^{vii}	2.9133 (5)	Sn4—Sn4 ^{xviii}	3.243 (2)
Sn2—Nb5 ^{viii}	2.9133 (5)	Nb5—Nb5 ^{viii}	2.8825
Sn2—Nb5 ^{ix}	2.9133 (5)	Nb5—Nb5 ^{xvi}	2.8825
Sn2—Nb5 ^x	2.9133 (5)	Nb5—Nb5 ^{ix}	2.8825
Sn3—Nb5 ^{viii}	2.9027 (5)	Nb5—Nb5 ^{xix}	2.8825
Sn3—Nb5 ^{iv}	2.9027 (5)	Nb5—Sn3 ^{iv}	2.9027 (5)
Sn3—Nb5 ^{xi}	2.9027 (5)	Nb5—Sn2 ^{vii}	2.9133 (5)
Sn3—Nb5 ^{xii}	2.9027 (5)	Nb5—Sn4 ^{xiii}	2.9835 (3)
Sn4—Tb1—Sn4 ⁱ	180.0	Nb5—Sn3—Tb1	73.341 (3)
Sn4—Tb1—Sn3 ⁱⁱ	90.0	Tb1 ^{xiii} —Sn3—Tb1	120.0
Sn4 ⁱ —Tb1—Sn3 ⁱⁱ	90.0	Tb1 ^{xiv} —Sn3—Tb1	120.0
Sn4—Tb1—Sn3 ⁱⁱⁱ	90.0	Nb5—Sn4—Nb5 ^{xv}	113.586 (17)
Sn4 ⁱ —Tb1—Sn3 ⁱⁱⁱ	90.0	Nb5—Sn4—Nb5 ^{ix}	57.772 (6)
Sn3 ⁱⁱ —Tb1—Sn3 ⁱⁱⁱ	180.0	Nb5 ^{xv} —Sn4—Nb5 ^{ix}	150.09 (4)
Sn4—Tb1—Sn3 ⁱ	90.0	Nb5—Sn4—Nb5 ^{xvi}	57.772 (6)
Sn4 ⁱ —Tb1—Sn3 ⁱ	90.0	Nb5 ^{xv} —Sn4—Nb5 ^{xvi}	57.772 (6)
Sn3 ⁱⁱ —Tb1—Sn3 ⁱ	120.0	Nb5 ^{ix} —Sn4—Nb5 ^{xvi}	113.586 (17)
Sn3 ⁱⁱⁱ —Tb1—Sn3 ⁱ	60.0	Nb5—Sn4—Nb5 ^v	150.09 (4)
Sn4—Tb1—Sn3	90.0	Nb5 ^{xv} —Sn4—Nb5 ^v	57.772 (6)
Sn4 ⁱ —Tb1—Sn3	90.0	Nb5 ^{ix} —Sn4—Nb5 ^v	113.586 (17)

Sn3 ⁱⁱ —Tb1—Sn3	60.0	Nb5 ^{xvi} —Sn4—Nb5 ^v	113.586 (17)
Sn3 ⁱⁱⁱ —Tb1—Sn3	120.0	Nb5—Sn4—Nb5 ^{xvii}	113.586 (17)
Sn3 ⁱ —Tb1—Sn3	180.0	Nb5 ^{xv} —Sn4—Nb5 ^{xvii}	113.586 (17)
Sn4—Tb1—Sn3 ^{iv}	90.0	Nb5 ^{ix} —Sn4—Nb5 ^{xvii}	57.772 (6)
Sn4 ⁱ —Tb1—Sn3 ^{iv}	90.0	Nb5 ^{xvi} —Sn4—Nb5 ^{xvii}	150.09 (4)
Sn3 ⁱⁱ —Tb1—Sn3 ^{iv}	120.0	Nb5 ^v —Sn4—Nb5 ^{xvii}	57.772 (6)
Sn3 ⁱⁱⁱ —Tb1—Sn3 ^{iv}	60.0	Nb5—Sn4—Tb1	75.05 (2)
Sn3 ⁱ —Tb1—Sn3 ^{iv}	120.0	Nb5 ^{xv} —Sn4—Tb1	75.05 (2)
Sn3—Tb1—Sn3 ^{iv}	60.0	Nb5 ^{ix} —Sn4—Tb1	75.05 (2)
Sn4—Tb1—Sn3 ^v	90.0	Nb5 ^{xvi} —Sn4—Tb1	75.05 (2)
Sn4 ⁱ —Tb1—Sn3 ^v	90.0	Nb5 ^v —Sn4—Tb1	75.05 (2)
Sn3 ⁱⁱ —Tb1—Sn3 ^v	60.0	Nb5 ^{xvii} —Sn4—Tb1	75.05 (2)
Sn3 ⁱⁱⁱ —Tb1—Sn3 ^v	120.0	Nb5—Sn4—Sn4 ^{xviii}	104.95 (2)
Sn3 ⁱ —Tb1—Sn3 ^v	60.0	Nb5 ^{xv} —Sn4—Sn4 ^{xviii}	104.95 (2)
Sn3—Tb1—Sn3 ^v	120.0	Nb5 ^{ix} —Sn4—Sn4 ^{xviii}	104.95 (2)
Sn3 ^{iv} —Tb1—Sn3 ^v	180.0	Nb5 ^{xvi} —Sn4—Sn4 ^{xviii}	104.95 (2)
Nb5—Sn2—Nb5 ^{vi}	146.807 (6)	Nb5 ^v —Sn4—Sn4 ^{xviii}	104.95 (2)
Nb5—Sn2—Nb5 ^{vii}	110.325 (14)	Nb5 ^{xvii} —Sn4—Sn4 ^{xviii}	104.95 (2)
Nb5 ^{vi} —Sn2—Nb5 ^{vii}	59.302 (11)	Tb1—Sn4—Sn4 ^{xviii}	180.0
Nb5—Sn2—Nb5 ^{viii}	59.302 (11)	Nb5 ^{viii} —Nb5—Nb5 ^{xvi}	180.0
Nb5 ^{vi} —Sn2—Nb5 ^{viii}	110.325 (14)	Nb5 ^{viii} —Nb5—Nb5 ^{ix}	60.0
Nb5 ^{vii} —Sn2—Nb5 ^{viii}	146.808 (6)	Nb5 ^{xvi} —Nb5—Nb5 ^{ix}	120.0
Nb5—Sn2—Nb5 ^{ix}	59.302 (11)	Nb5 ^{viii} —Nb5—Nb5 ^{xix}	120.0
Nb5 ^{vi} —Sn2—Nb5 ^{ix}	146.808 (6)	Nb5 ^{xvi} —Nb5—Nb5 ^{xix}	60.0
Nb5 ^{vii} —Sn2—Nb5 ^{ix}	146.808 (6)	Nb5 ^{ix} —Nb5—Nb5 ^{xix}	180.0
Nb5 ^{viii} —Sn2—Nb5 ^{ix}	59.302 (11)	Nb5 ^{viii} —Nb5—Sn3	60.229 (6)
Nb5—Sn2—Nb5 ^x	146.807 (6)	Nb5 ^{xvi} —Nb5—Sn3	119.770 (6)
Nb5 ^{vi} —Sn2—Nb5 ^x	59.302 (11)	Nb5 ^{ix} —Nb5—Sn3	60.229 (6)
Nb5 ^{vii} —Sn2—Nb5 ^x	59.302 (11)	Nb5 ^{xix} —Nb5—Sn3	119.770 (6)
Nb5 ^{viii} —Sn2—Nb5 ^x	146.808 (6)	Nb5 ^{viii} —Nb5—Sn3 ^{iv}	119.770 (6)
Nb5 ^{ix} —Sn2—Nb5 ^x	110.325 (14)	Nb5 ^{xvi} —Nb5—Sn3 ^{iv}	60.229 (6)
Nb5 ^{viii} —Sn3—Nb5 ^{iv}	146.683 (6)	Nb5 ^{ix} —Nb5—Sn3 ^{iv}	119.771 (6)
Nb5 ^{viii} —Sn3—Nb5 ^{xi}	110.033 (14)	Nb5 ^{xix} —Nb5—Sn3 ^{iv}	60.229 (6)
Nb5 ^{iv} —Sn3—Nb5 ^{xi}	59.541 (11)	Sn3—Nb5—Sn3 ^{iv}	69.967 (14)
Nb5 ^{viii} —Sn3—Nb5 ^{xii}	146.683 (6)	Nb5 ^{viii} —Nb5—Sn2	60.349 (6)
Nb5 ^{iv} —Sn3—Nb5 ^{xii}	59.541 (12)	Nb5 ^{xvi} —Nb5—Sn2	119.652 (6)
Nb5 ^{xi} —Sn3—Nb5 ^{xii}	59.541 (11)	Nb5 ^{ix} —Nb5—Sn2	60.349 (6)
Nb5 ^{viii} —Sn3—Nb5 ^{ix}	59.541 (11)	Nb5 ^{xix} —Nb5—Sn2	119.652 (6)
Nb5 ^{iv} —Sn3—Nb5 ^{ix}	146.683 (6)	Sn3 ^{iv} —Nb5—Sn2	179.854 (14)
Nb5 ^{xi} —Sn3—Nb5 ^{ix}	146.683 (6)	Nb5 ^{viii} —Nb5—Sn2 ^{vii}	119.651 (6)
Nb5 ^{xii} —Sn3—Nb5 ^{ix}	110.033 (14)	Nb5 ^{xvi} —Nb5—Sn2 ^{vii}	60.349 (6)

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Nb5 ^{viii} —Sn3—Nb5	59.541 (12)	Nb5 ^{ix} —Nb5—Sn2 ^{vii}	119.652 (6)
Nb5 ^{iv} —Sn3—Nb5	110.033 (14)	Nb5 ^{xix} —Nb5—Sn2 ^{vii}	60.349 (6)
Nb5 ^{xi} —Sn3—Nb5	146.683 (6)	Sn3—Nb5—Sn2 ^{vii}	179.855 (14)
Nb5 ^{xii} —Sn3—Nb5	146.683 (6)	Sn3 ^{iv} —Nb5—Sn2 ^{vii}	110.179 (2)
Nb5 ^{ix} —Sn3—Nb5	59.541 (11)	Sn2—Nb5—Sn2 ^{vii}	69.676 (14)
Nb5 ^{viii} —Sn3—Tb1 ^{xiii}	73.341 (3)	Nb5 ^{viii} —Nb5—Sn4	118.886 (3)
Nb5 ^{iv} —Sn3—Tb1 ^{xiii}	73.341 (3)	Nb5 ^{xvi} —Nb5—Sn4	61.114 (3)
Nb5 ^{xi} —Sn3—Tb1 ^{xiii}	73.341 (3)	Nb5 ^{ix} —Nb5—Sn4	61.114 (3)
Nb5 ^{xii} —Sn3—Tb1 ^{xiii}	124.984 (7)	Nb5 ^{xix} —Nb5—Sn4	118.886 (3)
Nb5 ^{ix} —Sn3—Tb1 ^{xiii}	124.984 (7)	Sn3—Nb5—Sn4	102.205 (16)
Nb5—Sn3—Tb1 ^{xiii}	73.341 (3)	Sn3 ^{iv} —Nb5—Sn4	102.205 (17)
Nb5 ^{viii} —Sn3—Tb1 ^{xiv}	73.341 (3)	Sn2—Nb5—Sn4	77.773 (17)
Nb5 ^{iv} —Sn3—Tb1 ^{xiv}	124.984 (7)	Sn2 ^{vii} —Nb5—Sn4	77.773 (17)
Nb5 ^{xi} —Sn3—Tb1 ^{xiv}	73.341 (3)	Nb5 ^{viii} —Nb5—Sn4 ^{xiii}	61.114 (3)
Nb5 ^{xii} —Sn3—Tb1 ^{xiv}	73.341 (3)	Nb5 ^{xvi} —Nb5—Sn4 ^{xiii}	118.886 (3)
Nb5 ^{ix} —Sn3—Tb1 ^{xiv}	73.341 (3)	Nb5 ^{ix} —Nb5—Sn4 ^{xiii}	118.886 (3)
Nb5—Sn3—Tb1 ^{xiv}	124.983 (7)	Nb5 ^{xix} —Nb5—Sn4 ^{xiii}	61.114 (3)
Tb1 ^{xiii} —Sn3—Tb1 ^{xiv}	120.0	Sn3—Nb5—Sn4 ^{xiii}	102.205 (17)
Nb5 ^{viii} —Sn3—Tb1	124.984 (7)	Sn3 ^{iv} —Nb5—Sn4 ^{xiii}	102.205 (16)
Nb5 ^{iv} —Sn3—Tb1	73.341 (3)	Sn2—Nb5—Sn4 ^{xiii}	77.773 (17)
Nb5 ^{xi} —Sn3—Tb1	124.983 (7)	Sn2 ^{vii} —Nb5—Sn4 ^{xiii}	77.772 (17)
Nb5 ^{xii} —Sn3—Tb1	73.341 (3)	Sn4—Nb5—Sn4 ^{xiii}	150.09 (4)
Nb5 ^{ix} —Sn3—Tb1	73.341 (3)		

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

Fig. 1

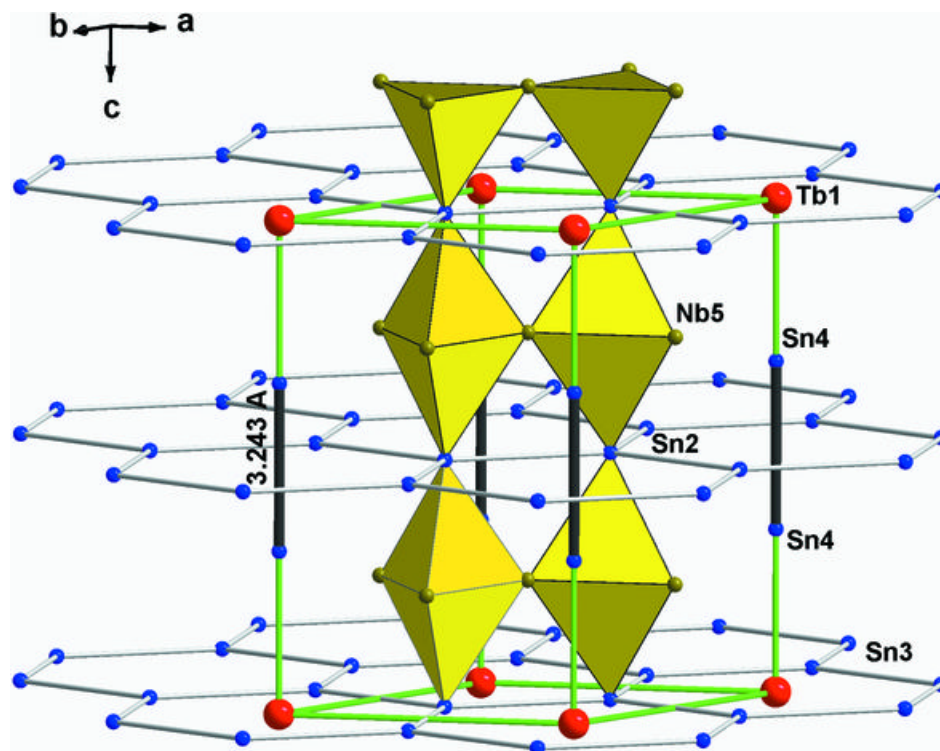


Fig. 2

