HP-Bi_2O_3 Structure: A2B3_hP20_159_bc_2c-001

This structure originally had the label `A2B3_hP20_159_bc_2c`. Calls to that address will be redirected here.

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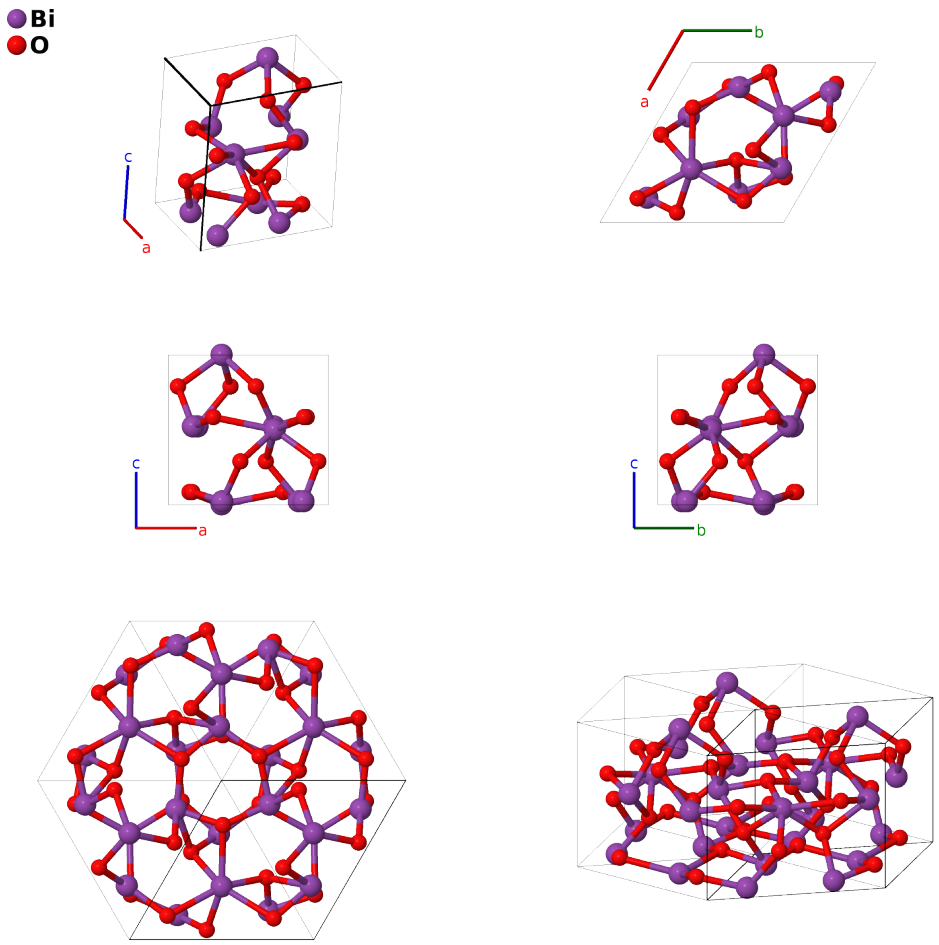
https://aflow.org/p/XT2J

https://aflow.org/p/A2B3_hP20_159_bc_2c-001

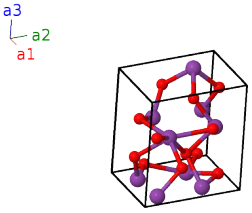


Prototype	Bi_2O_3
AFLOW prototype label	A2B3_hP20_159_bc_2c-001
ICSD	183150
Pearson symbol	hP20
Space group number	159
Space group symbol	$P31c$
AFLOW prototype command	`aflow --proto=A2B3_hP20_159_bc_2c-001 --params=`$a, c/a, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4$

- 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°C,
  - 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°C up to the melting point at 824°C,
  - a high-pressure HP-Bi_2O_3 (this structure), and
  - a second "nonquenchable" high-pressure structure, HPC-Bi_2O_3.
- We use the ambient pressure data of (Locherer, 2011) for our description of HP-Bi_2O_3.
- Space group $P3c1$ #159 allows an arbitary choice of the origin of the z-axis. We used this to set $z_1 = 0$ for the Bi-I (2b) atoms.

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
$\mathbf{B_1}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(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
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 + y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_2 - y_2)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(6c)	Bi II
$\mathbf{B_4}$	=	$-y_2\,\mathbf{a}_1 + (x_2 - y_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - 2y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(6c)	Bi II
$\mathbf{B_5}$	=	$-(x_2 - y_2)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_2 - y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(6c)	Bi II
$\mathbf{B_6}$	=	$y_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 + y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_2 - y_2)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Bi II
$\mathbf{B_7}$	=	$(x_2 - y_2)\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - 2y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Bi II
$\mathbf{B_8}$	=	$-x_2\,\mathbf{a}_1 - (x_2 - y_2)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_2 - y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	Bi II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 + y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_3 - y_3)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{10}}$	=	$-y_3\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - 2y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{11}}$	=	$-(x_3 - y_3)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{12}}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 + y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_3 - y_3)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{13}}$	=	$(x_3 - y_3)\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - 2y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{14}}$	=	$-x_3\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{15}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{16}}$	=	$-y_4\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - 2y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6c)	O II

$\mathbf{B_{17}}$	=	$-\left(x_4-y_4\right)\,\mathbf{a}_1-x_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_4-y_4\right)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{18}}$	=	$y_4\,\mathbf{a}_1+x_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4+y_4\right)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\left(x_4-y_4\right)\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{19}}$	=	$\left(x_4-y_4\right)\,\mathbf{a}_1-y_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4-2y_4\right)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{20}}$	=	$-x_4\,\mathbf{a}_1-\left(x_4-y_4\right)\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_4-y_4\right)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.