

β -Ga₂O₃ Structure:

A2B3_mC20_12_2i_3i-001

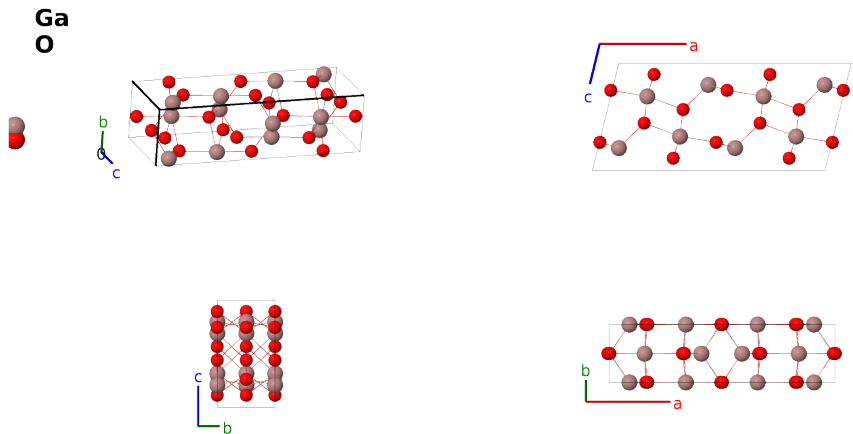
This structure previously used the label(s) **A2B3_mC20_12_2i_3i**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/LKDZ>

https://aflow.org/prototype-encyclopedia/A2B3_mC20_12_2i_3i-001



Prototype	Ga ₂ O ₃
AFLOW prototype label	A2B3_mC20_12_2i_3i-001
ICSD	83645
CCDC	1643685
Pearson symbol	mC20
Space group number	12
Space group symbol	<i>C</i> 2/ <i>m</i>
AFLOW prototype command	<code>aflow --proto=A2B3_mC20_12_2i_3i-001</code> <code>--params=<i>a</i>, <i>b</i>/<i>a</i>, <i>c</i>/<i>a</i>, β, <i>x</i>₁, <i>z</i>₁, <i>x</i>₂, <i>z</i>₂, <i>x</i>₃, <i>z</i>₃, <i>x</i>₄, <i>z</i>₄, <i>x</i>₅, <i>z</i>₅</code>

Other compounds with this structure

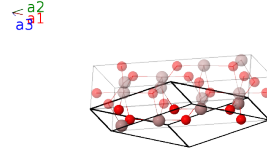
Al₂O₃

- Ga₂O₃ exhibits a variety of structures:
 - α -Ga₂O₃, which has the corundum (*D*5₁) structure,
 - β -Ga₂O₃ (this structure),
 - γ -Ga₂O₃, and

- $\epsilon\text{-Ga}_2\text{O}_3$, 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:
 - * $\beta\text{-Ga}_2\text{O}_3$ (this structure)
 - * $\alpha\text{-As}_2\text{Te}_3$
 - Prototypes with the label A3B2_mC20_12_3i_2i:
 - * Mo_2As_3
 - * Gd_2Cl_3

Base-centered Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



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.

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