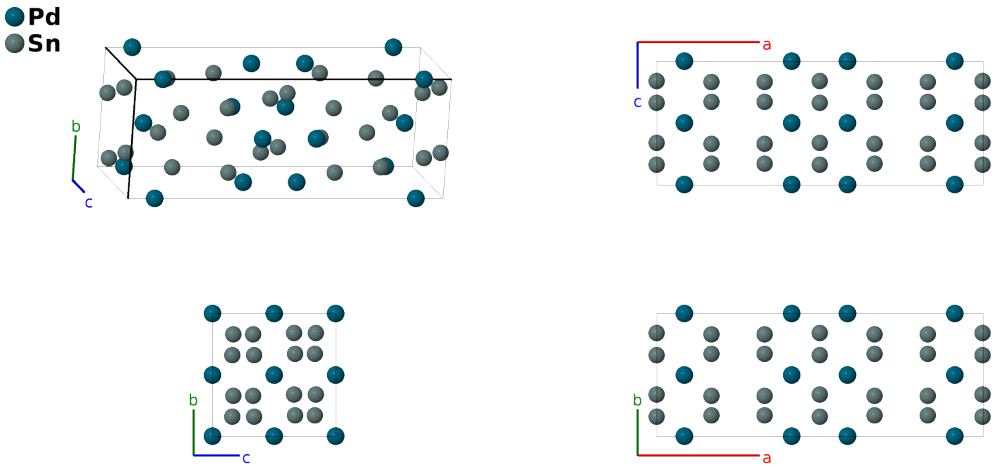
$PdSn_3$ Structure: AB3_oC32_64_d_fg-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/J38S

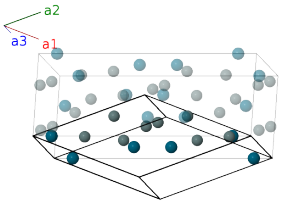
https://aflow.org/p/AB3_oC32_64_d_fg-001



Prototype	$PdSn_3$
AFLOW prototype label	AB3_oC32_64_d_fg-001
ICSD	413279
Pearson symbol	oC32
Space group number	64
Space group symbol	*Cmce*
AFLOW prototype command	`aflow --proto=AB3_oC32_64_d_fg-001 --params=`$a, b/a, c/a, x_1, y_2, z_2, x_3, y_3, z_3$

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{x}}$	(8d)	Pd I

$\mathbf{B_2}$	=	$-\left(x_1-\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_1-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8d)	Pd I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1-x_1\,\mathbf{a}_2$	=	$-ax_1\,\hat{\mathbf{x}}$	(8d)	Pd I
$\mathbf{B_4}$	=	$\left(x_1+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_1+\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8d)	Pd I
$\mathbf{B_5}$	=	$-y_2\,\mathbf{a}_1+y_2\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(8f)	Sn I
$\mathbf{B_6}$	=	$\left(y_2+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_2-\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-by_2\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Sn I
$\mathbf{B_7}$	=	$-\left(y_2-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_2+\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+by_2\,\hat{\mathbf{y}}-c\left(z_2-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Sn I
$\mathbf{B_8}$	=	$y_2\,\mathbf{a}_1-y_2\,\mathbf{a}_2-z_2\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}}-cz_2\,\hat{\mathbf{z}}$	(8f)	Sn I
$\mathbf{B_9}$	=	$(x_3-y_3)\,\mathbf{a}_1+(x_3+y_3)\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}+by_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(16g)	Sn II
$\mathbf{B_{10}}$	=	$\left(-x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_3+y_3-\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}}-by_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	Sn II
$\mathbf{B_{11}}$	=	$-\left(x_3+y_3-\frac{1}{2}\right)\,\mathbf{a}_1+\left(-x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}}+by_3\,\hat{\mathbf{y}}-c\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	Sn II
$\mathbf{B_{12}}$	=	$(x_3+y_3)\,\mathbf{a}_1+(x_3-y_3)\,\mathbf{a}_2-z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}-by_3\,\hat{\mathbf{y}}-cz_3\,\hat{\mathbf{z}}$	(16g)	Sn II
$\mathbf{B_{13}}$	=	$-(x_3-y_3)\,\mathbf{a}_1-(x_3+y_3)\,\mathbf{a}_2-z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}-by_3\,\hat{\mathbf{y}}-cz_3\,\hat{\mathbf{z}}$	(16g)	Sn II
$\mathbf{B_{14}}$	=	$\left(x_3-y_3+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}}+by_3\,\hat{\mathbf{y}}-c\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	Sn II
$\mathbf{B_{15}}$	=	$\left(x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_3-y_3+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}}-by_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	Sn II
$\mathbf{B_{16}}$	=	$-(x_3+y_3)\,\mathbf{a}_1-(x_3-y_3)\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}+by_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(16g)	Sn II

References

[1] J. Nylén, F. J. G. Garcìà, 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] A. Jain, S. Ping, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, and K. A. Persson, *Commentary: The Materials Project: A materials genome approach to accelerating materials innovation*, APL Materials **1**, 011002 (2013), doi:10.1063/1.4812323.