

Nd₆Ni₁₄P₁₀*hP*62(176) *P*6₃/*m* – h¹⁰c**Nd₃Ni₇P₅** [1]

Structural features: Infinite columns of base-linked PNd₆Ni₃, P(Nd₄Ni₂)Ni₃ and P(Nd₂Ni₄)Ni₃ tricapped trigonal prisms share atoms to form a 3D-framework with AlB₂-type columns (13 prisms in the dented triangular cross-section).

Chykhrii S.I. et al. (1989) [1]

Nd₆Ni_{14.01}P₁₀*a* = 1.6679, *c* = 0.3891 nm, *c/a* = 0.233, *V* = 0.9374 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ni1	6 <i>h</i>	<i>m</i> ..	0.0116	0.5665	¹ / ₄	0.67	cuboctahedron P ₄ Ni ₄ Nd ₄
P2	6 <i>h</i>	<i>m</i> ..	0.025	0.203	¹ / ₄		monocapped trigonal prism Ni ₇
P3	6 <i>h</i>	<i>m</i> ..	0.075	0.464	¹ / ₄		tricapped trigonal prism Ni ₅ Nd ₄
Ni4	6 <i>h</i>	<i>m</i> ..	0.1475	0.0882	¹ / ₄		11-vertex polyhedron P ₃ Ni ₇ Nd
Ni5	6 <i>h</i>	<i>m</i> ..	0.1765	0.2474	¹ / ₄		cuboctahedron P ₄ Ni ₅ Nd ₃
Ni6	6 <i>h</i>	<i>m</i> ..	0.2272	0.5113	¹ / ₄		tricapped trigonal prism P ₃ Nd ₆
P7	6 <i>h</i>	<i>m</i> ..	0.273	0.411	¹ / ₄		tricapped trigonal prism Ni ₅ Nd ₄
Ni8	6 <i>h</i>	<i>m</i> ..	0.3472	0.0432	¹ / ₄		cuboctahedron P ₄ Ni ₄ Nd ₄
Nd9	6 <i>h</i>	<i>m</i> ..	0.3582	0.2373	¹ / ₄		22-vertex polyhedron P ₈ Ni ₁₀ Nd ₄
Nd10	6 <i>h</i>	<i>m</i> ..	0.5606	0.1748	¹ / ₄		21-vertex polyhedron P ₇ Ni ₈ Nd ₆
P11	2 <i>c</i>	-6..	¹ / ₃	² / ₃	¹ / ₄		tricapped trigonal prism Ni ₃ Nd ₆

Transformation from published data: *y*,*x*,*-z*; origin shift 0 0 ¹/₂

Experimental: single crystal, diffractometer, X-rays, R = 0.061

References: [1] Chykhrii S.I., Oryshchyn S.V., Kuz'ma Y.B., Glowiak T. (1989), Sov. Phys. Crystallogr. 34, 681-684 (Kristallografiya 34, 1131-1135).