

Pr₁₅Ni₇Si₁₀*hP*64(176) *P*6₃/*m* – h¹⁰cb**Pr₁₅Ni₇Si₁₀** [1]; Ce₁₅Ni₄Si₁₃ [2]

Structural features: Infinite columns of base-linked SiPr₆Ni₃, SiPr₆(PrNi₂) and SiPr₆(Pr₂Ni) tricapped trigonal prisms share atoms to form a 3D-framework with AlB₂-type (BaLiSi) columns (16 prisms in the triangular cross-section); additional Ni in channels of hexagonal cross-section parallel to [001].

Hovestreydt E., Parthé E. (1985) [1]

Ni₇Pr₁₅Si₁₀*a* = 1.9881, *c* = 0.42554 nm, *c/a* = 0.214, *V* = 1.4566 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> ..	0.0609	0.2559	1/4		tricapped trigonal prism NiPr ₈
Si2	6 <i>h</i>	<i>m</i> ..	0.1081	0.4843	1/4		tricapped trigonal prism Ni ₂ Pr ₇
Pr3	6 <i>h</i>	<i>m</i> ..	0.1303	0.1474	1/4		square pyramid Ni ₂ Si ₃
Ni4	6 <i>h</i>	<i>m</i> ..	0.1529	0.3935	1/4		tricapped trigonal prism Si ₃ Pr ₆
Ni5	6 <i>h</i>	<i>m</i> ..	0.1989	0.6205	1/4		tricapped trigonal prism Si ₃ Pr ₆
Si6	6 <i>h</i>	<i>m</i> ..	0.2899	0.4424	1/4		tricapped trigonal prism Ni ₂ Pr ₇
Pr7	6 <i>h</i>	<i>m</i> ..	0.3204	0.1242	1/4		7-capped pentagonal prism Ni ₂ Si ₅ Pr ₁₀
Pr8	6 <i>h</i>	<i>m</i> ..	0.3549	0.3212	1/4		7-capped pentagonal prism Ni ₂ Si ₅ Pr ₁₀
Pr9	6 <i>h</i>	<i>m</i> ..	0.5017	0.0818	1/4		7-capped pentagonal prism Ni ₂ Si ₅ Pr ₁₀
Pr10	6 <i>h</i>	<i>m</i> ..	0.5332	0.2886	1/4		pseudo Frank-Kasper Ni ₆ Si ₆ Pr ₈
Si11	2 <i>c</i>	-6..	1/3	2/3	1/4		tricapped trigonal prism Ni ₃ Pr ₆
Ni12	2 <i>b</i>	-3..	0	0	0		square prism (cube) Ni ₂ Pr ₆

Experimental: single crystal, diffractometer, X-rays, R = 0.054

Remarks: The authors state that Ni atoms are delocalized along the *c*-axis; the *z*-coordinate of site Ni12 was arbitrarily set to 0. The structure type was originally defined on Ce₁₅Ni₄Si₁₃ [2], for which, however, a questionable distribution of Ni and Si was proposed.

References: [1] Hovestreydt E., Parthé E. (1985), Acta Crystallogr. C 41, 310-313. [2] Myskiv M.G., Bodak O.I., Gladyshevskii E.I. (1974), Sov. Phys. Crystallogr. 18, 450-453 (Kristallografiya 18, 715-719).