

Ce₅Ni₂Si₃*hP*40(176) *P*6₃/*m* – h⁶db**Ce₂NiSi** [1]

Structural features: Infinite columns of base-linked NiCe₆Si₃, SiCe₆(Ni₂Ce) and SiCe₆(NiCe₂) tricapped trigonal prisms (partial disorder Ni/Si ignored) share atoms to form a 3D-framework with AlB₂-type (BaLiSi) columns (9 prisms in the triangular cross-section); additional Ni in channels of hexagonal cross-section parallel to [001].

Bodak O.I. et al. (1972) [1]

Ce₅Ni₂Si₃*a* = 1.612, *c* = 0.4309 nm, *c/a* = 0.267, *V* = 0.9697 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ce1	6 <i>h</i>	<i>m</i> ..	0.0117	0.1795	1/4		square pyramid Ni ₂ Si ₃
Si2	6 <i>h</i>	<i>m</i> ..	0.1672	0.5472	1/4		tricapped trigonal prism Ni ₂ Ce ₇
M3	6 <i>h</i>	<i>m</i> ..	0.2416	0.3333	1/4		tricapped trigonal prism NiCe ₈
M4	6 <i>h</i>	<i>m</i> ..	0.2834	0.5021	1/4		tricapped trigonal prism Si ₃ Ce ₆
Ce5	6 <i>h</i>	<i>m</i> ..	0.3978	0.2618	1/4		7-capped pentagonal prism Ni ₂ Si ₅ Ce ₁₀
Ce6	6 <i>h</i>	<i>m</i> ..	0.4542	0.0671	1/4		7-capped pentagonal prism Ni ₂ Si ₅ Ce ₁₀
Ce7	2 <i>d</i>	-6..	2/3	1/3	1/4		pseudo Frank-Kasper Ni ₆ Si ₆ Ce ₈
Ni8	2 <i>b</i>	-3..	0	0	0		square prism (cube) Ni ₂ Ce ₆

M3 = 0.7Si + 0.3Ni; M4 = 0.7Ni + 0.3Si

Transformation from published data: *y*,*x*,*-z*; origin shift 0 0 1/2Experimental: single crystal, Weissenberg and rotation photographs, X-rays, *R* = 0.152

Remarks: Short interatomic distances *d*(Ni8-Ni8) = 0.216 nm. Homogeneity range Ce₂Ni_{1+x}Si_{1-x}, -0.2 < *x* < 0.2. A fully ordered atom arrangement is suggested in [2].

References: [1] Bodak O.I., Gladyshevskii E.I., Mis'kiv M.G. (1972), Sov. Phys. Crystallogr. 17, 439-441 (Kristallografiya 17, 439-441). [2] Parthé E., Hovestreydt E. (1985), J. Less-Common Met. 110, 307-313.