

β -AlF₃ Structure:

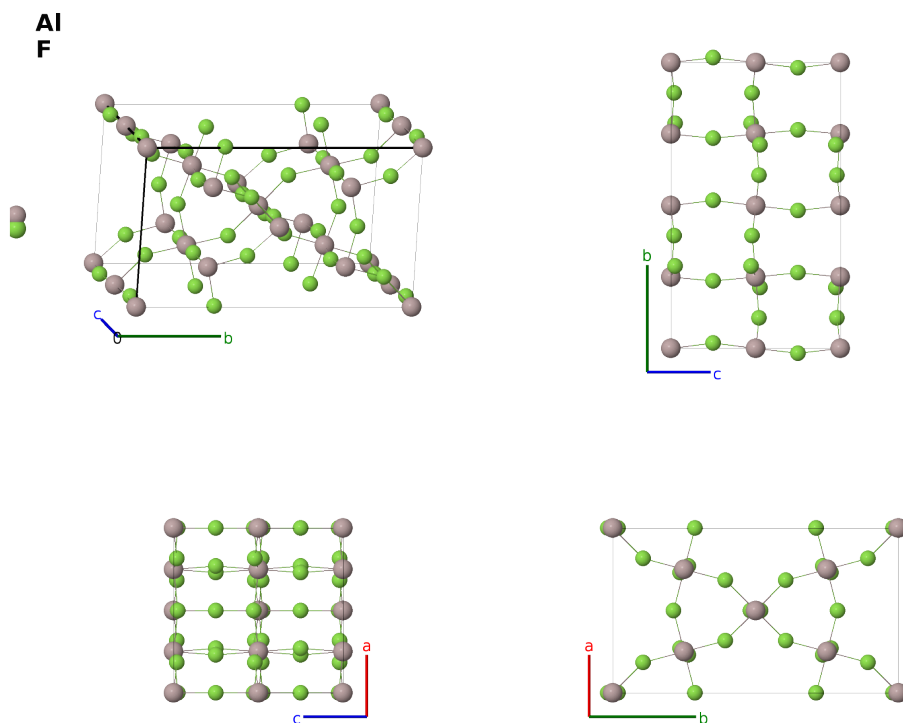
AB3_oC48_63_ad_cfgh-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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/W7TS>

https://aflow.org/prototype-encyclopedia/AB3_oC48_63_ad_cfgh-001



Prototype	AlF ₃
AFLOW prototype label	AB3_oC48_63_ad_cfgh-001
ICSD	202681
CCDC	1707247
Pearson symbol	oC48
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	<code>aflow --proto=AB3_oC48_63_ad_cfgh-001</code> <code>--params=a, b/a, c/a, y₂, y₄, z₄, x₅, y₅, x₆, y₆, z₆</code>

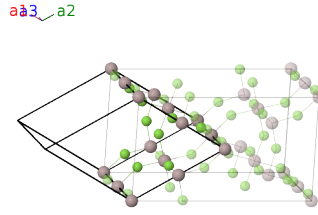
Other compounds with this structure

α' -AlH₃, β -GaF₃, β -InF₃

- AlF₃ has a variety of polymorphs (Le Bail, 2006) including:
 - α -AlF₃, which takes the rhombohedral FeF₃ ($D0_{12}$) structure.
 - β -AlF₃ is this body-centered orthorhombic structure.
 - η -AlF₃ has the β -AlH₃ structure.
 - κ -AlF₃ is a tetragonal structure.
 - θ -AlF₃, also known as τ -AlF₃, is a larger tetragonal structure.
 - Above 713K AlF₃ transforms into the cubic ReO₃ ($D0_9$) structure (Morelock, 2014).
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Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(4a)	Al I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B}_3$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	F I
$\mathbf{B}_4$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	F I
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}}$	(8d)	Al II
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8d)	Al II
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8d)	Al II
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}}$	(8d)	Al II
$\mathbf{B}_9$	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8f)	F II
$\mathbf{B}_{10}$	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	F II
$\mathbf{B}_{11}$	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	F II
$\mathbf{B}_{12}$	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8f)	F II
$\mathbf{B}_{13}$	$= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	F III
$\mathbf{B}_{14}$	$= -(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	F III
$\mathbf{B}_{15}$	$= -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	F III
$\mathbf{B}_{16}$	$= (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	F III

$$\begin{aligned}
\mathbf{B}_{17} &= \begin{matrix} (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + \\ z_6 \mathbf{a}_3 \end{matrix} = ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (16h) & \text{F IV} \\
\mathbf{B}_{18} &= \begin{matrix} -(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 + \\ (z_6 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}} & (16h) & \text{F IV} \\
\mathbf{B}_{19} &= \begin{matrix} -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - \\ (z_6 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}} & (16h) & \text{F IV} \\
\mathbf{B}_{20} &= \begin{matrix} (x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 - \\ z_6 \mathbf{a}_3 \end{matrix} = ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (16h) & \text{F IV} \\
\mathbf{B}_{21} &= \begin{matrix} -(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 - \\ z_6 \mathbf{a}_3 \end{matrix} = -ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (16h) & \text{F IV} \\
\mathbf{B}_{22} &= \begin{matrix} (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 - \\ (z_6 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}} & (16h) & \text{F IV} \\
\mathbf{B}_{23} &= \begin{matrix} (x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \\ (z_6 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}} & (16h) & \text{F IV} \\
\mathbf{B}_{24} &= \begin{matrix} -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 + \\ z_6 \mathbf{a}_3 \end{matrix} = -ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (16h) & \text{F IV}
\end{aligned}$$

References

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First cited in

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