Stibiopalladinite (Pd_5Sb_2) Structure: A5B2_hP42_185_ab4c_abc-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.

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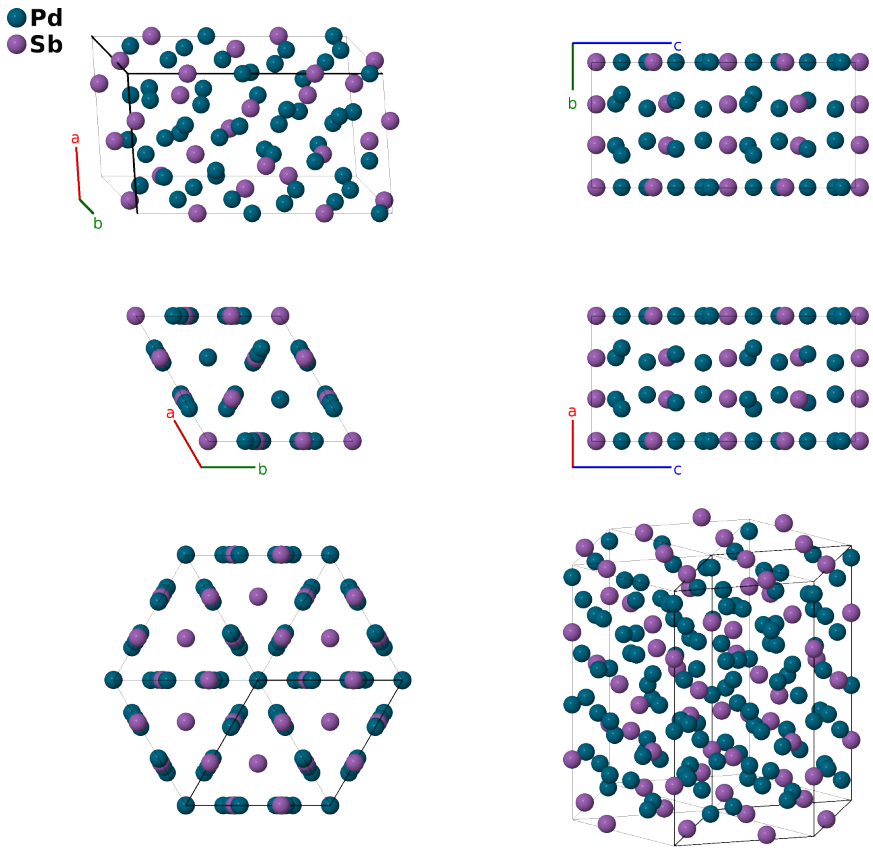
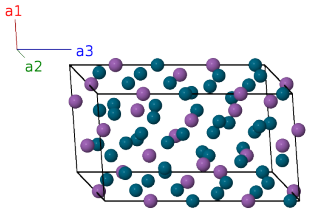


Prototype	Pd_5Sb_2
AFLOW prototype label	A5B2_hP42_185_ab4c_abc-001
Mineral name	stibiopalladinite
ICSD	648776
Pearson symbol	hP42
Space group number	185
Space group symbol	$P6_3cm$
AFLOW prototype command	`aflow --proto=A5B2_hP42_185_ab4c_abc-001 --params=`$a, c/a, z_1, z_2, z_3, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9$

Other compounds with this structure
Ni_5As_2 (orcelite)

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(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
$\mathbf{B_3}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(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
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(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
$\mathbf{B_8}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(4b)	Pd II
$\mathbf{B_9}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{12}}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(4b)	Sb II
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1+z_5\,\mathbf{a}_3$	=	$\frac{1}{2}ax_5\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(6c)	Pd III
$\mathbf{B_{14}}$	=	$x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$\frac{1}{2}ax_5\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(6c)	Pd III
$\mathbf{B_{15}}$	=	$-x_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}+cz_5\,\hat{\mathbf{z}}$	(6c)	Pd III
$\mathbf{B_{16}}$	=	$-x_5\,\mathbf{a}_1+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_5\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Pd III
$\mathbf{B_{17}}$	=	$-x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_5\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Pd III
$\mathbf{B_{18}}$	=	$x_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Pd III
$\mathbf{B_{19}}$	=	$x_6\,\mathbf{a}_1+z_6\,\mathbf{a}_3$	=	$\frac{1}{2}ax_6\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a}_1+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_6\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Pd IV
$\mathbf{B_{23}}$	=	$-x_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_6\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Pd IV
$\mathbf{B_{24}}$	=	$x_6\,\mathbf{a}_1+x_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{28}}$	=	$-x_7\,\mathbf{a}_1+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_7\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Pd V
$\mathbf{B_{29}}$	=	$-x_7\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_7\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Pd V
$\mathbf{B_{30}}$	=	$x_7\,\mathbf{a}_1+x_7\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}}+c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{34}}$	$=$	$-x_8\,\mathbf{a}_1 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{1}{2}ax_8\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Pd VI
$\mathbf{B_{35}}$	$=$	$-x_8\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{1}{2}ax_8\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Pd VI
$\mathbf{B_{36}}$	$=$	$x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$ax_8\,\hat{\mathbf{x}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{40}}$	$=$	$-x_9\,\mathbf{a}_1 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{1}{2}ax_9\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Sb III
$\mathbf{B_{41}}$	$=$	$-x_9\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\frac{1}{2}ax_9\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Sb III
$\mathbf{B_{42}}$	$=$	$x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$ax_9\,\hat{\mathbf{x}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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.