

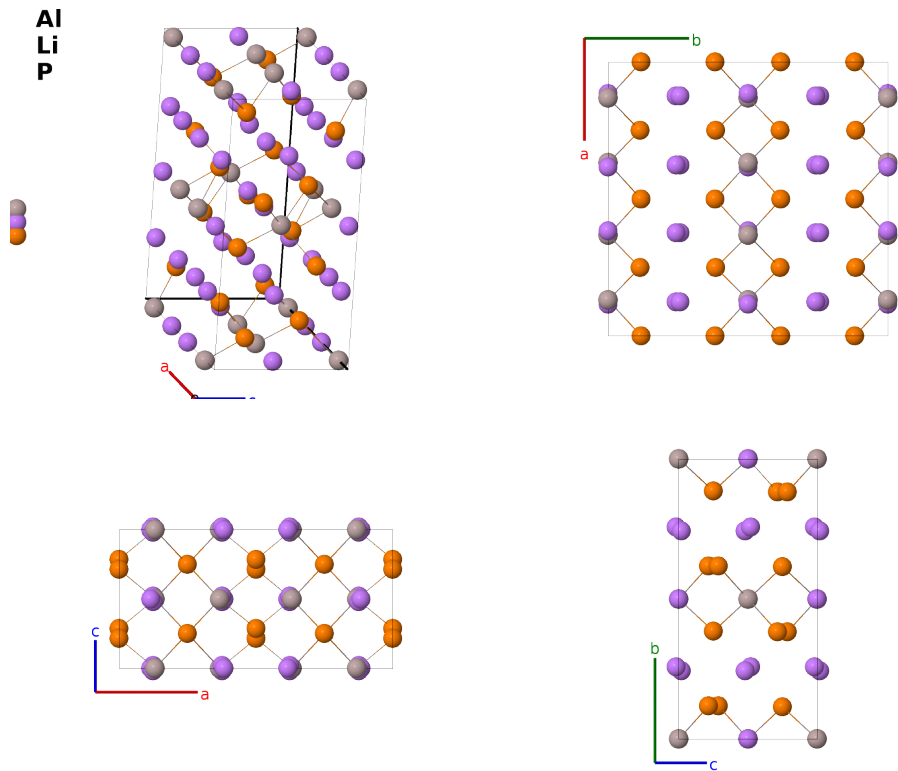
Experimental Li_3AlP_2 Structure: AB3C2_oC48_64_d_dg_ef-001

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<https://aflow.org/prototype-encyclopedia/94E5>

https://aflow.org/prototype-encyclopedia/AB3C2_oC48_64_d_dg_ef-001



Prototype	AlLi_3P_2
AFLOW prototype label	AB3C2_oC48_64_d_dg_ef-001
ICSD	17639
CCDC	1979150
Pearson symbol	oC48
Space group number	64
Space group symbol	$Cmce$
AFLOW prototype command	<code>aflow --proto=AB3C2_oC48_64_d_dg_ef-001</code> <code>--params=a, b/a, c/a, x₁, x₂, y₃, y₄, z₄, x₅, y₅, z₅</code>

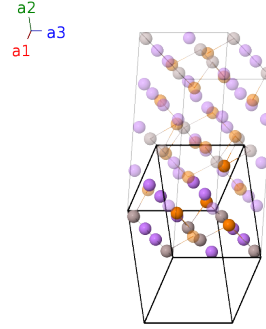
Other compounds with this structure

Li_3GaP_2

- The first experimental information we have for this structure is from (Juza, 1952), who placed the system in space group *Ibca* #71 but could not locate the lithium atoms, except to note that they are on a (16f) site.
- (Dadsetani, 2011) used this work as the starting point for first-principles calculations to minimize the total energy of the structure, including the positions of the lithium atoms, keeping the structure in space group *Ibca*.
- (Restle, 2020) used ball milling and annealing to produce samples of Li_3AlP_2 and Li_3GaP_2 and found them to be in space group *Cmce* #64, shown here. While we believe that this work is correct, we present both structures.

Base-centered Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 =$		$ax_1 \hat{\mathbf{x}}$	(8d)	Al I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$		$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8d)	Al I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 =$		$-ax_1 \hat{\mathbf{x}}$	(8d)	Al I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$		$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8d)	Al I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 =$		$ax_2 \hat{\mathbf{x}}$	(8d)	Li I
$\mathbf{B}_6$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$		$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8d)	Li I
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 =$		$-ax_2 \hat{\mathbf{x}}$	(8d)	Li I
$\mathbf{B}_8$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$		$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8d)	Li I
$\mathbf{B}_9$	$= -\left(y_3 - \frac{1}{4}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{4}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 =$		$\frac{1}{4}a \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8e)	P I
$\mathbf{B}_{10}$	$= \left(y_3 + \frac{1}{4}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{4}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 =$		$\frac{1}{4}a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8e)	P I
$\mathbf{B}_{11}$	$= \left(y_3 + \frac{3}{4}\right) \mathbf{a}_1 - \left(y_3 - \frac{3}{4}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 =$		$\frac{3}{4}a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8e)	P I
$\mathbf{B}_{12}$	$= -\left(y_3 - \frac{3}{4}\right) \mathbf{a}_1 + \left(y_3 + \frac{3}{4}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 =$		$\frac{3}{4}a \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8e)	P I
$\mathbf{B}_{13}$	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 =$		$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8f)	P II
$\mathbf{B}_{14}$	$= \left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 =$		$\frac{1}{2}a \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	P II
$\mathbf{B}_{15}$	$= -\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 =$		$\frac{1}{2}a \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	P II

$$\begin{aligned}
\mathbf{B}_{16} &= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (8f) & \text{P II} \\
\mathbf{B}_{17} &= (x_5 - y_5) \mathbf{a}_1 + (x_5 + 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}} & (16g) & \text{Li II} \\
\mathbf{B}_{18} &= \left(-x_5 + y_5 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_5 + y_5 - \frac{1}{2}\right) \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}} & (16g) & \text{Li II} \\
\mathbf{B}_{19} &= -\left(x_5 + y_5 - \frac{1}{2}\right) \mathbf{a}_1 + \left(-x_5 + y_5 + \frac{1}{2}\right) \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}} & (16g) & \text{Li II} \\
\mathbf{B}_{20} &= (x_5 + y_5) \mathbf{a}_1 + (x_5 - 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}} & (16g) & \text{Li II} \\
\mathbf{B}_{21} &= -(x_5 - y_5) \mathbf{a}_1 - (x_5 + 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}} & (16g) & \text{Li II} \\
\mathbf{B}_{22} &= \left(x_5 - y_5 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_5 + y_5 + \frac{1}{2}\right) \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}} & (16g) & \text{Li II} \\
\mathbf{B}_{23} &= \left(x_5 + y_5 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_5 - y_5 + \frac{1}{2}\right) \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}} & (16g) & \text{Li II} \\
\mathbf{B}_{24} &= -(x_5 + y_5) \mathbf{a}_1 - (x_5 - 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}} & (16g) & \text{Li II}
\end{aligned}$$

References

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