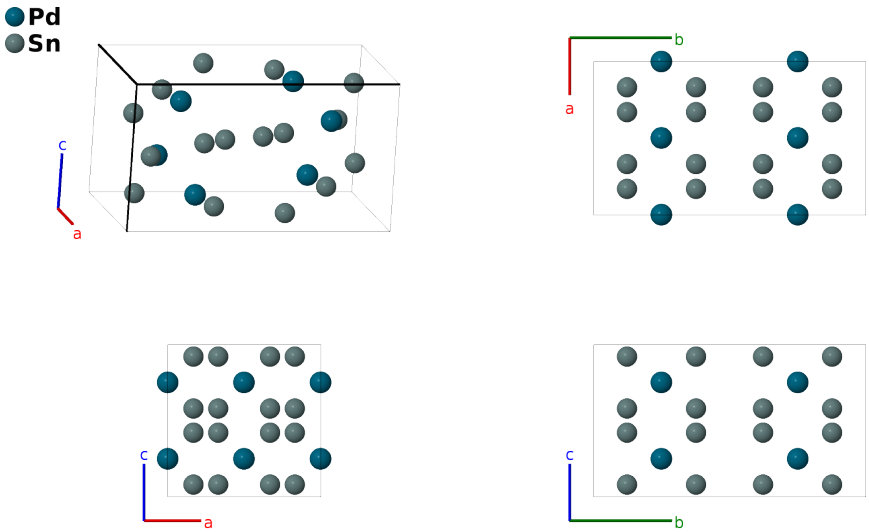
$PdSn_4$ Structure: AB4_oC20_68_a_i-001

This structure originally had the label `AB4_oC20_68_a_i`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

https://aflow.org/p/LGPW

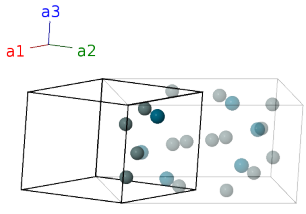
https://aflow.org/p/AB4_oC20_68_a_i-001



Prototype	$PdSn_4$
AFLOW prototype label	AB4_oC20_68_a_i-001
ICSD	413280
Pearson symbol	oC20
Space group number	68
Space group symbol	$Ccce$
AFLOW prototype command	`aflow --proto=AB4_oC20_68_a_i-001 --params=`$a, b/a, c/a, x_2, y_2, z_2$

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	Pd I
$\mathbf{B_2}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4a)	Pd I
$\mathbf{B_3}$	=	$(x_2 - y_2)\,\mathbf{a}_1 + (x_2 + y_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(16i)	Sn I
$\mathbf{B_4}$	=	$\left(-x_2 + y_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 + y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(16i)	Sn I
$\mathbf{B_5}$	=	$-(x_2 + y_2)\,\mathbf{a}_1 - (x_2 - y_2)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	Sn I
$\mathbf{B_6}$	=	$\left(x_2 + y_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 - y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	Sn I
$\mathbf{B_7}$	=	$-(x_2 - y_2)\,\mathbf{a}_1 - (x_2 + y_2)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(16i)	Sn I
$\mathbf{B_8}$	=	$\left(x_2 - y_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(16i)	Sn I
$\mathbf{B_9}$	=	$(x_2 + y_2)\,\mathbf{a}_1 + (x_2 - y_2)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	Sn I
$\mathbf{B_{10}}$	=	$-\left(x_2 + y_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_2 + y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	Sn I

References

[1] J. Nylén, F. J. G. Garcıà, B. D. Mosel, R. Pöttgen, and U. Häussermann, *Structural relationships, phase stability and bonding of compounds $PdSn_n$ (n=2, 3, 4)*, Solid State Sci. **6**, 147–155 (2004), doi:10.1016/j.solidstatesciences.2003.09.011.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.