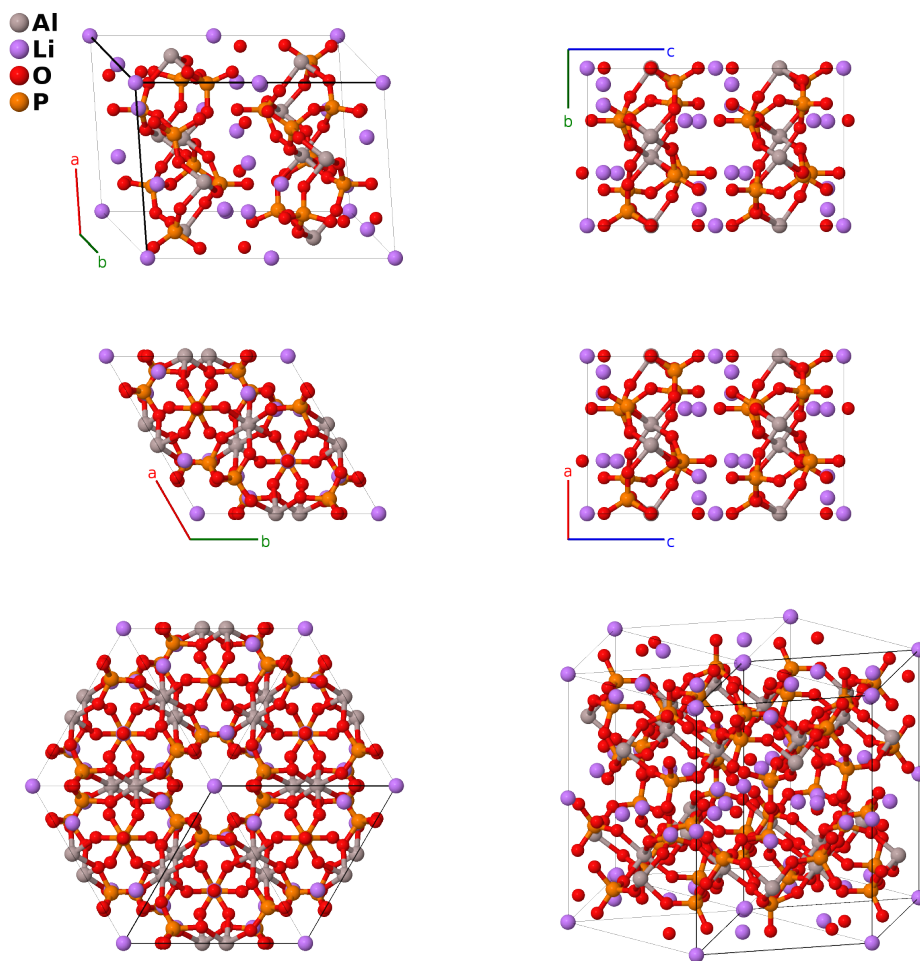


Li₉Al₃(P₂O₇)₃(PO₄)₂ Structure: A3B9C29D8_hP98_165_f_bdg_df4g_dg-001

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<https://aflow.org/p/JRX6>

https://aflow.org/p/A3B9C29D8_hP98_165_f_bdg_df4g_dg-001



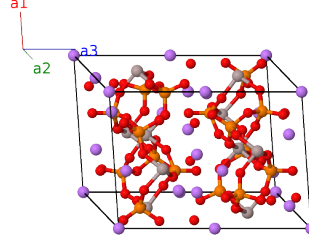
Prototype	Al ₃ Li ₉ O ₂₉ P ₈
AFLOW prototype label	A3B9C29D8_hP98_165_f_bdg_df4g_dg-001
ICSD	50957
Pearson symbol	hP98
Space group number	165
Space group symbol	$P\bar{3}c1$
AFLOW prototype command	aflow --proto=A3B9C29D8_hP98_165_f_bdg_df4g_dg-001 --params=a, c/a, z ₂ , z ₃ , z ₄ , x ₅ , x ₆ , x ₇ , y ₇ , z 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 , x ₁₂ , y ₁₂ , z ₁₂

Other compounds with this structure

$\text{Li}_9\text{Cr}_3(\text{P}_2\text{O}_7)_3(\text{PO}_4)_2$, $\text{Li}_9\text{Ga}_3(\text{P}_2\text{O}_7)_3(\text{PO}_4)_2$, $\text{Li}_9\text{Fe}_3(\text{P}_2\text{O}_7)_3(\text{PO}_4)_2$

Trigonal (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	0	$=$	0	(2b)	Li I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(2b)	Li I
\mathbf{B}_3	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4d)	Li II
\mathbf{B}_4	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	Li II
\mathbf{B}_5	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4d)	Li II
\mathbf{B}_6	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	Li II
\mathbf{B}_7	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4d)	O I
\mathbf{B}_8	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	O I
\mathbf{B}_9	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4d)	O I
\mathbf{B}_{10}	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	O I
\mathbf{B}_{11}	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4d)	P I
\mathbf{B}_{12}	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	P I
\mathbf{B}_{13}	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4d)	P I
\mathbf{B}_{14}	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	P I
\mathbf{B}_{15}	$x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6f)	Al I
\mathbf{B}_{16}	$x_5 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6f)	Al I
\mathbf{B}_{17}	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6f)	Al I
\mathbf{B}_{18}	$-x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6f)	Al I
\mathbf{B}_{19}	$-x_5 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6f)	Al I
\mathbf{B}_{20}	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6f)	Al I
\mathbf{B}_{21}	$x_6 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6f)	O II
\mathbf{B}_{22}	$x_6 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6f)	O II
\mathbf{B}_{23}	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6f)	O II
\mathbf{B}_{24}	$-x_6 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6f)	O II
\mathbf{B}_{25}	$-x_6 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6f)	O II
\mathbf{B}_{26}	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6f)	O II
\mathbf{B}_{27}	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 + y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_7 - y_7) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(12g)	Li III
\mathbf{B}_{28}	$-y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(12g)	Li III

$$\begin{aligned}
\mathbf{B}_{90} &= y_{12} \mathbf{a}_1 + x_{12} \mathbf{a}_2 - \left(z_{12} - \frac{1}{2}\right) \mathbf{a}_3 = \frac{1}{2}a(x_{12} + y_{12}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{12} - y_{12}) \hat{\mathbf{y}} - c\left(z_{12} - \frac{1}{2}\right) \hat{\mathbf{z}} & (12g) & \text{P II} \\
\mathbf{B}_{91} &= \begin{pmatrix} (x_{12} - y_{12}) \mathbf{a}_1 - y_{12} \mathbf{a}_2 - \\ (z_{12} - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \frac{1}{2}a(x_{12} - 2y_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{12} \hat{\mathbf{y}} - c\left(z_{12} - \frac{1}{2}\right) \hat{\mathbf{z}} & (12g) & \text{P II} \\
\mathbf{B}_{92} &= \begin{pmatrix} -x_{12} \mathbf{a}_1 - (x_{12} - y_{12}) \mathbf{a}_2 - \\ (z_{12} - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -\frac{1}{2}a(2x_{12} - y_{12}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{12} \hat{\mathbf{y}} - c\left(z_{12} - \frac{1}{2}\right) \hat{\mathbf{z}} & (12g) & \text{P II} \\
\mathbf{B}_{93} &= -x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3 = -\frac{1}{2}a(x_{12} + y_{12}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{12} - y_{12}) \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}} & (12g) & \text{P II} \\
\mathbf{B}_{94} &= y_{12} \mathbf{a}_1 - (x_{12} - y_{12}) \mathbf{a}_2 - z_{12} \mathbf{a}_3 = \frac{1}{2}a(-x_{12} + 2y_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{12} \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}} & (12g) & \text{P II} \\
\mathbf{B}_{95} &= \begin{pmatrix} (x_{12} - y_{12}) \mathbf{a}_1 + x_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3 \end{pmatrix} = \frac{1}{2}a(2x_{12} - y_{12}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{12} \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}} & (12g) & \text{P II} \\
\mathbf{B}_{96} &= \begin{pmatrix} -y_{12} \mathbf{a}_1 - x_{12} \mathbf{a}_2 + (z_{12} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -\frac{1}{2}a(x_{12} + y_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{12} - y_{12}) \hat{\mathbf{y}} + c\left(z_{12} + \frac{1}{2}\right) \hat{\mathbf{z}} & (12g) & \text{P II} \\
\mathbf{B}_{97} &= \begin{pmatrix} -(x_{12} - y_{12}) \mathbf{a}_1 + y_{12} \mathbf{a}_2 + \\ (z_{12} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \frac{1}{2}a(-x_{12} + 2y_{12}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{12} \hat{\mathbf{y}} + c\left(z_{12} + \frac{1}{2}\right) \hat{\mathbf{z}} & (12g) & \text{P II} \\
\mathbf{B}_{98} &= \begin{pmatrix} x_{12} \mathbf{a}_1 + (x_{12} - y_{12}) \mathbf{a}_2 + \\ (z_{12} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \frac{1}{2}a(2x_{12} - y_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{12} \hat{\mathbf{y}} + c\left(z_{12} + \frac{1}{2}\right) \hat{\mathbf{z}} & (12g) & \text{P II}
\end{aligned}$$

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