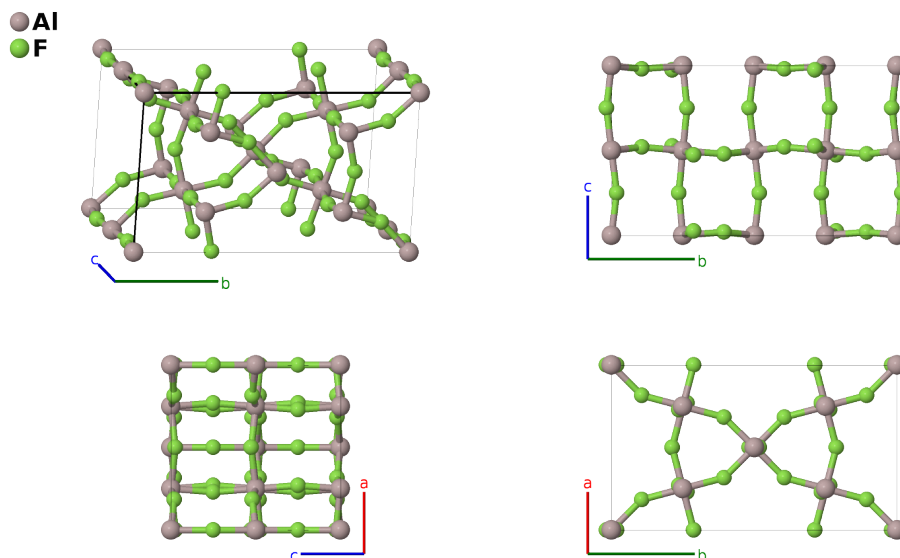


β -AlF₃ Structure: AB3_oC48_63_ad_cfgh-001

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<https://aflow.org/p/W7TS>

https://aflow.org/p/AB3_oC48_63_ad_cfgh-001



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

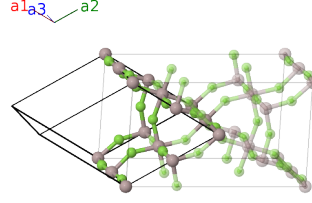
Other compounds with this structure

α' -AlH₃, β -GaF₃, β -InF₃

- AlF₃ has a variety of polymorphs (Le Bail, 2006) including:
 - α -AlF₃, which takes the rhombohedral FeF₃ (*D*₀₁₂) 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 (*D*₀₉) structure (Morelock, 2014).

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

$$\mathbf{B}_{24} = \begin{matrix} -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 + \\ z_6 \mathbf{a}_3 \end{matrix} = -ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} \quad (16h) \quad \text{F IV}$$

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