

Trigonal $\text{Li}_4\text{P}_2\text{O}_7$ Structure:

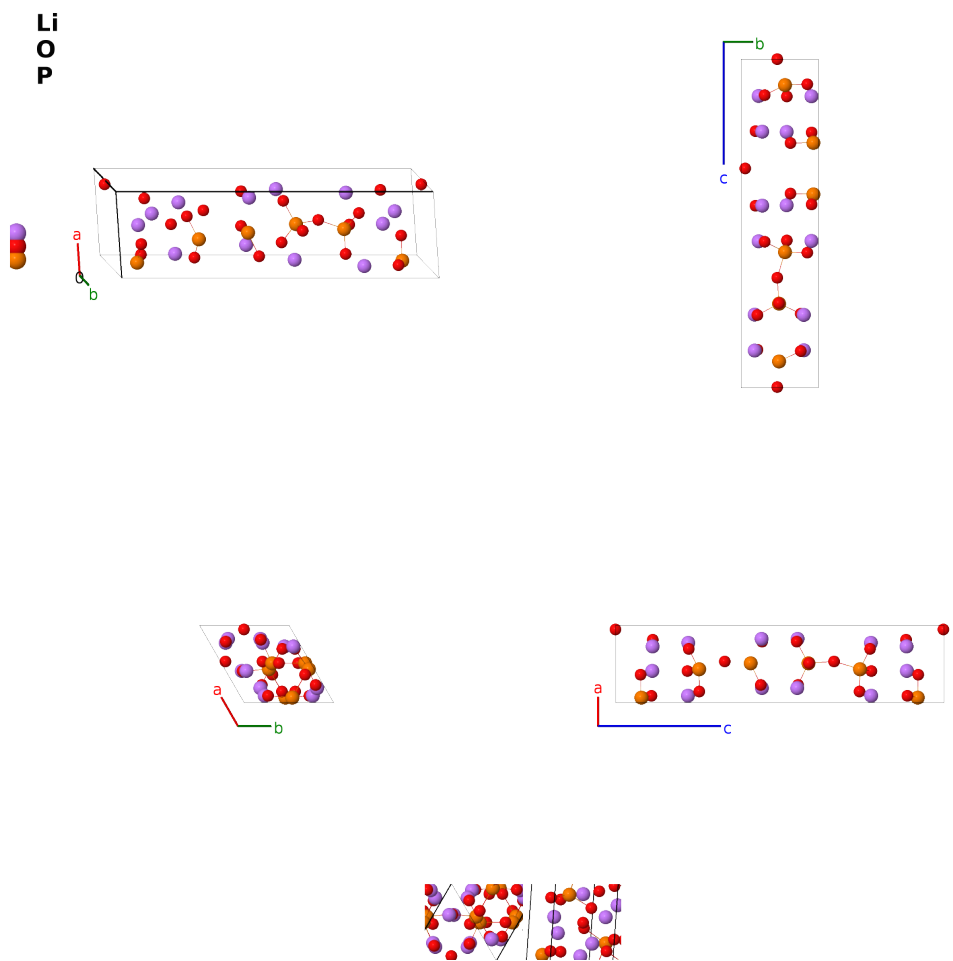
A4B7C2_hP39_153_2c_a3c_c-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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/prototype-encyclopedia/E8GQ>

https://aflow.org/prototype-encyclopedia/A4B7C2_hP39_153_2c_a3c_c-001

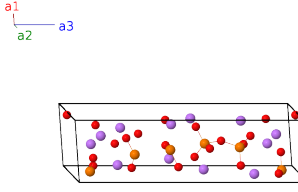


Prototype	$\text{Li}_4\text{O}_7\text{P}_2$
AFLOW prototype label	A4B7C2_hP39_153_2c_a3c_c-001
ICSD	130427
CCDC	1867263
Pearson symbol	hP39
Space group number	153
Space group symbol	$P3_212$

AFLOW prototype command `aflow --proto=A4B7C2_hP39_153_2c_a3c_c-001`
 `--params=a, c/a, x1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7`

- This is a metastable state prepared from the melt. (Raguž, 2019) also found a triclinic phase.
- Space group $P3_212$ #153 is chiral, Sohncke Class 2, and so this structure should also appear in the enantiomorphic space group $P3_112$ #151, but we have not found any references to that structure in the literature.

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
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_1 \hat{\mathbf{y}} + \frac{2}{3}c \hat{\mathbf{z}}$	(3a)	O I
$\mathbf{B}_2$	$= x_1 \mathbf{a}_1 + 2x_1 \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3a)	O I
$\mathbf{B}_3$	$= -2x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2$	$=$	$-\frac{3}{2}ax_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}}$	(3a)	O I
$\mathbf{B}_4$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(6c)	Li I
$\mathbf{B}_5$	$= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 - 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{1}{3}c(3z_2 + 2) \hat{\mathbf{z}}$	(6c)	Li I
$\mathbf{B}_6$	$= -(x_2 - y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + (z_2 + \frac{1}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	Li I
$\mathbf{B}_7$	$= -y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - (z_2 - \frac{1}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} - c(z_2 - \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	Li I
$\mathbf{B}_8$	$= -(x_2 - y_2) \mathbf{a}_1 + y_2 \mathbf{a}_2 - (z_2 - \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_2 + 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} - \frac{1}{3}c(3z_2 - 2) \hat{\mathbf{z}}$	(6c)	Li I
$\mathbf{B}_9$	$= x_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(6c)	Li I
$\mathbf{B}_{10}$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6c)	Li II
$\mathbf{B}_{11}$	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{3}c(3z_3 + 2) \hat{\mathbf{z}}$	(6c)	Li II
$\mathbf{B}_{12}$	$= -(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{1}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	Li II
$\mathbf{B}_{13}$	$= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - (z_3 - \frac{1}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} - c(z_3 - \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	Li II
$\mathbf{B}_{14}$	$= -(x_3 - y_3) \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_3 + 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} - \frac{1}{3}c(3z_3 - 2) \hat{\mathbf{z}}$	(6c)	Li II
$\mathbf{B}_{15}$	$= x_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(6c)	Li II
$\mathbf{B}_{16}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6c)	O II

$$\begin{aligned}
\mathbf{B}_{17} &= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{1}{(z_4 + \frac{2}{3})} \mathbf{a}_3 &= \frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{3}c(3z_4 + 2) \hat{\mathbf{z}} &(6c) & \text{O II} \\
\mathbf{B}_{18} &= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{(z_4 + \frac{1}{3})} \mathbf{a}_3 &= -\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{3}) \hat{\mathbf{z}} &(6c) & \text{O II} \\
\mathbf{B}_{19} &= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - (z_4 - \frac{1}{3}) \mathbf{a}_3 &= -\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} - c(z_4 - \frac{1}{3}) \hat{\mathbf{z}} &(6c) & \text{O II} \\
\mathbf{B}_{20} &= -(x_4 - y_4) \mathbf{a}_1 + y_4 \mathbf{a}_2 - \frac{1}{(z_4 - \frac{2}{3})} \mathbf{a}_3 &= \frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - \frac{1}{3}c(3z_4 - 2) \hat{\mathbf{z}} &(6c) & \text{O II} \\
\mathbf{B}_{21} &= x_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} &(6c) & \text{O II} \\
\mathbf{B}_{22} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= \frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} &(6c) & \text{O III} \\
\mathbf{B}_{23} &= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \frac{1}{(z_5 + \frac{2}{3})} \mathbf{a}_3 &= \frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{3}c(3z_5 + 2) \hat{\mathbf{z}} &(6c) & \text{O III} \\
\mathbf{B}_{24} &= -(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{1}{(z_5 + \frac{1}{3})} \mathbf{a}_3 &= -\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{3}) \hat{\mathbf{z}} &(6c) & \text{O III} \\
\mathbf{B}_{25} &= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - (z_5 - \frac{1}{3}) \mathbf{a}_3 &= -\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} - c(z_5 - \frac{1}{3}) \hat{\mathbf{z}} &(6c) & \text{O III} \\
\mathbf{B}_{26} &= -(x_5 - y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 - \frac{1}{(z_5 - \frac{2}{3})} \mathbf{a}_3 &= \frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - \frac{1}{3}c(3z_5 - 2) \hat{\mathbf{z}} &(6c) & \text{O III} \\
\mathbf{B}_{27} &= x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3 &= \frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} &(6c) & \text{O III} \\
\mathbf{B}_{28} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= \frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} &(6c) & \text{O IV} \\
\mathbf{B}_{29} &= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \frac{1}{(z_6 + \frac{2}{3})} \mathbf{a}_3 &= \frac{1}{2}a(x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + \frac{1}{3}c(3z_6 + 2) \hat{\mathbf{z}} &(6c) & \text{O IV} \\
\mathbf{B}_{30} &= -(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + \frac{1}{(z_6 + \frac{1}{3})} \mathbf{a}_3 &= -\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{3}) \hat{\mathbf{z}} &(6c) & \text{O IV} \\
\mathbf{B}_{31} &= -y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - (z_6 - \frac{1}{3}) \mathbf{a}_3 &= -\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} - c(z_6 - \frac{1}{3}) \hat{\mathbf{z}} &(6c) & \text{O IV} \\
\mathbf{B}_{32} &= -(x_6 - y_6) \mathbf{a}_1 + y_6 \mathbf{a}_2 - \frac{1}{(z_6 - \frac{2}{3})} \mathbf{a}_3 &= \frac{1}{2}a(-x_6 + 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - \frac{1}{3}c(3z_6 - 2) \hat{\mathbf{z}} &(6c) & \text{O IV} \\
\mathbf{B}_{33} &= x_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3 &= \frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(6c) & \text{O IV} \\
\mathbf{B}_{34} &= 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}} &(6c) & \text{P I} \\
\mathbf{B}_{35} &= -y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \frac{1}{(z_7 + \frac{2}{3})} \mathbf{a}_3 &= \frac{1}{2}a(x_7 - 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + \frac{1}{3}c(3z_7 + 2) \hat{\mathbf{z}} &(6c) & \text{P I} \\
\mathbf{B}_{36} &= -(x_7 - y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2 + \frac{1}{(z_7 + \frac{1}{3})} \mathbf{a}_3 &= -\frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{3}) \hat{\mathbf{z}} &(6c) & \text{P I} \\
\mathbf{B}_{37} &= -y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - (z_7 - \frac{1}{3}) \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}} - c(z_7 - \frac{1}{3}) \hat{\mathbf{z}} &(6c) & \text{P I} \\
\mathbf{B}_{38} &= -(x_7 - y_7) \mathbf{a}_1 + y_7 \mathbf{a}_2 - \frac{1}{(z_7 - \frac{2}{3})} \mathbf{a}_3 &= \frac{1}{2}a(-x_7 + 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} - \frac{1}{3}c(3z_7 - 2) \hat{\mathbf{z}} &(6c) & \text{P I} \\
\mathbf{B}_{39} &= x_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3 &= \frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} &(6c) & \text{P I}
\end{aligned}$$

References

- [1] B. Raguž, K. Wittich, and R. Glaum, *Two New, Metastable Polymorphs of Lithium Pyrophosphate $\text{Li}_4\text{P}_2\text{O}_7$* , Eur. J. Inorg. Chem. **2019**, 1688–1696 (2019), doi:10.1002/ejic.201801100.

Found in

- [1] *Inorganic Crystal Structure Database*. Entry 130427 ($\text{Li}_2\text{P}_2\text{O}_7$).

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