α-Bi_2Pd Structure: A2B_mC12_12_2i_i-006

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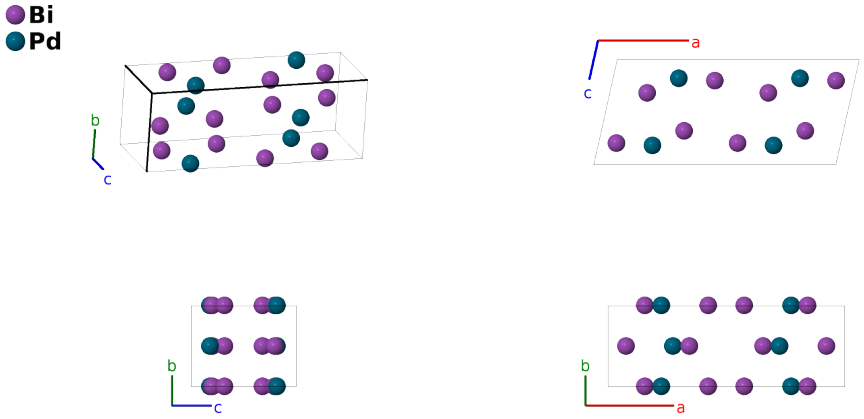
https://aflow.org/p/0NDQ

https://aflow.org/p/A2B_mC12_12_2i_i-006

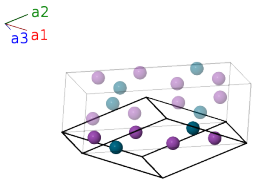


Prototype	Bi_2Pd
AFLOW prototype label	A2B_mC12_12_2i_i-006
ICSD	42565
Pearson symbol	mC12
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=A2B_mC12_12_2i_i-006 --params=`$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3$

- This is the room-temperature structure of Bi_2Pd. Above 380-390°C, depending on the exact composition, this transforms into β-Bi_2Pd, which has the tetragonal $MoSi_2$ ($C11_b$) structure (Villars, 2018).
- α-Ba_2Pd shares the same AFLOW label, A2B_mC12_12_2i_i, with CaC_2-III and $OsGe_2$. 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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



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.