

PtBi₂ Structure:

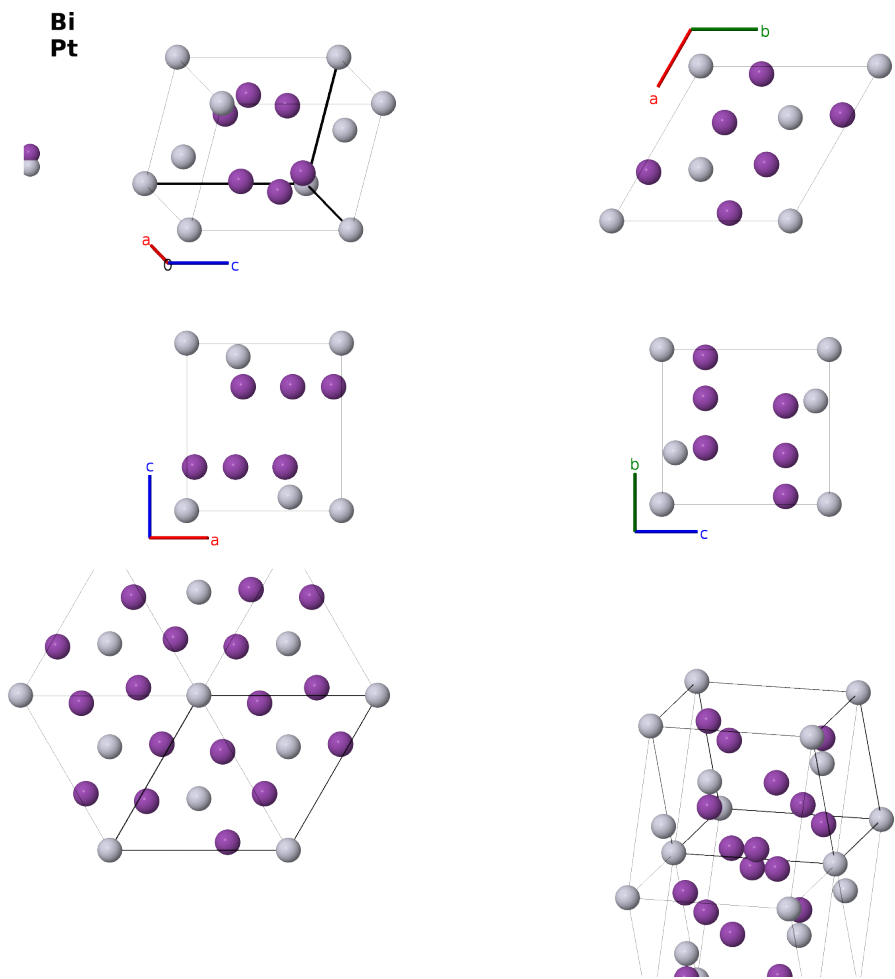
A2B_hP9_147_g_ad-002

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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

https://aflow.org/prototype-encyclopedia/A2B_hP9_147_g_ad-002

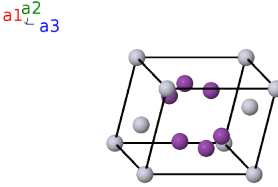


Prototype	Bi ₂ Pt
AFLOW prototype label	A2B_hP9_147_g_ad-002
ICSD	58847
CCDC	1622845
Pearson symbol	hP9
Space group number	147
Space group symbol	$P\bar{3}$

AFLOW prototype command `aflow --proto=A2B_hP9_147_g_ad-002`
 `--params=a, c/a, z2, x3, y3, z3`

- PtBi₂ can also be found in the pyrite (*C*2) structure.
- γ -AgZn (*B_b*) and PtBi₂ 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

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$


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
$\mathbf{B}_4$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_3 - y_3) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6g)	Bi I
$\mathbf{B}_5$	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6g)	Bi I
$\mathbf{B}_6$	$= -(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6g)	Bi I
$\mathbf{B}_7$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a (x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_3 - y_3) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(6g)	Bi I
$\mathbf{B}_8$	$= y_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a (-x_3 + 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(6g)	Bi I
$\mathbf{B}_9$	$= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(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 PtBi₂*, Phys. Rev. B **94**, 165119 (2016), doi:10.1103/PhysRevB.94.165119.

First cited in

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