

PdSn₂ (*C_e*) Structure: AB2_oC24_41_2a_2b-001

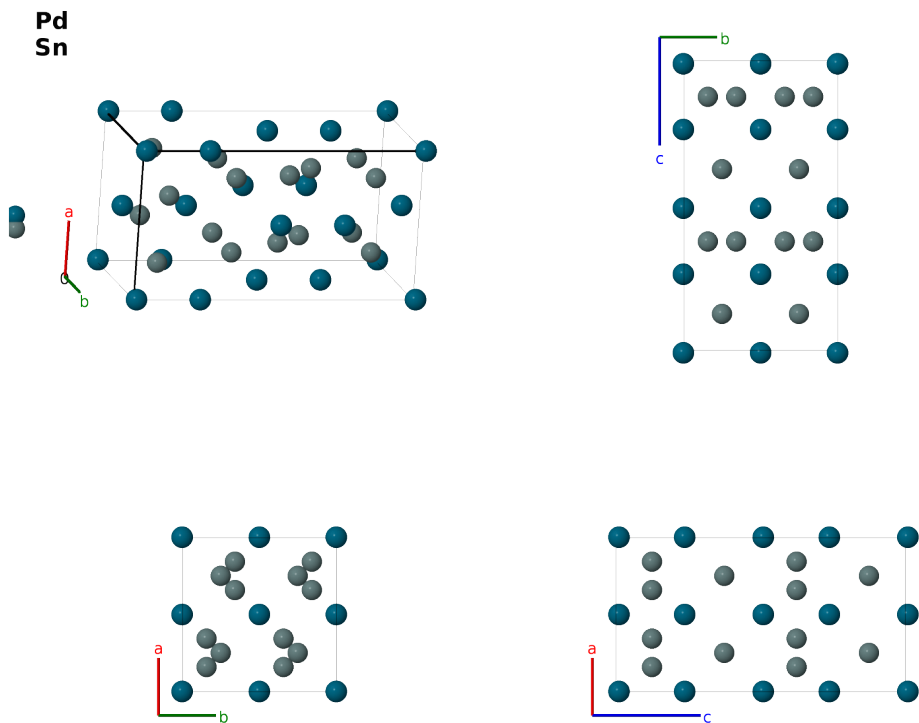
This structure previously used the label(s) **AB2_oC24_41_2a_2b**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/BVS7>

https://aflow.org/prototype-encyclopedia/AB2_oC24_41_2a_2b-001



Prototype	PdSn ₂
AFLOW prototype label	AB2_oC24_41_2a_2b-001
<i>Strukturbericht</i> designation	<i>C_e</i>
ICSD	105684
CCDC	1663562
Pearson symbol	oC24
Space group number	41
Space group symbol	<i>Aea</i> 2

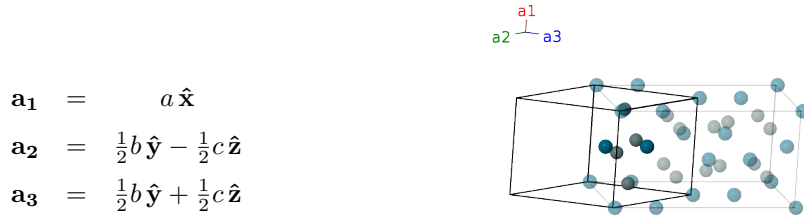
AFLOW prototype command `aflow --proto=AB2_oC24_41_2a_2b-001`
 `--params=a,b/a,c/a,z1,z2,x3,y3,z3,x4,y4,z4`

Other compounds with this structure

CoGe₂, GaGe₃Ni₂, RhSn₂

- PdSn₂ can also be found in the tetragonal α -PdSn₂ structure.
- In fact, AFLOW will place this form of PdSn₂ in that structure unless we tighten the tolerance, using
- `aflow --proto=AB2_oC24_41_2a_2b:Pd:Sn --tolerance=0.001 --params=a,b/a,c/a,z1,z2,x3,y3,z3,x4,y4,z4` .
- In the C_e structure the palladium sites have 89% occupation.

Base-centered Orthorhombic primitive vectors



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
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 - (z_1 - \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4a)	Pd I
$\mathbf{B}_3$	$= -z_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$cz_2 \hat{\mathbf{z}}$	(4a)	Pd II
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 - (z_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(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
$\mathbf{B}_7$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 + z_3 - \frac{1}{2}) \mathbf{a}_2 + (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8b)	Sn I
$\mathbf{B}_8$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_2 + (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{11}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 + z_4 - \frac{1}{2}) \mathbf{a}_2 + (-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8b)	Sn II
$\mathbf{B}_{12}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_2 + (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8b)	Sn II

References

- [1] K. Schubert and H. Pfisterer, *Zur Kristallchemie der B-Metall-reichsten Phasen in Legierungen von Übergangsmetallen 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.

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- M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017