PtBi₂ Structure:
A2B_hP9_147_g_ad-002

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

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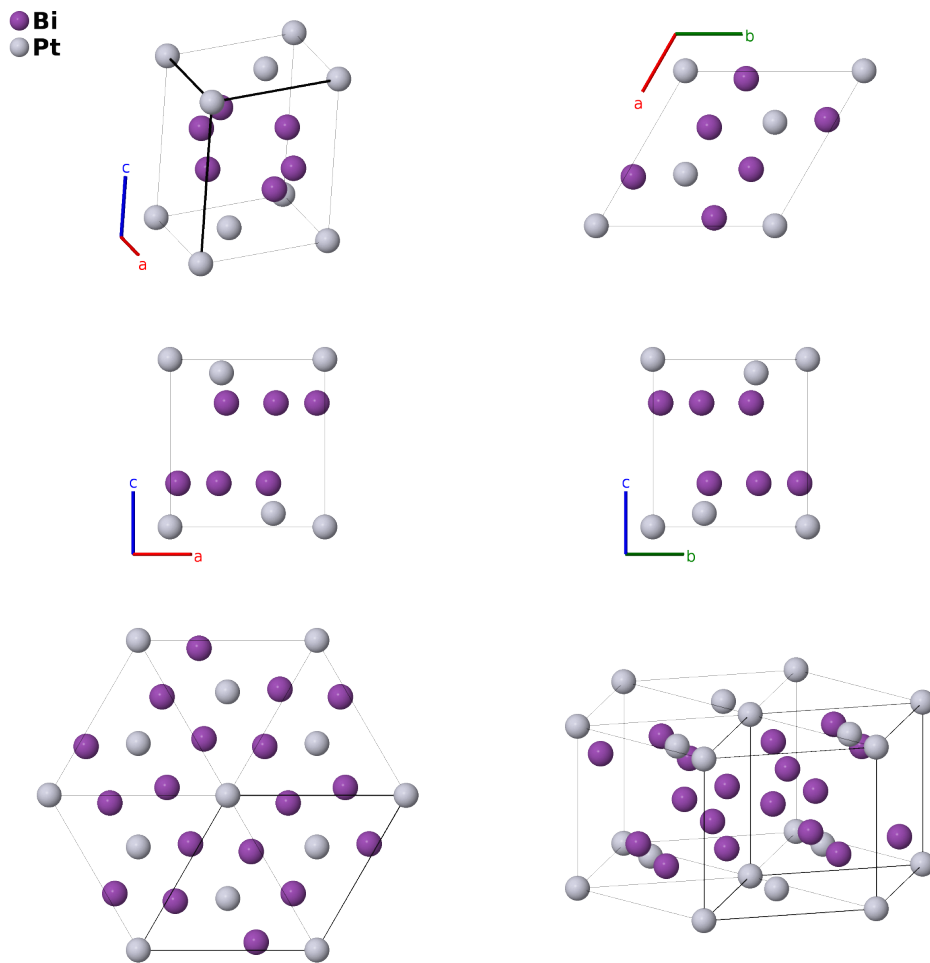
Prototype	Bi₂Pt
AFLOW prototype label	A2B_hP9_147_g_ad-002
ICSD	58847
Pearson symbol	hP9
Space group number	147
Space group symbol	$P\bar{3}$
AFLOW prototype command	aflow --proto=A2B_hP9_147_g_ad-002 --params=$a, c/a, z_2, x_3, y_3, z_3$

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- PtBi$_2$ can also be found in the pyrite ($C2$) structure.

- γ-AgZn (B_b) and PtBi$_2$ have the same AFLOW label, A2B_hP9_147_g_ad. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
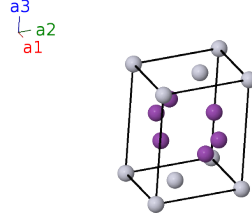
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	0	$=$	0	(1a)	Pt I
$\mathbf{B_2}$	$=$	$\frac{1}{3}\,\mathbf{a_1} + \frac{2}{3}\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2d)	Pt II
$\mathbf{B_3}$	$=$	$\frac{2}{3}\,\mathbf{a_1} + \frac{1}{3}\,\mathbf{a_2} - z_2\,\mathbf{a_3}$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2d)	Pt II
$\mathbf{B_4}$	$=$	$x_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$\frac{1}{2}a\left(x_3 + y_3\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_3 - y_3\right)\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6g)	Bi I
$\mathbf{B_5}$	$=$	$-y_3\,\mathbf{a_1} + \left(x_3 - y_3\right)\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$\frac{1}{2}a\left(x_3 - 2y_3\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6g)	Bi I
$\mathbf{B_6}$	$=$	$-\left(x_3 - y_3\right)\mathbf{a_1} - x_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$-\frac{1}{2}a\left(2x_3 - y_3\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6g)	Bi I
$\mathbf{B_7}$	$=$	$-x_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$-\frac{1}{2}a\left(x_3 + y_3\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\left(x_3 - y_3\right)\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(6g)	Bi I
$\mathbf{B_8}$	$=$	$y_3\,\mathbf{a_1} - \left(x_3 - y_3\right)\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$\frac{1}{2}a\left(-x_3 + 2y_3\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(6g)	Bi I
$\mathbf{B_9}$	$=$	$\left(x_3 - y_3\right)\mathbf{a_1} + x_3\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$\frac{1}{2}a\left(2x_3 - y_3\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(6g)	Bi I

References

[1] T. Biswas and K. Schubert, *Strukturuntersuchungen in den mischungen Pt-Tl-Pb und Pt-Pb-Bi*, J. Less-Common Met. **19**, 223–243 (1969), doi:10.1016/0022-5088(69)90099-X.

Found in

[1] C. Q. Xu, X. Z. Xing, X. Xu, B. Li, B. Chen, L. Q. Che, X. Lu, J. Dai, and Z. X. Shi, *Synthesis, physical properties, and band structure of the layered bismuthide PtBi$_2$*, Phys. Rev. B **94**, 165119 (2016), doi:10.1103/PhysRevB.94.165119.