

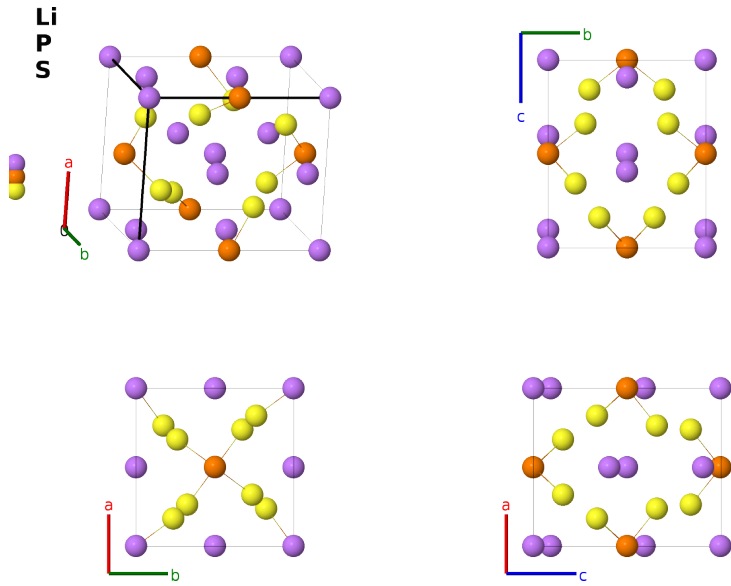
Theoretical δ -Li₃PS₄ Structure: A3BC4_tP16_114_ad_b_e-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, 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/KJ7L>

https://aflow.org/prototype-encyclopedia/A3BC4_tP16_114_ad_b_e-001



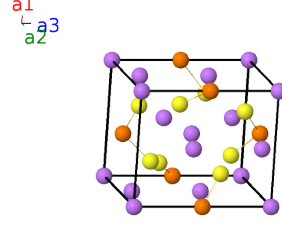
Prototype	Li ₃ PS ₄
AFLOW prototype label	A3BC4_tP16_114_ad_b_e-001
Pearson symbol	tP16
Space group number	114
Space group symbol	$P\bar{4}2_1c$
AFLOW prototype command	<code>aflow --proto=A3BC4_tP16_114_ad_b_e-001 --params=a, c/a, z₃, x₄, y₄, z₄</code>

- Li₃PS₄ is known to exist in four forms (Homma, 2011):
 - γ -Li₃PS₄, the ground state, is stable below 573K in the enargite ($H2_5$) structure.
 - β -Li₃PS₄ is stable between 573 and 746K.
 - α -Li₃PS₄ is stable above 746K.
 - δ -Li₃PS₄ (this structure) is a predicted high-pressure phase.
- This is a computational prediction of the δ -Li₃PS₄ structure, calculated at 10 GPa.

- AFLOW shifts the origin by $c/2$ along the $\hat{z}$ -axis, moving the Li I atoms from the (2b) to the (2a) Wyckoff positions.

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(2a)	Li I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2a)	Li I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	(2b)	P I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(2b)	P I
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4d)	Li II
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_3 \hat{\mathbf{z}}$	(4d)	Li II
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_1 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	Li II
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	Li II
$\mathbf{B}_9$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8e)	S I
$\mathbf{B}_{10}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8e)	S I
$\mathbf{B}_{11}$	$= y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8e)	S I
$\mathbf{B}_{12}$	$= -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8e)	S I
$\mathbf{B}_{13}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	S I
$\mathbf{B}_{14}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	S I
$\mathbf{B}_{15}$	$= -(y_4 - \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	S I
$\mathbf{B}_{16}$	$= (y_4 + \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(y_4 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	S I

References

- [1] S. Iikubo, K. Shimoyama, S. Kawano, M. Fujii, K. Yamamoto, M. Matsushita, T. Shinmei, Y. Higo, and H. Ohtani, *Novel stable structure of Li_3PS_4 predicted by evolutionary algorithm under high-pressure*, AIP Adv. **8**, 015008 (2018), doi:10.1063/1.5011401.
- [2] 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.

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5*. Submitted to Computational Materials Science (2026).