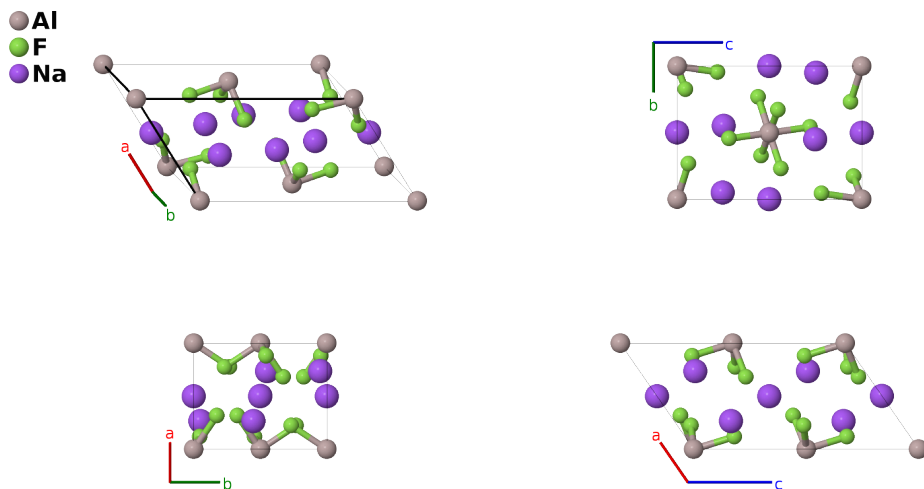# Cryolite (Na_3AlF_6, $J2_6$) Structure: AB6C3_mP20_14_a_3e_be-001

This structure originally had the label `AB6C3_mP20_14_a_3e_de`. Calls to that address will be redirected here.

https://aflow.org/p/G2BV

https://aflow.org/p/AB6C3_mP20_14_a_3e_be-001

Prototype	AlF_6Na_3
AFLOW prototype label	AB6C3_mP20_14_a_3e_be-001
***Strukturbericht* designation**	$J2_6$
Mineral name	cryolite
ICSD	74200
Pearson symbol	mP20
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	`aflow --proto=AB6C3_mP20_14_a_3e_be-001` `--params=`$a, b/a, c/a, \beta, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

- Cryolite undergoes a phase transition to an orthorhombic $Immm$ #71 phase at 890K. Here we use structural data taken at 295K.

- (Yang, 1993) gives the Wyckoff positions for the orientation $P2_1/n$ of space group #14. We used FINDSYM to change this to the standard $P2_1/c$ orientation. This included a change in the primitive vectors and the shift of the sodium atom on the (1b) site to the (1d) site.

Simple Monoclinic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$
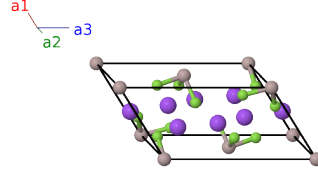
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	0	$=$	0	(2a)	Al I
$\mathbf{B_2}$	$=$	$\frac{1}{2}\mathbf{a_2} + \frac{1}{2}\mathbf{a_3}$	$=$	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2a)	Al I
$\mathbf{B_3}$	$=$	$\frac{1}{2}\mathbf{a_1}$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(2b)	Na I
$\mathbf{B_4}$	$=$	$\frac{1}{2}\mathbf{a_1} + \frac{1}{2}\mathbf{a_2} + \frac{1}{2}\mathbf{a_3}$	$=$	$\frac{1}{2}\left(a + c\cos\beta\right)\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2b)	Na I
$\mathbf{B_5}$	$=$	$x_3\mathbf{a_1} + y_3\mathbf{a_2} + z_3\mathbf{a_3}$	$=$	$\left(ax_3 + cz_3\cos\beta\right)\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_6}$	$=$	$-x_3\mathbf{a_1} + \left(y_3 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_3 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_7}$	$=$	$-x_3\mathbf{a_1} - y_3\mathbf{a_2} - z_3\mathbf{a_3}$	$=$	$-\left(ax_3 + cz_3\cos\beta\right)\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_8}$	$=$	$x_3\mathbf{a_1} - \left(y_3 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_3 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_9}$	$=$	$x_4\mathbf{a_1} + y_4\mathbf{a_2} + z_4\mathbf{a_3}$	$=$	$\left(ax_4 + cz_4\cos\beta\right)\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	F II
$\mathbf{B_{10}}$	$=$	$-x_4\mathbf{a_1} + \left(y_4 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_4 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F II
$\mathbf{B_{11}}$	$=$	$-x_4\mathbf{a_1} - y_4\mathbf{a_2} - z_4\mathbf{a_3}$	$=$	$-\left(ax_4 + cz_4\cos\beta\right)\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	F II
$\mathbf{B_{12}}$	$=$	$x_4\mathbf{a_1} - \left(y_4 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_4 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F II
$\mathbf{B_{13}}$	$=$	$x_5\mathbf{a_1} + y_5\mathbf{a_2} + z_5\mathbf{a_3}$	$=$	$\left(ax_5 + cz_5\cos\beta\right)\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	F III
$\mathbf{B_{14}}$	$=$	$-x_5\mathbf{a_1} + \left(y_5 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_5 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_5 + c\left(z_5 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F III
$\mathbf{B_{15}}$	$=$	$-x_5\mathbf{a_1} - y_5\mathbf{a_2} - z_5\mathbf{a_3}$	$=$	$-\left(ax_5 + cz_5\cos\beta\right)\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	F III
$\mathbf{B_{16}}$	$=$	$x_5\mathbf{a_1} - \left(y_5 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_5 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_5 + c\left(z_5 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F III
$\mathbf{B_{17}}$	$=$	$x_6\mathbf{a_1} + y_6\mathbf{a_2} + z_6\mathbf{a_3}$	$=$	$\left(ax_6 + cz_6\cos\beta\right)\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	Na II
$\mathbf{B_{18}}$	$=$	$-x_6\mathbf{a_1} + \left(y_6 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_6 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_6 + c\left(z_6 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Na II
$\mathbf{B_{19}}$	$=$	$-x_6\mathbf{a_1} - y_6\mathbf{a_2} - z_6\mathbf{a_3}$	$=$	$-\left(ax_6 + cz_6\cos\beta\right)\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	Na II
$\mathbf{B_{20}}$	$=$	$x_6\mathbf{a_1} - \left(y_6 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_6 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_6 + c\left(z_6 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Na II

References

[1] H. Yang, S. Ghose, and D. M. Hatch, *Ferroelastic phase transition in cryolite, Na_3AlF_6, a mixed fluoride perovskite: High temperature single crystal X-ray diffraction study and symmetry analysis of the transition mechanism*, Phys. Chem. Minerals **19**, 528–544 (1993), doi:10.1007/BF00203053.

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