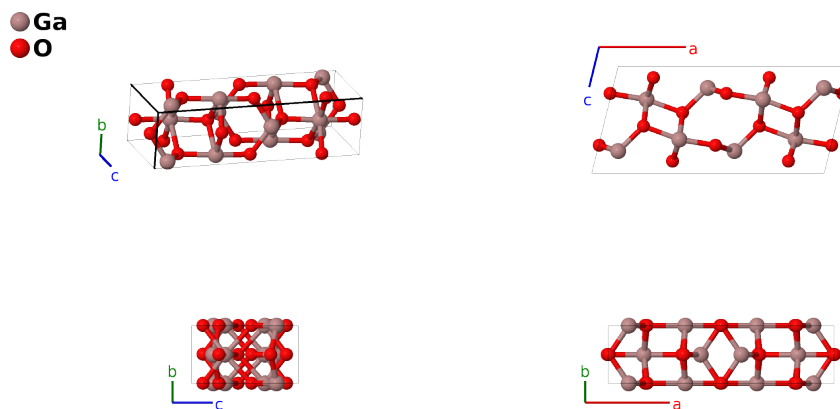# β-Ga$_2$O$_3$ Structure: A2B3_mC20_12_2i_3i-001

This structure originally had the label `A2B3_mC20_12_2i_3i`. Calls to that address will be redirected here.

https://aflow.org/p/LKDZ

https://aflow.org/p/A2B3_mC20_12_2i_3i-001

Prototype	Ga$_2$O$_3$
AFLOW prototype label	A2B3_mC20_12_2i_3i-001
ICSD	83645
Pearson symbol	mC20
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	aflow --proto=A2B3_mC20_12_2i_3i-001 --params=$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5$

Other compounds with this structure

Al$_2$O$_3$

- Ga$_2$O$_3$ exhibits a variety of structures:

    - αGa$_2$O$_3$, which has the corundum ($D5_1$) structure,

    - βGa$_2$O$_3$ (this structure),

    - γGa$_2$O$_3$, and

    - ϵGa$_2$O$_3$, a structure with many vacancies which can be approximated by the κ alumina structure.

- There are numerous structures with the AFLOW prototype label A2B3_mC20_12_2i_3i or A3B2_mC20_12_3i_2i. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
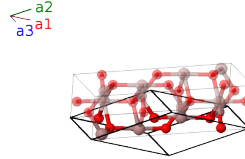
- We have identified the following structures as sufficiently different to warrant their own prototypes:

  - Prototypes with the label A2B3_mC20_12_2i_3i:
    * β-Ga_2O_3 (this structure)
    * α-As_2Te_3
  - Prototypes with the label A3B2_mC20_12_3i_2i:
    * Mo_2As_3
    * Gd_2Cl_3

Base-centered Monoclinic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\mathbf{a_1} + x_1\mathbf{a_2} + z_1\mathbf{a_3}$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ga I
$\mathbf{B_2}$	=	$-x_1\mathbf{a_1} - x_1\mathbf{a_2} - z_1\mathbf{a_3}$	=	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ga I
$\mathbf{B_3}$	=	$x_2\mathbf{a_1} + x_2\mathbf{a_2} + z_2\mathbf{a_3}$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ga II
$\mathbf{B_4}$	=	$-x_2\mathbf{a_1} - x_2\mathbf{a_2} - z_2\mathbf{a_3}$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ga II
$\mathbf{B_5}$	=	$x_3\mathbf{a_1} + x_3\mathbf{a_2} + z_3\mathbf{a_3}$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	O I
$\mathbf{B_6}$	=	$-x_3\mathbf{a_1} - x_3\mathbf{a_2} - z_3\mathbf{a_3}$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	O I
$\mathbf{B_7}$	=	$x_4\mathbf{a_1} + x_4\mathbf{a_2} + z_4\mathbf{a_3}$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	O II
$\mathbf{B_8}$	=	$-x_4\mathbf{a_1} - x_4\mathbf{a_2} - z_4\mathbf{a_3}$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	O II
$\mathbf{B_9}$	=	$x_5\mathbf{a_1} + x_5\mathbf{a_2} + z_5\mathbf{a_3}$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	O III
$\mathbf{B_{10}}$	=	$-x_5\mathbf{a_1} - x_5\mathbf{a_2} - z_5\mathbf{a_3}$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	O III

References

[1] J. Åhman, G. Svensson, and J. Albertsson, *A Reinvestigation of β-Gallium Oxide*, Acta Crystallogr. Sect. C **52**, 1336–1338 (1996), doi:10.1107/S0108270195016404.