γ-Bi_2O_3 Structure: A13B20_cI66_197_af_2cf-001

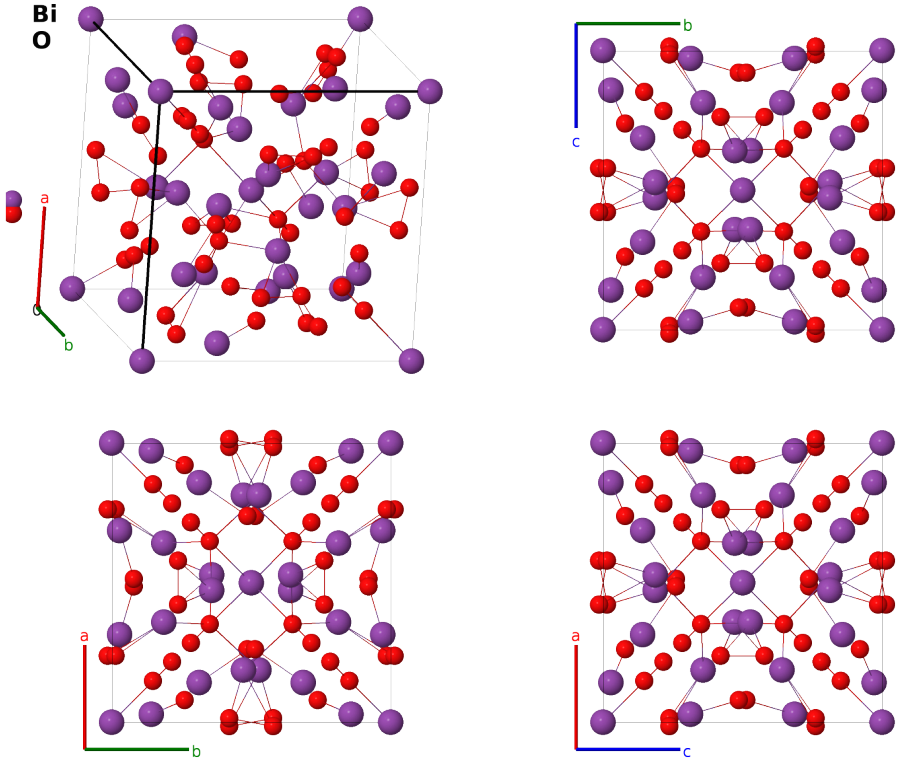
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

https://aflow.org/prototype-encyclopedia/8111

https://aflow.org/prototype-encyclopedia/A13B20_cI66_197_af_2cf-001



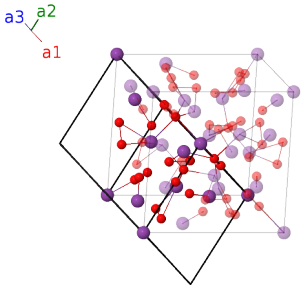
Prototype	Bi_2O_3
AFLOW prototype label	A13B20_cI66_197_af_2cf-001
ICSD	2376
CCDC	1592278
Pearson symbol	cI66
Space group number	197
Space group symbol	$I23$
AFLOW prototype command	`aflow --proto=A13B20_cI66_197_af_2cf-001 --params=`$a, x_2, x_3, x_4, y_4, z_4, x_5, y_5, z_5$

Other compounds with this structure
$Bi_{12}GeO_{20}$, $Bi_{38}ZnO_{60}$

- 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 (this structure),
  - 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.
- The Bi-I (2a) site is 97.5% occupied, making the actual composition of this structure $Bi_{1.95}O_3$. The Bi-I site may be occupied by germanium or zinc atoms, *e.g.* $Bi_{12}GeO_{20}$.

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Bi I
$\mathbf{B_2}$	=	$2x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2 + 2x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_3}$	=	$-2x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_4}$	=	$-2x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_5}$	=	$-2x_2\,\mathbf{a}_1$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_6}$	=	$2x_3\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2 + 2x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_7}$	=	$-2x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_8}$	=	$-2x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_9}$	=	$-2x_3\,\mathbf{a}_1$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_{10}}$	=	$(y_4 + z_4)\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + (x_4 + y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(24f)	Bi II
$\mathbf{B_{11}}$	=	$-(y_4 - z_4)\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - (x_4 + y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(24f)	Bi II
$\mathbf{B_{12}}$	=	$(y_4 - z_4)\,\mathbf{a}_1 - (x_4 + z_4)\,\mathbf{a}_2 - (x_4 - y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}}$	(24f)	Bi II
$\mathbf{B_{13}}$	=	$-(y_4 + z_4)\,\mathbf{a}_1 + (x_4 - z_4)\,\mathbf{a}_2 + (x_4 - y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}}$	(24f)	Bi II
$\mathbf{B_{14}}$	=	$(x_4 + y_4)\,\mathbf{a}_1 + (y_4 + z_4)\,\mathbf{a}_2 + (x_4 + z_4)\,\mathbf{a}_3$	=	$az_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ay_4\,\hat{\mathbf{z}}$	(24f)	Bi II
$\mathbf{B_{15}}$	=	$-(x_4 + y_4)\,\mathbf{a}_1 - (y_4 - z_4)\,\mathbf{a}_2 - (x_4 - z_4)\,\mathbf{a}_3$	=	$az_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ay_4\,\hat{\mathbf{z}}$	(24f)	Bi II

$$\mathbf{B_{16}} = -(x_4 - y_4)\,\mathbf{a}_1 + (y_4 - z_4)\,\mathbf{a}_2 - (x_4 + z_4)\,\mathbf{a}_3 = -az_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + ay_4\,\hat{\mathbf{z}} \quad (24f) \quad \text{Bi II}$$

$$\mathbf{B_{17}} = (x_4 - y_4)\,\mathbf{a}_1 - (y_4 + z_4)\,\mathbf{a}_2 + (x_4 - z_4)\,\mathbf{a}_3 = -az_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - ay_4\,\hat{\mathbf{z}} \quad (24f) \quad \text{Bi II}$$

$$\mathbf{B_{18}} = (x_4 + z_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + (y_4 + z_4)\,\mathbf{a}_3 = ay_4\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}} \quad (24f) \quad \text{Bi II}$$

$$\mathbf{B_{19}} = -(x_4 - z_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 - (y_4 - z_4)\,\mathbf{a}_3 = -ay_4\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}} \quad (24f) \quad \text{Bi II}$$

$$\mathbf{B_{20}} = -(x_4 + z_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 + (y_4 - z_4)\,\mathbf{a}_3 = ay_4\,\hat{\mathbf{x}} - az_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}} \quad (24f) \quad \text{Bi II}$$

$$\mathbf{B_{21}} = (x_4 - z_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 - (y_4 + z_4)\,\mathbf{a}_3 = -ay_4\,\hat{\mathbf{x}} - az_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}} \quad (24f) \quad \text{Bi II}$$

$$\mathbf{B_{22}} = (y_5 + z_5)\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + (x_5 + y_5)\,\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{O III}$$

$$\mathbf{B_{23}} = -(y_5 - z_5)\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - (x_5 + y_5)\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{O III}$$

$$\mathbf{B_{24}} = (y_5 - z_5)\,\mathbf{a}_1 - (x_5 + z_5)\,\mathbf{a}_2 - (x_5 - y_5)\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{O III}$$

$$\mathbf{B_{25}} = -(y_5 + z_5)\,\mathbf{a}_1 + (x_5 - z_5)\,\mathbf{a}_2 + (x_5 - y_5)\,\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{O III}$$

$$\mathbf{B_{26}} = (x_5 + y_5)\,\mathbf{a}_1 + (y_5 + z_5)\,\mathbf{a}_2 + (x_5 + z_5)\,\mathbf{a}_3 = az_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + ay_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{O III}$$

$$\mathbf{B_{27}} = -(x_5 + y_5)\,\mathbf{a}_1 - (y_5 - z_5)\,\mathbf{a}_2 - (x_5 - z_5)\,\mathbf{a}_3 = az_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - ay_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{O III}$$

$$\mathbf{B_{28}} = -(x_5 - y_5)\,\mathbf{a}_1 + (y_5 - z_5)\,\mathbf{a}_2 - (x_5 + z_5)\,\mathbf{a}_3 = -az_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + ay_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{O III}$$

$$\mathbf{B_{29}} = (x_5 - y_5)\,\mathbf{a}_1 - (y_5 + z_5)\,\mathbf{a}_2 + (x_5 - z_5)\,\mathbf{a}_3 = -az_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - ay_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{O III}$$

$$\mathbf{B_{30}} = (x_5 + z_5)\,\mathbf{a}_1 + (x_5 + y_5)\,\mathbf{a}_2 + (y_5 + z_5)\,\mathbf{a}_3 = ay_5\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{O III}$$

$$\mathbf{B_{31}} = -(x_5 - z_5)\,\mathbf{a}_1 - (x_5 + y_5)\,\mathbf{a}_2 - (y_5 - z_5)\,\mathbf{a}_3 = -ay_5\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{O III}$$

$$\mathbf{B_{32}} = -(x_5 + z_5)\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 + (y_5 - z_5)\,\mathbf{a}_3 = ay_5\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{O III}$$

$$\mathbf{B_{33}} = (x_5 - z_5)\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 - (y_5 + z_5)\,\mathbf{a}_3 = -ay_5\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{O III}$$

References

[1] 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.

[2] D. A. Keen and S. Hull, *The high-temperature structural behaviour of copper(I) iodide*, J. Phys.: Condens. Matter **7**, 5793–5804 (1995), doi:10.1088/0953-8984/7/29/007.

[3] 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.

Found in

[1] D. Risold, B. Hallstedt, L. J. Gauckler, H. L. Lukas, and S. G. Fries, *The Bismuth-Oxygen System*, J. Phase Eq **16**, 223 (1995), doi:10.1007/BF02667306.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.