α-$PdSn_2$ Structure: AB2_tI48_142_d_ef-001

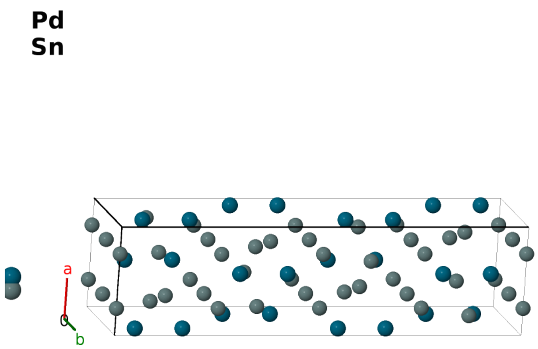
Cite this page as:

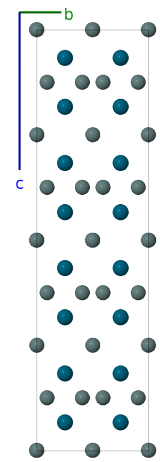
- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

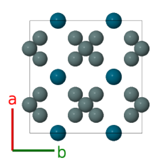
---

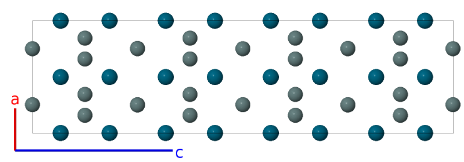
https://aflow.org/prototype-encyclopedia/FUUU

https://aflow.org/prototype-encyclopedia/AB2_tI48_142_d_ef-001









Prototype	$PdSn_2$
AFLOW prototype label	AB2_tI48_142_d_ef-001
ICSD	30235
CCDC	1604605
Pearson symbol	tI48

Space group number 142

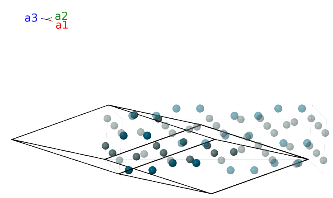
Space group symbol $I4_1/acd$

AFLOW prototype command `aflow --proto=AB2_tI48_142_d_ef-001`
`--params=`$a, c/a, z_1, x_2, x_3$

- This structure is stable up to 600°C. (Villars, 2016)
- $PdSn_2$ has also been found in the orthorhombic C_e structure.
- The ICSD entry is from (Hellner, 1956), but we use the refined data from (Künnen, 2000), which has no ICSD or CCDC listing, for this presentation.

Body-centered Tetragonal primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\left(z_1+\frac{1}{4}\right)\mathbf{a}_1 + z_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(16d)	Pd I
$\mathbf{B_2}$	=	$z_1\,\mathbf{a}_1 + \left(z_1+\frac{1}{4}\right)\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_1-\frac{1}{4}\right)\hat{\mathbf{z}}$	(16d)	Pd I
$\mathbf{B_3}$	=	$-\left(z_1-\frac{1}{4}\right)\mathbf{a}_1 - \left(z_1-\frac{1}{2}\right)\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(16d)	Pd I
$\mathbf{B_4}$	=	$-\left(z_1-\frac{1}{2}\right)\mathbf{a}_1 - \left(z_1-\frac{1}{4}\right)\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_1-\frac{1}{4}\right)\hat{\mathbf{z}}$	(16d)	Pd I
$\mathbf{B_5}$	=	$-\left(z_1-\frac{3}{4}\right)\mathbf{a}_1 - z_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(16d)	Pd I
$\mathbf{B_6}$	=	$-z_1\,\mathbf{a}_1 - \left(z_1-\frac{3}{4}\right)\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_1-\frac{1}{4}\right)\hat{\mathbf{z}}$	(16d)	Pd I
$\mathbf{B_7}$	=	$\left(z_1+\frac{3}{4}\right)\mathbf{a}_1 + \left(z_1+\frac{1}{2}\right)\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\hat{\mathbf{z}}$	(16d)	Pd I
$\mathbf{B_8}$	=	$\left(z_1+\frac{1}{2}\right)\mathbf{a}_1 + \left(z_1+\frac{3}{4}\right)\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16d)	Pd I
$\mathbf{B_9}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_2+\frac{1}{4}\right)\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16e)	Sn I
$\mathbf{B_{10}}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_2-\frac{1}{4}\right)\mathbf{a}_2 - \left(x_2-\frac{1}{2}\right)\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16e)	Sn I
$\mathbf{B_{11}}$	=	$\left(x_2+\frac{1}{4}\right)\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_2-\frac{1}{4}\right)\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(16e)	Sn I
$\mathbf{B_{12}}$	=	$-\left(x_2-\frac{1}{4}\right)\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(x_2-\frac{1}{2}\right)\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_2-\frac{1}{4}\right)\hat{\mathbf{y}}$	(16e)	Sn I
$\mathbf{B_{13}}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_2-\frac{3}{4}\right)\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(16e)	Sn I
$\mathbf{B_{14}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_2+\frac{3}{4}\right)\mathbf{a}_2 + \left(x_2+\frac{1}{2}\right)\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16e)	Sn I
$\mathbf{B_{15}}$	=	$-\left(x_2-\frac{3}{4}\right)\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_2-\frac{1}{4}\right)\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(16e)	Sn I
$\mathbf{B_{16}}$	=	$\left(x_2+\frac{3}{4}\right)\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(x_2+\frac{1}{2}\right)\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_2+\frac{1}{4}\right)\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(16e)	Sn I

$$\mathbf{B_{17}} = \left(x_3+\tfrac{3}{8}\right)\mathbf{a}_1 + \left(x_3+\tfrac{1}{8}\right)\mathbf{a}_2 + \left(2x_3+\tfrac{1}{4}\right)\mathbf{a}_3 = ax_3\,\hat{\mathbf{x}} + a\left(x_3+\tfrac{1}{4}\right)\hat{\mathbf{y}} + \tfrac{1}{8}c\,\hat{\mathbf{z}} \qquad \text{(16f)} \qquad \text{Sn II}$$

$$\mathbf{B_{18}} = -\left(x_3-\tfrac{3}{8}\right)\mathbf{a}_1 - \left(x_3-\tfrac{1}{8}\right)\mathbf{a}_2 - \left(2x_3-\tfrac{1}{4}\right)\mathbf{a}_3 = -ax_3\,\hat{\mathbf{x}} - a\left(x_3-\tfrac{1}{4}\right)\hat{\mathbf{y}} + \tfrac{1}{8}c\,\hat{\mathbf{z}} \qquad \text{(16f)} \qquad \text{Sn II}$$

$$\mathbf{B_{19}} = \left(x_3+\tfrac{1}{8}\right)\mathbf{a}_1 - \left(x_3-\tfrac{3}{8}\right)\mathbf{a}_2 + \tfrac{3}{4}\,\mathbf{a}_3 = -a\left(x_3-\tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_3+\tfrac{1}{4}\right)\hat{\mathbf{y}} - \tfrac{1}{8}c\,\hat{\mathbf{z}} \qquad \text{(16f)} \qquad \text{Sn II}$$

$$\mathbf{B_{20}} = -\left(x_3-\tfrac{1}{8}\right)\mathbf{a}_1 + \left(x_3+\tfrac{3}{8}\right)\mathbf{a}_2 + \tfrac{3}{4}\,\mathbf{a}_3 = a\left(x_3+\tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_3-\tfrac{1}{4}\right)\hat{\mathbf{y}} - \tfrac{1}{8}c\,\hat{\mathbf{z}} \qquad \text{(16f)} \qquad \text{Sn II}$$

$$\mathbf{B_{21}} = -\left(x_3-\tfrac{5}{8}\right)\mathbf{a}_1 - \left(x_3-\tfrac{7}{8}\right)\mathbf{a}_2 - \left(2x_3-\tfrac{3}{4}\right)\mathbf{a}_3 = -a\left(x_3-\tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_3-\tfrac{1}{4}\right)\hat{\mathbf{y}} + \tfrac{3}{8}c\,\hat{\mathbf{z}} \qquad \text{(16f)} \qquad \text{Sn II}$$

$$\mathbf{B_{22}} = \left(x_3+\tfrac{5}{8}\right)\mathbf{a}_1 + \left(x_3+\tfrac{7}{8}\right)\mathbf{a}_2 + \left(2x_3+\tfrac{3}{4}\right)\mathbf{a}_3 = a\left(x_3+\tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_3+\tfrac{1}{4}\right)\hat{\mathbf{y}} + \tfrac{3}{8}c\,\hat{\mathbf{z}} \qquad \text{(16f)} \qquad \text{Sn II}$$

$$\mathbf{B_{23}} = -\left(x_3-\tfrac{7}{8}\right)\mathbf{a}_1 + \left(x_3+\tfrac{5}{8}\right)\mathbf{a}_2 + \tfrac{1}{4}\,\mathbf{a}_3 = ax_3\,\hat{\mathbf{x}} - a\left(x_3-\tfrac{1}{4}\right)\hat{\mathbf{y}} + \tfrac{5}{8}c\,\hat{\mathbf{z}} \qquad \text{(16f)} \qquad \text{Sn II}$$

$$\mathbf{B_{24}} = \left(x_3+\tfrac{7}{8}\right)\mathbf{a}_1 - \left(x_3-\tfrac{5}{8}\right)\mathbf{a}_2 + \tfrac{1}{4}\,\mathbf{a}_3 = -ax_3\,\hat{\mathbf{x}} + a\left(x_3+\tfrac{1}{4}\right)\hat{\mathbf{y}} + \tfrac{5}{8}c\,\hat{\mathbf{z}} \qquad \text{(16f)} \qquad \text{Sn II}$$

References

[1] E. Hellner, *Flu-Misch-Typen*, Zeitschrift für Kristallographie **107**, 99–123 (1956), doi:10.1524/zkri.1956.107.16.99.

[2] P. Villars, ed., *PAULING FILE* (Springer, 2016), chap. Pd-Sn Binary Phase Diagram 0-100 at.% Sn.

Found in

[1] B. Künnen, D. Niepmann, and W. Jeitschko, *Structure refinements and some properties of the transition metal stannides Os_3Sn_7, Ir_5Sn_7, $Ni_{0.402(4)}Pd_{0.598}Sn_4$, α-$PdSn_2$ and $PtSn_4$*, J. Alloys Compd. **309**, 1–9 (2000), doi:10.1016/S0925-8388(00)01042-2.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.