

β -LiSn Structure:

AB_tI24_141_ae_be-001

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<https://aflow.org/prototype-encyclopedia/1GTY>

https://aflow.org/prototype-encyclopedia/AB_tI24_141_ae_be-001

Prototype	LiSn
AFLOW prototype label	AB_tI24_141_ae_be-001
ICSD	107516
CCDC	1665239
Pearson symbol	tI24
Space group number	141
Space group symbol	$I4_1/amd$
AFLOW prototype command	<code>aflow --proto=AB_tI24_141_ae_be-001 --params=a, c/a, z₃, z₄</code>

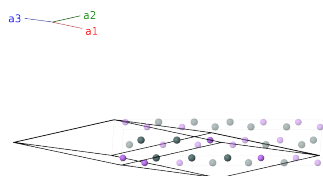
Other compounds with this structure

LiGe

- This is apparently the high-temperature structure of LiSn. Below 470K LiSn is in the monoclinic α -LiSn structure (Villars, 2018).
- We have shifted the origin so that a lithium atom is on the (4a) site.

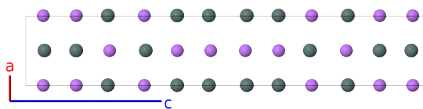
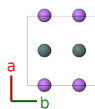
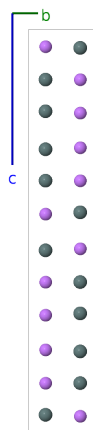
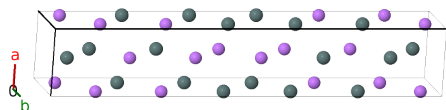
Body-centered Tetragonal primitive vectors

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



Basis vectors

Li
Sn



	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{7}{8} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{8} c \hat{\mathbf{z}}$	(4a)	Li I
$\mathbf{B}_2$	$= \frac{1}{8} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{8} c \hat{\mathbf{z}}$	(4a)	Li I
$\mathbf{B}_3$	$= \frac{5}{8} \mathbf{a}_1 + \frac{3}{8} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{8} c \hat{\mathbf{z}}$	(4b)	Sn I
$\mathbf{B}_4$	$= \frac{3}{8} \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{8} c \hat{\mathbf{z}}$	(4b)	Sn I
$\mathbf{B}_5$	$= \left(z_3 + \frac{1}{4}\right) \mathbf{a}_1 + z_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(8e)	Li II
$\mathbf{B}_6$	$= z_3 \mathbf{a}_1 + \left(z_3 + \frac{1}{4}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + c \left(z_3 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(8e)	Li II
$\mathbf{B}_7$	$= -\left(z_3 - \frac{3}{4}\right) \mathbf{a}_1 - z_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(8e)	Li II
$\mathbf{B}_8$	$= -z_3 \mathbf{a}_1 - \left(z_3 - \frac{3}{4}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{4} a \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(8e)	Li II
$\mathbf{B}_9$	$= \left(z_4 + \frac{1}{4}\right) \mathbf{a}_1 + z_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(8e)	Sn II
$\mathbf{B}_{10}$	$= z_4 \mathbf{a}_1 + \left(z_4 + \frac{1}{4}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + c \left(z_4 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(8e)	Sn II
$\mathbf{B}_{11}$	$= -\left(z_4 - \frac{3}{4}\right) \mathbf{a}_1 - z_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{y}} - c z_4 \hat{\mathbf{z}}$	(8e)	Sn II
$\mathbf{B}_{12}$	$= -z_4 \mathbf{a}_1 - \left(z_4 - \frac{3}{4}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{4} a \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(8e)	Sn II

References

- [1] W. Blase and G. Cordier, *Crystal structure of β -Lithium stannide, β -LiSn*, Z. Kristallogr. **193**, 317–318 (1990), doi:10.1524/zkri.1990.193.14.317.
- [2] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. Lithium-Tin Binary Phase Diagram (1998 Sangster J.). Copyright ©2006-2018 ASM International.

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