

Tb₃Sn₇ Structure:

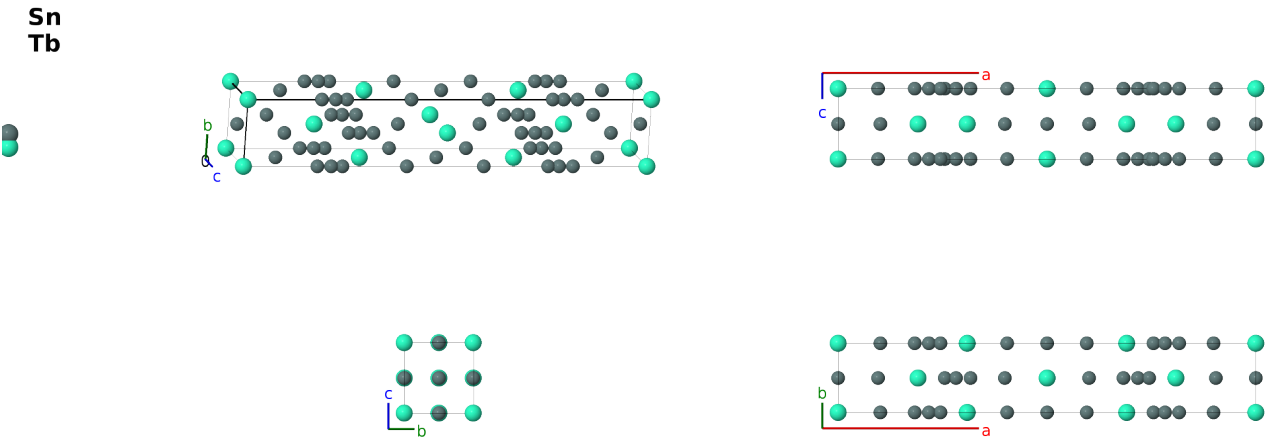
A11B3_oC28_65_c4gh_ah-001

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<https://aflow.org/prototype-encyclopedia/2ATW>

https://aflow.org/prototype-encyclopedia/A11B3_oC28_65_c4gh_ah-001



Prototype	Sn ₇ Tb ₃
AFLOW prototype label	A11B3_oC28_65_c4gh_ah-001
ICSD	54357
CCDC	1618929
Pearson symbol	oC28
Space group number	65
Space group symbol	<i>Cmmm</i>
AFLOW prototype command	<code>aflow --proto=A11B3_oC28_65_c4gh_ah-001</code> <code>--params=a, b/a, c/a, x₃, x₄, x₅, x₆, x₇, x₈</code>

Other compounds with this structure

Dy₃Sn₇, Gd₃Sn₇

- This is the low temperature phase of Tb₃Sn₇. (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.

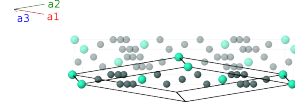
- We shifted the coordinate system so that the Tb-I atom is at the origin and the longest primitive vector is along $\mathbf{a}_1$, rather than $\mathbf{a}_2$ as given in (Palenzona, 1993).

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* ($R = \text{Gd}, \text{Tb}, \text{Dy}, \text{Ho}, \text{Er}, \text{Tm}, \text{Lu}$ and Y), J. Alloys Compd. **201**, 43–47 (1993), doi:10.1016/0925-8388(93)90859-L.

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