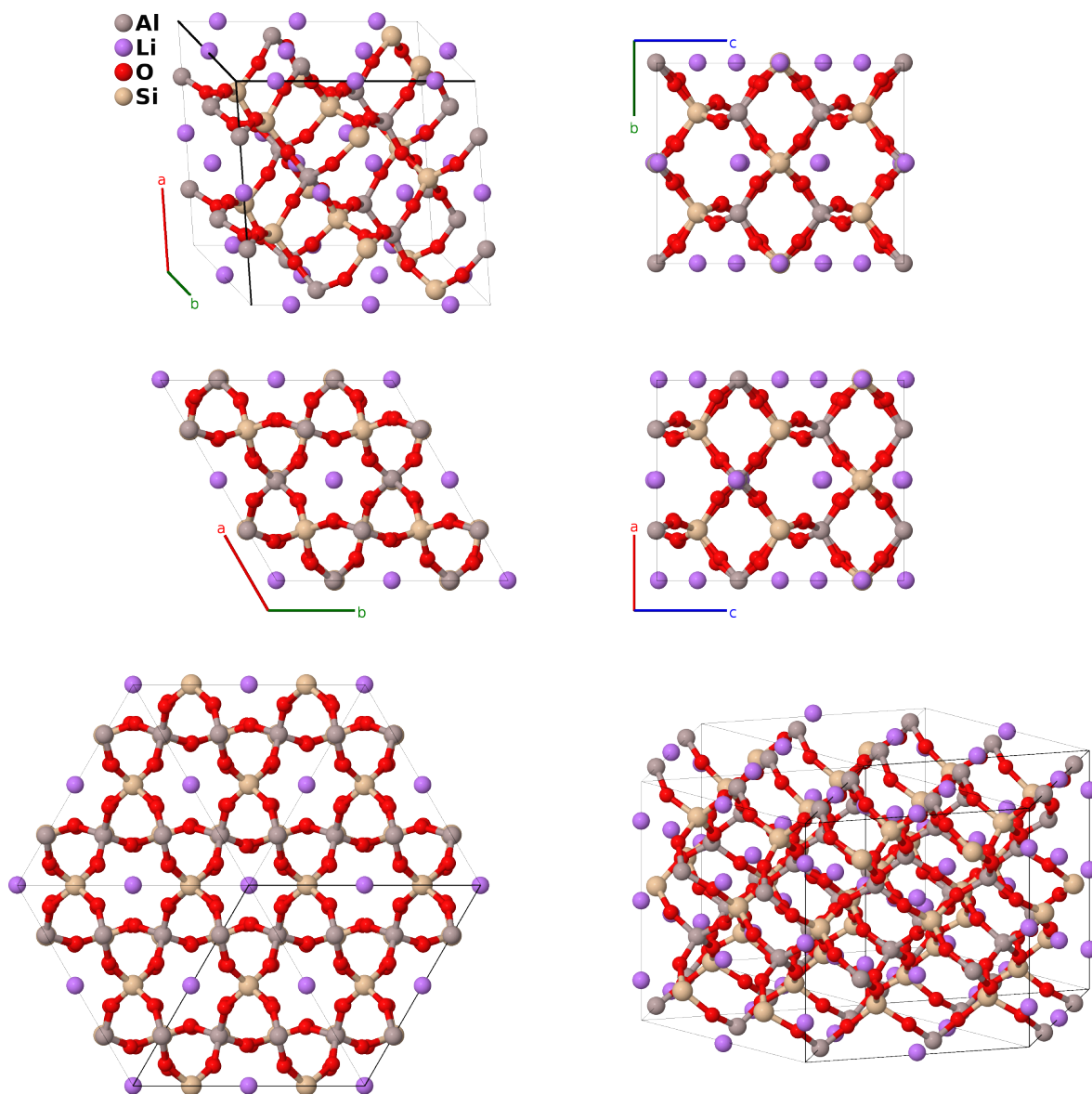


β -Eucryptite (LiAlSiO_4) Structure: ABC4D_hP84_181_gi_bcf_4k_hj-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

<https://aflow.org/p/N1MQ>

https://aflow.org/p/ABC4D_hP84_181_gi_bcf_4k_hj-001



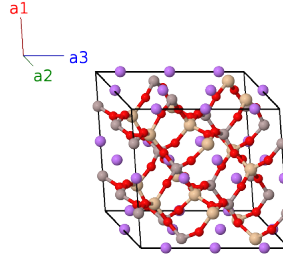
Prototype	AlLiO_4Si
AFLOW prototype label	ABC4D_hP84_181_gi_bcf_4k_hj-001
Mineral name	eucryptite
ICSD	22010

Pearson symbol	hP84
Space group number	181
Space group symbol	$P6_422$
AFLOW prototype command	aflow --proto=ABC4D_hP84_181_gi_bcf_4k_hj-001 --params= $a, c/a, z_3, x_4, x_5, x_6, x_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}$

- We use the data taken by (Pillars, 1973) at 23°C.
- α -eucryptite takes on the rhombohedral LiZnPO_4 structure (Daniels, 2001).
- This structure can also be found in the enantiomorphic space group $P6_222$ #180.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(3b)	Li I
\mathbf{B}_2	$= \frac{5}{6} \mathbf{a}_3$	$=$	$\frac{5}{6}c \hat{\mathbf{z}}$	(3b)	Li I
\mathbf{B}_3	$= \frac{1}{6} \mathbf{a}_3$	$=$	$\frac{1}{6}c \hat{\mathbf{z}}$	(3b)	Li I
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}}$	(3c)	Li II
\mathbf{B}_5	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3c)	Li II
\mathbf{B}_6	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{2}{3}c \hat{\mathbf{z}}$	(3c)	Li II
\mathbf{B}_7	$= \frac{1}{2} \mathbf{a}_1 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6f)	Li III
\mathbf{B}_8	$= \frac{1}{2} \mathbf{a}_2 + (z_3 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + c(z_3 + \frac{1}{3}) \hat{\mathbf{z}}$	(6f)	Li III
\mathbf{B}_9	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_3 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{3}c(3z_3 + 2) \hat{\mathbf{z}}$	(6f)	Li III
\mathbf{B}_{10}	$= \frac{1}{2} \mathbf{a}_2 - (z_3 - \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} - c(z_3 - \frac{1}{3}) \hat{\mathbf{z}}$	(6f)	Li III
\mathbf{B}_{11}	$= \frac{1}{2} \mathbf{a}_1 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(6f)	Li III
\mathbf{B}_{12}	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_3 - \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{3}c(3z_3 - 2) \hat{\mathbf{z}}$	(6f)	Li III
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1$	$=$	$\frac{1}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}}$	(6g)	Al I
\mathbf{B}_{14}	$= x_4 \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(6g)	Al I
\mathbf{B}_{15}	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{2}{3}c \hat{\mathbf{z}}$	(6g)	Al I
\mathbf{B}_{16}	$= -x_4 \mathbf{a}_1$	$=$	$-\frac{1}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}}$	(6g)	Al I
\mathbf{B}_{17}	$= -x_4 \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(6g)	Al I
\mathbf{B}_{18}	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{2}{3}c \hat{\mathbf{z}}$	(6g)	Al I
\mathbf{B}_{19}	$= x_5 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6h)	Si I

$$\mathbf{B}_{81} = \begin{matrix} -x_{11} \mathbf{a}_1 - (x_{11} - y_{11}) \mathbf{a}_2 - \\ (z_{11} - \frac{2}{3}) \mathbf{a}_3 \end{matrix} = \begin{matrix} -\frac{1}{2}a(2x_{11} - y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{11} \hat{\mathbf{y}} - \\ \frac{1}{3}c(3z_{11} - 2) \hat{\mathbf{z}} \end{matrix} \quad (12k) \quad \text{O IV}$$

$$\mathbf{B}_{82} = -y_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 - (z_{11} - \frac{1}{3}) \mathbf{a}_3 = \begin{matrix} -\frac{1}{2}a(x_{11} + y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{11} - y_{11}) \hat{\mathbf{y}} - \\ c(z_{11} - \frac{1}{3}) \hat{\mathbf{z}} \end{matrix} \quad (12k) \quad \text{O IV}$$

$$\mathbf{B}_{83} = -(x_{11} - y_{11}) \mathbf{a}_1 + y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 = \begin{matrix} \frac{1}{2}a(-x_{11} + 2y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} \end{matrix} \quad (12k) \quad \text{O IV}$$

$$\mathbf{B}_{84} = \begin{matrix} x_{11} \mathbf{a}_1 + (x_{11} - y_{11}) \mathbf{a}_2 - \\ (z_{11} - \frac{2}{3}) \mathbf{a}_3 \end{matrix} = \begin{matrix} \frac{1}{2}a(2x_{11} - y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{11} \hat{\mathbf{y}} - \\ \frac{1}{3}c(3z_{11} - 2) \hat{\mathbf{z}} \end{matrix} \quad (12k) \quad \text{O IV}$$

References

- [1] W. W. Pillaras and D. R. Peacor, *The Crystal Structure of Beta Eucryptite as a Function of Temperature*, Am. Mineral. **58**, 681–690 (1973).
- [2] P. Daniels and C. A. Fyfe, *Al, Si order in the crystal structure of α -eucryptite (LiAlSiO_4)*, Am. Mineral. **86**, 279–283 (2001).

Found in

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