κ-AlF_3 Structure: AB3_tP40_127_di_cg2ij-001

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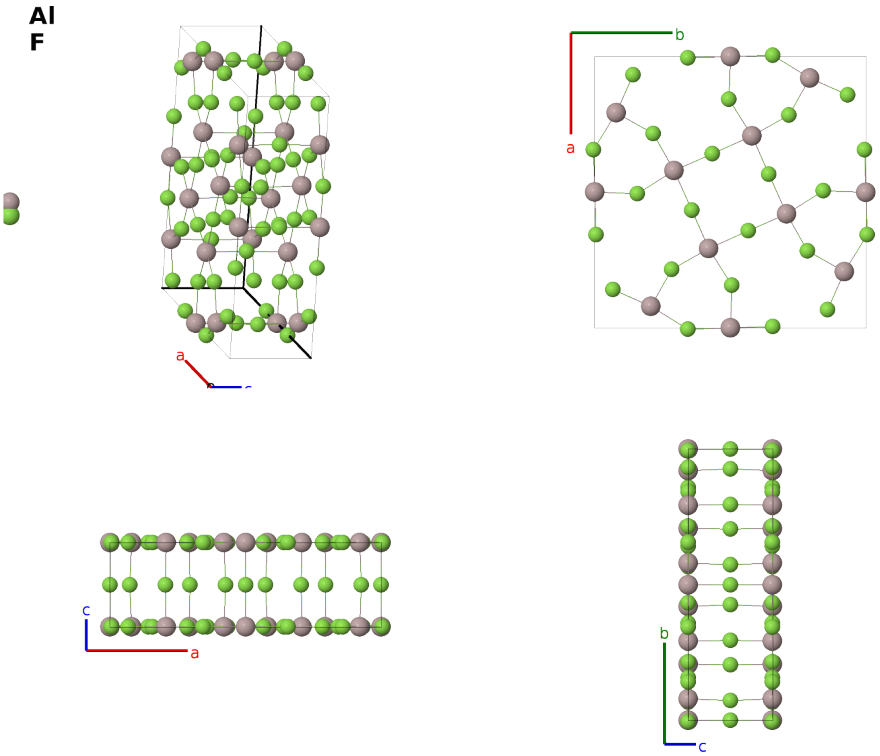
https://aflow.org/prototype-encyclopedia/46QF

https://aflow.org/prototype-encyclopedia/AB3_tP40_127_di_cg2ij-001



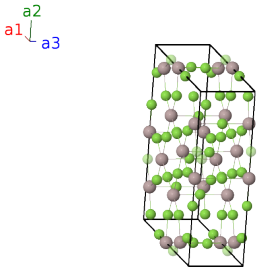
Prototype	AlF_3
AFLOW prototype label	AB3_tP40_127_di_cg2ij-001
ICSD	79816
CCDC	1640051
Pearson symbol	tP40
Space group number	127
Space group symbol	$P4/mbm$
AFLOW prototype command	`aflow --proto=AB3_tP40_127_di_cg2ij-001 --params=`$a, c/a, x_3, x_4, y_4, x_5, y_5, x_6, y_6, x_7, y_7$

- AlF_3 has a variety of polymorphs (Le Bail, 2006) including:

– α-AlF_3, which takes the rhombohedral FeF_3 ($D0_{12}$) structure.
– β-AlF_3 has a body-centered orthorhombic structure.
– η-AlF_3 has the β-AlH_3 structure.
– κ-AlF_3 is this tetragonal structure.
– θ-AlF_3, also known as τ-AlF_3, is a larger tetragonal structure.
– Above 713K AlF_3 transforms into the cubic ReO_3 ($D0_9$) structure (Morelock, 2014).

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	F I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	F I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(2d)	Al I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(2d)	Al I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	F II
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	F II
$\mathbf{B_7}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(4g)	F II
$\mathbf{B_8}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(4g)	F II
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}}$	(8i)	Al II
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}}$	(8i)	Al II
$\mathbf{B_{11}}$	=	$-y_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2$	=	$-ay_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(8i)	Al II
$\mathbf{B_{12}}$	=	$y_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$ay_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(8i)	Al II
$\mathbf{B_{13}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8i)	Al II
$\mathbf{B_{14}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8i)	Al II
$\mathbf{B_{15}}$	=	$\left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8i)	Al II
$\mathbf{B_{16}}$	=	$-\left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8i)	Al II
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}}$	(8i)	F III
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2$	=	$-ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}}$	(8i)	F III
$\mathbf{B_{19}}$	=	$-y_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2$	=	$-ay_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}}$	(8i)	F III
$\mathbf{B_{20}}$	=	$y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2$	=	$ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}}$	(8i)	F III
$\mathbf{B_{21}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8i)	F III
$\mathbf{B_{22}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8i)	F III

$\mathbf{B_{23}}$	=	$\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8i)	F III
$\mathbf{B_{24}}$	=	$-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8i)	F III
$\mathbf{B_{25}}$	=	$x_6\,\mathbf{a}_1+y_6\,\mathbf{a}_2$	=	$ax_6\,\hat{\mathbf{x}}+ay_6\,\hat{\mathbf{y}}$	(8i)	F IV
$\mathbf{B_{26}}$	=	$-x_6\,\mathbf{a}_1-y_6\,\mathbf{a}_2$	=	$-ax_6\,\hat{\mathbf{x}}-ay_6\,\hat{\mathbf{y}}$	(8i)	F IV
$\mathbf{B_{27}}$	=	$-y_6\,\mathbf{a}_1+x_6\,\mathbf{a}_2$	=	$-ay_6\,\hat{\mathbf{x}}+ax_6\,\hat{\mathbf{y}}$	(8i)	F IV
$\mathbf{B_{28}}$	=	$y_6\,\mathbf{a}_1-x_6\,\mathbf{a}_2$	=	$ay_6\,\hat{\mathbf{x}}-ax_6\,\hat{\mathbf{y}}$	(8i)	F IV
$\mathbf{B_{29}}$	=	$-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_6+\frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8i)	F IV
$\mathbf{B_{30}}$	=	$\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8i)	F IV
$\mathbf{B_{31}}$	=	$\left(y_6+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8i)	F IV
$\mathbf{B_{32}}$	=	$-\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8i)	F IV
$\mathbf{B_{33}}$	=	$x_7\,\mathbf{a}_1+y_7\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}}+ay_7\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8j)	F V
$\mathbf{B_{34}}$	=	$-x_7\,\mathbf{a}_1-y_7\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}}-ay_7\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8j)	F V
$\mathbf{B_{35}}$	=	$-y_7\,\mathbf{a}_1+x_7\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$-ay_7\,\hat{\mathbf{x}}+ax_7\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8j)	F V
$\mathbf{B_{36}}$	=	$y_7\,\mathbf{a}_1-x_7\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$ay_7\,\hat{\mathbf{x}}-ax_7\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8j)	F V
$\mathbf{B_{37}}$	=	$-\left(x_7-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_7+\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_7-\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_7+\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8j)	F V
$\mathbf{B_{38}}$	=	$\left(x_7+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_7-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_7+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_7-\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8j)	F V
$\mathbf{B_{39}}$	=	$\left(y_7+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_7+\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$a\left(y_7+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_7+\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8j)	F V
$\mathbf{B_{40}}$	=	$-\left(y_7-\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_7-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(y_7-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_7-\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8j)	F V

References

[1] N. Herron, D. L. Thorn, R. L. Harlow, G. A. Jones, J. B. Parise, J. A. Fernandez-Baca, and T. Vogt, *Preparation and Structural Characterization of Two New Phases of Aluminum Trifluoride*, Chem. Mater. **7**, 75–83 (1995), doi:10.1021/cm00049a013.

[2] C. R. Morelock, J. C. Hancock, and A. P. Wilkinson, *Thermal expansion and phase transitions of α-AlF_3*, J. Solid State Chem. **219**, 143–147 (2014), doi:10.1016/j.jssc.2014.07.031.

Found in

[1] A. L. Bail and F. Calvayrac, *Hypothetical AlF_3 crystal structures*, J. Solid State Chem. **179**, 3159–3166 (2006), doi:10.1016/j.jssc.2006.06.010.

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