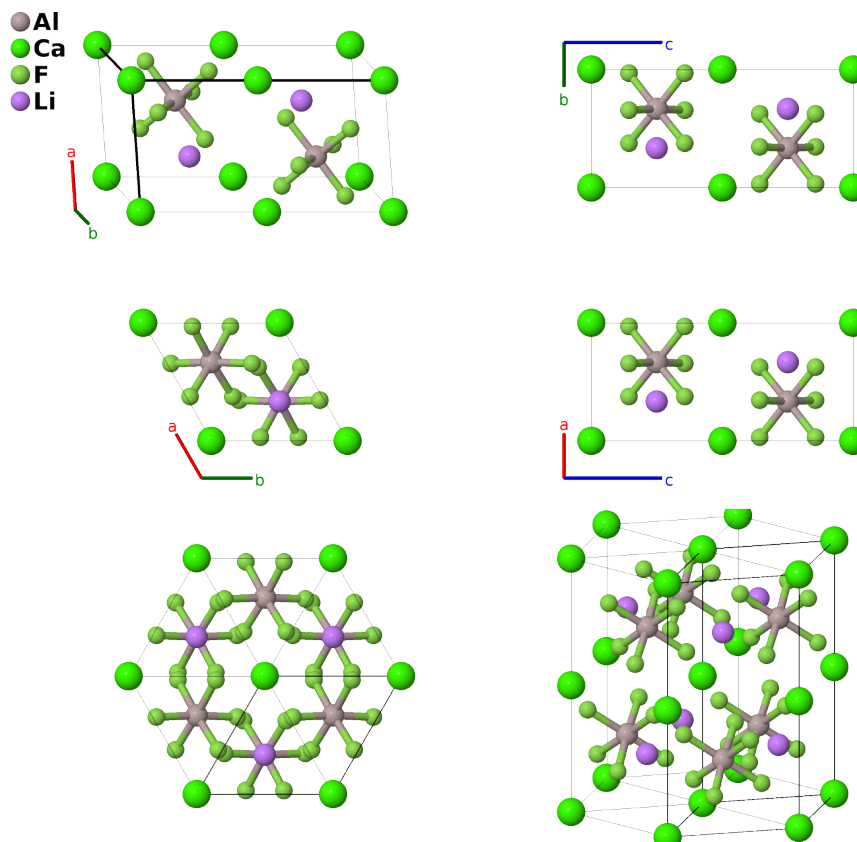# Colquiriite (LiCaAlF$_6$) Structure: ABC6D_hP18_163_c_b_i_d-001

This structure originally had the label `ABC6D_hP18_163_d_b_i_c`. Calls to that address will be redirected here.

https://aflow.org/p/8D1V

https://aflow.org/p/ABC6D_hP18_163_c_b_i_d-001

Prototype	AlCaF$_6$Li
AFLOW prototype label	ABC6D_hP18_163_c_b_i_d-001
Mineral name	colquiriite
ICSD	150332
Pearson symbol	hP18
Space group number	163
Space group symbol	$P\bar{3}1c$
AFLOW prototype command	aflow --proto=ABC6D_hP18_163_c_b_i_d-001 --params=$a, c/a, x_4, y_4, z_4$

Other compounds with this structure

LiSrAlF$_6$

- This is the low-temperature standard-pressure structure of LiCaAlF$_6$. We used the data taken at 300K and ambient pressure.

Trigonal (Hexagonal) primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}
$$
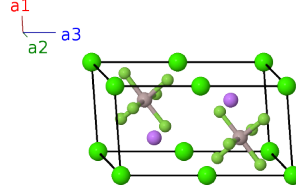
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2b)	Ca I
$\mathbf{B_2}$	=	$\tfrac{1}{2}\mathbf{a_3}$	=	$\tfrac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Ca I
$\mathbf{B_3}$	=	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Al I
$\mathbf{B_4}$	=	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Al I
$\mathbf{B_5}$	=	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(2d)	Li I
$\mathbf{B_6}$	=	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(2d)	Li I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	=	$\tfrac{1}{2}a\,(x_4+y_4)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_4-y_4)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12i)	F I
$\mathbf{B_8}$	=	$-y_4\,\mathbf{a_1} + (x_4-y_4)\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	=	$\tfrac{1}{2}a\,(x_4-2y_4)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12i)	F I
$\mathbf{B_9}$	=	$-(x_4-y_4)\,\mathbf{a_1} - x_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	=	$-\tfrac{1}{2}a\,(2x_4-y_4)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12i)	F I
$\mathbf{B_{10}}$	=	$-y_4\,\mathbf{a_1} - x_4\,\mathbf{a_2} - \left(z_4-\tfrac{1}{2}\right)\mathbf{a_3}$	=	$-\tfrac{1}{2}a\,(x_4+y_4)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_4-y_4)\,\hat{\mathbf{y}} - c\left(z_4-\tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	F I
$\mathbf{B_{11}}$	=	$-(x_4-y_4)\,\mathbf{a_1} + y_4\,\mathbf{a_2} - \left(z_4-\tfrac{1}{2}\right)\mathbf{a_3}$	=	$\tfrac{1}{2}a\,(-x_4+2y_4)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - c\left(z_4-\tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	F I
$\mathbf{B_{12}}$	=	$x_4\,\mathbf{a_1} + (x_4-y_4)\,\mathbf{a_2} - \left(z_4-\tfrac{1}{2}\right)\mathbf{a_3}$	=	$\tfrac{1}{2}a\,(2x_4-y_4)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} - c\left(z_4-\tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	F I
$\mathbf{B_{13}}$	=	$-x_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	=	$-\tfrac{1}{2}a\,(x_4+y_4)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_4-y_4)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12i)	F I
$\mathbf{B_{14}}$	=	$y_4\,\mathbf{a_1} - (x_4-y_4)\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	=	$\tfrac{1}{2}a\,(-x_4+2y_4)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12i)	F I
$\mathbf{B_{15}}$	=	$(x_4-y_4)\,\mathbf{a_1} + x_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	=	$\tfrac{1}{2}a\,(2x_4-y_4)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12i)	F I
$\mathbf{B_{16}}$	=	$y_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} + \left(z_4+\tfrac{1}{2}\right)\mathbf{a_3}$	=	$\tfrac{1}{2}a\,(x_4+y_4)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_4-y_4)\,\hat{\mathbf{y}} + c\left(z_4+\tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	F I
$\mathbf{B_{17}}$	=	$(x_4-y_4)\,\mathbf{a_1} - y_4\,\mathbf{a_2} + \left(z_4+\tfrac{1}{2}\right)\mathbf{a_3}$	=	$\tfrac{1}{2}a\,(x_4-2y_4)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4+\tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	F I
$\mathbf{B_{18}}$	=	$-x_4\,\mathbf{a_1} - (x_4-y_4)\,\mathbf{a_2} + \left(z_4+\tfrac{1}{2}\right)\mathbf{a_3}$	=	$-\tfrac{1}{2}a\,(2x_4-y_4)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + c\left(z_4+\tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12i)	F I

References

[1] S. Kuze, D. du Boulay, N. Ishizawa, N. Kodama, M. Yamaga, and B. Henderson, *Structures of LiCaAlF$_6$ and LiSrAlF$_6$ at 120 and 300 K by synchrotron X-ray single-crystal diffraction*, J. Solid State Chem. **177**, 3505–3513 (2004), doi:10.1016/j.jssc.2004.04.039.