

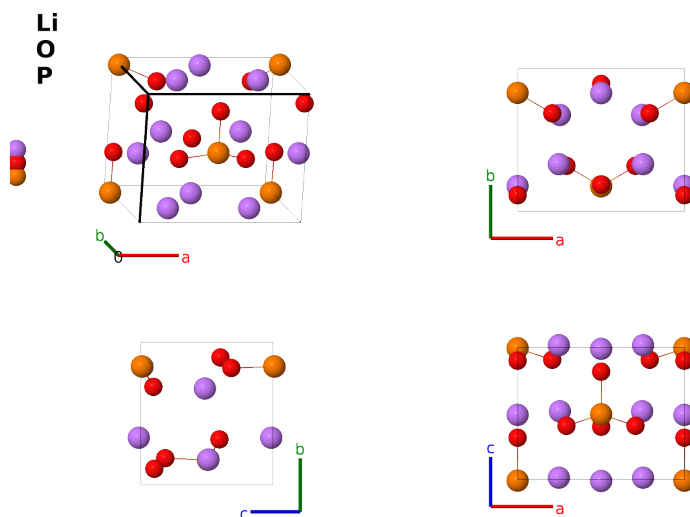
β -Li₃PO₄ Structure: A3B4C_oP16_31_ab_2ab_a-002

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<https://aflow.org/prototype-encyclopedia/0L2F>

https://aflow.org/prototype-encyclopedia/A3B4C_oP16_31_ab_2ab_a-002



Prototype	Li ₃ O ₄ P
AFLOW prototype label	A3B4C_oP16_31_ab_2ab_a-002
ICSD	257439
CCDC	1928155
Pearson symbol	oP16
Space group number	31
Space group symbol	$Pmn2_1$
AFLOW prototype command	<pre>aflow --proto=A3B4C_oP16_31_ab_2ab_a-002 --params=a,b/a,c/a,y1,z1,y2,z2,y3,z3,y4,z4,x5,y5,z5,x6,y6,z6</pre>

Other compounds with this structure

Li₂CoSiO₄, Li₂FeSiO₄, Li₂MnSiO₄

- Li₃PO₄ exists in three known phases (Popović, 2003):
 - α -Li₃PO₄, stable from 1170°C to the melting point at 1220°C, has an uncertain crystal structure.
 - β -Li₃PO₄ (this structure) is the ground state and is stable up to 500°.
 - γ -Li₃PO₄ (Li₂CdSiO₄ structure) is the intermediate phase, and is metastable at room temperature.

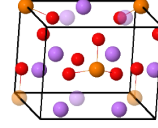
Simple Orthorhombic primitive vectors



$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(2a)	Li I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Li I
$\mathbf{B}_3$	$= y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_5$	$= y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B}_7$	$= y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2a)	P I
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	P I
$\mathbf{B}_9$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4b)	Li II
$\mathbf{B}_{10}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Li II
$\mathbf{B}_{11}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Li II
$\mathbf{B}_{12}$	$= -x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4b)	Li II
$\mathbf{B}_{13}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4b)	O III
$\mathbf{B}_{14}$	$= -(x_6 - \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	O III
$\mathbf{B}_{15}$	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	O III
$\mathbf{B}_{16}$	$= -x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4b)	O III

References

- [1] N. I. P. Ayu, E. Kartini, L. D. Prayogi, M. Faisal, and Supardi, *Crystal structure analysis of Li_3PO_4 powder prepared by wet chemical reaction and solid-state reaction by using X-ray diffraction (XRD)*, *Ionics* **22**, 1051–1057 (2016), doi:10.1007/s11581-016-1643-z.
- [2] L. Popović, B. Manoun, D. de Waal, M. K. Nieuwoudt, and J. D. Comins, *Raman spectroscopic study of phase transitions in Li_3PO_4* , *J. Raman Spectrosc.* **34**, 77–83 (2003), doi:10.1002/jrs.954.

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