

**La<sub>5</sub>Ni<sub>1.75</sub>Si<sub>3</sub>***hP44*(176) *P6<sub>3</sub>/m – h<sup>6</sup>eda***La<sub>5</sub>Ni<sub>1.75</sub>Si<sub>3</sub> [1]**

Structural features: Infinite columns of base-linked NiLa<sub>6</sub>Si<sub>3</sub>, SiLa<sub>6</sub>(Ni<sub>2</sub>La) and SiLa<sub>6</sub>(NiLa<sub>2</sub>) tricapped trigonal prisms share atoms to form a 3D-framework with AlB<sub>2</sub>-type (BaLiSi) columns (9 prisms in the triangular cross-section); additional Ni (partial disorder) in channels of hexagonal cross-section parallel to [001].

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

**La<sub>5</sub>Ni<sub>1.75</sub>Si<sub>3</sub>***a* = 1.6244, *c* = 0.4344 nm, *c/a* = 0.267, *V* = 0.9927 nm<sup>3</sup>, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
La1	6 <i>h</i>	<i>m</i> ..	0.00996	0.18316	<sup>1</sup> / <sub>4</sub>		
Si2	6 <i>h</i>	<i>m</i> ..	0.1677	0.5522	<sup>1</sup> / <sub>4</sub>		tricapped trigonal prism Ni <sub>2</sub> La <sub>7</sub>
Si3	6 <i>h</i>	<i>m</i> ..	0.2329	0.3293	<sup>1</sup> / <sub>4</sub>		tricapped trigonal prism NiLa <sub>8</sub>
Ni4	6 <i>h</i>	<i>m</i> ..	0.2821	0.4991	<sup>1</sup> / <sub>4</sub>		tricapped trigonal prism Si <sub>3</sub> La <sub>6</sub>
La5	6 <i>h</i>	<i>m</i> ..	0.40055	0.26433	<sup>1</sup> / <sub>4</sub>		7-capped pentagonal prism Ni <sub>2</sub> Si <sub>5</sub> La <sub>10</sub>
La6	6 <i>h</i>	<i>m</i> ..	0.45525	0.06803	<sup>1</sup> / <sub>4</sub>		7-capped pentagonal prism Ni <sub>2</sub> Si <sub>5</sub> La <sub>10</sub>
Ni7	4 <i>e</i>	3..	0	0	0.114	0.083	
La8	2 <i>d</i>	-6..	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		pseudo Frank-Kasper Si <sub>6</sub> Ni <sub>6</sub> La <sub>8</sub>
Ni9	2 <i>a</i>	-6..	0	0	<sup>1</sup> / <sub>4</sub>	0.335	

Experimental: single crystal, diffractometer, X-rays, *R* = 0.026, *T* = 295 K

Remarks: Short interatomic distances for partly occupied site(s). In table 2 of [1] the *z*-coordinate of former La4 is misprinted as <sup>1</sup>/<sub>4</sub> instead of <sup>3</sup>/<sub>4</sub> and the corresponding Wyckoff position as 2*c* instead of 2*d* (from the description of the structure, checked on interatomic distances).

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