

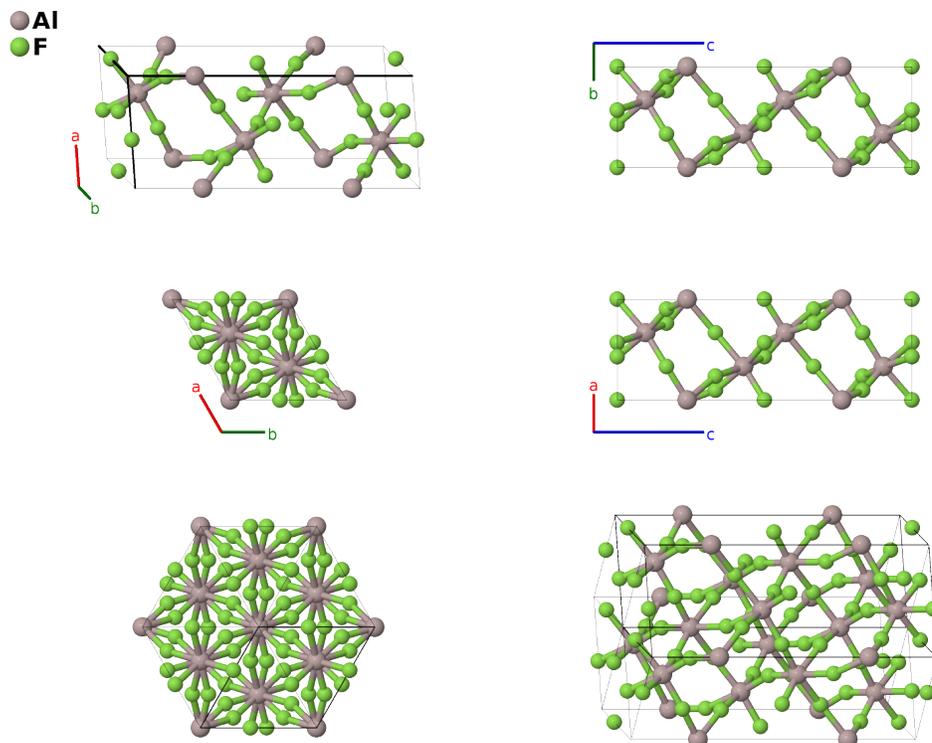
AlF₃ (*D*₀₁₄) Structure: AB3_hR8_155_c_de-001

This structure originally had the label **AB3_hR8_155_c_de**. Calls to that address will be redirected here.

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<https://aflow.org/p/QG2U>

https://aflow.org/p/AB3_hR8_155_c_de-001



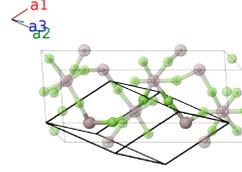
Prototype	AlF ₃
AFLOW prototype label	AB3_hR8_155_c_de-001
<i>Strukturbericht</i> designation	<i>D</i> ₀₁₄
ICSD	30274
Pearson symbol	hR8
Space group number	155
Space group symbol	<i>R</i> 32
AFLOW prototype command	<code>aflow --proto=AB3_hR8_155_c_de-001 --params=a, c/a, x₁, y₂, y₃</code>

Other compounds with this structure
FeF₃

- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	=	$cx_1 \hat{\mathbf{z}}$	(2c)	Al I
\mathbf{B}_2	$-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	=	$-cx_1 \hat{\mathbf{z}}$	(2c)	Al I
\mathbf{B}_3	$y_2 \mathbf{a}_2 - y_2 \mathbf{a}_3$	=	$\frac{1}{2}ay_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}}$	(3d)	F I
\mathbf{B}_4	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_3$	=	$-ay_2 \hat{\mathbf{x}}$	(3d)	F I
\mathbf{B}_5	$y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	=	$\frac{1}{2}ay_2 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}}$	(3d)	F I
\mathbf{B}_6	$\frac{1}{2} \mathbf{a}_1 + y_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	=	$\frac{1}{4}a(2y_3 + 1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a(6y_3 - 1) \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3e)	F II
\mathbf{B}_7	$-y_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + y_3 \mathbf{a}_3$	=	$-ay_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3e)	F II
\mathbf{B}_8	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{4}a(2y_3 - 1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a(6y_3 + 1) \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3e)	F II

References

- [1] J. A. A. Ketelaar, *Die Kristallstruktur der Aluminiumhalogenide: I. Die Kristallstruktur von AlF_3* , Z. Kristallogr. **85**, 119–131 (1933), doi:10.1524/zkri.1933.85.1.119.
- [2] R. Hoppe and D. Kissel, *Zur Kenntnis von AlF_3 und InF_3 [1]*, J. Fluorine Chem. **24**, 324–340 (1984), doi:10.1016/S0022-1139(00)81321-4.

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).