HPC-Bi_2O_3 Structure: A2B3_hP20_186_bc_2c-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

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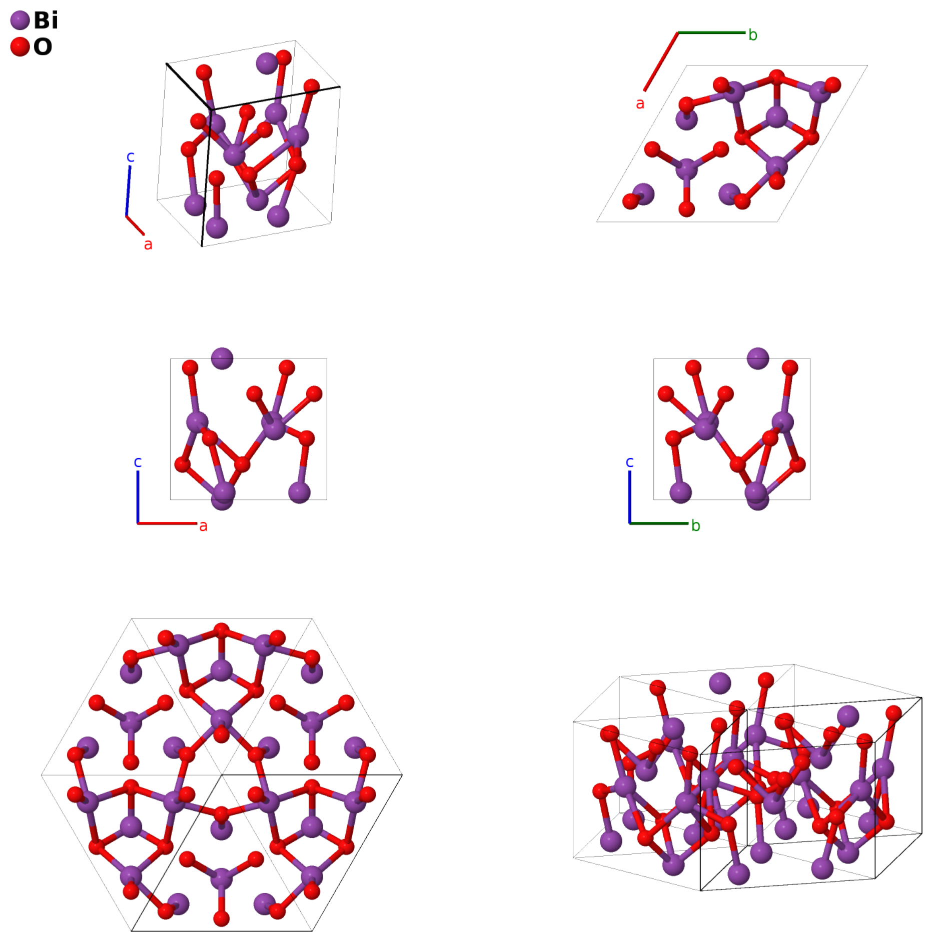
https://aflow.org/p/14M3

https://aflow.org/p/A2B3_hP20_186_bc_2c-001

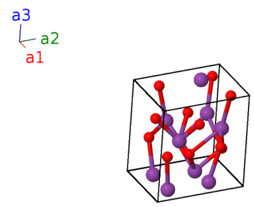


Prototype	Bi_2O_3
AFLOW prototype label	A2B3_hP20_186_bc_2c-001
ICSD	422451
Pearson symbol	hP20
Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	`aflow --proto=A2B3_hP20_186_bc_2c-001` `--params=`$a, c/a, z_1, x_2, z_2, x_3, z_3, x_4, z_4$

- Bi_2O_3 can be found in at least six forms (Harwig, 1978; Locherer, 2011):
  - monoclinic α-Bi_2O_3, the ground state, stable up to 729°,
  - tetragonal β-Bi_2O_3, $D5_{12}$, a metastable state observed at 650°C,
  - body-centered cubic γ-Bi_2O_3, another metastable phase observed at 639°C,
  - face-centered cubic δ-Bi_2O_3, the stable phase from 729° up to the melting point at 824°C,
  - a high-pressure HP-Bi_2O_3, and
  - a second "non-quenchable" high-pressure structure, HPC-Bi_2O_3 (this structure).
- We use the $P = 2.8$ GPa data of (Locherer, 2011) for our description of HP-Bi_2O_3.

Hexagonal primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(2b)	Bi I
$\mathbf{B_2}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Bi I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-\sqrt{3}ax_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(6c)	Bi II
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{3}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(6c)	Bi II
$\mathbf{B_5}$	=	$-2x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(6c)	Bi II
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\sqrt{3}ax_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Bi II
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 - 2x_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Bi II
$\mathbf{B_8}$	=	$2x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Bi II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-\sqrt{3}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{10}}$	=	$x_3\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{11}}$	=	$-2x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{12}}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\sqrt{3}ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{13}}$	=	$-x_3\,\mathbf{a}_1 - 2x_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{14}}$	=	$2x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{15}}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-\sqrt{3}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{16}}$	=	$x_4\,\mathbf{a}_1 + 2x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{17}}$	=	$-2x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{18}}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\sqrt{3}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{19}}$	=	$-x_4\,\mathbf{a}_1 - 2x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{20}}$	=	$2x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II

References

[1] T. Locherer, D. L. V. K. Prasad, R. Dinnebier, U. Wedig, M. Jansen, G. Garbarino, and T. Hansen, *High-pressure structural evolution of HP-Bi_2O_3*, Phys. Rev. B **83**, 214102 (2011), doi:10.1103/PhysRevB.83.214102.

[2] H. A. Harwig, *On the Structure of Bismuthsesquioxide: The α, β, γ, and δ-phase*, Z. Anorganische und Allgemeine Chemie **444**, 151–166 (1978), doi:10.1002/zaac.19784440118.