Orthorhombic B_2O_3 Structure: A2B3_oC20_36_b_ab-001

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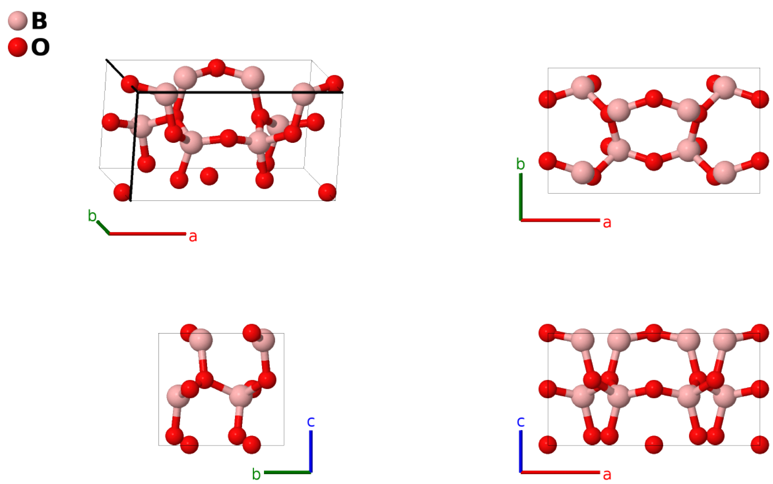
https://aflow.org/p/KLS9

https://aflow.org/p/A2B3_oC20_36_b_ab-001

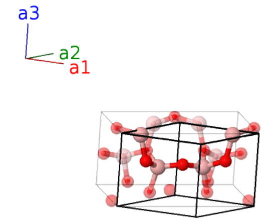


Prototype	B_2O_3
AFLOW prototype label	A2B3_oC20_36_b_ab-001
ICSD	34685
Pearson symbol	oC20
Space group number	36
Space group symbol	$Cmc2_1$
AFLOW prototype command	`aflow --proto=A2B3_oC20_36_b_ab-001` `--params=`$a, b/a, c/a, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3$

- This is the high-pressure structure of B_2O_3, stable above ≈ 2 GPa. The ground state is trigonal.
- Data was taken a 6.5 GPa. (Prewitt, 1968) give the structure in the $Ccm2_1$ setting of space group #36. We used FINDSYM to transform it to the standard $Cmc2_1$ setting. This space group allows for an arbitrary placement of the origin of the z-axis, which we fixed by setting $z_1 = 0$ for the O-I (2a) Wyckoff position.
- The ICSD 34685 website entry for this structure states that it was refined at ambient pressure, but the data is consistent with the high-pressure structure shown here.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_3}$	=	$(x_2 - y_2)\,\mathbf{a}_1 + (x_2 + y_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8b)	B I
$\mathbf{B_4}$	=	$-(x_2 - y_2)\,\mathbf{a}_1 - (x_2 + y_2)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	B I
$\mathbf{B_5}$	=	$(x_2 + y_2)\,\mathbf{a}_1 + (x_2 - y_2)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	B I
$\mathbf{B_6}$	=	$-(x_2 + y_2)\,\mathbf{a}_1 - (x_2 - y_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8b)	B I
$\mathbf{B_7}$	=	$(x_3 - y_3)\,\mathbf{a}_1 + (x_3 + y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_8}$	=	$-(x_3 - y_3)\,\mathbf{a}_1 - (x_3 + y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_9}$	=	$(x_3 + y_3)\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_{10}}$	=	$-(x_3 + y_3)\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8b)	O II

References

[1] 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] H. Effenberger, C. L. Lengauer, and E. Parthé, *Trigonal B_2O_3 with Higher Space-Group Symmetry: Results of a Reevaluation*, Monatsh. Chem. **132**, 1515–1517 (2001), doi:10.1007/s007060170008.