β-Bi_2O_3 ($D5_{12}$) Structure: A2B3_tP20_117_i_adgh-001

This structure originally had the label `A2B3_tP20_117_i_adgh`. Calls to that address will be redirected here.

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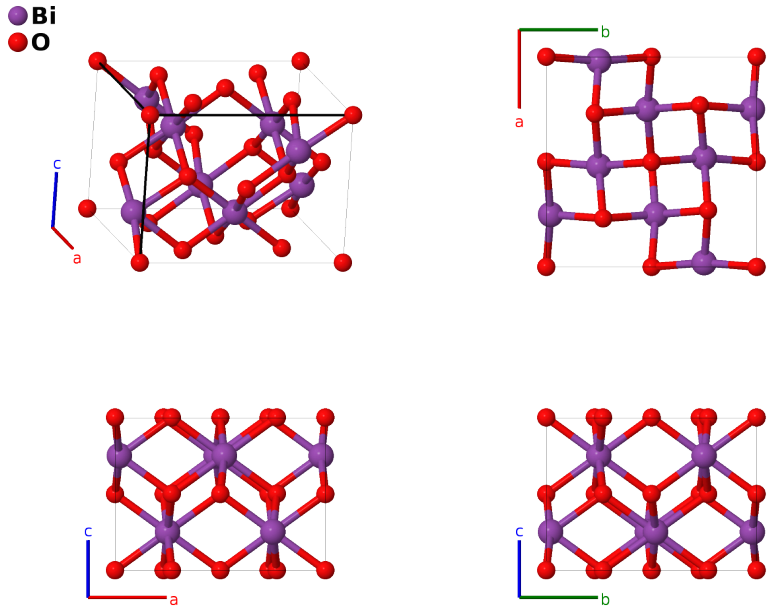
https://aflow.org/p/B48H

https://aflow.org/p/A2B3_tP20_117_i_adgh-001



Prototype	Bi_2O_3
AFLOW prototype label	A2B3_tP20_117_i_adgh-001
***Strukturbericht* designation**	$D5_{12}$
ICSD	27151
Pearson symbol	tP20
Space group number	117
Space group symbol	$P\bar{4}b2$
AFLOW prototype command	`aflow --proto=A2B3_tP20_117_i_adgh-001 --params=`$a, c/a, x_3, x_4, x_5, y_5, z_5$

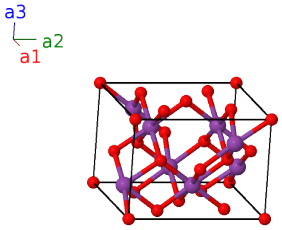
- Bi_2O_3 can be found in at least six forms (Harwig, 1978; Locherer, 2011):
  - monoclinic α-Bi_2O_3, the ground state, stable up to 729°,
  - tetragonal β-Bi_2O_3, $D5_{12}$, a metastable state observed at 650°C (this structure),
  - body-centered cubic γ-Bi_2O_3, another metastable phase observed 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 "nonquenchable" high-pressure structure, HPC-Bi_2O_3.

- (Sillén, 1937) presented this structure in the doubled-unit cell $C\bar{4}2b$ setting of space group #117, and the ICSD entry is from that paper. We follow (Harwig, 1978) and use the standard $P\bar{4}b2$ setting. We have shifted the origin so that the O-I atom is at the (2a) site.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	O I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(2a)	O I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2d)	O II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2d)	O II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	O III
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	O III
$\mathbf{B_7}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(4g)	O III
$\mathbf{B_8}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(4g)	O III
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O IV
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O IV
$\mathbf{B_{11}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O IV
$\mathbf{B_{12}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O IV
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8i)	Bi I
$\mathbf{B_{14}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8i)	Bi I
$\mathbf{B_{15}}$	=	$y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8i)	Bi I
$\mathbf{B_{16}}$	=	$-y_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8i)	Bi I
$\mathbf{B_{17}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8i)	Bi I
$\mathbf{B_{18}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8i)	Bi I
$\mathbf{B_{19}}$	=	$\left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$a\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8i)	Bi I
$\mathbf{B_{20}}$	=	$-\left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-a\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8i)	Bi I

References

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Found in

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