Tb_3Sn_7 Structure: A11B3_oC28_65_c4gh_ah-001

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https://aflow.org/p/2ATW

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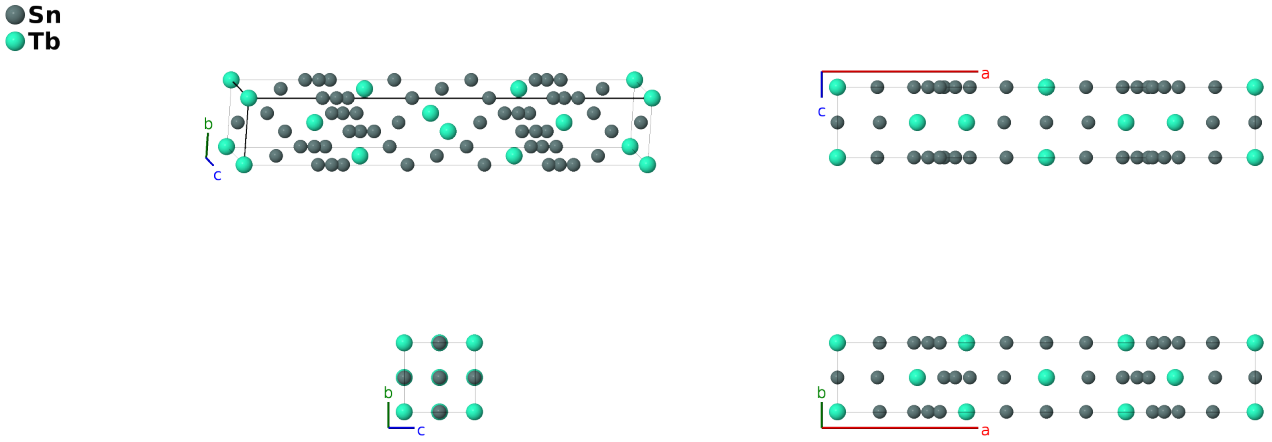


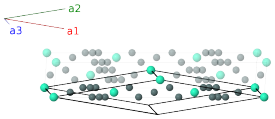
Prototype	Sn_7Tb_3
AFLOW prototype label	A11B3_oC28_65_c4gh_ah-001
ICSD	54357
Pearson symbol	oC28
Space group number	65
Space group symbol	$Cmmm$
AFLOW prototype command	`aflow --proto=A11B3_oC28_65_c4gh_ah-001 --params=`$a, b/a, c/a, x_3, x_4, x_5, x_6, x_7, x_8$

Other compounds with this structure
Dy_3Sn_7, Gd_3Sn_7

- This is the low temperature phase of Tb_3Sn_7. (Palenzona, 1993) describe a high temperature phase but do not give enough information to determine the structure.
- The Sn-III (80%), Sn-IV (13%), and Sn-V (7%) sites are only partially occupied. These three Wyckoff positions are very close together, so presumably only one of the sites is occupied at any location in the crystal.
- We shifted the coordinate system so that the Tb-I atom is at the origin and the longest primitive vector is along $\mathbf{a}_1$, rather than $\mathbf{a}_2$ as given in (Palenzona, 1993).

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Tb I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	Sn I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}}$	(4g)	Sn II
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}}$	(4g)	Sn II
$\mathbf{B_5}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}}$	(4g)	Sn III
$\mathbf{B_6}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}}$	(4g)	Sn III
$\mathbf{B_7}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2$	=	$ax_5\,\hat{\mathbf{x}}$	(4g)	Sn IV
$\mathbf{B_8}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2$	=	$-ax_5\,\hat{\mathbf{x}}$	(4g)	Sn IV
$\mathbf{B_9}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2$	=	$ax_6\,\hat{\mathbf{x}}$	(4g)	Sn V
$\mathbf{B_{10}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2$	=	$-ax_6\,\hat{\mathbf{x}}$	(4g)	Sn V
$\mathbf{B_{11}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Sn VI
$\mathbf{B_{12}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Sn VI
$\mathbf{B_{13}}$	=	$x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Tb II
$\mathbf{B_{14}}$	=	$-x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Tb II

References

[1] A. Palenzona and P. Manfrinetti, *The tin-rich side of the rare earth-tin systems (R = Gd, Tb, Dy, Ho, Er, Tm, Lu and Y)*, J. Alloys Compd. **201**, 43–47 (1993), doi:10.1016/0925-8388(93)90859-L.