

PdSn₄ Structure:

AB4_oC20_68_a_i-001

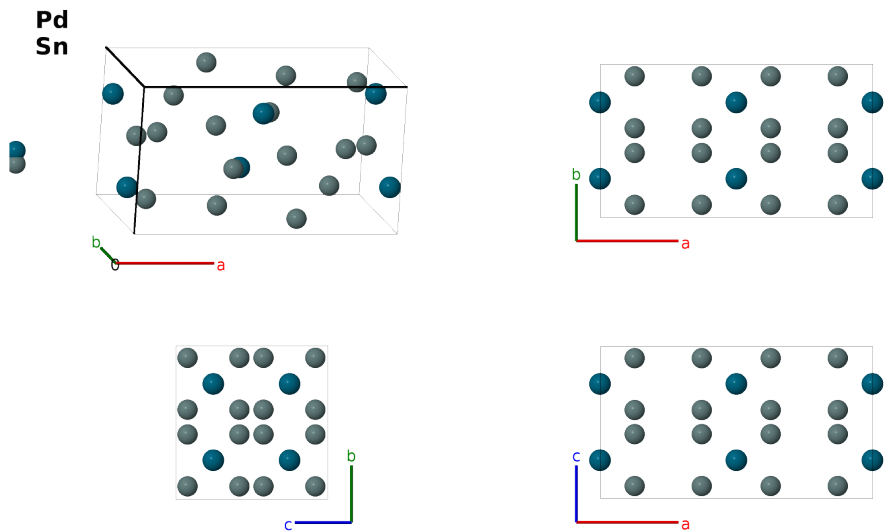
This structure previously used the label(s) **AB4_oC20_68_a_i**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/AB4_oC20_68_a_i-001



Prototype	PdSn ₄
AFLOW prototype label	AB4_oC20_68_a_i-001
ICSD	413280
CCDC	1728312
Pearson symbol	oC20
Space group number	68
Space group symbol	<i>Ccce</i>
AFLOW prototype command	<code>aflow --proto=AB4_oC20_68_a_i-001</code> <code>--params=<i>a</i>, <i>b/a</i>, <i>c/a</i>, <i>x</i>₂, <i>y</i>₂, <i>z</i>₂</code>

Base-centered Orthorhombic primitive vectors



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
$\mathbf{B}_4$	$= \begin{pmatrix} -x_2 + y_2 + \frac{1}{2} \\ x_2 + y_2 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_2 + y_2 - \frac{1}{2} \\ z_2 \end{pmatrix} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(16i)	Sn I
$\mathbf{B}_5$	$= -\begin{pmatrix} x_2 + y_2 \\ z_2 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_2 - y_2 \\ z_2 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_2 + y_2 + \frac{1}{2} \\ x_2 - y_2 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(16i)	Sn I
$\mathbf{B}_6$	$= \begin{pmatrix} x_2 + y_2 + \frac{1}{2} \\ x_2 - y_2 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_2 + y_2 + \frac{1}{2} \\ x_2 - y_2 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_2 - y_2 + \frac{1}{2} \\ z_2 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(16i)	Sn I
$\mathbf{B}_7$	$= -\begin{pmatrix} x_2 - y_2 \\ z_2 \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_2 + y_2 \\ z_2 \end{pmatrix} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(16i)	Sn I
$\mathbf{B}_8$	$= \begin{pmatrix} x_2 - y_2 + \frac{1}{2} \\ x_2 + y_2 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_2 + y_2 + \frac{1}{2} \\ x_2 - y_2 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(16i)	Sn I
$\mathbf{B}_9$	$= \begin{pmatrix} x_2 + y_2 \\ z_2 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_2 - y_2 \\ z_2 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_2 + y_2 + \frac{1}{2} \\ x_2 - y_2 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(16i)	Sn I
$\mathbf{B}_{10}$	$= \begin{pmatrix} -x_2 + y_2 - \frac{1}{2} \\ -x_2 + y_2 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} -x_2 + y_2 - \frac{1}{2} \\ -x_2 + y_2 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_2 + y_2 + \frac{1}{2} \\ x_2 - y_2 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(16i)	Sn I

References

- [1] J. Nylén, F. J. G. Garcìa, 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.

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- 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