

Li₇Sn₃ Structure:

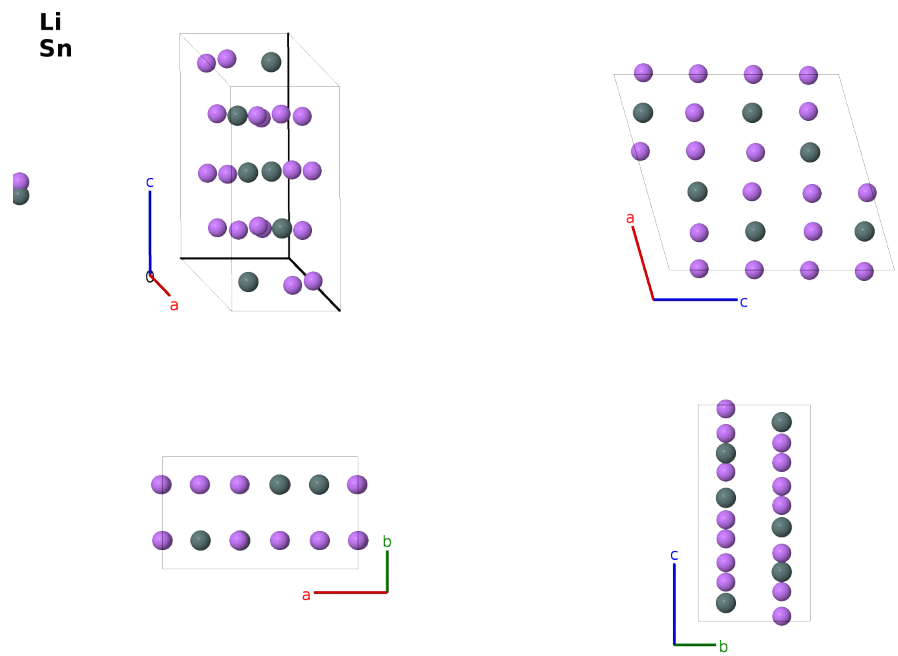
A7B3_mP20_11_7e_3e-001

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<https://aflow.org/prototype-encyclopedia/YDAL>

https://aflow.org/prototype-encyclopedia/A7B3_mP20_11_7e_3e-001

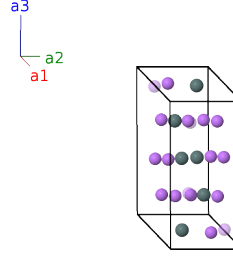


Prototype	Li ₇ Sn ₃
AFLOW prototype label	A7B3_mP20_11_7e_3e-001
ICSD	104785
CCDC	1662686
Pearson symbol	mP20
Space group number	11
Space group symbol	$P2_1/m$
AFLOW prototype command	<pre>aflow --proto=A7B3_mP20_11_7e_3e-001 --params=a,b/a,c/a,β,x₁,z₁,x₂,z₂,x₃,z₃,x₄,z₄,x₅,z₅,x₆,z₆,x₇,z₇,x₈,z₈,x₉,z₉,x₁₀,z₁₀</pre>

- (Müller, 1974) gives this structure in the “unique axis-*c*” setting of space group $P2_1/m$ #11. We used FINDSYM to transform this to the standard “unique axis-*b*” setting.

Simple Monoclinic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(2e)	Li I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(2e)	Li I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(2e)	Li II
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(2e)	Li II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(2e)	Li III
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(2e)	Li III
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(2e)	Li IV
$\mathbf{B}_8$	$= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(2e)	Li IV
$\mathbf{B}_9$	$= x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(2e)	Li V
$\mathbf{B}_{10}$	$= -x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(2e)	Li V
$\mathbf{B}_{11}$	$= x_6 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(2e)	Li VI
$\mathbf{B}_{12}$	$= -x_6 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(2e)	Li VI
$\mathbf{B}_{13}$	$= x_7 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(2e)	Li VII
$\mathbf{B}_{14}$	$= -x_7 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(2e)	Li VII
$\mathbf{B}_{15}$	$= x_8 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(2e)	Sn I
$\mathbf{B}_{16}$	$= -x_8 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(2e)	Sn I
$\mathbf{B}_{17}$	$= x_9 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(2e)	Sn II
$\mathbf{B}_{18}$	$= -x_9 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(2e)	Sn II
$\mathbf{B}_{19}$	$= x_{10} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(2e)	Sn III
$\mathbf{B}_{20}$	$= -x_{10} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_{10} \sin \beta \hat{\mathbf{z}}$	(2e)	Sn III

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