α-$BiPd_3$ Structure: AB3_oP16_51_af_behk-001

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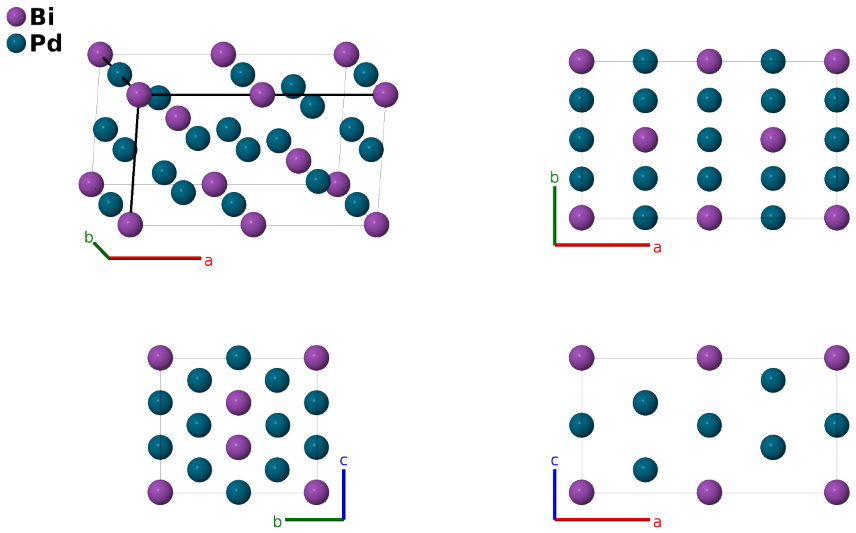
https://aflow.org/p/9W5L

https://aflow.org/p/AB3_oP16_51_af_behk-001

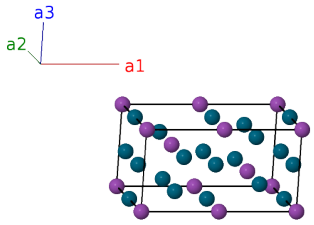


Prototype	$BiPd_3$
AFLOW prototype label	AB3_oP16_51_af_behk-001
ICSD	58839
Pearson symbol	oP16
Space group number	51
Space group symbol	*Pmma*
AFLOW prototype command	`aflow --proto=AB3_oP16_51_af_behk-001 --params=`$a, b/a, c/a, z_3, z_4, y_5, y_6, z_6$

- 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

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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

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