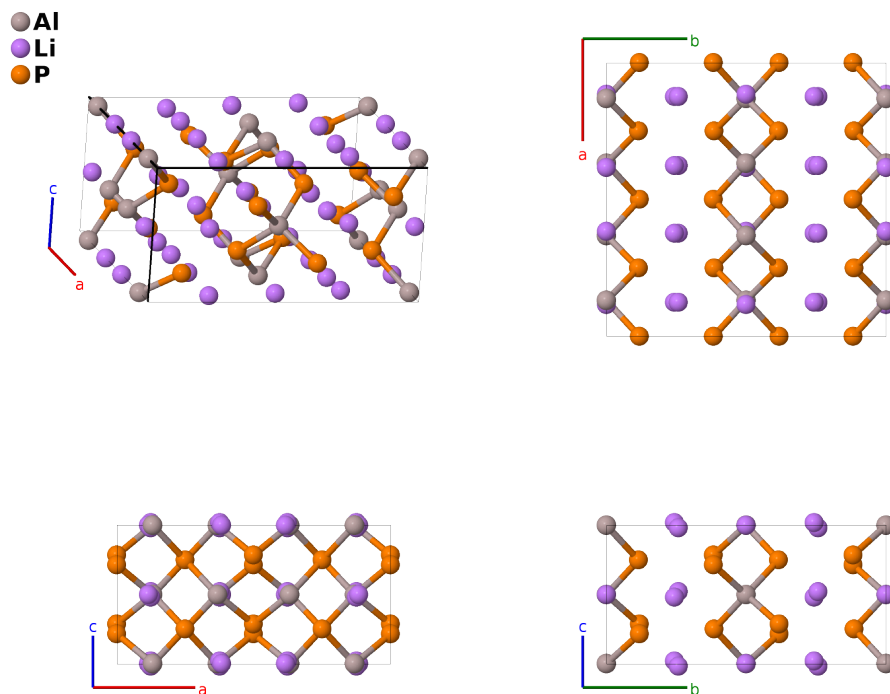


Experimental Li_3AlP_2 Structure: AB3C2_oC48_64_d_dg_ef-001

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<https://afLOW.org/p/94E5>

https://afLOW.org/p/AB3C2_oC48_64_d_dg_ef-001



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

Other compounds with this structure

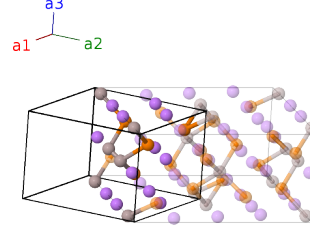
Li_3GaP_2

- 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
\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)	P II
\mathbf{B}_{17}	$= \left(x_5 - y_5\right) \mathbf{a}_1 + \left(x_5 + y_5\right) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5\hat{\mathbf{x}} + by_5\hat{\mathbf{y}} + cz_5\hat{\mathbf{z}}$	(16g)	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)	Li II

$$\begin{aligned}
\mathbf{B}_{19} &= \begin{matrix} -(x_5 + y_5 - \frac{1}{2}) \mathbf{a}_1 + \\ (-x_5 + y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}} & (16g) & \text{Li II} \\
\mathbf{B}_{20} &= \begin{matrix} (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 - \\ z_5 \mathbf{a}_3 \end{matrix} = ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} & (16g) & \text{Li II} \\
\mathbf{B}_{21} &= \begin{matrix} -(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 - \\ z_5 \mathbf{a}_3 \end{matrix} = -ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} & (16g) & \text{Li II} \\
\mathbf{B}_{22} &= \begin{matrix} (x_5 - y_5 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_5 + y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}} & (16g) & \text{Li II} \\
\mathbf{B}_{23} &= \begin{matrix} (x_5 + y_5 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_5 - y_5 + \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}} & (16g) & \text{Li II} \\
\mathbf{B}_{24} &= \begin{matrix} -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + \\ z_5 \mathbf{a}_3 \end{matrix} = -ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (16g) & \text{Li II}
\end{aligned}$$

References

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