

Ce₉Ni₂₆P₁₂*hP*47(187) *P*-6*m*2 – m²k⁵j⁴fa**Ce₉Ni₂₆P₁₂** [1]

Structural features: Infinite columns of base-linked P(Ce₂Ni₄)Ni₃, P(Ce₄Ni₂)Ni₃ and NiCe₆Ni₃ tricapped trigonal prisms share atoms to form a 3D-framework with two kinds of AlB₂-type column (6 and 10 prisms in the cross-section, respectively) and channels of hexagonal cross-section parallel to [001].

Babizhetskii V.S. et al. (1992) [1]

Ce₉Ni₂₆P₁₂*a* = 1.426, *c* = 0.3863 nm, *c/a* = 0.271, *V* = 0.6803 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ni1	6 <i>m</i>	<i>m</i> ..	0.37633	0.04667	1/2		cuboctahedron P ₄ Ni ₄ Ce ₄
P2	6 <i>l</i>	<i>m</i> ..	0.00433	0.26967	0		tricapped trigonal prism Ni ₅ Ce ₄
Ni3	6 <i>l</i>	<i>m</i> ..	0.07933	0.45947	0		13-vertex polyhedron Ni ₇ P ₃ Ce ₃
Ce4	3 <i>k</i>	<i>mm</i> 2	0.18703	0.81297	1/2		22-vertex polyhedron Ni ₁₂ P ₆ Ce ₄
Ni5	3 <i>k</i>	<i>mm</i> 2	0.39653	0.60347	1/2		13-vertex polyhedron PNi ₁₀ Ce ₂
P6	3 <i>k</i>	<i>mm</i> 2	0.48233	0.51767	1/2		tricapped trigonal prism Ni ₇ Ce ₂
P7	3 <i>k</i>	<i>mm</i> 2	0.75233	0.24767	1/2		tricapped trigonal prism Ni ₅ Ce ₄
Ce8	3 <i>k</i>	<i>mm</i> 2	0.90923	0.09077	1/2		21-vertex polyhedron P ₅ Ni ₁₀ Ce ₆
Ni9	3 <i>j</i>	<i>mm</i> 2	0.09163	0.90837	0		tricapped trigonal prism P ₂ NiCe ₆
Ni10	3 <i>j</i>	<i>mm</i> 2	0.27633	0.72367	0		square prism (cube) Ni ₈
Ce11	3 <i>j</i>	<i>mm</i> 2	0.57323	0.42677	0		22-vertex polyhedron P ₈ Ni ₁₀ Ce ₄
Ni12	3 <i>j</i>	<i>mm</i> 2	0.81073	0.18927	0		cuboctahedron P ₄ Ni ₄ Ce ₄
Ni13	1 <i>f</i>	-6 <i>m</i> 2	2/3	1/3	1/2		coplanar triangle P ₃
Ni14	1 <i>a</i>	-6 <i>m</i> 2	0	0	0		tricapped trigonal prism Ni ₃ Ce ₆

Transformation from published data: -*x*, -*y*, -*z*; origin shift 2/3 1/3 1/2Experimental: single crystal, diffractometer, X-rays, *R* = 0.069

References: [1] Babizhetskii V.S., Chykhrii S.I., Oryshchyn S.V., Kuz'ma Y.B. (1992), Russ. J. Inorg. Chem. 37, 1372-1374 (Zh. Neorg. Khim. 37, 2660-2662).