Low Temperature GdBO₃ Structure: ABC3_hR30_155_de_f_de2f-001

https://aflow.org/p/5YKD

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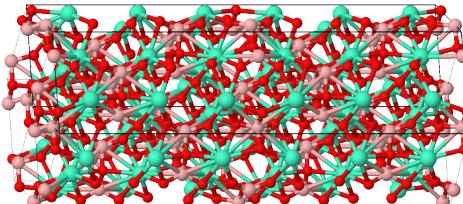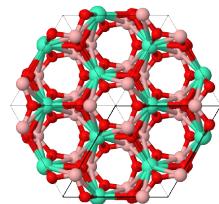
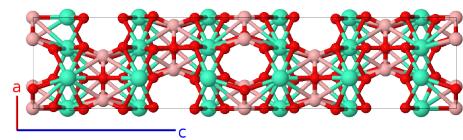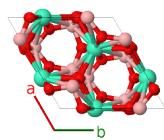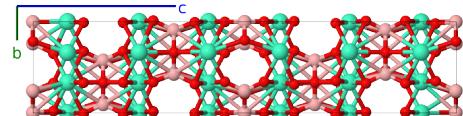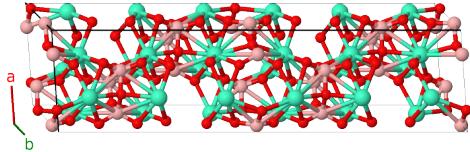| Prototype	BGdO₃
AFLOW prototype label	ABC3_hR30_155_de_f_de2f-001
ICSD	87778
Pearson symbol	hR30
Space group number	155
Space group symbol	$R32$
AFLOW prototype command	aflow --proto=ABC3_hR30_155_de_f_de2f-001 --params=$a, c/a, y_1, y_2, y_3, y_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

- (Ren, 1999) found two structures for GdBO₃: this low-temperature rhombohedral structure, and a high-temperature hexagonal structure.

- There is large thermal hysteresis in this system, with the LT $\to$ HT transition taking place at 1109K and the HT $\to$ LT transition at 819K.

- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$

$$\mathbf{a_2} = \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$

$$\mathbf{a_3} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$
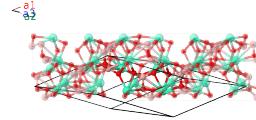
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$y_1\,\mathbf{a_2} - y_1\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}ay_1\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_1\,\hat{\mathbf{y}}$	(3d)	B I
$\mathbf{B_2}$	$=$	$-y_1\,\mathbf{a_1} + y_1\,\mathbf{a_3}$	$=$	$-ay_1\,\hat{\mathbf{x}}$	(3d)	B I
$\mathbf{B_3}$	$=$	$y_1\,\mathbf{a_1} - y_1\,\mathbf{a_2}$	$=$	$\tfrac{1}{2}ay_1\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_1\,\hat{\mathbf{y}}$	(3d)	B I
$\mathbf{B_4}$	$=$	$y_2\,\mathbf{a_2} - y_2\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}ay_2\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}}$	(3d)	O I
$\mathbf{B_5}$	$=$	$-y_2\,\mathbf{a_1} + y_2\,\mathbf{a_3}$	$=$	$-ay_2\,\hat{\mathbf{x}}$	(3d)	O I
$\mathbf{B_6}$	$=$	$y_2\,\mathbf{a_1} - y_2\,\mathbf{a_2}$	$=$	$\tfrac{1}{2}ay_2\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}}$	(3d)	O I
$\mathbf{B_7}$	$=$	$\tfrac{1}{2}\,\mathbf{a_1} + y_3\,\mathbf{a_2} - y_3\,\mathbf{a_3}$	$=$	$\tfrac{1}{4}a\,(2y_3 + 1)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{12}a\,(6y_3 - 1)\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,\hat{\mathbf{z}}$	(3e)	B II
$\mathbf{B_8}$	$=$	$-y_3\,\mathbf{a_1} + \tfrac{1}{2}\,\mathbf{a_2} + y_3\,\mathbf{a_3}$	$=$	$-ay_3\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,\hat{\mathbf{z}}$	(3e)	B II
$\mathbf{B_9}$	$=$	$y_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} + \tfrac{1}{2}\,\mathbf{a_3}$	$=$	$\tfrac{1}{4}a\,(2y_3 - 1)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{12}a\,(6y_3 + 1)\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,\hat{\mathbf{z}}$	(3e)	B II
$\mathbf{B_{10}}$	$=$	$\tfrac{1}{2}\,\mathbf{a_1} + y_4\,\mathbf{a_2} - y_4\,\mathbf{a_3}$	$=$	$\tfrac{1}{4}a\,(2y_4 + 1)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{12}a\,(6y_4 - 1)\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,\hat{\mathbf{z}}$	(3e)	O II
$\mathbf{B_{11}}$	$=$	$-y_4\,\mathbf{a_1} + \tfrac{1}{2}\,\mathbf{a_2} + y_4\,\mathbf{a_3}$	$=$	$-ay_4\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,\hat{\mathbf{z}}$	(3e)	O II
$\mathbf{B_{12}}$	$=$	$y_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} + \tfrac{1}{2}\,\mathbf{a_3}$	$=$	$\tfrac{1}{4}a\,(2y_4 - 1)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{12}a\,(6y_4 + 1)\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,\hat{\mathbf{z}}$	(3e)	O II
$\mathbf{B_{13}}$	$=$	$x_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,(x_5 - z_5)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_5 - 2y_5 + z_5)\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(6f)	Gd I
$\mathbf{B_{14}}$	$=$	$z_5\,\mathbf{a_1} + x_5\,\mathbf{a_2} + y_5\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\,(y_5 - z_5)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_5 - y_5 - z_5)\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(6f)	Gd I
$\mathbf{B_{15}}$	$=$	$y_5\,\mathbf{a_1} + z_5\,\mathbf{a_2} + x_5\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\,(x_5 - y_5)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_5 + y_5 - 2z_5)\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(6f)	Gd I
$\mathbf{B_{16}}$	$=$	$-z_5\,\mathbf{a_1} - y_5\,\mathbf{a_2} - x_5\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,(x_5 - z_5)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_5 - 2y_5 + z_5)\,\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(6f)	Gd I
$\mathbf{B_{17}}$	$=$	$-y_5\,\mathbf{a_1} - x_5\,\mathbf{a_2} - z_5\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\,(y_5 - z_5)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(2x_5 - y_5 - z_5)\,\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(6f)	Gd I
$\mathbf{B_{18}}$	$=$	$-x_5\,\mathbf{a_1} - z_5\,\mathbf{a_2} - y_5\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\,(x_5 - y_5)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_5 + y_5 - 2z_5)\,\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(6f)	Gd I
$\mathbf{B_{19}}$	$=$	$x_6\,\mathbf{a_1} + y_6\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B_{20}}$	$=$	$z_6\,\mathbf{a_1} + x_6\,\mathbf{a_2} + y_6\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\,(y_6 - z_6)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B_{21}}$	$=$	$y_6\,\mathbf{a_1} + z_6\,\mathbf{a_2} + x_6\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\,(x_6 - y_6)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B_{22}}$	$=$	$-z_6\,\mathbf{a_1} - y_6\,\mathbf{a_2} - x_6\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\,\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(6f)	O III

$$\mathbf{B_{23}} = -y_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_6 - z_6)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\,\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{O III}$$

$$\mathbf{B_{24}} = -x_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_2 - y_6\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_6 - y_6)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\,\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{O III}$$

$$\mathbf{B_{25}} = x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_7 - 2y_7 + z_7)\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{O IV}$$

$$\mathbf{B_{26}} = z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + y_7\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_7 - z_7)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(2x_7 - y_7 - z_7)\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{O IV}$$

$$\mathbf{B_{27}} = y_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_7 - y_7)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_7 + y_7 - 2z_7)\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{O IV}$$

$$\mathbf{B_{28}} = -z_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_7 - 2y_7 + z_7)\,\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{O IV}$$

$$\mathbf{B_{29}} = -y_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_7 - z_7)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(2x_7 - y_7 - z_7)\,\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{O IV}$$

$$\mathbf{B_{30}} = -x_7\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 - y_7\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_7 - y_7)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_7 + y_7 - 2z_7)\,\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_7 + y_7 + z_7)\,\hat{\mathbf{z}} \qquad \text{(6f)} \qquad \text{O IV}$$

References

[1] M. Ren, J. H. Lin, Y. Dong, L. Q. Yang, M. Z. Su, and L. P. You, *Structure and Phase Transition of GdBO$_3$*, Chem. Mater. **11**, 1576–1580 (1999), doi:10.1021/cm990022o.