

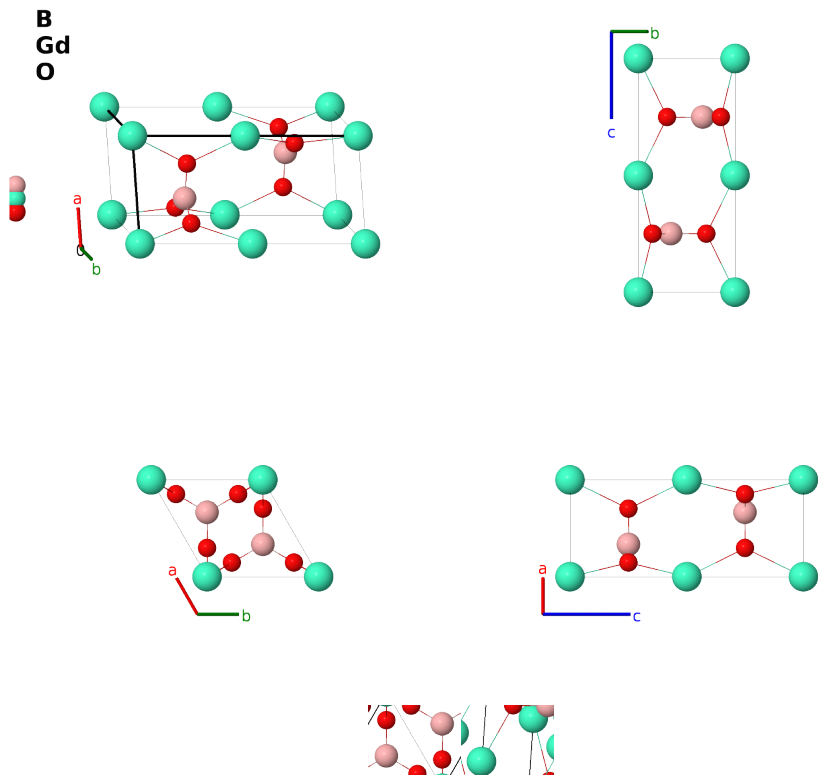
High Temperature GdBO_3 Structure: ABC3_hP10_194_c_a_h-002

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, 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/R6VB>

https://aflow.org/prototype-encyclopedia/ABC3_hP10_194_c_a_h-002



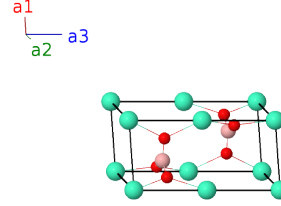
Prototype	BGdO ₃
AFLOW prototype label	ABC3_hP10_194_c_a_h-002
ICSD	87779
CCDC	1647554
Pearson symbol	hP10
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=ABC3_hP10_194_c_a_h-002 --params=a, c/a, x₃</code>

- (Ren, 1999) found two structures for GdBO_3 : a low-temperature rhombohedral structure, and this high-temperature hexagonal structure.

- There is large thermal hysteresis in this system, with the LT $\rightarrow$ HT transition taking place at 1109K and the HT $\rightarrow$ LT transition at 819K.
- (Ren, 1999) list YBO_3 as the prototype for this phase, but although related it differs from both our ordered and disordered YBO_3 structures.
- This structure has the same AFLOW label, ABC3_hP10_194_c_a_h, as the BaNiO_3 structure, but the c/a ration of GdBO_3 is more than twice that of BaNiO_3 , so we treat them as different structures. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

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
$\mathbf{B}_1$	=	0	=	0	(2a) Gd I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}c \hat{\mathbf{z}}$	(2a) Gd I
$\mathbf{B}_3$	=	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c) B I
$\mathbf{B}_4$	=	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c) B I
$\mathbf{B}_5$	=	$x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{3}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h) O I
$\mathbf{B}_6$	=	$-2x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$-\frac{3}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h) O I
$\mathbf{B}_7$	=	$x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$-\sqrt{3}ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h) O I
$\mathbf{B}_8$	=	$-x_3 \mathbf{a}_1 - 2x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$-\frac{3}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h) O I
$\mathbf{B}_9$	=	$2x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{3}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h) O I
$\mathbf{B}_{10}$	=	$-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\sqrt{3}ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h) O I

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.

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