

β -BiI Structure:

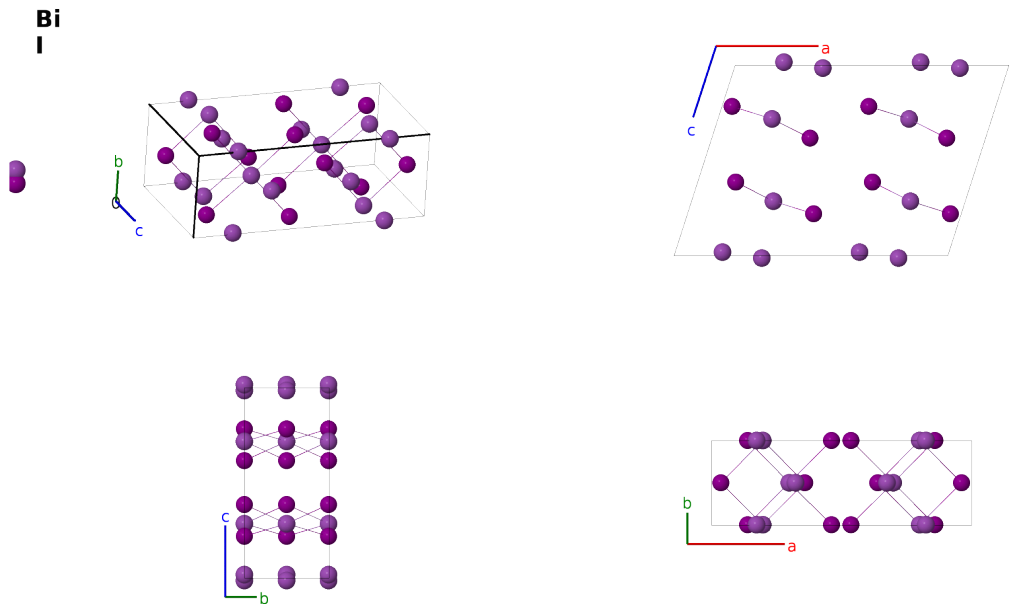
AB_mC16_12_2i_2i-002

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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/DA8J>

https://aflow.org/prototype-encyclopedia/AB_mC16_12_2i_2i-002



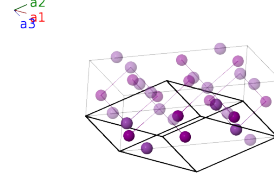
Prototype	BiI
AFLOW prototype label	AB_mC16_12_2i_2i-002
ICSD	1559
CCDC	1591665
Pearson symbol	mC16
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<code>aflow --proto=AB_mC16_12_2i_2i-002</code> <code>--params=a, b/a, c/a, β, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4</code>

- BiI occurs naturally in three phases, with high pressure phases predicted to occur (Deng, 2019). All of the natural phases are in space group $C2/m$ #12, with atoms on the (4i) Wyckoff positions. The only difference between the structures is the stacking of the atoms.
 - α -BiI is the ground state structure.

- β -BiI (this structure) is metastable at room temperature and stable above 564K.
- γ -BiI is formed at 580K.
- SrN, β -BiI, and γ -BiI share the same AFLOW prototype label, AB_mC16_12_2i_2i. 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)	I 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)	I I
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	I II
$\mathbf{B}_8$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	I II

References

- [1] H. G. von Schnering, H. von Benda, and C. Kalveram, *Wismutmonojodid BiI, eine Verbindung mit Bi(O) und Bi(II)*, Z. Anorganische und Allgemeine Chemie **438**, 37–52 (1978), doi:10.1002/zaac.19784380104.

Found in

- [1] S. Deng, X. Song, X. Shao, Q. Li, Y. Xie, C. Chen, and Y. Ma, *First-principles study of high-pressure phase stability and superconductivity of Bi₄I₄*, Phys. Rev. B **100**, 224108 (2019), doi:10.1103/PhysRevB.100.224108.

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