

$\text{Ce}_6\text{Ni}(\text{Ni}_{0.33}\text{Si}_{0.67})_3\text{Si}$ $hP22$ $(176) P6_3/m - h^3cb$ **Ce₆Ni₂Si₃** [1]

Structural features: Infinite columns of base-linked $\text{SiCe}_6(\text{Si},\text{Ni})_3$ and $(\text{Si},\text{Ni})\text{Ce}_6[\text{Ce}_2(\text{Si},\text{Ni})]$ tricapped trigonal prisms share atoms to form a 3D-framework with AlB_2 -type columns (4 prisms in the triangular cross-section); additional Ni (trigonal antiprismatic coordination) in channels of hexagonal cross-section parallel to [001].

Bodak O.I. et al. (1974) [1]

 $\text{Ce}_6\text{Ni}_2\text{Si}_3$ $a = 1.2112$, $c = 0.4323$ nm, $c/a = 0.357$, $V = 0.5492$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	6h	$m..$	0.165	0.456	$1/4$		single atom Si
Ce2	6h	$m..$	0.236	0.231	$1/4$		square pyramid Ni_2Si_3
Ce3	6h	$m..$	0.521	0.142	$1/4$		7-capped pentagonal prism $\text{Si}_7\text{Ce}_{10}$
Si4	2c	$-6..$	$1/3$	$2/3$	$1/4$		tricapped trigonal prism Si_3Ce_6
Ni5	2b	$-3..$	0	0	0		square prism (cube) Ni_2Ce_6

 $\text{M1} = 0.667\text{Si} + 0.333\text{Ni}$ Transformation from published data: $y, x, -z$ Experimental: single crystal, Weissenberg photographs, X-rays, $R = 0.115$

Remarks: A fully ordered atom arrangement is suggested in [2].

References: [1] Bodak O.I., Gladyshevskii E.I., Kharchenko O.I. (1974), Sov. Phys. Crystallogr. 19, 45-46 (Kristallografiya 19, 80-83). [2] Parthé E., Hovestreydt E. (1985), J. Less-Common Met. 110, 307-313.