

α -BiPd₃ Structure:

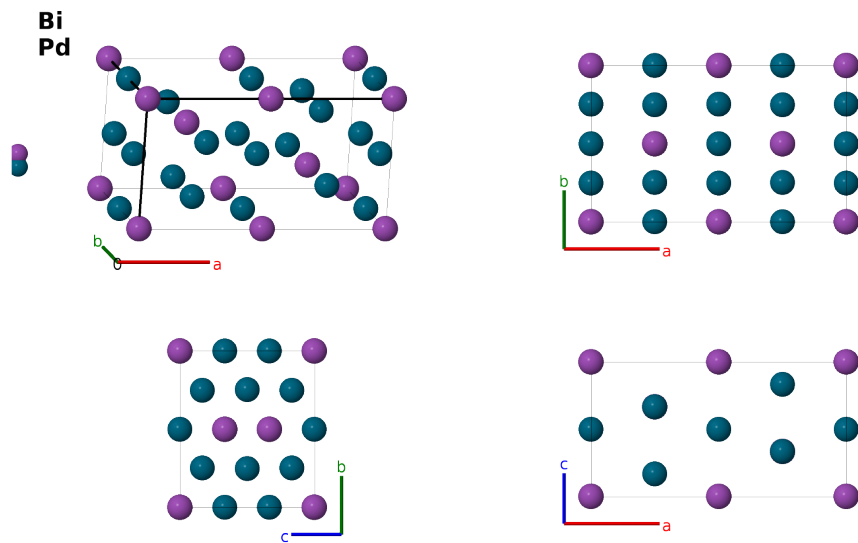
AB3_oP16_51_af_behk-001

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<https://aflow.org/prototype-encyclopedia/9W5L>

https://aflow.org/prototype-encyclopedia/AB3_oP16_51_af_behk-001

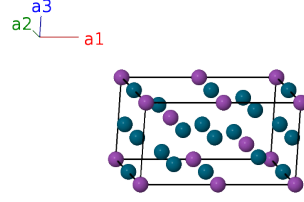


Prototype	BiPd ₃
AFLOW prototype label	AB3_oP16_51_af_behk-001
ICSD	58839
CCDC	1622837
Pearson symbol	oP16
Space group number	51
Space group symbol	$Pmma$
AFLOW prototype command	<code>aflow --proto=AB3_oP16_51_af_behk-001</code> <code>--params=a, b/a, c/a, z₃, z₄, y₅, y₆, z₆</code>

- This is the room temperature structure of BiPd.
- Okamoto's phase diagram (Villars, 2018) shows a transition to a high-temperature phase at 800°C, but says that no data is available for that structure.
- (Schubert, 1968) puts one bismuth atom on the (2c) (0 0 1/2) Wyckoff position. We shift this so that atom is at the origin, Wyckoff position (2a).

Simple Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(2a)	Bi I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2} a \hat{\mathbf{x}}$	(2a)	Bi I
$\mathbf{B}_3$	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} b \hat{\mathbf{y}}$	(2b)	Pd I
$\mathbf{B}_4$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$	(2b)	Pd I
$\mathbf{B}_5$	$\frac{1}{4} \mathbf{a}_1 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + cz_3 \hat{\mathbf{z}}$	(2e)	Pd II
$\mathbf{B}_6$	$\frac{3}{4} \mathbf{a}_1 - z_3 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - cz_3 \hat{\mathbf{z}}$	(2e)	Pd II
$\mathbf{B}_7$	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2f)	Bi II
$\mathbf{B}_8$	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(2f)	Bi II
$\mathbf{B}_9$	$y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$by_5 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Pd III
$\mathbf{B}_{10}$	$\frac{1}{2} \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Pd III
$\mathbf{B}_{11}$	$-y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-by_5 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Pd III
$\mathbf{B}_{12}$	$\frac{1}{2} \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Pd III
$\mathbf{B}_{13}$	$\frac{1}{4} \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4k)	Pd IV
$\mathbf{B}_{14}$	$\frac{1}{4} \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4k)	Pd IV
$\mathbf{B}_{15}$	$\frac{3}{4} \mathbf{a}_1 + y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4k)	Pd IV
$\mathbf{B}_{16}$	$\frac{3}{4} \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4k)	Pd IV

References

- [1] K. Schubert, S. Bhan, T. K. Biswas, K. Frank, and P. K. Panday, *Einige Strukturdaten metallischer Phasen*, Naturwissenschaften **55**, 542–543 (1968), doi:10.1007/BF00660131.
- [2] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. Bismuth-Palladium Binary Phase Diagram (1994 Okamoto H.). Copyright ©2006-2018 ASM International.

Found in

- [1] A. Götze, T. C. Hansen, and H. Kohlmann, *The reversible hydrogenation of BiPd3 followed by in situ methods and the crystal structure of PbPd3D_{0.13(1)}*, J. Alloys Compd. **731**, 1001–1008 (2018), doi:10.1016/j.jallcom.2017.10.107.

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