

β -BiPd Structure:

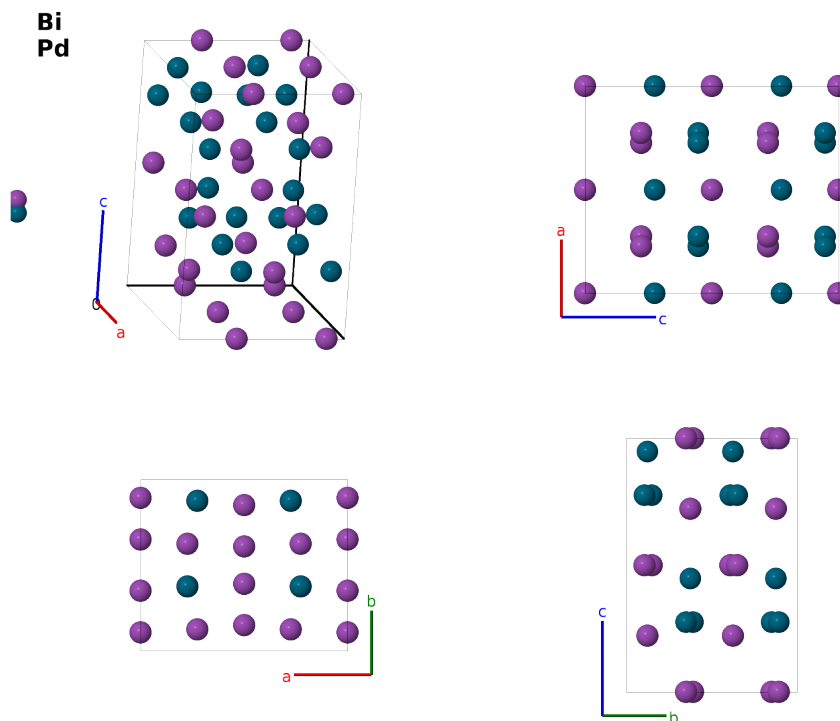
AB_oC32_36_2ab_2ab-001

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<https://aflow.org/prototype-encyclopedia/6W3L>

https://aflow.org/prototype-encyclopedia/AB_oC32_36_2ab_2ab-001



Prototype	BiPd
AFLOW prototype label	AB_oC32_36_2ab_2ab-001
ICSD	56279
CCDC	1620540
Pearson symbol	oC32
Space group number	36
Space group symbol	$Cmc2_1$
AFLOW prototype command	<code>aflow --proto=AB_oC32_36_2ab_2ab-001</code> <code>--params=a,b/a,c/a,y₁,z₁,y₂,z₂,y₃,z₃,y₄,z₄,x₅,y₅,z₅,x₆,y₆,z₆</code>

- This is the high-temperature structure of BiPd. Below 210°C it transforms into the monoclinic α -BiPd structure (Villars, 2018). (Zhuralvlev, 1957) gives the structure in the $Ccm2_1$ setting of space group #36. We used FINDSYM to transform this to the standard $Cmc2_1$ setting.

- Space group $Cmc2_1$ allows an arbitrary definition of the origin of the z -axis. Here we follow (Zhuravlev, 1957) and set $z_1 = 0$ for the first bismuth atom, Bi I. Zhuravlev also finds $z_2 = 0$ for Bi II, probably due to the low resolution of the experimental data.

Base-centered Orthorhombic primitive vectors



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4a)	Bi I
$\mathbf{B}_2$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Bi I
$\mathbf{B}_3$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4a)	Bi II
$\mathbf{B}_4$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Bi II
$\mathbf{B}_5$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4a)	Pd I
$\mathbf{B}_6$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Pd I
$\mathbf{B}_7$	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4a)	Pd II
$\mathbf{B}_8$	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Pd II
$\mathbf{B}_9$	$= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8b)	Bi III
$\mathbf{B}_{10}$	$= -(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	Bi III
$\mathbf{B}_{11}$	$= (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	Bi III
$\mathbf{B}_{12}$	$= -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8b)	Bi III
$\mathbf{B}_{13}$	$= (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8b)	Pd III
$\mathbf{B}_{14}$	$= -(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	Pd III
$\mathbf{B}_{15}$	$= (x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	Pd III
$\mathbf{B}_{16}$	$= -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8b)	Pd III

References

- [1] N. N. Zhuravlev, *Structure of Superconductors, X. Thermal, Microscopic, and X-ray Investigation of the Bismuth-Palladium System*, Sov. Phys. JETP **5**, 1064–1072 (1957).

Found in

- [1] 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.

First cited in

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