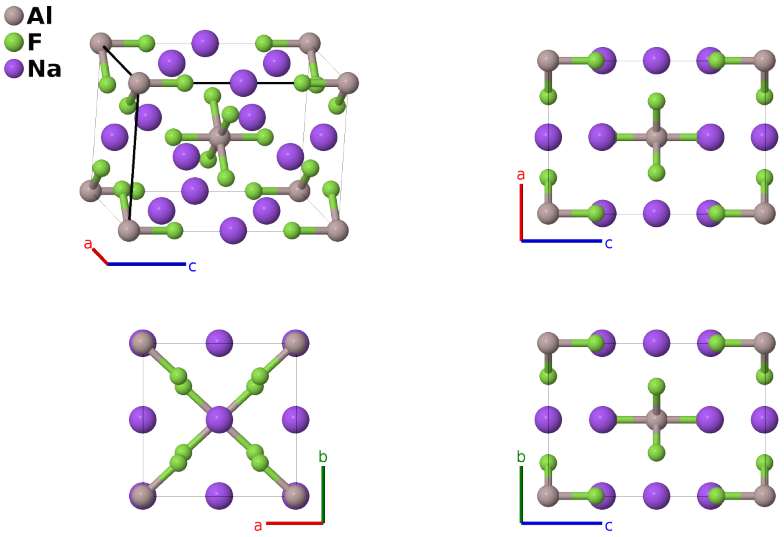
High-Temperature Cryolite (Na_3AlF_6) Structure: AB6C3_oI20_71_a_el_bf-001

This structure originally had the label `AB6C3_oI20_71_a_in_cj`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

https://aflow.org/p/6BL9

https://aflow.org/p/AB6C3_oI20_71_a_el_bf-001

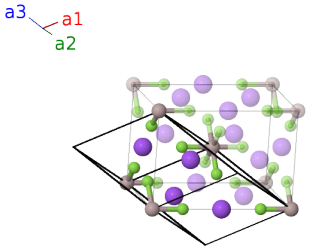


Prototype	AlF_6Na_3
AFLOW prototype label	AB6C3_oI20_71_a_el_bf-001
Mineral name	cryolite
ICSD	74211
Pearson symbol	oI20
Space group number	71
Space group symbol	$Immm$
AFLOW prototype command	`aflow --proto=AB6C3_oI20_71_a_el_bf-001 --params=`$a, b/a, c/a, x_3, x_4, y_5, z_5$

- Cryolite undergoes a phase transition from the monoclinic $J2_6$ phase, space group $P2_1/c$ #14, to this orthorhombic phase at 890K. We show structural data taken at 900K.

Body-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(2b)	Na I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}$	(4e)	F I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}$	(4e)	F I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(4f)	Na II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(4f)	Na II
$\mathbf{B_7}$	=	$(y_5 + z_5)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + y_5\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8l)	F II
$\mathbf{B_8}$	=	$-(y_5 - z_5)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 - y_5\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8l)	F II
$\mathbf{B_9}$	=	$(y_5 - z_5)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 + y_5\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8l)	F II
$\mathbf{B_{10}}$	=	$-(y_5 + z_5)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - y_5\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8l)	F 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.

Found in

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