

Nd<sub>6</sub>Ni<sub>1.66</sub>Si<sub>3</sub>*hP*26(176) *P*6<sub>3</sub>/*m* – h<sup>3</sup>eca**Nd<sub>6</sub>Ni<sub>2-x</sub>Si<sub>3</sub>** [1]

Structural features: Infinite columns of base-linked NiNd<sub>6</sub>Si<sub>3</sub> and SiNd<sub>6</sub>(Nd<sub>2</sub>Ni) tricapped trigonal prisms share atoms to form a 3D-framework with AlB<sub>2</sub>-type columns (4 prisms in the triangular cross-section); additional Ni (partial disorder) in channels of hexagonal cross-section parallel to [001]. Variant of Ce<sub>6</sub>Ni<sub>2</sub>Si<sub>3</sub>.

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

Nd<sub>6</sub>Ni<sub>1.66</sub>Si<sub>3</sub>*a* = 1.1939, *c* = 0.4266 nm, *c/a* = 0.357, *V* = 0.5266 nm<sup>3</sup>, *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> ..	0.1607	0.4423	1/4		tricapped trigonal prism NiNd <sub>8</sub>
Nd2	6 <i>h</i>	<i>m</i> ..	0.24038	0.22947	1/4		
Nd3	6 <i>h</i>	<i>m</i> ..	0.51988	0.13899	1/4		7-capped pentagonal prism Ni <sub>2</sub> Si <sub>5</sub> Nd <sub>10</sub>
Ni4	4 <i>e</i>	3..	0	0	0.091	0.203	
Ni5	2 <i>c</i>	-6..	1/3	2/3	1/4		tricapped trigonal prism Si <sub>3</sub> Nd <sub>6</sub>
Ni6	2 <i>a</i>	-6..	0	0	1/4	0.25	

Experimental: single crystal, diffractometer, X-rays, *R* = 0.028

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

References: [1] Prots' Y.M., Jeitschko W. (1998), J. Solid State Chem. 137, 302-310.