β-BiI Structure: AB_mC16_12_2i_2i-002

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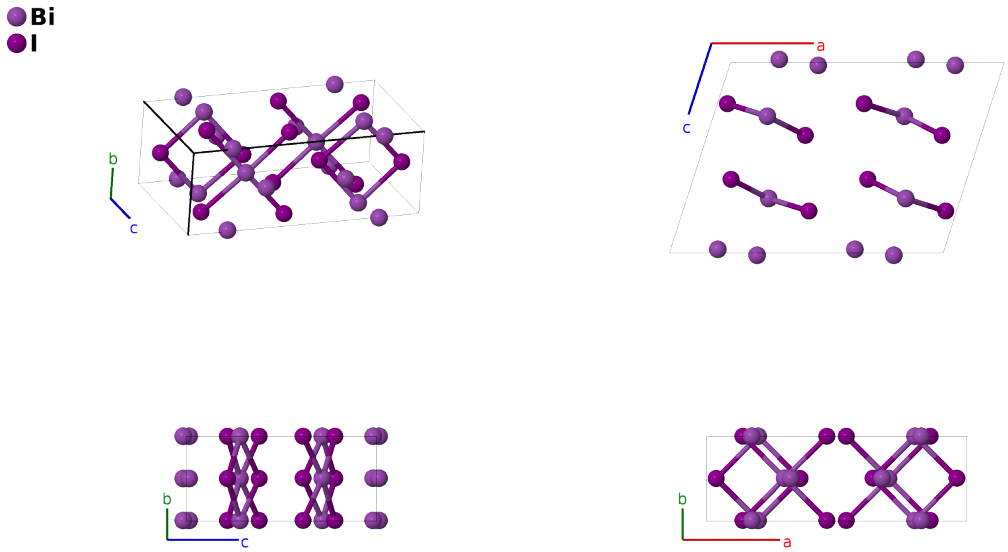
https://aflow.org/p/DA8J

https://aflow.org/p/AB_mC16_12_2i_2i-002

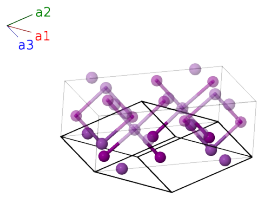


Prototype	BiI
AFLOW prototype label	AB_mC16_12_2i_2i-002
ICSD	1559
Pearson symbol	mC16
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=AB_mC16_12_2i_2i-002 --params=`$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4$

- 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 BiJ, 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 Bi_4I_4*, Phys. Rev. B **100**, 224108 (2019), doi:10.1103/PhysRevB.100.224108.