$PdSn_2$ (C_e) Structure: AB2_oC24_41_2a_2b-001

This structure originally had the label `AB2_oC24_41_2a_2b`. Calls to that address will be redirected here.

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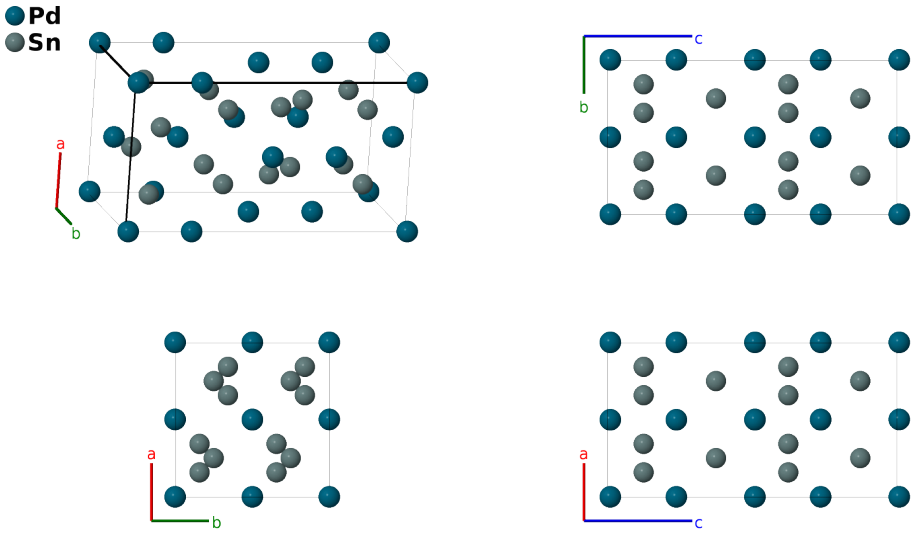
https://aflow.org/p/BVS7

https://aflow.org/p/AB2_oC24_41_2a_2b-001



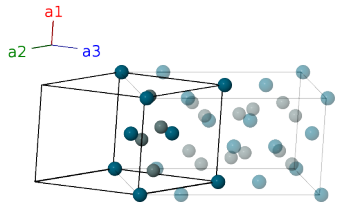
Prototype	$PdSn_2$
AFLOW prototype label	AB2_oC24_41_2a_2b-001
***Strukturbericht* designation**	C_e
ICSD	105684
Pearson symbol	oC24
Space group number	41
Space group symbol	$Aea2$
AFLOW prototype command	`aflow --proto=AB2_oC24_41_2a_2b-001 --params=`$a, b/a, c/a, z_1, z_2, x_3, y_3, z_3, x_4, y_4, z_4$

Other compounds with this structure
$CoGe_2$, $GaGe_3Ni_2$, $RhSn_2$

- $PdSn_2$ can also be found in the tetragonal α-$PdSn_2$ structure.
- In fact, AFLOW will place $PdSn_2$ in that structure unless we lower the tolerance, using
- aflow --proto=AB2_oC24_41_2a_2b:Pd:Sn --tolerance=0.001 --params=a,b/a,c/a,z_1,z_2,x_3,y_3,z_3,x_4,y_4,z_4 .
- In the C_e structure the palladium sites have 89% occupation.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-z_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(4a)	Pd I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	Pd I
$\mathbf{B_3}$	=	$-z_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(4a)	Pd II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	Pd II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + (y_3 - z_3)\,\mathbf{a}_2 + (y_3 + z_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8b)	Sn I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - (y_3 + z_3)\,\mathbf{a}_2 - (y_3 - z_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8b)	Sn I
$\mathbf{B_7}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8b)	Sn I
$\mathbf{B_8}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8b)	Sn I
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 + (y_4 - z_4)\,\mathbf{a}_2 + (y_4 + z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8b)	Sn II
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 - (y_4 + z_4)\,\mathbf{a}_2 - (y_4 - z_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8b)	Sn II
$\mathbf{B_{11}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-y_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8b)	Sn II
$\mathbf{B_{12}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 - z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8b)	Sn II

References

[1] K. Schubert and H. Pfisterer, *Zur Kristallchemie der B-Metall-reichsten Phasen in Legierungen von Ü"bergangsmetallen der Eisen- und Platintriaden mit Elementen der vierten Nebengruppe*, Z. Metallkd. **41**, 433–441 (1950).

Found in

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.