

LiSmAlF₆*hP*18(182) *P*6₃22 – idca**LiSmAlF₆** [1]; RbSnIO₆ [2]

Structural features: Close-packed F layers in BBCC stacking; Al and Li in octahedral, Sm in trigonal prismatic voids. Infinite slabs of edge-linked AlF₆ and LiF₆ octahedra are interconnected via common vertices with SmF₆ trigonal prisms to form a 3D-framework.

Köhler J., Müller B.G. (1991) [1]

AlF₆LiSm*a* = 0.5079, *c* = 1.0405 nm, *c/a* = 2.049, *V* = 0.2324 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	12 <i>i</i>	1	0.0314	0.3882	0.1502		non-colinear AlLi
Li2	2 <i>d</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		octahedron F ₆
Al3	2 <i>c</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		octahedron F ₆
Sm4	2 <i>a</i>	32.	0	0	0		trigonal prism F ₆

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, wR = 0.016

References: [1] Köhler J., Müller B.G. (1991), Z. Anorg. Allg. Chem. 606, 169-176. [2] Currie D.B., Levason W., Oldroyd R.D., Weller M.T. (1993), J. Mater. Chem. 3, 447-451.