

La₁₅Ni_{6.62}Si₁₀*hP*68(176) *P*6₃/*m* – h¹⁰eca**La₁₅Ni_{6.62}Si₁₀** [1]

Structural features: Infinite columns of base-linked SiLa₆Ni₃, SiLa₆(LaNi₂) and SiLa₆(La₂Ni) tricapped trigonal prisms share atoms to form a 3D-framework with AlB₂-type (BaLiSi) columns (16 prisms in the triangular cross-section); additional Ni and Si in channels of hexagonal cross-section parallel to [001] (partial disorder). Variant of Pr₁₅Ni₇Si₁₀.

Prots' Y.M., Jeitschko W. (1998) [1]

La₁₅Ni_{6.62}Si₁₀*a* = 2.0212, *c* = 0.4351 nm, *c/a* = 0.215, *V* = 1.5394 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Si1	6 <i>h</i>	<i>m</i> ..	0.0623	0.2584	1/4		tricapped trigonal prism NiLa ₈
Si2	6 <i>h</i>	<i>m</i> ..	0.1103	0.4851	1/4		tricapped trigonal prism Ni ₂ La ₇
La3	6 <i>h</i>	<i>m</i> ..	0.13183	0.14868	1/4		
Ni4	6 <i>h</i>	<i>m</i> ..	0.1542	0.39517	1/4		tricapped trigonal prism Si ₃ La ₆
Ni5	6 <i>h</i>	<i>m</i> ..	0.19972	0.62056	1/4		tricapped trigonal prism Si ₃ La ₆
Si6	6 <i>h</i>	<i>m</i> ..	0.2899	0.4448	1/4		tricapped trigonal prism Ni ₂ La ₇
La7	6 <i>h</i>	<i>m</i> ..	0.32182	0.12395	1/4		7-capped pentagonal prism Ni ₂ Si ₅ La ₁₀
La8	6 <i>h</i>	<i>m</i> ..	0.35616	0.32177	1/4		7-capped pentagonal prism Ni ₂ Si ₅ La ₁₀
La9	6 <i>h</i>	<i>m</i> ..	0.50191	0.0817	1/4		7-capped pentagonal prism Ni ₂ Si ₅ La ₁₀
La10	6 <i>h</i>	<i>m</i> ..	0.534	0.28881	1/4		pseudo Frank-Kasper Ni ₆ Si ₆ La ₈
Ni11	4 <i>e</i>	3..	0	0	0.09	0.156	
Si12	2 <i>c</i>	-6..	1/3	2/3	1/4		tricapped trigonal prism Ni ₃ La ₆
Ni13	2 <i>a</i>	-6..	0	0	1/4	0.306	

Experimental: single crystal, diffractometer, X-rays, *R* = 0.024, *T* = 295 K

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Prots' Y.M., Jeitschko W. (1998), *Inorg. Chem.* 37, 5431-5438.