

RbLi₇Ge₈*hP*64(186) *P*6₃*mc* – dc⁷b³a²**RbLi₇Ge₈** [1]

Structural features: Ge₁₂ truncated tetrahedra (four six- and four three-membered rings) and Ge₄ tetrahedra; Li at the centers of the truncated tetrahedra, above its hexagonal faces (Friauf polyhedron) and between the units.

Bobev S., Sevov S.C. (2001) [1]

Ge₈Li₇Rb*a* = 0.98946, *c* = 1.6269 nm, *c/a* = 1.644, *V* = 1.3794 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ge1	12 <i>d</i>	1	0.26075	0.00235	0.08845		8-vertex polyhedron Ge ₃ Li ₅
Ge2	6 <i>c</i>	. <i>m</i> .	0.08716	0.91284	0.34133		tricapped trigonal prism Ge ₃ Li ₆
Ge3	6 <i>c</i>	. <i>m</i> .	0.17447	0.82553	0.2178		pseudo Frank-Kasper Ge ₃ Li ₇ Rb
Li4	6 <i>c</i>	. <i>m</i> .	0.431	0.569	0.306		7-vertex polyhedron Li ₃ Ge ₃ Rb
Li5	6 <i>c</i>	. <i>m</i> .	0.516	0.484	0.181		bicapped square prism Li ₃ Ge ₆ Rb
Ge6	6 <i>c</i>	. <i>m</i> .	0.58017	0.41983	0.35708		tricapped trigonal prism Ge ₃ Li ₆
Li7	6 <i>c</i>	. <i>m</i> .	0.8313	0.1687	0.2484		15-vertex Frank-Kasper Ge ₉ Li ₆
Li8	6 <i>c</i>	. <i>m</i> .	0.8402	0.1598	0.4318		square antiprism Ge ₆ Li ₂
Rb9	2 <i>b</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.07112		21-vertex polyhedron Li ₉ Ge ₁₂
Rb10	2 <i>b</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.4389		non-coplanar triangle Li ₃
Ge11	2 <i>b</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.7281		tricapped trigonal prism Ge ₃ Li ₆
Li12	2 <i>a</i>	3 <i>m</i> .	0	0	0.0		pseudo Frank-Kasper Ge ₉ Li ₄
Li13	2 <i>a</i>	3 <i>m</i> .	0	0	0.183		16-vertex Frank-Kasper Li ₄ Ge ₁₂

Transformation from published data: origin shift 0 0 0.149

Experimental: single crystal, diffractometer, X-rays, *R* = 0.036

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions.

References: [1] Bobev S., Sevov S.C. (2001), *Angew. Chem. Int. Ed.* 40, 1507-1510.