

Sm₁₀Ni_{20.8}P₁₅*hP*98(176) *P*6₃/*m* – h¹⁶d**Sm₂₀Ni_{41.6}P₃₀** [1]

Structural features: Infinite columns of base-linked PSm₆Ni₃, P(Sm₄Ni₂)Ni₃ and P(Sm₂Ni₄)Ni₃ tricapped trigonal prisms (split site for the latter) share atoms to form a 3D-framework with AlB₂-type columns (21 prisms in the dented triangular cross-section) and channels of hexagonal cross-section parallel to [001].

Chykhrii S.I. et al. (1993) [1]

Ni_{20.85}P₁₅Sm₁₀*a* = 2.0448, *c* = 0.3877 nm, *c/a* = 0.190, *V* = 1.4039 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> ..	0.0274	0.3708	1/4		cuboctahedron P ₄ Ni ₄ Sm ₄
Ni2	6 <i>h</i>	<i>m</i> ..	0.0661	0.2051	1/4		
P3	6 <i>h</i>	<i>m</i> ..	0.082	0.509	1/4		square pyramid Ni ₅
Ni4	6 <i>h</i>	<i>m</i> ..	0.098	0.0047	1/4	0.18	
P5	6 <i>h</i>	<i>m</i> ..	0.116	0.332	1/4		square pyramid Ni ₅
Ni6	6 <i>h</i>	<i>m</i> ..	0.1274	0.0486	1/4	0.77	
P7	6 <i>h</i>	<i>m</i> ..	0.161	0.167	1/4		
Ni8	6 <i>h</i>	<i>m</i> ..	0.2061	0.5828	1/4		tricapped trigonal prism P ₃ Sm ₆
Ni9	6 <i>h</i>	<i>m</i> ..	0.2417	0.4126	1/4		tricapped trigonal prism P ₃ Sm ₆
Ni10	6 <i>h</i>	<i>m</i> ..	0.2876	0.2408	1/4		cuboctahedron P ₄ Ni ₄ Sm ₄
Sm11	6 <i>h</i>	<i>m</i> ..	0.2894	0.0897	1/4		
P12	6 <i>h</i>	<i>m</i> ..	0.294	0.547	1/4		tricapped trigonal prism Ni ₃ Sm ₆
P13	6 <i>h</i>	<i>m</i> ..	0.319	0.369	1/4		tricapped trigonal prism Ni ₅ Sm ₄
Sm14	6 <i>h</i>	<i>m</i> ..	0.4581	0.2981	1/4		21-vertex polyhedron Ni ₈ P ₇ Sm ₆
Sm15	6 <i>h</i>	<i>m</i> ..	0.4951	0.1219	1/4		21-vertex polyhedron P ₇ Ni ₈ Sm ₆
Ni16	6 <i>h</i>	<i>m</i> ..	0.5528	0.0098	1/4		cuboctahedron P ₄ Ni ₄ Sm ₄
Sm17	2 <i>d</i>	-6..	2/3	1/3	1/4		pseudo Frank-Kasper P ₆ Ni ₆ Sm ₈

Transformation from published data: origin shift 0 0 1/2

Experimental: single crystal, diffractometer, X-rays, wR = 0.046

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Chykhrii S.I., Babizhets'kii V.S., Oryshchyn S.V., Aksel'rud L.G., Kuz'ma Y.B. (1993), Crystallogr. Rep. 38, 569-571 (Kristallografiya 38(4), 262-265).