

PtSn₄ (*D*1_{*c*}) Structure: AB4_oC20_41_a_2b-001

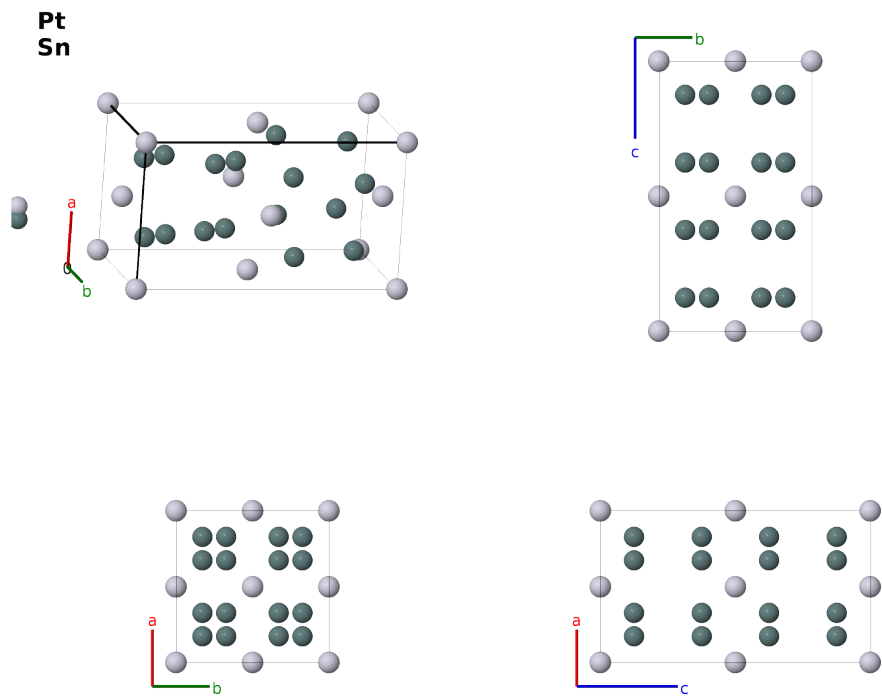
This structure previously used the label(s) **AB4_oC20_41_a_2b**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/AB4_oC20_41_a_2b-001



Prototype	PtSn ₄
AFLOW prototype label	AB4_oC20_41_a_2b-001
<i>Strukturbericht</i> designation	<i>D</i> 1 _{<i>c</i>}
ICSD	105793
CCDC	1663669
Pearson symbol	oC20
Space group number	41
Space group symbol	<i>Aea</i> 2
AFLOW prototype command	<code>aflow --proto=AB4_oC20_41_a_2b-001</code> <code>--params=<i>a</i>,<i>b</i>/<i>a</i>,<i>c</i>/<i>a</i>,<i>z</i>₁,<i>x</i>₂,<i>y</i>₂,<i>z</i>₂,<i>x</i>₃,<i>y</i>₃,<i>z</i>₃</code>

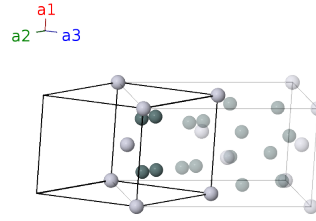
Other compounds with this structure

AuSn₄, IrSn₄, PdSn₄

- The published atomic positions have $x_2 = y_3$, $x_3 = y_2$ and $z_2 = -z_3$. This puts the system into space group *Ccce* #68, very similar to PdSn₄.
- To get space group *Aba2* #41 we shifted the y_2 and z_3 positions slightly. Even then we could not place this in space group *Aba2* until we adjusted the tolerance. The original structure can be recovered using the command:
- `afLOW --proto=AB4.oC20_41_a_2b:Pt:Sn --tolerance=0.001 --params=a,b/a,c/a,x2,y2,z2,x3,y3,z3`
- (Schubert, 1950) give the lattice constants in kX units. We used the factor of 1.00202Å/kX from (Wood, 1947) to convert to Ångströms.

Base-centered Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= \frac{1}{2}b \hat{\mathbf{y}} - \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}\end{aligned}$$



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)	Pt 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)	Pt I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + (y_2 - z_2) \mathbf{a}_2 + (y_2 + z_2) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8b)	Sn I
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - (y_2 + z_2) \mathbf{a}_2 - (y_2 - z_2) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8b)	Sn I
$\mathbf{B}_5$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 + z_2 - \frac{1}{2}) \mathbf{a}_2 + (-y_2 + z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8b)	Sn I
$\mathbf{B}_6$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 - z_2 + \frac{1}{2}) \mathbf{a}_2 + (y_2 + z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8b)	Sn I
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 + (y_3 + z_3) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8b)	Sn II
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 - (y_3 + z_3) \mathbf{a}_2 - (y_3 - z_3) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8b)	Sn II
$\mathbf{B}_9$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 + z_3 - \frac{1}{2}) \mathbf{a}_2 + (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8b)	Sn II
$\mathbf{B}_{10}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_2 + (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8b)	Sn II

References

- [1] K. Schubert and U. Rösler, *Die Kristallstruktur von $PtSn_4$* , Z. Metallkd. **41**, 298–300 (1950).
- [2] E. A. Wood, *The Conversion Factor for kX Units to Angström Units*, J. Appl. Phys. **18**, 929–930 (1947), doi:10.1063/1.1697570.

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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