

Tb₈Ni₁₈P₁₁*hP*74(187) *P*-6*m*2 – *m*³*l*³*k*⁷*j*⁵*ca***Tb₁₆Ni₃₆P₂₂** [1]

Structural features: Infinite columns of base-linked PTb₆Ni₃, P(Tb₄Ni₂)Ni₃, P(Tb₂Ni₄)Ni₃ tricapped trigonal prisms share atoms to form a 3D-framework with two kinds of AlB₂-type column (13 and 18 columns in the dented triangular cross-section, respectively) and channels of hexagonal cross-section parallel to [001].

Chykhrii S.I. et al. (1997) [1]

Ni₁₈P₁₁Tb₈*a* = 1.8049, *c* = 0.38154 nm, *c/a* = 0.211, *V* = 1.0764 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ni1	6 <i>m</i>	<i>m</i> ..	0.06807	0.35503	¹ / ₂		10-vertex polyhedron P ₄ Ni ₄ Tb ₂
P2	6 <i>m</i>	<i>m</i> ..	0.35667	0.07533	¹ / ₂		tricapped trigonal prism Ni ₅ Tb ₄
Ni3	6 <i>m</i>	<i>m</i> ..	0.49267	0.13993	¹ / ₂		11-vertex polyhedron P ₃ Ni ₆ Tb ₂
Tb4	6 <i>l</i>	<i>m</i> ..	0.00147	0.21583	0		21-vertex polyhedron Ni ₈ P ₇ Tb ₆
P5	6 <i>l</i>	<i>m</i> ..	0.10767	0.44533	0		square pyramid Ni ₅
Ni6	6 <i>l</i>	<i>m</i> ..	0.38877	0.02903	0		cuboctahedron P ₄ Ni ₄ Tb ₄
Ni7	3 <i>k</i>	<i>mm</i> 2	0.06967	0.93033	¹ / ₂		tricapped trigonal prism P ₃ Tb ₆
P8	3 <i>k</i>	<i>mm</i> 2	0.14167	0.85833	¹ / ₂		tricapped trigonal prism Ni ₅ Tb ₄
Tb9	3 <i>k</i>	<i>mm</i> 2	0.26617	0.73383	¹ / ₂		21-vertex polyhedron P ₇ Ni ₈ Tb ₆
Tb10	3 <i>k</i>	<i>mm</i> 2	0.47737	0.52263	¹ / ₂		22-vertex polyhedron P ₈ Ni ₁₀ Tb ₄
Ni11	3 <i>k</i>	<i>mm</i> 2	0.70827	0.29173	¹ / ₂		square prism (cube) Ni ₈
Ni12	3 <i>k</i>	<i>mm</i> 2	0.85347	0.14653	¹ / ₂		tricapped trigonal prism P ₃ Tb ₆
P13	3 <i>k</i>	<i>mm</i> 2	0.92867	0.07133	¹ / ₂		tricapped trigonal prism Ni ₃ Tb ₆
Ni14	3 <i>j</i>	<i>mm</i> 2	0.18217	0.81783	0		cuboctahedron P ₄ Ni ₄ Tb ₄
Ni15	3 <i>j</i>	<i>mm</i> 2	0.40667	0.59333	0		tricapped trigonal prism P ₃ Tb ₆
P16	3 <i>j</i>	<i>mm</i> 2	0.55467	0.44533	0		tricapped trigonal prism Ni ₇ Tb ₂
Ni17	3 <i>j</i>	<i>mm</i> 2	0.62447	0.37553	0		monocapped trigonal prism PNi ₆
Tb18	3 <i>j</i>	<i>mm</i> 2	0.78257	0.21743	0		22-vertex polyhedron Ni ₁₂ P ₆ Tb ₄
P19	1 <i>c</i>	-6 <i>m</i> 2	¹ / ₃	² / ₃	0		tricapped trigonal prism Ni ₃ Tb ₆
Tb20	1 <i>a</i>	-6 <i>m</i> 2	0	0	0		pseudo Frank-Kasper Ni ₆ P ₆ Tb ₈

Transformation from published data: origin shift ¹/₃ ²/₃ ¹/₂Experimental: powder, diffractometer, X-rays, R_B = 0.095

Remarks: In table 3 of [1] the *y*-coordinates of former Tb2 and Ni2 are misprinted as 0.2308 and 0.1031 instead of 0.2318 and 1.0310, respectively (agreement with Wyckoff position 3*k*; checked on interatomic distances), and the Wyckoff position of former P1 as 1*e* instead of 1*f*.

References: [1] Chykhrii S.I., Babizhets'kii V.S., Oryshchyn S.V., Kuz'ma Y.B., Aksel'rud L.G. (1997), J. Alloys Compd. 259, 186-190.