Trigonal B_2O_3 Structure: A2B3_hP15_152_c_ac-001

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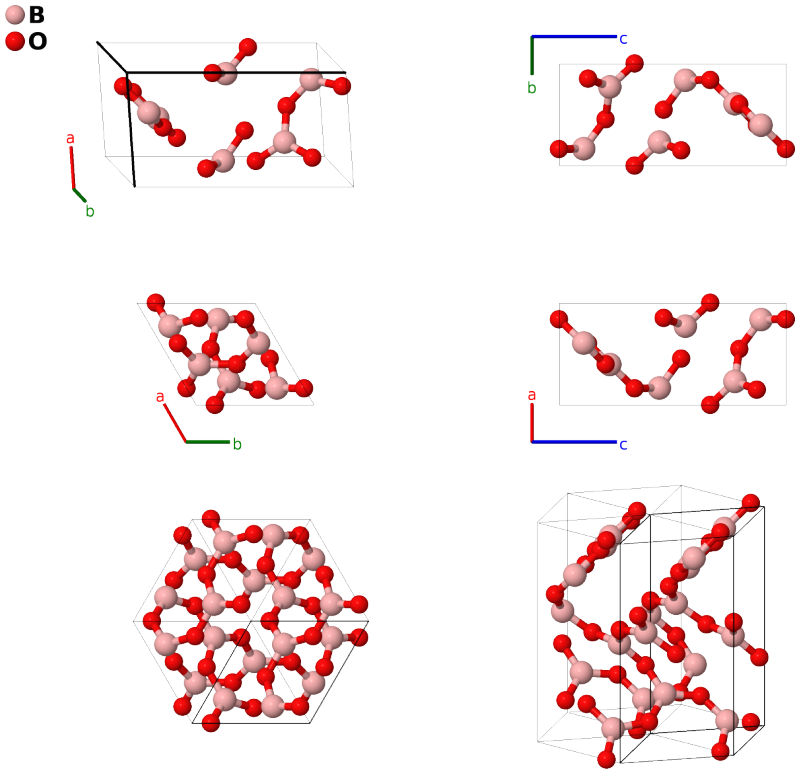
https://aflow.org/p/A2B3_hP15_152_c_ac-001

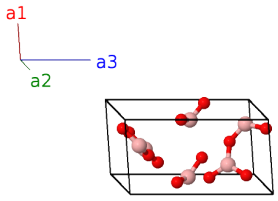


Prototype	B_2O_3
AFLOW prototype label	A2B3_hP15_152_c_ac-001
ICSD	51575
Pearson symbol	hP15
Space group number	152
Space group symbol	$P3_121$
AFLOW prototype command	`aflow --proto=A2B3_hP15_152_c_ac-001 --params=`$a, c/a, x_1, x_2, y_2, z_2, x_3, y_3, z_3$

- This is the ground state structure of B_2O_3. 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 B_2O_3, see (Prewitt, 1968).
- Space group $P3_221$ #154 is the enantiomorph of $P3_121$ #152, so this structure could exist in that space group as well.

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_5}$	=	$-y_2\,\mathbf{a}_1 + (x_2 - y_2)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - 2y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(6c)	B I
$\mathbf{B_6}$	=	$-(x_2 - y_2)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(z_2 + \frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_2 - y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_2 + 2)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_8}$	=	$(x_2 - y_2)\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - \left(z_2 - \frac{2}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - 2y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} - \frac{1}{3}c\,(3z_2 - 2)\,\hat{\mathbf{z}}$	(6c)	B I
$\mathbf{B_9}$	=	$-x_2\,\mathbf{a}_1 - (x_2 - y_2)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_2 - y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{11}}$	=	$-y_3\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - 2y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{12}}$	=	$-(x_3 - y_3)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(z_3 + \frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_3 + 2)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{14}}$	=	$(x_3 - y_3)\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - \left(z_3 - \frac{2}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - 2y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - \frac{1}{3}c\,(3z_3 - 2)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{15}}$	=	$-x_3\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(6c)	O II

References

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