

LiAl[SiO<sub>4</sub>]*hP*84(180) *P*6<sub>2</sub>22 – k<sup>4</sup>jihgfda**LiAlSiO<sub>4</sub> β rt** [2], eucryptite β rtStructural features: AlO<sub>4</sub> and SiO<sub>4</sub> tetrahedra share vertices to form a quartz-like framework with twisted chains; Li in narrow channels of hexagonal cross-section parallel to [001].

Khosrovani N., Sleight A.W. (1999) [1]

AlLiO<sub>4</sub>Si*a* = 1.0498, *c* = 1.118 nm, *c/a* = 1.065, *V* = 1.0671 nm<sup>3</sup>, *Z* = 12

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	1	0.1	0.401	0.09233		non-colinear SiAl
O2	12 <i>k</i>	1	0.111	0.2	0.257		single atom Al
O3	12 <i>k</i>	1	0.401	0.105	0.09833		single atom Si
O4	12 <i>k</i>	1	0.608	0.2	0.25		non-colinear AlSi
Si5	6 <i>j</i>	..2	0.249	0.498	<sup>1</sup> / <sub>2</sub>		tetrahedron O <sub>4</sub>
Al6	6 <i>i</i>	..2	0.252	0.504	0		tetrahedron O <sub>4</sub>
Si7	6 <i>h</i>	..2	0.245	0	<sup>1</sup> / <sub>2</sub>		tetrahedron O <sub>4</sub>
Al8	6 <i>g</i>	..2	0.249	0	0		tetrahedron O <sub>4</sub>
Li9	6 <i>f</i>	2..	<sup>1</sup> / <sub>2</sub>	0	0.172		tetrahedron O <sub>4</sub>
Li10	3 <i>d</i>	222	<sup>1</sup> / <sub>2</sub>	0	<sup>1</sup> / <sub>2</sub>		tetrahedron O <sub>4</sub>
Li11	3 <i>a</i>	222	0	0	0		tetrahedron O <sub>4</sub>

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

Experimental: powder, diffractometer, neutrons, T = 298 K

Remarks: Phase stable at T &lt; 760 K. Cell parameters taken from figure. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions.

References: [1] Khosrovani N., Sleight A.W. (1999), Int. J. Inorg. Mater. 1, 3-10. [2] Tscherry V., Schulz H. (1970), Naturwissenschaften 57, 194.