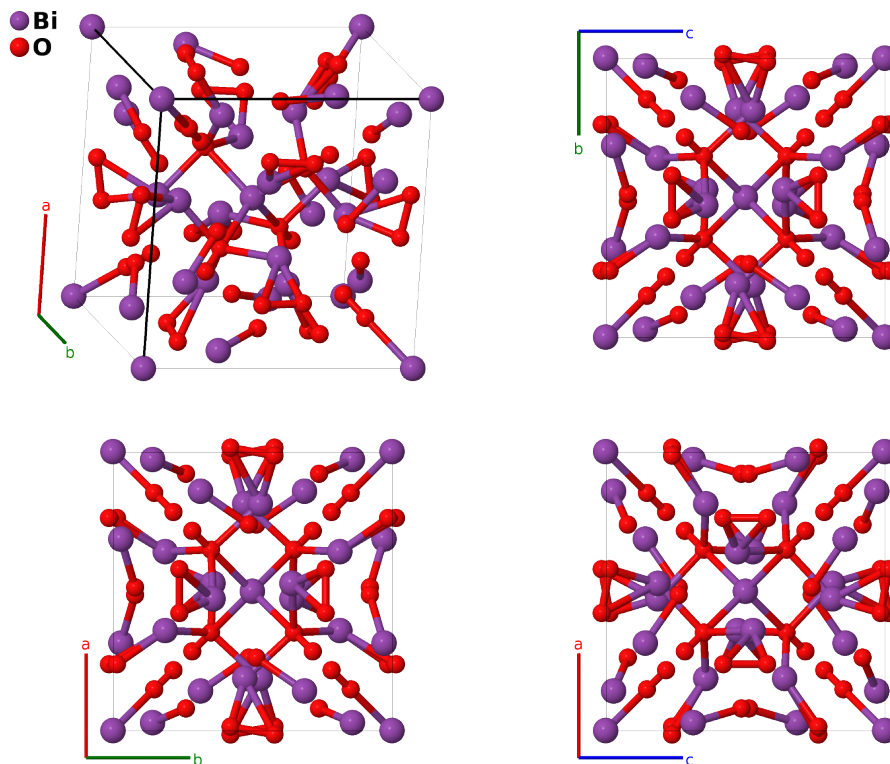


γ -Bi₂O₃ Structure: A13B20_cI66_197_af_2cf-001

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<https://aflow.org/p/8111>

https://aflow.org/p/A13B20_cI66_197_af_2cf-001



| | |
|-------------------------|--|
| Prototype | Bi ₂ O ₃ |
| AFLOW prototype label | A13B20_cI66_197_af_2cf-001 |
| ICSD | 2376 |
| Pearson symbol | cI66 |
| Space group number | 197 |
| Space group symbol | <i>I</i> 23 |
| AFLOW prototype command | <code>aflow --proto=A13B20_cI66_197_af_2cf-001 --params=a, x₂, x₃, x₄, y₄, z₄, x₅, y₅, z₅</code> |

Other compounds with this structure

Bi₁₂GeO₂₀, Bi₃₈ZnO₆₀

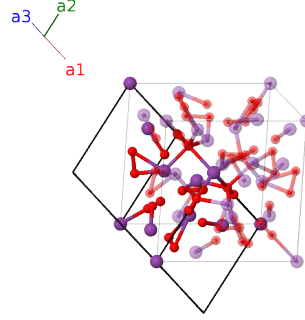
- Bi₂O₃ can be found in at least six forms (Harwig, 1978; Locherer, 2011):
 - monoclinic α -Bi₂O₃, the ground state, stable up to 729°,

- tetragonal β -Bi₂O₃, D_{5h} , a metastable state observed at 650°C,
- body-centered cubic γ -Bi₂O₃, another metastable phase observed at 639°C (this structure),
- 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 “non-quenchable” high-pressure structure, HPC-Bi₂O₃.

- The Bi-I (2a) site is 97.5% occupied, making the actual composition of this structure Bi_{1.95}O₃. The Bi-I site may be occupied by germanium or zinc atoms, *e.g.* Bi₁₂GeO₂₀.

Body-centered Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{y} + \frac{1}{2}a\hat{z} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{x} - \frac{1}{2}a\hat{y} + \frac{1}{2}a\hat{z} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{y} - \frac{1}{2}a\hat{z}\end{aligned}$$



Basis vectors

| | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|-------------------|---|-----|---|------------------|-----------|
| \mathbf{B}_1 | 0 | $=$ | 0 | (2a) | Bi I |
| \mathbf{B}_2 | $2x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + 2x_2 \mathbf{a}_3$ | $=$ | $ax_2 \hat{x} + ax_2 \hat{y} + ax_2 \hat{z}$ | (8c) | O I |
| \mathbf{B}_3 | $-2x_2 \mathbf{a}_3$ | $=$ | $-ax_2 \hat{x} - ax_2 \hat{y} + ax_2 \hat{z}$ | (8c) | O I |
| \mathbf{B}_4 | $-2x_2 \mathbf{a}_2$ | $=$ | $-ax_2 \hat{x} + ax_2 \hat{y} - ax_2 \hat{z}$ | (8c) | O I |
| \mathbf{B}_5 | $-2x_2 \mathbf{a}_1$ | $=$ | $ax_2 \hat{x} - ax_2 \hat{y} - ax_2 \hat{z}$ | (8c) | O I |
| \mathbf{B}_6 | $2x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2 + 2x_3 \mathbf{a}_3$ | $=$ | $ax_3 \hat{x} + ax_3 \hat{y} + ax_3 \hat{z}$ | (8c) | O II |
| \mathbf{B}_7 | $-2x_3 \mathbf{a}_3$ | $=$ | $-ax_3 \hat{x} - ax_3 \hat{y} + ax_3 \hat{z}$ | (8c) | O II |
| \mathbf{B}_8 | $-2x_3 \mathbf{a}_2$ | $=$ | $-ax_3 \hat{x} + ax_3 \hat{y} - ax_3 \hat{z}$ | (8c) | O II |
| \mathbf{B}_9 | $-2x_3 \mathbf{a}_1$ | $=$ | $ax_3 \hat{x} - ax_3 \hat{y} - ax_3 \hat{z}$ | (8c) | O II |
| \mathbf{B}_{10} | $(y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3$ | $=$ | $ax_4 \hat{x} + ay_4 \hat{y} + az_4 \hat{z}$ | (24f) | Bi II |
| \mathbf{B}_{11} | $-(y_4 - z_4) \mathbf{a}_1 - (x_4 - z_4) \mathbf{a}_2 - (x_4 + y_4) \mathbf{a}_3$ | $=$ | $-ax_4 \hat{x} - ay_4 \hat{y} + az_4 \hat{z}$ | (24f) | Bi II |
| \mathbf{B}_{12} | $(y_4 - z_4) \mathbf{a}_1 - (x_4 + z_4) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3$ | $=$ | $-ax_4 \hat{x} + ay_4 \hat{y} - az_4 \hat{z}$ | (24f) | Bi II |
| \mathbf{B}_{13} | $-(y_4 + z_4) \mathbf{a}_1 + (x_4 - z_4) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3$ | $=$ | $ax_4 \hat{x} - ay_4 \hat{y} - az_4 \hat{z}$ | (24f) | Bi II |
| \mathbf{B}_{14} | $(x_4 + y_4) \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 + (x_4 + z_4) \mathbf{a}_3$ | $=$ | $az_4 \hat{x} + ax_4 \hat{y} + ay_4 \hat{z}$ | (24f) | Bi II |
| \mathbf{B}_{15} | $-(x_4 + y_4) \mathbf{a}_1 - (y_4 - z_4) \mathbf{a}_2 - (x_4 - z_4) \mathbf{a}_3$ | $=$ | $az_4 \hat{x} - ax_4 \hat{y} - ay_4 \hat{z}$ | (24f) | Bi II |
| \mathbf{B}_{16} | $-(x_4 - y_4) \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 - (x_4 + z_4) \mathbf{a}_3$ | $=$ | $-az_4 \hat{x} - ax_4 \hat{y} + ay_4 \hat{z}$ | (24f) | Bi II |

$$\begin{aligned}
\mathbf{B}_{17} &= \begin{pmatrix} (x_4 - y_4) \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 + \\ (x_4 - z_4) \mathbf{a}_3 \end{pmatrix} = -az_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}} & (24f) & \text{Bi II} \\
\mathbf{B}_{18} &= \begin{pmatrix} (x_4 + z_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + \\ (y_4 + z_4) \mathbf{a}_3 \end{pmatrix} = ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} & (24f) & \text{Bi II} \\
\mathbf{B}_{19} &= \begin{pmatrix} -(x_4 - z_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 - \\ (y_4 - z_4) \mathbf{a}_3 \end{pmatrix} = -ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} & (24f) & \text{Bi II} \\
\mathbf{B}_{20} &= \begin{pmatrix} -(x_4 + z_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + \\ (y_4 - z_4) \mathbf{a}_3 \end{pmatrix} = ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} & (24f) & \text{Bi II} \\
\mathbf{B}_{21} &= \begin{pmatrix} (x_4 - z_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 - \\ (y_4 + z_4) \mathbf{a}_3 \end{pmatrix} = -ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} & (24f) & \text{Bi II} \\
\mathbf{B}_{22} &= \begin{pmatrix} (y_5 + z_5) \mathbf{a}_1 + (x_5 + z_5) \mathbf{a}_2 + \\ (x_5 + y_5) \mathbf{a}_3 \end{pmatrix} = ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + az_5 \hat{\mathbf{z}} & (24f) & \text{O III} \\
\mathbf{B}_{23} &= \begin{pmatrix} -(y_5 - z_5) \mathbf{a}_1 - (x_5 - z_5) \mathbf{a}_2 - \\ (x_5 + y_5) \mathbf{a}_3 \end{pmatrix} = -ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + az_5 \hat{\mathbf{z}} & (24f) & \text{O III} \\
\mathbf{B}_{24} &= \begin{pmatrix} (y_5 - z_5) \mathbf{a}_1 - (x_5 + z_5) \mathbf{a}_2 - \\ (x_5 - y_5) \mathbf{a}_3 \end{pmatrix} = -ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}} & (24f) & \text{O III} \\
\mathbf{B}_{25} &= \begin{pmatrix} -(y_5 + z_5) \mathbf{a}_1 + (x_5 - z_5) \mathbf{a}_2 + \\ (x_5 - y_5) \mathbf{a}_3 \end{pmatrix} = ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}} & (24f) & \text{O III} \\
\mathbf{B}_{26} &= \begin{pmatrix} (x_5 + y_5) \mathbf{a}_1 + (y_5 + z_5) \mathbf{a}_2 + \\ (x_5 + z_5) \mathbf{a}_3 \end{pmatrix} = az_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}} & (24f) & \text{O III} \\
\mathbf{B}_{27} &= \begin{pmatrix} -(x_5 + y_5) \mathbf{a}_1 - (y_5 - z_5) \mathbf{a}_2 - \\ (x_5 - z_5) \mathbf{a}_3 \end{pmatrix} = az_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}} & (24f) & \text{O III} \\
\mathbf{B}_{28} &= \begin{pmatrix} -(x_5 - y_5) \mathbf{a}_1 + (y_5 - z_5) \mathbf{a}_2 - \\ (x_5 + z_5) \mathbf{a}_3 \end{pmatrix} = -az_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}} & (24f) & \text{O III} \\
\mathbf{B}_{29} &= \begin{pmatrix} (x_5 - y_5) \mathbf{a}_1 - (y_5 + z_5) \mathbf{a}_2 + \\ (x_5 - z_5) \mathbf{a}_3 \end{pmatrix} = -az_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}} & (24f) & \text{O III} \\
\mathbf{B}_{30} &= \begin{pmatrix} (x_5 + z_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + \\ (y_5 + z_5) \mathbf{a}_3 \end{pmatrix} = ay_5 \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}} & (24f) & \text{O III} \\
\mathbf{B}_{31} &= \begin{pmatrix} -(x_5 - z_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 - \\ (y_5 - z_5) \mathbf{a}_3 \end{pmatrix} = -ay_5 \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}} & (24f) & \text{O III} \\
\mathbf{B}_{32} &= \begin{pmatrix} -(x_5 + z_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + \\ (y_5 - z_5) \mathbf{a}_3 \end{pmatrix} = ay_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}} & (24f) & \text{O III} \\
\mathbf{B}_{33} &= \begin{pmatrix} (x_5 - z_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 - \\ (y_5 + z_5) \mathbf{a}_3 \end{pmatrix} = -ay_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}} & (24f) & \text{O III}
\end{aligned}$$

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