Rhombohedral BiI_3 ($D0_5$) Structure: AB3_hR8_148_c_f-001

This structure previously used the label(s) `AB3_hR8_148_c_f`. Calls to these addresses will be redirected here.

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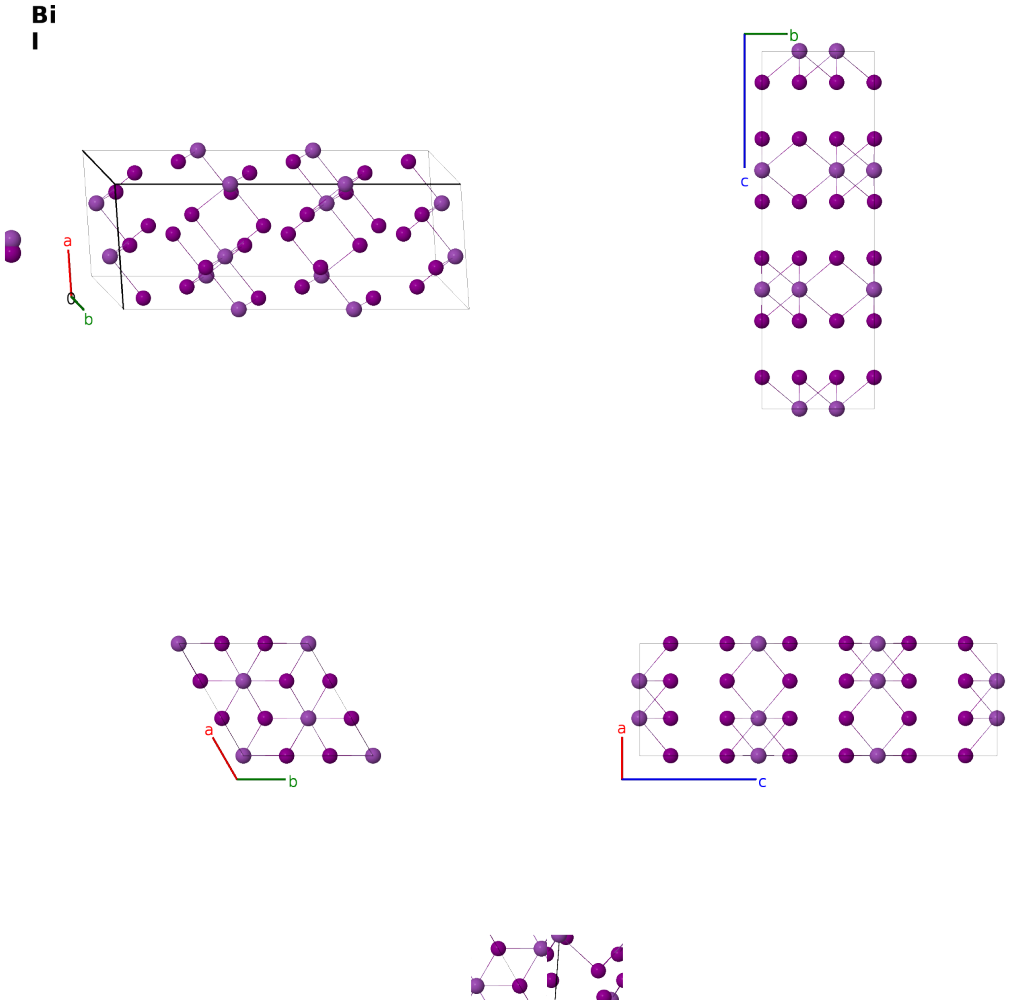
https://aflow.org/prototype-encyclopedia/TZC0

https://aflow.org/prototype-encyclopedia/AB3_hR8_148_c_f-001



Prototype	BiI_3
AFLOW prototype label	AB3_hR8_148_c_f-001
***Strukturbericht* designation**	$D0_5$
ICSD	36182
CCDC	1607956

Pearson symbol	hR8
Space group number	148
Space group symbol	$R\bar{3}$
AFLOW prototype command	`aflow --proto=AB3_hR8_148_c_f-001 --params=`$a, c/a, x_1, x_2, y_2, z_2$

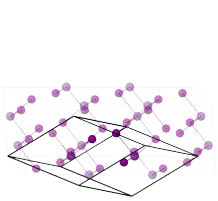
Other compounds with this structure

AsI_3, BrI_3, CmI_3, $CrBr_3$, $CrCl_3$, CrI_3, $FeBr_3$, $FeCl_3$, $RhBr_3$, $RuBr_3$, SbI_3, $ScCl_3$, $TiBr_3$, $TiCl_3$, VBr_3, VCl_3, VI_3, YI_3, YbI_3

- BiI_3 has also been reported in a hexagonal (trigonal) structure. The Bi-I bonds are similar in both structures, with the only difference being the stacing of the layers.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(2c)	Bi I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-cx_1\,\hat{\mathbf{z}}$	(2c)	Bi I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_2 - 2y_2 + z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	I I
$\mathbf{B_4}$	=	$z_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + y_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_2 - z_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_2 - y_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	I I
$\mathbf{B_5}$	=	$y_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2 - y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_2 + y_2 - 2z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	I I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_2 - 2y_2 + z_2)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	I I
$\mathbf{B_7}$	=	$-z_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - y_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_2 - z_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_2 - y_2 - z_2)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	I I
$\mathbf{B_8}$	=	$-y_2\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_2 + y_2 - 2z_2)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_2 + y_2 + z_2)\,\hat{\mathbf{z}}$	(6f)	I I

References

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Found in

[1] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

First cited in

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