

Ce₆Ni₁₅P₁₀*hP*68(176) *P*6₃/*m* – h¹¹c**Ce₆Ni₁₅P₁₀** [1]

Structural features: Infinite columns of base-linked PCe₆Ni₃, P(Ce₄Ni₂)Ni₃ and P(Ce₂Ni₄)Ni₃ tricapped trigonal prisms share atoms to form a 3D-framework with AlB₂-type columns (13 prisms in the dented triangular cross-section).

Babizhetskii V.S. et al. (1993) [1]

Ce₆Ni₁₅P₁₀*a* = 1.6637, *c* = 0.3878 nm, *c/a* = 0.233, *V* = 0.9296 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> ..	0.0133	0.5645	¹ / ₄		cuboctahedron P ₄ Ni ₄ Ce ₄
P2	6 <i>h</i>	<i>m</i> ..	0.02	0.2093	¹ / ₄		monocapped trigonal prism Ni ₇
Ni3	6 <i>h</i>	<i>m</i> ..	0.0634	0.0412	¹ / ₄	0.21	
P4	6 <i>h</i>	<i>m</i> ..	0.072	0.4627	¹ / ₄		square pyramid Ni ₅
Ni5	6 <i>h</i>	<i>m</i> ..	0.1464	0.0879	¹ / ₄	0.79	
Ni6	6 <i>h</i>	<i>m</i> ..	0.1767	0.2496	¹ / ₄		trigonal bipyramid P ₄ Ni
Ni7	6 <i>h</i>	<i>m</i> ..	0.2263	0.5099	¹ / ₄		tricapped trigonal prism P ₃ Ce ₆
P8	6 <i>h</i>	<i>m</i> ..	0.2793	0.408	¹ / ₄		tricapped trigonal prism Ni ₅ Ce ₄
Ni9	6 <i>h</i>	<i>m</i> ..	0.3473	0.0419	¹ / ₄		cuboctahedron P ₄ Ni ₄ Ce ₄
Ce10	6 <i>h</i>	<i>m</i> ..	0.3575	0.2356	¹ / ₄		22-vertex polyhedron P ₈ Ni ₁₀ Ce ₄
Ce11	6 <i>h</i>	<i>m</i> ..	0.5599	0.1759	¹ / ₄		21-vertex polyhedron P ₇ Ni ₈ Ce ₆
P12	2 <i>c</i>	-6..	¹ / ₃	² / ₃	¹ / ₄		tricapped trigonal prism Ni ₃ Ce ₆

Transformation from published data: *y*,*x*,*-z*; origin shift 0 0 ¹/₂Experimental: single crystal, diffractometer, X-rays, *R* = 0.042

Remarks: When relevant, we changed the last digit of partial site occupancies to obtain total occupancy 1. Short interatomic distances for partly occupied site(s).

References: [1] Babizhetskii V.S., Chykhrii S.I., Oryshchyn S.V., Kuz'ma Y.B. (1993), Ukr. Khim. Zh. (Ukr. Ed.) 59, 240-242.