α-LiSn Structure: AB_mP6_10_bn_cm-001

This structure originally had the label `AB_mP6_10_en_am`. Calls to that address will be redirected here.

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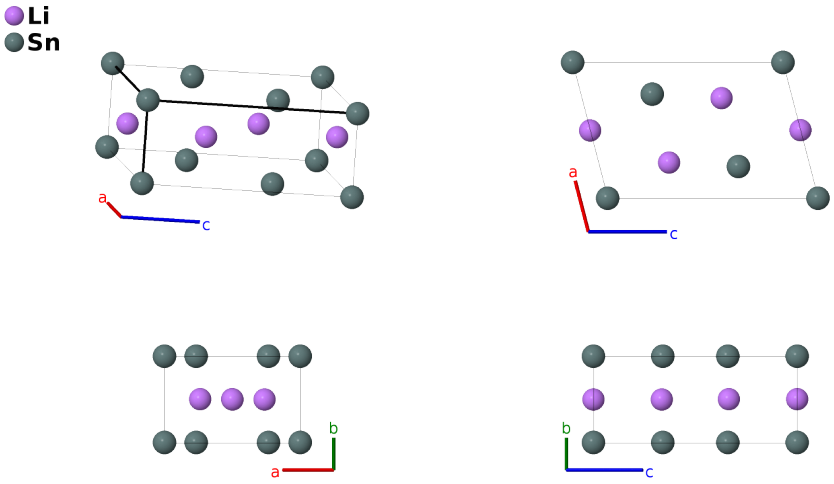
https://aflow.org/p/QVV1

https://aflow.org/p/AB_mP6_10_bn_cm-001

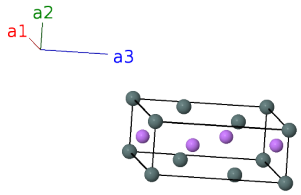


Prototype	LiSn
AFLOW prototype label	AB_mP6_10_bn_cm-001
ICSD	104782
Pearson symbol	mP6
Space group number	10
Space group symbol	$P2/m$
AFLOW prototype command	`aflow --proto=AB_mP6_10_bn_cm-001 --params=`$a, b/a, c/a, \beta, x_3, z_3, x_4, z_4$

- This is the low-temperature structure of LiSn. Above 470K LiSn may transform into the tetragonal β-LiSn structure (Villars, 2018). This structure is apparently metastable at room temperature (Blase, 1990).
- (Müller, 1973) give 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. This involves an origin shift.

Simple Monoclinic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}b\,\hat{\mathbf{y}}$	(1b)	Li I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(1c)	Sn I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(2m)	Sn II
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(2m)	Sn II
$\mathbf{B_5}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(2n)	Li II
$\mathbf{B_6}$	=	$-x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(2n)	Li II

References

[1] W. Müller and H. Schäfer, *Die Kristallstruktur der Phase LiSn*, Z. Naturforsch. B **28**, 246–248 (1973), doi:10.1515/znb-1973-5-604.

[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.