

Trigonal B₂O₃ Structure:

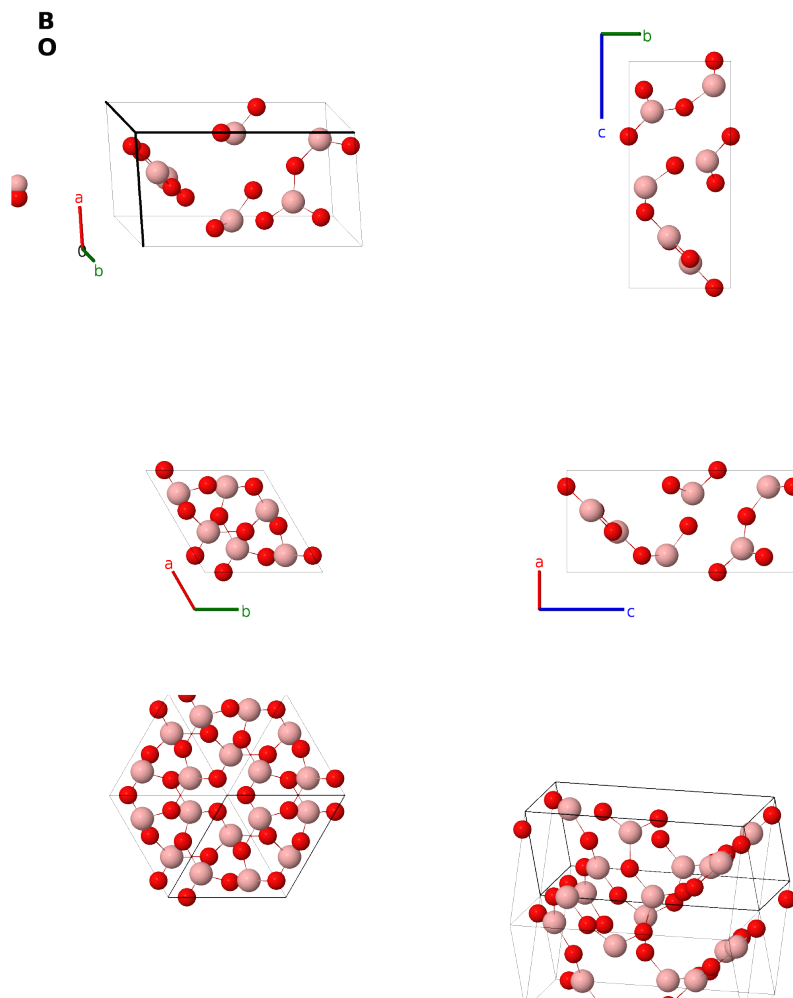
A2B3_hP15_152_c_ac-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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/MKFS>

https://aflow.org/prototype-encyclopedia/A2B3_hP15_152_c_ac-001



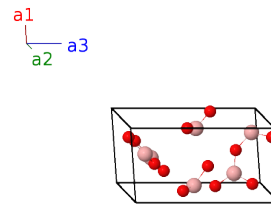
Prototype	B ₂ O ₃
AFLOW prototype label	A2B3_hP15_152_c_ac-001
ICSD	51575
CCDC	1616450
Pearson symbol	hP15
Space group number	152

Space group symbol $P3_121$

AFLOW prototype command `aflow --proto=A2B3_hP15_152_c_ac-001`
`--params=a, c/a, x1, x2, y2, z2, x3, y3, z3`

- This is the ground state structure of B₂O₃. At approximately 2 GPa it transforms to a high-pressure orthorhombic phase.
- Originally this phase was thought to be in space group $P3_1$ #144, but reanalysis by (Effenberger, 2001) showed that the higher symmetry group matches that data at least as well. For more history on the determination of the structure of B₂O₃, see (Prewitt, 1968).
- Space group $P3_221$ #154 is the enantiomorph of $P3_121$ #152, so the mirror image of this structure could exist in that space group as well.

Trigonal (Hexagonal) primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_3$	=	$\frac{1}{2}ax_1 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3a)	O I
$\mathbf{B}_2$	$x_1 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	=	$\frac{1}{2}ax_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{2}{3}c \hat{\mathbf{z}}$	(3a)	O I
$\mathbf{B}_3$	$-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2$	=	$-ax_1 \hat{\mathbf{x}}$	(3a)	O I
$\mathbf{B}_4$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$\frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(6c)	B I
$\mathbf{B}_5$	$-y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{3}) \mathbf{a}_3$	=	$\frac{1}{2}a(x_2 - 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	B I
$\mathbf{B}_6$	$-(x_2 - y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + (z_2 + \frac{2}{3}) \mathbf{a}_3$	=	$-\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + \frac{1}{3}c(3z_2 + 2) \hat{\mathbf{z}}$	(6c)	B I
$\mathbf{B}_7$	$y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$\frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(6c)	B I
$\mathbf{B}_8$	$(x_2 - y_2) \mathbf{a}_1 - y_2 \mathbf{a}_2 - (z_2 - \frac{2}{3}) \mathbf{a}_3$	=	$\frac{1}{2}a(x_2 - 2y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} - \frac{1}{3}c(3z_2 - 2) \hat{\mathbf{z}}$	(6c)	B I
$\mathbf{B}_9$	$-x_2 \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 - (z_2 - \frac{1}{3}) \mathbf{a}_3$	=	$-\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	B I
$\mathbf{B}_{10}$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B}_{11}$	$-y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{3}) \mathbf{a}_3$	=	$\frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B}_{12}$	$-(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{2}{3}) \mathbf{a}_3$	=	$-\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + \frac{1}{3}c(3z_3 + 2) \hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B}_{13}$	$y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B}_{14}$	$(x_3 - y_3) \mathbf{a}_1 - y_3 \mathbf{a}_2 - (z_3 - \frac{2}{3}) \mathbf{a}_3$	=	$\frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} - \frac{1}{3}c(3z_3 - 2) \hat{\mathbf{z}}$	(6c)	O II

$$\mathbf{B}_{15} = \begin{matrix} -x_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - \\ (z_3 - \frac{1}{3}) \mathbf{a}_3 \end{matrix} = -\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{3}) \hat{\mathbf{z}} \quad (6c) \quad \text{O II}$$

References

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- [2] C. T. Prewitt and R. D. Shannon, *Crystal Structure of a High-Pressure Form of B_2O_3* , *Acta Crystallogr. Sect. B* **24**, 869–874 (1968), doi:10.1107/S0567740868003304.

Found in

- [1] A. Jain, S. P. Ong, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, G. D. Ceder, and K. A. Persson, *Commentary: The Materials Project: A materials genome approach to accelerating materials innovation*, *APL Materials* **1**, 011002 (2013), doi:10.1063/1.4812323.

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