

α -Bi₂Pd Structure:

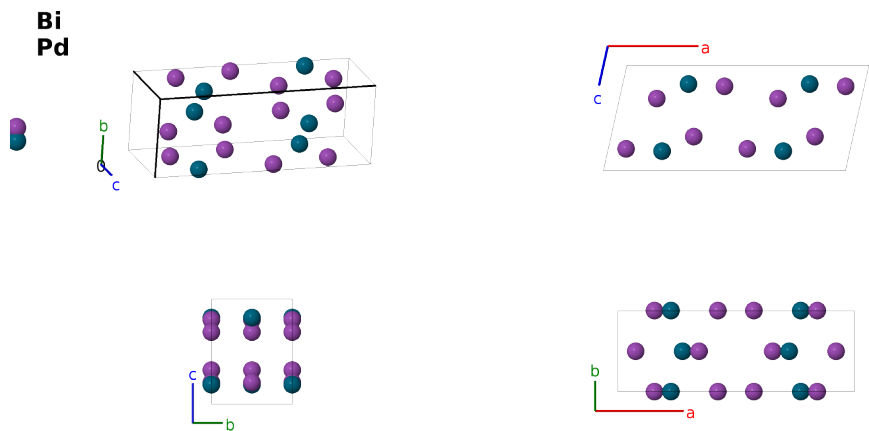
A2B_mC12_12_2i_i-006

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<https://aflow.org/prototype-encyclopedia/0NDQ>

https://aflow.org/prototype-encyclopedia/A2B_mC12_12_2i_i-006

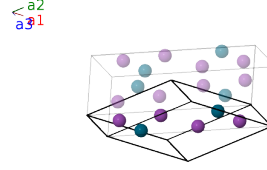


Prototype	Bi ₂ Pd
AFLOW prototype label	A2B_mC12_12_2i_i-006
ICSD	42565
CCDC	1612221
Pearson symbol	mC12
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<code>aflow --proto=A2B_mC12_12_2i_i-006</code> <code>--params=a, b/a, c/a, β, x_1, z_1, x_2, z_2, x_3, z_3</code>

- This is the room-temperature structure of Bi₂Pd. Above 380-390°C, depending on the exact composition, this transforms into β -Bi₂Pd, which has the tetragonal MoSi₂ ($C11_b$) structure (Villars, 2018).
- α -Ba₂Pd shares the same AFLOW label, A2B_mC12_12_2i_i, with CaC₂-III and OsGe₂. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Base-centered Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(4i)	Bi I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(4i)	Bi I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4i)	Bi II
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4i)	Bi II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	Pd I
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	Pd I

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.

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