α-$PdSn_2$ Structure: AB2_tI48_142_d_ef-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

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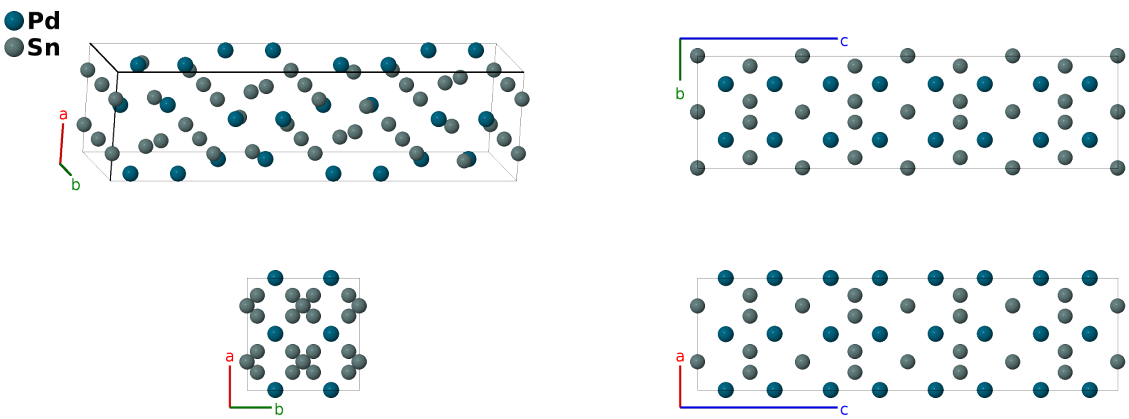
https://aflow.org/p/AB2_tI48_142_d_ef-001

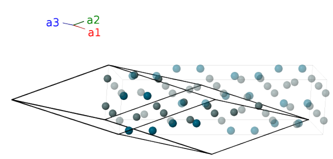


Prototype	$PdSn_2$
AFLOW prototype label	AB2_tI48_142_d_ef-001
ICSD	30235
Pearson symbol	tI48
Space group number	142
Space group symbol	$I4_1/acd$
AFLOW prototype command	`aflow --proto=AB2_tI48_142_d_ef-001 --params=`$a, c/a, z_1, x_2, x_3$

- 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) for this presentation.

Body-centered Tetragonal primitive vectors

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



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
$\mathbf{B_{17}}$	=	$\left(x_3+\frac{3}{8}\right)\,\mathbf{a}_1+\left(x_3+\frac{1}{8}\right)\,\mathbf{a}_2+\left(2x_3+\frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}+a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	Sn II
$\mathbf{B_{18}}$	=	$-\left(x_3-\frac{3}{8}\right)\,\mathbf{a}_1-\left(x_3-\frac{1}{8}\right)\,\mathbf{a}_2-\left(2x_3-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}-a\left(x_3-\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	Sn II
$\mathbf{B_{19}}$	=	$\left(x_3+\frac{1}{8}\right)\,\mathbf{a}_1-\left(x_3-\frac{3}{8}\right)\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}-\frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	Sn II
$\mathbf{B_{20}}$	=	$-\left(x_3-\frac{1}{8}\right)\,\mathbf{a}_1+\left(x_3+\frac{3}{8}\right)\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_3-\frac{1}{4}\right)\,\hat{\mathbf{y}}-\frac{1}{8}c\,\hat{\mathbf{z}}$	(16f)	Sn II
$\mathbf{B_{21}}$	=	$-\left(x_3-\frac{5}{8}\right)\,\mathbf{a}_1-\left(x_3-\frac{7}{8}\right)\,\mathbf{a}_2-\left(2x_3-\frac{3}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_3-\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{3}{8}c\,\hat{\mathbf{z}}$	(16f)	Sn II
$\mathbf{B_{22}}$	=	$\left(x_3+\frac{5}{8}\right)\,\mathbf{a}_1+\left(x_3+\frac{7}{8}\right)\,\mathbf{a}_2+\left(2x_3+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{3}{8}c\,\hat{\mathbf{z}}$	(16f)	Sn II
$\mathbf{B_{23}}$	=	$-\left(x_3-\frac{7}{8}\right)\,\mathbf{a}_1+\left(x_3+\frac{5}{8}\right)\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}-a\left(x_3-\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{5}{8}c\,\hat{\mathbf{z}}$	(16f)	Sn II
$\mathbf{B_{24}}$	=	$\left(x_3+\frac{7}{8}\right)\,\mathbf{a}_1-\left(x_3-\frac{5}{8}\right)\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}+a\left(x_3+\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{5}{8}c\,\hat{\mathbf{z}}$	(16f)	Sn II

References

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