

LiScI<sub>3</sub>*hP10*(188) *P-6c2* – kca**LiScI<sub>3</sub>** [1]

Structural features: Close-packed I layers in h stacking; Sc and Li in octahedral voids. ScI<sub>6</sub> octahedra share faces to form infinite columns parallel to [001].

Lachgar A. et al. (1991) [1]

I<sub>3</sub>LiSc $a = 0.72861$ ,  $c = 0.6768$  nm,  $c/a = 0.929$ ,  $V = 0.3112$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
I1	6 <i>k</i>	<i>m</i> ..	0.0041	0.32685	<sup>1</sup> / <sub>4</sub>		non-coplanar square Sc <sub>2</sub> Li <sub>2</sub>
Li2	2 <i>c</i>	3.2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0		octahedron I <sub>6</sub>
Sc3	2 <i>a</i>	3.2	0	0	0		octahedron I <sub>6</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.010

References: [1] Lachgar A., Dudis D.S., Dorhout P.K., Corbett J.D. (1991), Inorg. Chem. 30, 3321-3326.