Hexagonal BiI_3 Structure: AB3_hP8_162_c_k-001

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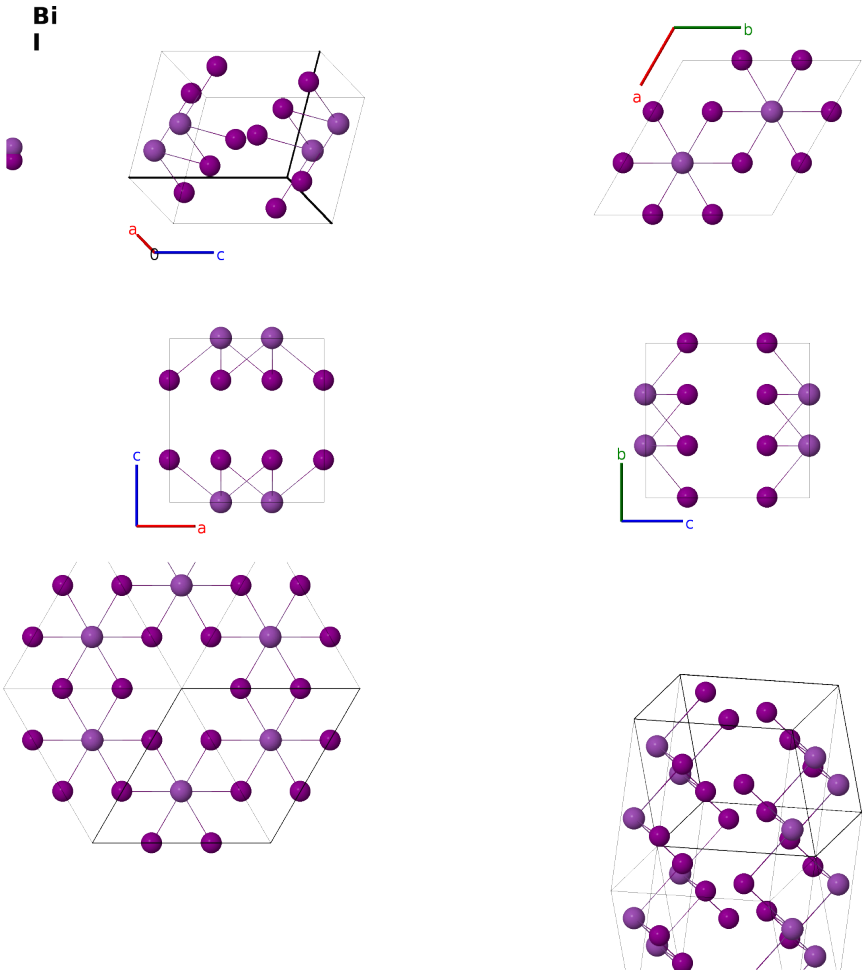
https://aflow.org/prototype-encyclopedia/D8KY

https://aflow.org/prototype-encyclopedia/AB3_hP8_162_c_k-001



Prototype	BiI_3
AFLOW prototype label	AB3_hP8_162_c_k-001
ICSD	20676
CCDC	1598437
Pearson symbol	hP8
Space group number	162
Space group symbol	$P\bar{3}1m$

AFLOW prototype command `aflow --proto=AB3_hP8_162_c_k-001 --params=`$a, c/a, x_2, z_2$

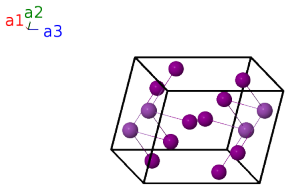
Other compounds with this structure

$TiCl_3$

- BiI_3 has also been reported in the rhombohedral $D0_5$ structure. The Bi-I bonds are similar in both structures, with the only difference being the stacing of the layers.
- Note that although the lattice is hexagonal, the symmetry is trigonal.

Trigonal (Hexagonal) primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	Bi I
$\mathbf{B_2}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	Bi I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(6k)	I I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(6k)	I I
$\mathbf{B_5}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + cz_2\,\hat{\mathbf{z}}$	(6k)	I I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(6k)	I I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 - z_2\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(6k)	I I
$\mathbf{B_8}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - cz_2\,\hat{\mathbf{z}}$	(6k)	I I

References

[1] Z. G. Pinkser, *The electron diffraction analysis of BiI_3 and the modern ideas on the structure of the layered lattices*, Trudy Instituta Kristallografii, Akademiya Nauk SSSR **7**, 35–48 (1952).

Found in

[1] *Inorganic Crystal Structure Database*. Entry 20676 (BiI3).

First cited in

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