β-Li_3PO_4 Structure: A3B4C_oP16_31_ab_2ab_a-002

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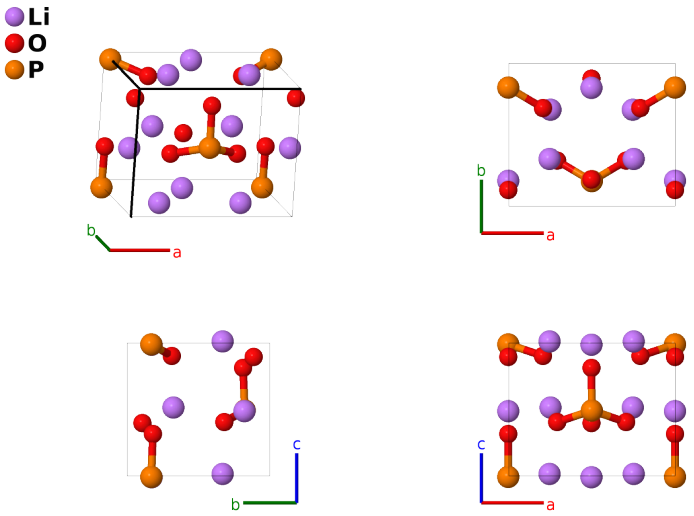
https://aflow.org/p/0L2F

https://aflow.org/p/A3B4C_oP16_31_ab_2ab_a-002



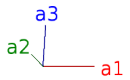
Prototype	Li_3O_4P
AFLOW prototype label	A3B4C_oP16_31_ab_2ab_a-002
ICSD	257439
Pearson symbol	oP16
Space group number	31
Space group symbol	$Pmn2_1$
AFLOW prototype command	`aflow --proto=A3B4C_oP16_31_ab_2ab_a-002 --params=`$a, b/a, c/a, y_1, z_1, y_2, z_2, y_3, z_3, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

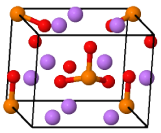
Other compounds with this structure
Li_2CoSiO_4, Li_2FeSiO_4, Li_2MnSiO_4

- Li_3PO_4 exists in three known phases (Popović, 2003):
  - α-Li_3PO_4, stable from 1170°C to the melting point at 1220°C, has an uncertain crystal structure.
  - β-Li_3PO_4 (this structure) is the ground state and is stable up to 500°.
  - γ-Li_3PO_4 (Li_2CdSiO_4 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
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{10}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4b)	Li II
$\mathbf{B_{11}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{14}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4b)	O III
$\mathbf{B_{15}}$	=	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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.