

PdSn₃ Structure:

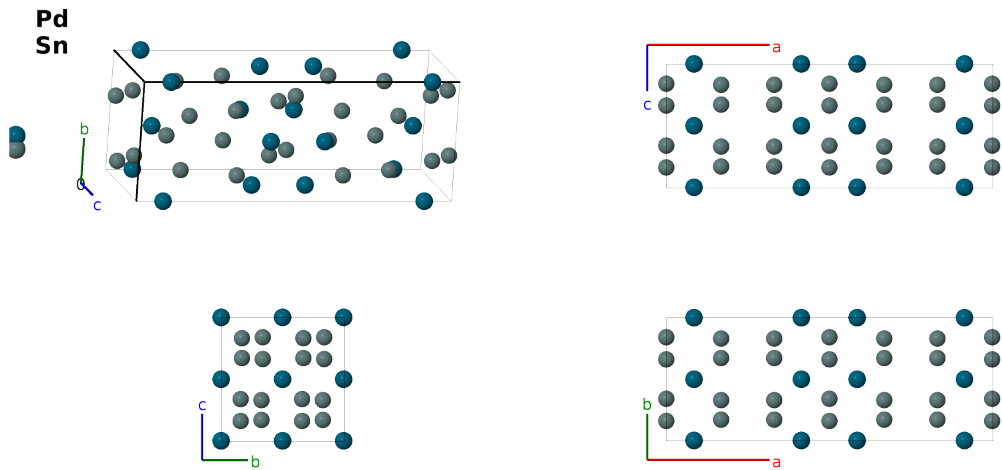
AB3_oC32_64_d_fg-001

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<https://aflow.org/prototype-encyclopedia/J38S>

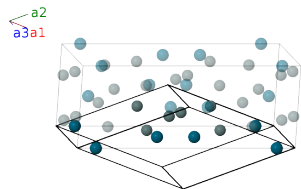
https://aflow.org/prototype-encyclopedia/AB3_oC32_64_d_fg-001



Prototype	PdSn ₃
AFLOW prototype label	AB3_oC32_64_d_fg-001
ICSD	413279
CCDC	1728311
Pearson symbol	oC32
Space group number	64
Space group symbol	<i>Cmce</i>
AFLOW prototype command	<code>aflow --proto=AB3_oC32_64_d_fg-001</code> <code>--params=a, b/a, c/a, x₁, y₂, z₂, x₃, y₃, z₃</code>

Base-centered Orthorhombic primitive vectors

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



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

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