

β -LiIO₃ Structure:

ABC3_tP40_86_g_g_3g-001

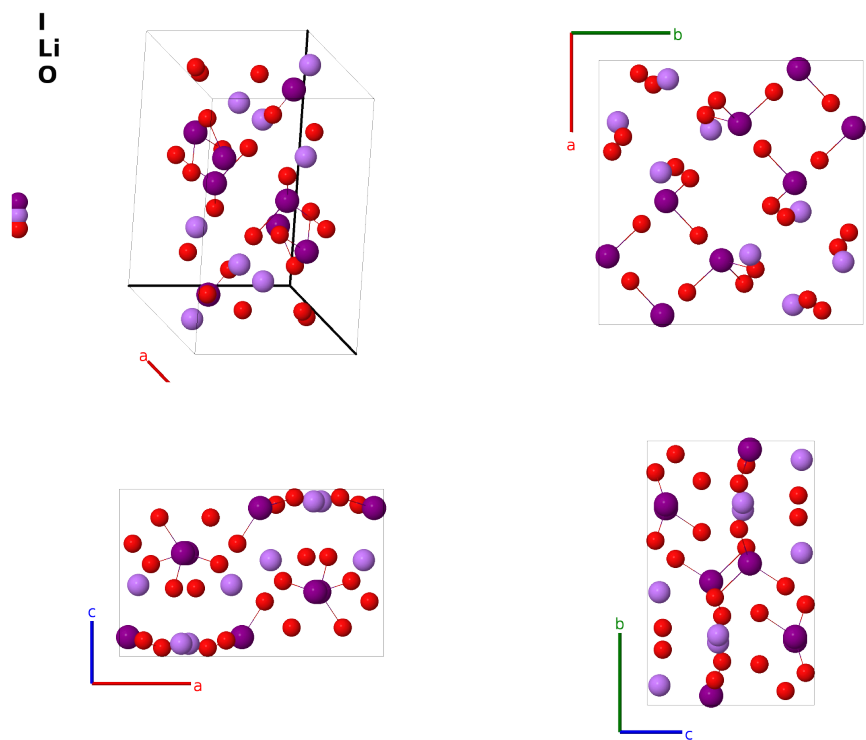
This structure previously used the label(s) **ABC3_tP40_86_g_g_3g**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/9SQG>

https://aflow.org/prototype-encyclopedia/ABC3_tP40_86_g_g_3g-001

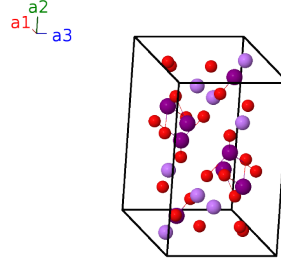


Prototype	ILiO ₃
AFLOW prototype label	ABC3_tP40_86_g_g_3g-001
ICSD	2642
CCDC	1592510
Pearson symbol	tP40
Space group number	86
Space group symbol	$P4_2/n$
AFLOW prototype command	<code>aflow --proto=ABC3_tP40_86_g_g_3g-001</code> <code>--params=a,c/a,x₁,y₁,z₁,x₂,y₂,z₂,x₃,y₃,z₃,x₄,y₄,z₄,x₅,y₅,z₅</code>

- LiIO_3 is known to exist in three forms:
- $\alpha\text{-LiIO}_3$, stable below 470K:
 - (Zachariasen, 1931) originally determined that the structure of $\alpha\text{-LiIO}_3$ was in space group $P6_322$ #182, which (Hermann, 1937) designated *Strukturbericht* $E2_3$.
 - (Rosenzweig, 1966) subsequently determined that this structure was incorrect because of the small sample size, and determined that the true structure was in space group $P6_3$ #173.
- $\beta\text{-LiIO}_3$, stable from 573K up to the melting point at 708K. (this structure)
- $\gamma\text{-LiIO}_3$, stable between the α - and β -phases, with an orthorhombic structure in space group $Pna2_1$ #33.

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
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$a x_1 \hat{\mathbf{x}} + a y_1 \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(8g)	I I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(8g)	I I
$\mathbf{B}_3$	$= -y_1 \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a y_1 \hat{\mathbf{x}} + a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	I I
$\mathbf{B}_4$	$= \left(y_1 + \frac{1}{2}\right) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(y_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a x_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	I I
$\mathbf{B}_5$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-a x_1 \hat{\mathbf{x}} - a y_1 \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(8g)	I I
$\mathbf{B}_6$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(8g)	I I
$\mathbf{B}_7$	$= y_1 \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a y_1 \hat{\mathbf{x}} - a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	I I
$\mathbf{B}_8$	$= -\left(y_1 - \frac{1}{2}\right) \mathbf{a}_1 + x_1 \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(y_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + a x_1 \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	I I
$\mathbf{B}_9$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} + a y_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(8g)	Li I
$\mathbf{B}_{10}$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(8g)	Li I
$\mathbf{B}_{11}$	$= -y_2 \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a y_2 \hat{\mathbf{x}} + a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	Li I
$\mathbf{B}_{12}$	$= \left(y_2 + \frac{1}{2}\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(y_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a x_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	Li I
$\mathbf{B}_{13}$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} - a y_2 \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(8g)	Li I
$\mathbf{B}_{14}$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(8g)	Li I
$\mathbf{B}_{15}$	$= y_2 \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a y_2 \hat{\mathbf{x}} - a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	Li I

$\mathbf{B}_{16}$	$=$	$-\left(y_2 - \frac{1}{2}\right) \mathbf{a}_1 + x_2 \mathbf{a}_2 -$	$=$	$-a\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	Li I
		$\left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$				
$\mathbf{B}_{17}$	$=$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_{18}$	$=$	$-\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 +$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8g)	O I
		$z_3 \mathbf{a}_3$				
$\mathbf{B}_{19}$	$=$	$-y_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 +$	$=$	$-ay_3 \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	O I
		$\left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$				
$\mathbf{B}_{20}$	$=$	$\left(y_3 + \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_{21}$	$=$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_{22}$	$=$	$\left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_{23}$	$=$	$y_3 \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	O I
$\mathbf{B}_{24}$	$=$	$-\left(y_3 - \frac{1}{2}\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 -$	$=$	$-a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	O I
		$\left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$				
$\mathbf{B}_{25}$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B}_{26}$	$=$	$-\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 +$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	O II
		$z_4 \mathbf{a}_3$				
$\mathbf{B}_{27}$	$=$	$-y_4 \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 +$	$=$	$-ay_4 \hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	O II
		$\left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$				
$\mathbf{B}_{28}$	$=$	$\left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B}_{29}$	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B}_{30}$	$=$	$\left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B}_{31}$	$=$	$y_4 \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	O II
$\mathbf{B}_{32}$	$=$	$-\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 -$	$=$	$-a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	O II
		$\left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$				
$\mathbf{B}_{33}$	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B}_{34}$	$=$	$-\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right) \mathbf{a}_2 +$	$=$	$-a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_5 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8g)	O III
		$z_5 \mathbf{a}_3$				
$\mathbf{B}_{35}$	$=$	$-y_5 \mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_2 +$	$=$	$-ay_5 \hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	O III
		$\left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$				
$\mathbf{B}_{36}$	$=$	$\left(y_5 + \frac{1}{2}\right) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(y_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B}_{37}$	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B}_{38}$	$=$	$\left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B}_{39}$	$=$	$y_5 \mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B}_{40}$	$=$	$-\left(y_5 - \frac{1}{2}\right) \mathbf{a}_1 + x_5 \mathbf{a}_2 -$	$=$	$-a\left(y_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8g)	O III
		$\left(z_5 - \frac{1}{2}\right) \mathbf{a}_3$				

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