

LiYSn	<i>hP24</i>	(186) $P6_3mc - c^3b^2a$
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LiYSn [1]

Structural features: 3D-framework of fused Y₆ trigonal prisms centered alternatively by Li and Sn. Li and Sn form a distorted wurtzite-type (ZnO) sublattice. Deformation derivative of ZrBeSi.

Steinberg G., Schuster H.U. (1979) [1]

LiSnY

$a = 0.9296$, $c = 0.7346$ nm, $c/a = 0.790$, $V = 0.5498$ nm³, $Z = 8$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Sn1	6 <i>c</i>	. <i>m</i> .	0.17	0.83	0.258		fourcapped trigonal prism Li ₄ Y ₆
Y2	6 <i>c</i>	. <i>m</i> .	0.482	0.518	0.0		16-vertex polyhedron Li ₆ Sn ₆ Y ₄
Li3	6 <i>c</i>	. <i>m</i> .	0.826	0.174	0.18		pseudo Frank-Kasper Sn ₄ Y ₆ Li
Li4	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.312		13-vertex polyhedron Sn ₄ Y ₆ Li ₃
Sn5	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.719		bicapped square prism Li ₄ Y ₆
Y6	2 <i>a</i>	3 <i>m</i> .	0	0	0.0		rhombic dodecahedron Li ₆ Sn ₆ Y ₂

Transformation from published data: origin shift 0 0 0.5

Experimental: single crystal, diffractometer, X-rays, R = 0.096

References: [1] Steinberg G., Schuster H.U. (1979), Z. Naturforsch. B 34, 1165-1166.