γ-Ga_2O_3 Structure: A11B4_cF120_227_acdf_e-001

This structure originally had the label `A11B4_cF120_227_acdf_e`. Calls to that address will be redirected here.

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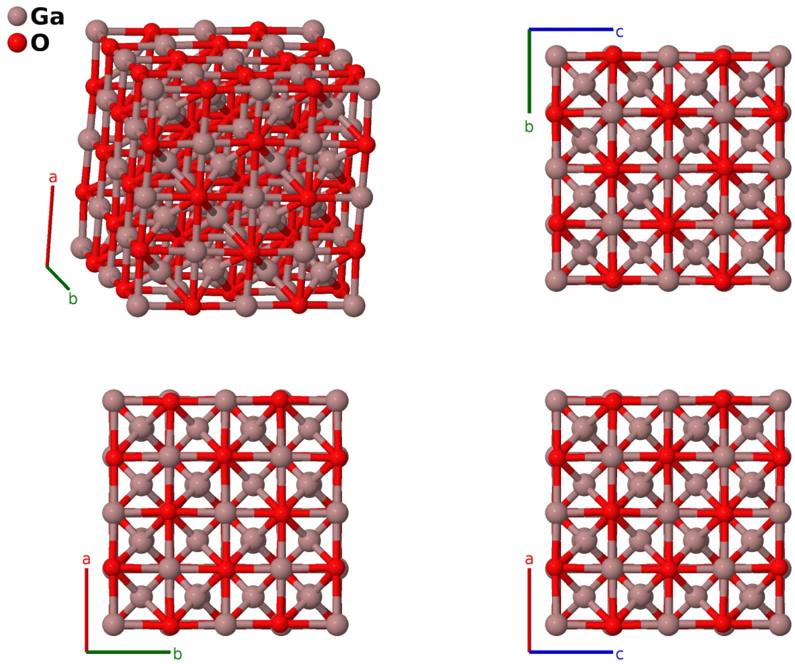
https://aflow.org/p/VTDR

https://aflow.org/p/A11B4_cF120_227_acdf_e-001



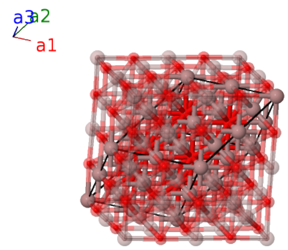
Prototype	Ga_2O_3
AFLOW prototype label	A11B4_cF120_227_acdf_e-001
ICSD	236276
Pearson symbol	cF120
Space group number	227
Space group symbol	$Fd\overline{3}m$
AFLOW prototype command	`aflow --proto=A11B4_cF120_227_acdf_e-001` `--params=`a, x_4, x_5

- Ga_2O_3 exhibits a variety of structures:
  - αGa_2O_3, which has the corundum ($D5_1$) structure ,
  - βGa_2O_3,
  - γGa_2O_3, this structure, and
  - ϵGa_2O_3, a structure with many vacancies which can be approximated by the κ alumina structure.

- In γGa_2O_3 none of the gallium sites have full occupancy. Ga-I and Ga-II are 74.1% occupied, Ga-III is 6.6% occupied, and Ga-IV is only 2.4% occupied.

Face-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(8a)	Ga I
$\mathbf{B_2}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$\frac{7}{8}a\,\hat{\mathbf{x}} + \frac{7}{8}a\,\hat{\mathbf{y}} + \frac{7}{8}a\,\hat{\mathbf{z}}$	(8a)	Ga I
$\mathbf{B_3}$	=	0	=	0	(16c)	Ga II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(16c)	Ga II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	Ga II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	Ga II
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(16d)	Ga III
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(16d)	Ga III
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16d)	Ga III
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16d)	Ga III
$\mathbf{B_{11}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B_{12}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - \left(3x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 - \left(3x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B_{14}}$	=	$-\left(3x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(3x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B_{16}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B_{17}}$	=	$-x_4\,\mathbf{a}_1 + \left(3x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B_{18}}$	=	$\left(3x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	O I
$\mathbf{B_{19}}$	=	$-\left(x_5 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	Ga IV
$\mathbf{B_{20}}$	=	$x_5\,\mathbf{a}_1 - \left(x_5 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_5 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	Ga IV
$\mathbf{B_{21}}$	=	$x_5\,\mathbf{a}_1 - \left(x_5 - \frac{1}{4}\right)\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	Ga IV
$\mathbf{B_{22}}$	=	$-\left(x_5 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - \left(x_5 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	Ga IV
$\mathbf{B_{23}}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - \left(x_5 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(48f)	Ga IV
$\mathbf{B_{24}}$	=	$-\left(x_5 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_5 - \frac{1}{4}\right)\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} - a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48f)	Ga IV
$\mathbf{B_{25}}$	=	$\left(x_5 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \left(x_5 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + a\left(x_5 + \frac{3}{4}\right)\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	Ga IV

$\mathbf{B_{26}}$	=	$-x_5\,\mathbf{a}_1 + \left(x_5 + \frac{3}{4}\right)\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\mathbf{\hat{x}} - ax_5\,\mathbf{\hat{y}} + \frac{3}{8}a\,\mathbf{\hat{z}}$	(48f)	Ga IV
$\mathbf{B_{27}}$	=	$-x_5\,\mathbf{a}_1 + \left(x_5 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_5 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{3}{4}\right)\,\mathbf{\hat{x}} + \frac{3}{8}a\,\mathbf{\hat{y}} + \frac{3}{8}a\,\mathbf{\hat{z}}$	(48f)	Ga IV
$\mathbf{B_{28}}$	=	$\left(x_5 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\mathbf{\hat{x}} + \frac{3}{8}a\,\mathbf{\hat{y}} + \frac{3}{8}a\,\mathbf{\hat{z}}$	(48f)	Ga IV
$\mathbf{B_{29}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \left(x_5 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\mathbf{\hat{x}} + \frac{3}{8}a\,\mathbf{\hat{y}} - ax_5\,\mathbf{\hat{z}}$	(48f)	Ga IV
$\mathbf{B_{30}}$	=	$\left(x_5 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_5 + \frac{3}{4}\right)\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\mathbf{\hat{x}} + \frac{3}{8}a\,\mathbf{\hat{y}} + a\left(x_5 + \frac{3}{4}\right)\,\mathbf{\hat{z}}$	(48f)	Ga IV

References

[1] H. Y. Playford, A. C. Hannon, E. R. Barney, and R. I. Walton, *Structures of Uncharacterised Polymorphs of Gallium Oxide from Total Neutron Diffraction*, Chem. Euro. J. **19**, 2803–2813 (2013), doi:10.1002/chem.201203359.