Chiolite ($Na_5Al_3F_{14}$, $K7_5$) Structure: A3B14C5_tP44_128_ac_ehi_bg-001

This structure previously used the label(s) `A3B14C5_tP44_128_ac_ehi_bg`. Calls to these addresses will be redirected here.

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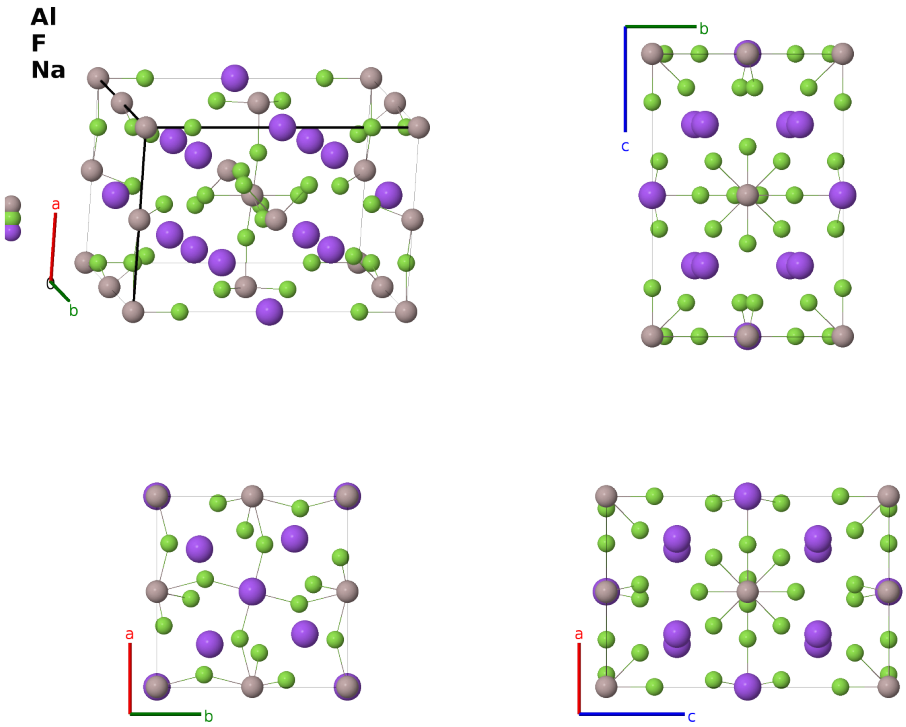
https://aflow.org/prototype-encyclopedia/GFQ6

https://aflow.org/prototype-encyclopedia/A3B14C5_tP44_128_ac_ehi_bg-001

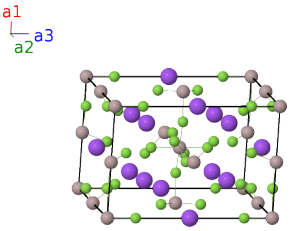


Prototype	$Al_3F_{14}Na_5$
AFLOW prototype label	A3B14C5_tP44_128_ac_ehi_bg-001
***Strukturbericht* designation**	$K7_5$
Mineral name	chiolite
ICSD	26419
CCDC	1601827
Pearson symbol	tP44
Space group number	128
Space group symbol	$P4/mnc$

AFLOW prototype command `aflow --proto=A3B14C5_tP44_128_ac_ehi_bg-001 --params=`$a, c/a, z_4, x_5, x_6, y_6, x_7, y_7, z_7$

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	Al I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Na I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(2b)	Na I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(4c)	Al II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(4c)	Al II
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4c)	Al II
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4c)	Al II
$\mathbf{B_9}$	=	$z_4\,\mathbf{a}_3$	=	$cz_4\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_{11}}$	=	$-z_4\,\mathbf{a}_3$	=	$-cz_4\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Na II
$\mathbf{B_{14}}$	=	$-x_5\,\mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Na II
$\mathbf{B_{15}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Na II
$\mathbf{B_{16}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Na II
$\mathbf{B_{17}}$	=	$-x_5\,\mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	Na II
$\mathbf{B_{18}}$	=	$x_5\,\mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	Na II
$\mathbf{B_{19}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	Na II
$\mathbf{B_{20}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	Na II
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2$	=	$ax_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}}$	(8h)	F II
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2$	=	$-ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}}$	(8h)	F II
$\mathbf{B_{23}}$	=	$-y_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2$	=	$-ay_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}}$	(8h)	F II
$\mathbf{B_{24}}$	=	$y_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2$	=	$ay_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}}$	(8h)	F II
$\mathbf{B_{25}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8h)	F II

$$\mathbf{B_{26}} = \left(x_6+\tfrac{1}{2}\right)\mathbf{a}_1-\left(y_6-\tfrac{1}{2}\right)\mathbf{a}_2+\tfrac{1}{2}\mathbf{a}_3 = a\left(x_6+\tfrac{1}{2}\right)\hat{\mathbf{x}}-a\left(y_6-\tfrac{1}{2}\right)\hat{\mathbf{y}}+\tfrac{1}{2}c\,\hat{\mathbf{z}} \quad (8h) \quad \text{F II}$$

$$\mathbf{B_{27}} = \left(y_6+\tfrac{1}{2}\right)\mathbf{a}_1+\left(x_6+\tfrac{1}{2}\right)\mathbf{a}_2+\tfrac{1}{2}\mathbf{a}_3 = a\left(y_6+\tfrac{1}{2}\right)\hat{\mathbf{x}}+a\left(x_6+\tfrac{1}{2}\right)\hat{\mathbf{y}}+\tfrac{1}{2}c\,\hat{\mathbf{z}} \quad (8h) \quad \text{F II}$$

$$\mathbf{B_{28}} = -\left(y_6-\tfrac{1}{2}\right)\mathbf{a}_1-\left(x_6-\tfrac{1}{2}\right)\mathbf{a}_2+\tfrac{1}{2}\mathbf{a}_3 = -a\left(y_6-\tfrac{1}{2}\right)\hat{\mathbf{x}}-a\left(x_6-\tfrac{1}{2}\right)\hat{\mathbf{y}}+\tfrac{1}{2}c\,\hat{\mathbf{z}} \quad (8h) \quad \text{F II}$$

$$\mathbf{B_{29}} = x_7\,\mathbf{a}_1+y_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}}+ay_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} \quad (16i) \quad \text{F III}$$

$$\mathbf{B_{30}} = -x_7\,\mathbf{a}_1-y_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}}-ay_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} \quad (16i) \quad \text{F III}$$

$$\mathbf{B_{31}} = -y_7\,\mathbf{a}_1+x_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3 = -ay_7\,\hat{\mathbf{x}}+ax_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} \quad (16i) \quad \text{F III}$$

$$\mathbf{B_{32}} = y_7\,\mathbf{a}_1-x_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3 = ay_7\,\hat{\mathbf{x}}-ax_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} \quad (16i) \quad \text{F III}$$

$$\mathbf{B_{33}} = -\left(x_7-\tfrac{1}{2}\right)\mathbf{a}_1+\left(y_7+\tfrac{1}{2}\right)\mathbf{a}_2-\left(z_7-\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_7-\tfrac{1}{2}\right)\hat{\mathbf{x}}+a\left(y_7+\tfrac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_7-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16i) \quad \text{F III}$$

$$\mathbf{B_{34}} = \left(x_7+\tfrac{1}{2}\right)\mathbf{a}_1-\left(y_7-\tfrac{1}{2}\right)\mathbf{a}_2-\left(z_7-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_7+\tfrac{1}{2}\right)\hat{\mathbf{x}}-a\left(y_7-\tfrac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_7-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16i) \quad \text{F III}$$

$$\mathbf{B_{35}} = \left(y_7+\tfrac{1}{2}\right)\mathbf{a}_1+\left(x_7+\tfrac{1}{2}\right)\mathbf{a}_2-\left(z_7-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(y_7+\tfrac{1}{2}\right)\hat{\mathbf{x}}+a\left(x_7+\tfrac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_7-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16i) \quad \text{F III}$$

$$\mathbf{B_{36}} = -\left(y_7-\tfrac{1}{2}\right)\mathbf{a}_1-\left(x_7-\tfrac{1}{2}\right)\mathbf{a}_2-\left(z_7-\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(y_7-\tfrac{1}{2}\right)\hat{\mathbf{x}}-a\left(x_7-\tfrac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_7-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16i) \quad \text{F III}$$

$$\mathbf{B_{37}} = -x_7\,\mathbf{a}_1-y_7\,\mathbf{a}_2-z_7\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}}-ay_7\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}} \quad (16i) \quad \text{F III}$$

$$\mathbf{B_{38}} = x_7\,\mathbf{a}_1+y_7\,\mathbf{a}_2-z_7\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}}+ay_7\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}} \quad (16i) \quad \text{F III}$$

$$\mathbf{B_{39}} = y_7\,\mathbf{a}_1-x_7\,\mathbf{a}_2-z_7\,\mathbf{a}_3 = ay_7\,\hat{\mathbf{x}}-ax_7\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}} \quad (16i) \quad \text{F III}$$

$$\mathbf{B_{40}} = -y_7\,\mathbf{a}_1+x_7\,\mathbf{a}_2-z_7\,\mathbf{a}_3 = -ay_7\,\hat{\mathbf{x}}+ax_7\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}} \quad (16i) \quad \text{F III}$$

$$\mathbf{B_{41}} = \left(x_7+\tfrac{1}{2}\right)\mathbf{a}_1-\left(y_7-\tfrac{1}{2}\right)\mathbf{a}_2+\left(z_7+\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_7+\tfrac{1}{2}\right)\hat{\mathbf{x}}-a\left(y_7-\tfrac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_7+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16i) \quad \text{F III}$$

$$\mathbf{B_{42}} = -\left(x_7-\tfrac{1}{2}\right)\mathbf{a}_1+\left(y_7+\tfrac{1}{2}\right)\mathbf{a}_2+\left(z_7+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_7-\tfrac{1}{2}\right)\hat{\mathbf{x}}+a\left(y_7+\tfrac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_7+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16i) \quad \text{F III}$$

$$\mathbf{B_{43}} = -\left(y_7-\tfrac{1}{2}\right)\mathbf{a}_1-\left(x_7-\tfrac{1}{2}\right)\mathbf{a}_2+\left(z_7+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(y_7-\tfrac{1}{2}\right)\hat{\mathbf{x}}-a\left(x_7-\tfrac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_7+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16i) \quad \text{F III}$$

$$\mathbf{B_{44}} = \left(y_7+\tfrac{1}{2}\right)\mathbf{a}_1+\left(x_7+\tfrac{1}{2}\right)\mathbf{a}_2+\left(z_7+\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(y_7+\tfrac{1}{2}\right)\hat{\mathbf{x}}+a\left(x_7+\tfrac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_7+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16i) \quad \text{F III}$$

References

[1] C. Jacoboni, A. Leble, and J. J. Rousseau, *Détermination précise de la structure de la chiolite $Na_5Al_3F_{14}$ et étude par R.P.E. de $Na_5Al_3F_{14}$:Cr^{3+}*, J. Solid State Chem. **36**, 297–304 (1981), doi:10.1016/0022-4596(81)90440-0.

Found in

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

First cited in

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.