AlF_3 ($D0_{14}$) Structure: AB3_hR8_155_c_de-001

This structure previously used the label(s) `AB3_hR8_155_c_de`. Calls to these addresses will be redirected here.

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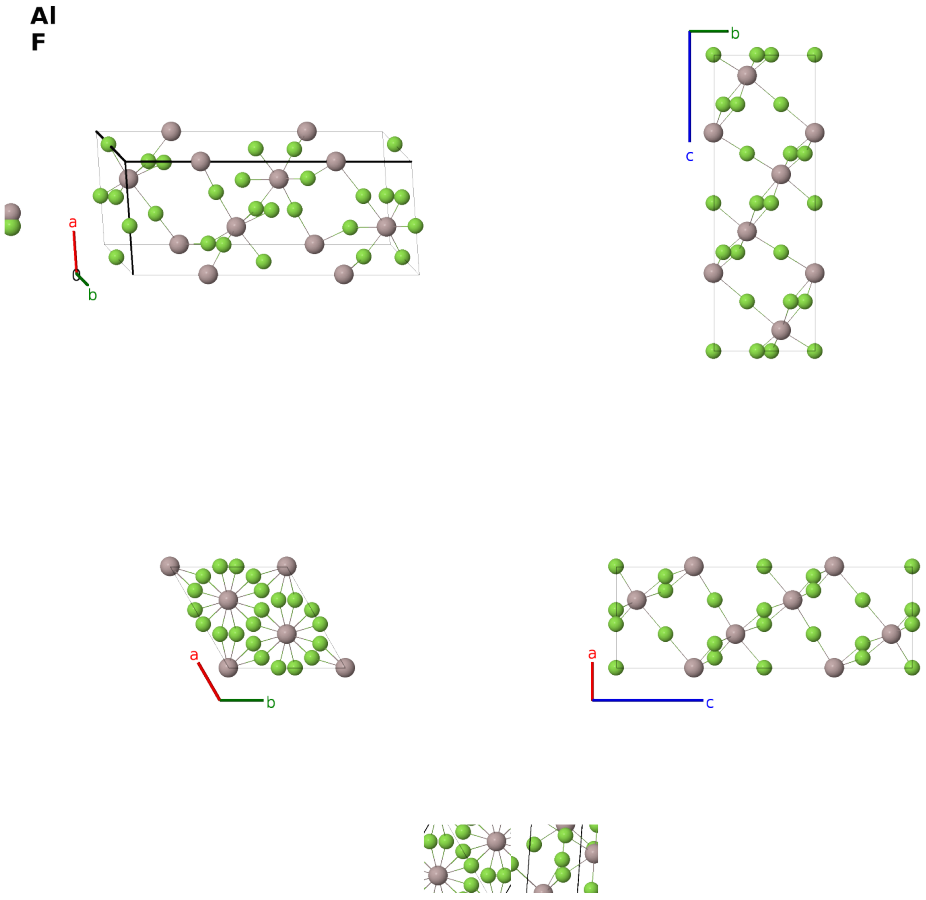
https://aflow.org/prototype-encyclopedia/QG2U

https://aflow.org/prototype-encyclopedia/AB3_hR8_155_c_de-001



Prototype	AlF_3
AFLOW prototype label	AB3_hR8_155_c_de-001
***Strukturbericht* designation**	$D0_{14}$
ICSD	30274
CCDC	1604642
Pearson symbol	hR8
Space group number	155

Space group symbol $R32$

AFLOW prototype command `aflow --proto=AB3_hR8_155_c_de-001 --params=`$a, c/a, x_1, y_2, y_3$

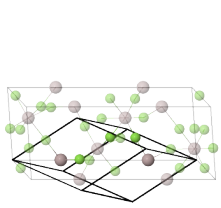
Other compounds with this structure

FeF_3

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

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



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. Flourine 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).

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