

β -Bi₂O₃ ($D_{5_{12}}$) Structure: A2B3_tP20_117_i_adgh-001

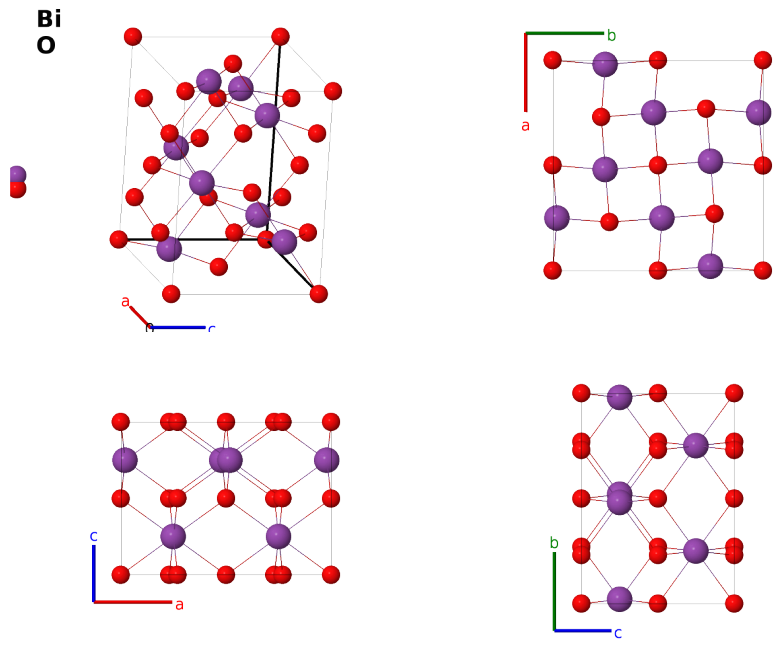
This structure previously used the label(s) **A2B3_tP20_117_i_adgh**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/B48H>

https://aflow.org/prototype-encyclopedia/A2B3_tP20_117_i_adgh-001



Prototype	Bi ₂ O ₃
AFLOW prototype label	A2B3_tP20_117_i_adgh-001
<i>Strukturbericht</i> designation	$D_{5_{12}}$
ICSD	27151
CCDC	1602473
Pearson symbol	tP20
Space group number	117
Space group symbol	$P\bar{4}b2$
AFLOW prototype command	<code>aflow --proto=A2B3_tP20_117_i_adgh-001 --params=a, c/a, x₃, x₄, x₅, y₅, z₅</code>

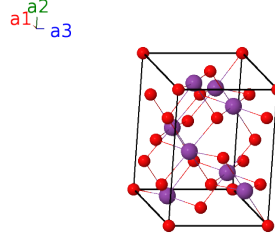
- Bi₂O₃ can be found in at least six forms (Harwig, 1978; Locherer, 2011):

- monoclinic α -Bi₂O₃, the ground state, stable up to 729°,
- tetragonal β -Bi₂O₃, $D5_{12}$, a metastable state observed at 650°C (this structure),
- body-centered cubic γ -Bi₂O₃, another metastable phase observed at 639°C,
- face-centered cubic δ -Bi₂O₃, the stable phase from 729° up to the melting point at 824°C,
- a high-pressure HP-Bi₂O₃, and
- a second “nonquenchable” high-pressure structure, HPC-Bi₂O₃.

- (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

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	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
$\mathbf{B}_5$	$=$	$x_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g) O III
$\mathbf{B}_6$	$=$	$-x_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g) O III
$\mathbf{B}_7$	$=$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}}$	(4g) O III
$\mathbf{B}_8$	$=$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}}$	(4g) O III
$\mathbf{B}_9$	$=$	$x_4 \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) O IV
$\mathbf{B}_{10}$	$=$	$-x_4 \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) O IV
$\mathbf{B}_{11}$	$=$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) O IV
$\mathbf{B}_{12}$	$=$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(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
$\mathbf{B}_{17}$	$=$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8i) Bi I
$\mathbf{B}_{18}$	$=$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8i) Bi I
$\mathbf{B}_{19}$	$=$	$(y_5 + \frac{1}{2}) \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a(y_5 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8i) Bi I

$$\mathbf{B}_{20} = -\left(y_5 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_2 - z_5 \mathbf{a}_3 = -a\left(y_5 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} \quad (8i) \quad \text{Bi I}$$

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First cited in

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