$PtSn_4$ ($D1_c$) Structure: AB4_oC20_41_a_2b-001

This structure originally had the label `AB4_oC20_41_a_2b`. Calls to that address will be redirected here.

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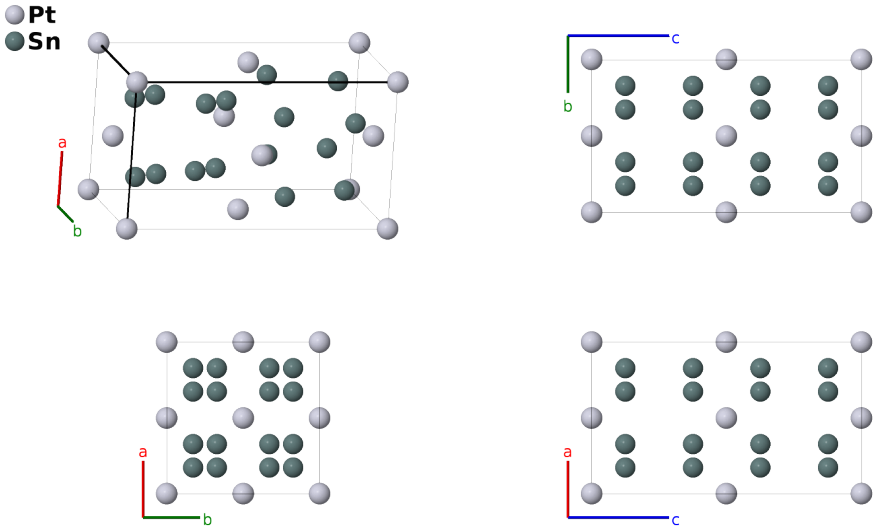
https://aflow.org/p/MALE

https://aflow.org/p/AB4_oC20_41_a_2b-001



Prototype	$PtSn_4$
AFLOW prototype label	AB4_oC20_41_a_2b-001
***Strukturbericht* designation**	$D1_c$
ICSD	105793
Pearson symbol	oC20
Space group number	41
Space group symbol	$Aea2$
AFLOW prototype command	`aflow --proto=AB4_oC20_41_a_2b-001 --params=`$a, b/a, c/a, z_1, x_2, y_2, z_2, x_3, y_3, z_3$

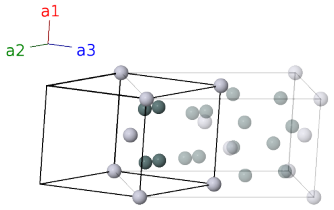
Other compounds with this structure
$AuSn_4$, $IrSn_4$, $PdSn_4$

- 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 $PdSn_4$.
- 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,x_2,y_2,z_2,x_3,y_3,z_3

- (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

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



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)	Pt 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)	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
$\mathbf{B_5}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 + z_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-y_2 + z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8b)	Sn I
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 - z_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_2 + z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(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
$\mathbf{B_9}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8b)	Sn II
$\mathbf{B_{10}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8b)	Sn 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.