

LiAl[SiO ₄]	<i>hP</i> 93	(180) <i>P</i> 6 ₂ 22 – k ⁴ jihgf ² dca
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LiAlSiO₄ β rt [1], eucryptite β rt

Structural features: AlO₄ and SiO₄ tetrahedra share vertices to form a quartz-like framework with twisted chains; Li in narrow channels of hexagonal cross-section parallel to [001] (partial disorder).

Tscherry V. et al. (1972) [1]

AlLiO₄Si

a = 1.04818, *c* = 1.1175 nm, *c/a* = 1.066, *V* = 1.0633 nm³, *Z* = 12

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	1	0.098	0.203	0.268		non-coplanar triangle SiAlLi
O2	12 <i>k</i>	1	0.112	0.41	0.08433		tetrahedron SiAlLi ₂
O3	12 <i>k</i>	1	0.392	0.088	0.08733		tetrahedron SiAlLi ₂
O4	12 <i>k</i>	1	0.602	0.205	0.258		tetrahedron SiAlLi ₂
Al5	6 <i>j</i>	.2	0.2489	0.4978	¹ / ₂		tetrahedron O ₄
Si6	6 <i>i</i>	.2	0.2526	0.5052	0		tetrahedron O ₄
Al7	6 <i>h</i>	.2	0.2489	0	¹ / ₂		tetrahedron O ₄
Si8	6 <i>g</i>	.2	0.2513	0	0		tetrahedron O ₄
Li9	6 <i>f</i>	2..	¹ / ₂	0	0.1667	0.5	octahedron Li ₂ O ₄
Li10	6 <i>f</i>	2..	¹ / ₂	0	0.3333	0.5	octahedron Li ₂ O ₄
Li11	3 <i>d</i>	222	¹ / ₂	0	¹ / ₂	0.5	octahedron Li ₂ O ₄
Li12	3 <i>c</i>	222	¹ / ₂	0	0	0.5	octahedron Li ₂ O ₄
Li13	3 <i>a</i>	222	0	0	0		tetrahedron O ₄

Transformation from published data (*P*6₄22): new axes -a,-b,-c

Experimental: single crystal, diffractometer, X-rays, R = 0.128

Remarks: Phase stable at T < ~760 K. We took the cell parameters from Part I of the same work [2]. Short interatomic distances for partly occupied site(s). A fully ordered model in the same space group is also proposed (R = 0.057).

References: [1] Tscherry V., Schulz H., Laves F. (1972), Z. Kristallogr. 135, 175-198. [2] Tscherry V., Schulz H., Laves F. (1972), Z. Kristallogr. 135, 161-174.