

Low Temperature GdBO₃ Structure: ABC3_hR30_155_de_f_de2f-001

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<https://aflow.org/prototype-encyclopedia/5YKD>

https://aflow.org/prototype-encyclopedia/ABC3_hR30_155_de_f_de2f-001

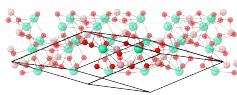
Prototype	BGdO ₃
AFLOW prototype label	ABC3_hR30_155_de_f_de2f-001
ICSD	87778
CCDC	1647553
Pearson symbol	hR30
Space group number	155
Space group symbol	<i>R</i> 32
AFLOW prototype command	<code>aflow --proto=ABC3_hR30_155_de_f_de2f-001 --params=a, c/a, y₁, y₂, y₃, y₄, x₅, y₅, z₅, x₆, y₆, z₆, x₇, y₇, z₇</code>

- (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 → HT transition taking place at 1109K and the HT → LT transition at 819K.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

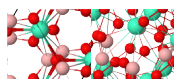
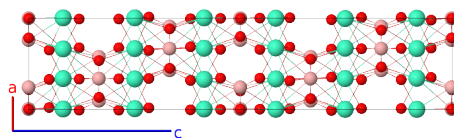
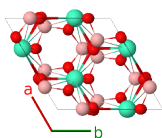
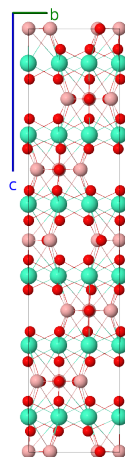
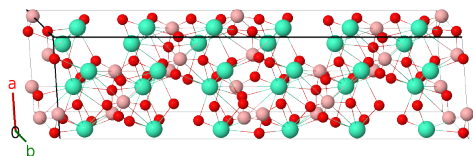
$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \end{aligned}$$

-81



Basis vectors

B
Gd
O



	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= y_1 \mathbf{a}_2 - y_1 \mathbf{a}_3$	$=$	$\frac{1}{2}ay_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_1 \hat{\mathbf{y}}$	(3d)	B I
$\mathbf{B}_2$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_3$	$=$	$-ay_1 \hat{\mathbf{x}}$	(3d)	B I
$\mathbf{B}_3$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2$	$=$	$\frac{1}{2}ay_1 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_1 \hat{\mathbf{y}}$	(3d)	B I
$\mathbf{B}_4$	$= y_2 \mathbf{a}_2 - y_2 \mathbf{a}_3$	$=$	$\frac{1}{2}ay_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}}$	(3d)	O I
$\mathbf{B}_5$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_3$	$=$	$-ay_2 \hat{\mathbf{x}}$	(3d)	O I
$\mathbf{B}_6$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	$=$	$\frac{1}{2}ay_2 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}}$	(3d)	O I
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_1 + y_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$\frac{1}{4}a(2y_3 + 1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a(6y_3 - 1) \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3e)	B II
$\mathbf{B}_8$	$= -y_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3e)	B II
$\mathbf{B}_9$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a(2y_3 - 1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a(6y_3 + 1) \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3e)	B II
$\mathbf{B}_{10}$	$= \frac{1}{2} \mathbf{a}_1 + y_4 \mathbf{a}_2 - y_4 \mathbf{a}_3$	$=$	$\frac{1}{4}a(2y_4 + 1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a(6y_4 - 1) \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3e)	O II
$\mathbf{B}_{11}$	$= -y_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3e)	O II
$\mathbf{B}_{12}$	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a(2y_4 - 1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a(6y_4 + 1) \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3e)	O II
$\mathbf{B}_{13}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 - 2y_5 + z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f)	Gd I
$\mathbf{B}_{14}$	$= z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_5 - y_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f)	Gd I
$\mathbf{B}_{15}$	$= y_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 + y_5 - 2z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f)	Gd I
$\mathbf{B}_{16}$	$= -z_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - 2y_5 + z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f)	Gd I
$\mathbf{B}_{17}$	$= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_5 - y_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f)	Gd I
$\mathbf{B}_{18}$	$= -x_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 + y_5 - 2z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f)	Gd I
$\mathbf{B}_{19}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B}_{20}$	$= z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B}_{21}$	$= y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B}_{22}$	$= -z_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - x_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} - \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B}_{23}$	$= -y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} - \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B}_{24}$	$= -x_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} - \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B}_{25}$	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 - 2y_7 + z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(6f)	O IV
$\mathbf{B}_{26}$	$= z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + y_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_7 - y_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(6f)	O IV
$\mathbf{B}_{27}$	$= y_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 + y_7 - 2z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(6f)	O IV
$\mathbf{B}_{28}$	$= -z_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 - 2y_7 + z_7) \hat{\mathbf{y}} - \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(6f)	O IV

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

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

References

- [1] M. Ren, J. H. Lin, Y. Dong, L. Q. Yang, M. Z. Su, and L. P. You, *Structure and Phase Transition of GdBO₃*, Chem. Mater. **11**, 1576–1580 (1999), doi:10.1021/cm990022o.

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