α-Li_3PS_4 Structure: A2BC4_oP28_60_d_c_2d-002

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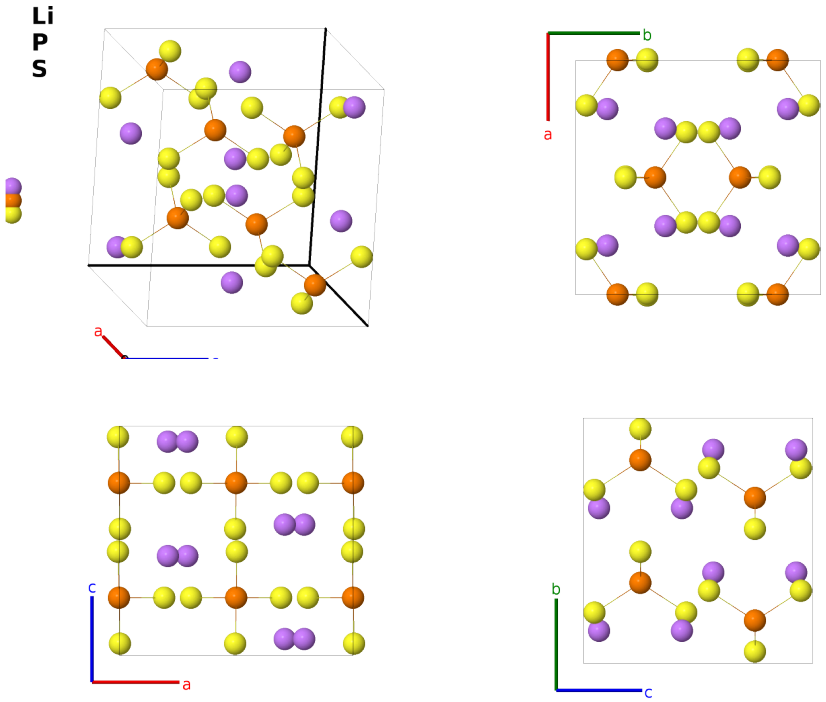
https://aflow.org/prototype-encyclopedia/7NXF

https://aflow.org/prototype-encyclopedia/A2BC4_oP28_60_d_c_2d-002



Prototype	Li_3PS_4
AFLOW prototype label	A2BC4_oP28_60_d_c_2d-002
Pearson symbol	oP28
Space group number	60
Space group symbol	*Pbcn*
AFLOW prototype command	`aflow --proto=A2BC4_oP28_60_d_c_2d-002 --params=`$a, b/a, c/a, y_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4$

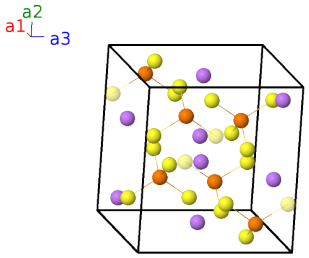
- Li_3PS_4 is known to exist in four forms (Homma, 2011):
  - γ-Li_3PS_4, the ground state, is stable below 573K in the enargite ($H2_5$) structure.
  - β-Li_3PS_4 is stable between 573 and 746K.
  - α-Li_3PS_4 (this structure) is stable above 746K.

  - δ-Li_3PS_4 is a predicted high-pressure phase.

- The astute reader will note that we have left 1/3 of the lithium atoms unaccounted for. (Homma, 2010) could not find the positions of these atoms. As Li_3PS_4 is a superionic conductor it is possible that these atoms move freely through the structure.
- Data for this structure was taken at 906K.
- CaB_2O_4 I and α-Li_3PO_4 have the same AFLOW prototype label, A2BC4_oP28_60_d_c_2d. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

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
$\mathbf{B_1}$	=	$y_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B_3}$	=	$-y_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8d)	Li I
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Li I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Li I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8d)	Li I
$\mathbf{B_9}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8d)	Li I
$\mathbf{B_{10}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Li I
$\mathbf{B_{11}}$	=	$x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Li I
$\mathbf{B_{12}}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8d)	Li I
$\mathbf{B_{13}}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8d)	S I
$\mathbf{B_{14}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	S I
$\mathbf{B_{15}}$	=	$-x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	S I
$\mathbf{B_{16}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8d)	S I
$\mathbf{B_{17}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8d)	S I

$$\mathbf{B_{18}} = \left(x_3+\tfrac{1}{2}\right)\mathbf{a}_1+\left(y_3+\tfrac{1}{2}\right)\mathbf{a}_2-\left(z_3-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_3+\tfrac{1}{2}\right)\hat{\mathbf{x}}+b\left(y_3+\tfrac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_3-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{S I}$$

$$\mathbf{B_{19}} = x_3\,\mathbf{a}_1-y_3\,\mathbf{a}_2+\left(z_3+\tfrac{1}{2}\right)\mathbf{a}_3 = ax_3\,\hat{\mathbf{x}}-by_3\,\hat{\mathbf{y}}+c\left(z_3+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{S I}$$

$$\mathbf{B_{20}} = -\left(x_3-\tfrac{1}{2}\right)\mathbf{a}_1+\left(y_3+\tfrac{1}{2}\right)\mathbf{a}_2+z_3\,\mathbf{a}_3 = -a\left(x_3-\tfrac{1}{2}\right)\hat{\mathbf{x}}+b\left(y_3+\tfrac{1}{2}\right)\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}} \quad (8d) \quad \text{S I}$$

$$\mathbf{B_{21}} = x_4\,\mathbf{a}_1+y_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3 = ax_4\,\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}} \quad (8d) \quad \text{S II}$$

$$\mathbf{B_{22}} = -\left(x_4-\tfrac{1}{2}\right)\mathbf{a}_1-\left(y_4-\tfrac{1}{2}\right)\mathbf{a}_2+\left(z_4+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_4-\tfrac{1}{2}\right)\hat{\mathbf{x}}-b\left(y_4-\tfrac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_4+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{S II}$$

$$\mathbf{B_{23}} = -x_4\,\mathbf{a}_1+y_4\,\mathbf{a}_2-\left(z_4-\tfrac{1}{2}\right)\mathbf{a}_3 = -ax_4\,\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}-c\left(z_4-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{S II}$$

$$\mathbf{B_{24}} = \left(x_4+\tfrac{1}{2}\right)\mathbf{a}_1-\left(y_4-\tfrac{1}{2}\right)\mathbf{a}_2-z_4\,\mathbf{a}_3 = a\left(x_4+\tfrac{1}{2}\right)\hat{\mathbf{x}}-b\left(y_4-\tfrac{1}{2}\right)\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}} \quad (8d) \quad \text{S II}$$

$$\mathbf{B_{25}} = -x_4\,\mathbf{a}_1-y_4\,\mathbf{a}_2-z_4\,\mathbf{a}_3 = -ax_4\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}} \quad (8d) \quad \text{S II}$$

$$\mathbf{B_{26}} = \left(x_4+\tfrac{1}{2}\right)\mathbf{a}_1+\left(y_4+\tfrac{1}{2}\right)\mathbf{a}_2-\left(z_4-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_4+\tfrac{1}{2}\right)\hat{\mathbf{x}}+b\left(y_4+\tfrac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_4-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{S II}$$

$$\mathbf{B_{27}} = x_4\,\mathbf{a}_1-y_4\,\mathbf{a}_2+\left(z_4+\tfrac{1}{2}\right)\mathbf{a}_3 = ax_4\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}+c\left(z_4+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8d) \quad \text{S II}$$

$$\mathbf{B_{28}} = -\left(x_4-\tfrac{1}{2}\right)\mathbf{a}_1+\left(y_4+\tfrac{1}{2}\right)\mathbf{a}_2+z_4\,\mathbf{a}_3 = -a\left(x_4-\tfrac{1}{2}\right)\hat{\mathbf{x}}+b\left(y_4+\tfrac{1}{2}\right)\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}} \quad (8d) \quad \text{S II}$$

References

[1] K. Homma, M. Yonemura, M. Nagao, M. Hirayama, and R. Kanno, *Crystal Structure of High-Temperature Phase of Lithium Ionic Conductor, Li_3PS_4*, J. Phys. Soc. Jpn. **79**, 90–93 (2010), doi:10.1143/JPSJS.79SA.90.

Found in

[1] K. Homma, M. Yonemura, T. Kobayashi, M. Nagao, M. Hirayama, and R. Kanno, *Crystal structure and phase transitions of the lithium ionic conductor Li_3PS_4*, Solid State Ionics **182**, 53–58 (2011), doi:10.1016/j.ssi.2010.10.001.

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