

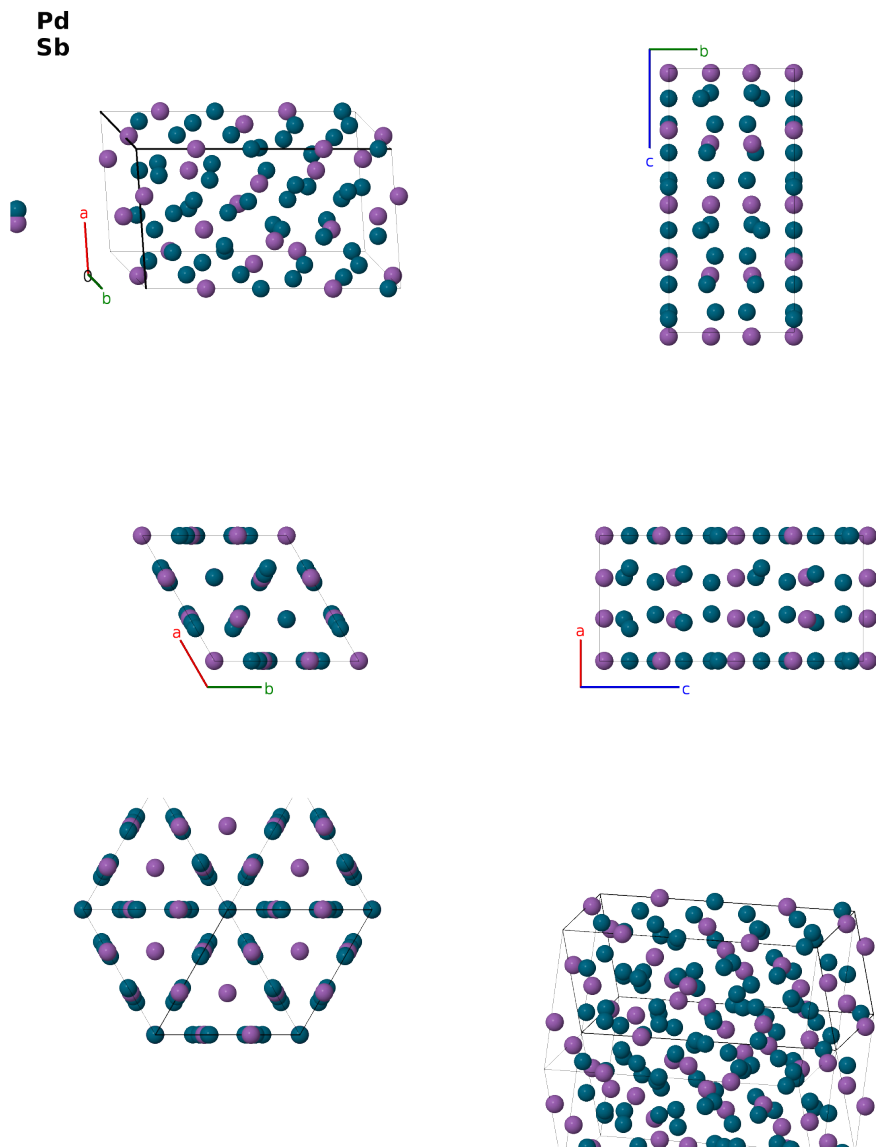
Stibiopalladinite (Pd_5Sb_2) Structure: A5B2_hP42_185_ab4c_abc-001

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<https://aflow.org/prototype-encyclopedia/04LT>

https://aflow.org/prototype-encyclopedia/A5B2_hP42_185_ab4c_abc-001



Prototype	Pd_5Sb_2
AFLOW prototype label	A5B2_hP42_185_ab4c_abc-001
Mineral name	stibiopalladinite
ICSD	648776

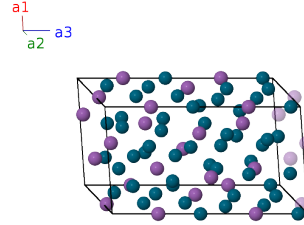
CCDC	1763412
Pearson symbol	hP42
Space group number	185
Space group symbol	$P6_3cm$
AFLOW prototype command	aflow --proto=A5B2_hP42_185_ab4c_abc-001 --params= $a, c/a, z_1, z_2, z_3, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9$

Other compounds with this structure

Ni₅As₂ (orcelite)

Hexagonal primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
\mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
\mathbf{a}_3 &= c \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(2a)	Pd I
$\mathbf{B}_2$	$= \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2a)	Pd I
$\mathbf{B}_3$	$= z_2 \mathbf{a}_3$	$=$	$c z_2 \hat{\mathbf{z}}$	(2a)	Sb I
$\mathbf{B}_4$	$= \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2a)	Sb I
$\mathbf{B}_5$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4b)	Pd II
$\mathbf{B}_6$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4b)	Pd II
$\mathbf{B}_7$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4b)	Pd II
$\mathbf{B}_8$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4b)	Pd II
$\mathbf{B}_9$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4b)	Sb II
$\mathbf{B}_{10}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4b)	Sb II
$\mathbf{B}_{11}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4b)	Sb II
$\mathbf{B}_{12}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4b)	Sb II
$\mathbf{B}_{13}$	$= x_5 \mathbf{a}_1 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a x_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(6c)	Pd III
$\mathbf{B}_{14}$	$= x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a x_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(6c)	Pd III
$\mathbf{B}_{15}$	$= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a x_5 \hat{\mathbf{x}} + c z_5 \hat{\mathbf{z}}$	(6c)	Pd III
$\mathbf{B}_{16}$	$= -x_5 \mathbf{a}_1 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}a x_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(6c)	Pd III
$\mathbf{B}_{17}$	$= -x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}a x_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(6c)	Pd III
$\mathbf{B}_{18}$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a x_5 \hat{\mathbf{x}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(6c)	Pd III
$\mathbf{B}_{19}$	$= x_6 \mathbf{a}_1 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a x_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(6c)	Pd IV

$\mathbf{B}_{20} =$	$x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(6c)	Pd IV
$\mathbf{B}_{21} =$	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + cz_6 \hat{\mathbf{z}}$	(6c)	Pd IV
$\mathbf{B}_{22} =$	$-x_6 \mathbf{a}_1 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Pd IV
$\mathbf{B}_{23} =$	$-x_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Pd IV
$\mathbf{B}_{24} =$	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Pd IV
$\mathbf{B}_{25} =$	$x_7 \mathbf{a}_1 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_7 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(6c)	Pd V
$\mathbf{B}_{26} =$	$x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_7 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(6c)	Pd V
$\mathbf{B}_{27} =$	$-x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + cz_7 \hat{\mathbf{z}}$	(6c)	Pd V
$\mathbf{B}_{28} =$	$-x_7 \mathbf{a}_1 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_7 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Pd V
$\mathbf{B}_{29} =$	$-x_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_7 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Pd V
$\mathbf{B}_{30} =$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Pd V
$\mathbf{B}_{31} =$	$x_8 \mathbf{a}_1 + z_8 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_8 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(6c)	Pd VI
$\mathbf{B}_{32} =$	$x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_8 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(6c)	Pd VI
$\mathbf{B}_{33} =$	$-x_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} + cz_8 \hat{\mathbf{z}}$	(6c)	Pd VI
$\mathbf{B}_{34} =$	$-x_8 \mathbf{a}_1 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_8 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Pd VI
$\mathbf{B}_{35} =$	$-x_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_8 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Pd VI
$\mathbf{B}_{36} =$	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Pd VI
$\mathbf{B}_{37} =$	$x_9 \mathbf{a}_1 + z_9 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_9 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(6c)	Sb III
$\mathbf{B}_{38} =$	$x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_9 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(6c)	Sb III
$\mathbf{B}_{39} =$	$-x_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} + cz_9 \hat{\mathbf{z}}$	(6c)	Sb III
$\mathbf{B}_{40} =$	$-x_9 \mathbf{a}_1 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_9 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Sb III
$\mathbf{B}_{41} =$	$-x_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_9 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Sb III
$\mathbf{B}_{42} =$	$x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Sb III

References

- [1] M. El-Boragy, S. Bhan, and K. Schubert, *Kristallstruktur von Pd_5Sb_2 und Ni_5As_2 und einigen varianten*, J. Less-Common Met. **22**, 445–458 (1970), doi:10.1016/0022-5088(70)90132-3.

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