

Tb₁₅Ni₂₈P₂₁*hP*128(176) *P*6₃/*m* – h²¹c**Tb₁₅Ni₂₈P₂₁** [1]

Structural features: Infinite columns of base-linked PTb₆Ni₃, P(Tb₄Ni₂)Ni₃ and P(Tb₂Ni₄)Ni₃ tricapped trigonal prisms share atoms to form a 3D-framework with AlB₂-type (BaLiSi) columns (31 prisms in the dented triangular cross-section) and channels of hexagonal cross-section parallel to [001].

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

Ni₂₈P₂₁Tb₁₅*a* = 2.417, *c* = 0.3825 nm, *c/a* = 0.158, *V* = 1.9352 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
P1	6 <i>h</i>	<i>m</i> ..	0.006	0.14	¹ / ₄		tricapped trigonal prism Ni ₇ Tb ₂
Ni2	6 <i>h</i>	<i>m</i> ..	0.0093	0.545	¹ / ₄		tetrahedron P ₄
P3	6 <i>h</i>	<i>m</i> ..	0.031	0.305	¹ / ₄		square pyramid Ni ₅
P4	6 <i>h</i>	<i>m</i> ..	0.055	0.48	¹ / ₄		square pyramid Ni ₅
Ni5	6 <i>h</i>	<i>m</i> ..	0.1029	0.068	¹ / ₄		11-vertex polyhedron P ₃ Ni ₇ Tb
Ni6	6 <i>h</i>	<i>m</i> ..	0.1155	0.1714	¹ / ₄		cuboctahedron P ₄ Ni ₅ Tb ₃
Ni7	6 <i>h</i>	<i>m</i> ..	0.1353	0.3476	¹ / ₄		tricapped trigonal prism P ₃ Tb ₆
Ni8	6 <i>h</i>	<i>m</i> ..	0.16	0.5189	¹ / ₄		tricapped trigonal prism P ₃ Tb ₆
P9	6 <i>h</i>	<i>m</i> ..	0.178	0.285	¹ / ₄		tricapped trigonal prism Ni ₅ Tb ₄
P10	6 <i>h</i>	<i>m</i> ..	0.204	0.459	¹ / ₄		tricapped trigonal prism Ni ₃ Tb ₆
P11	6 <i>h</i>	<i>m</i> ..	0.222	0.62	¹ / ₄		tricapped trigonal prism Ni ₃ Tb ₆
Tb12	6 <i>h</i>	<i>m</i> ..	0.2417	0.1732	¹ / ₄		22-vertex polyhedron P ₈ Ni ₁₀ Tb ₄
Ni13	6 <i>h</i>	<i>m</i> ..	0.2437	0.0425	¹ / ₄		cuboctahedron P ₄ Ni ₄ Tb ₄
Ni14	6 <i>h</i>	<i>m</i> ..	0.2858	0.3174	¹ / ₄		cuboctahedron P ₄ Ni ₄ Tb ₄
Ni15	6 <i>h</i>	<i>m</i> ..	0.3056	0.4917	¹ / ₄		tricapped trigonal prism P ₃ Tb ₆
P16	6 <i>h</i>	<i>m</i> ..	0.348	0.425	¹ / ₄		square pyramid Ni ₅
Tb17	6 <i>h</i>	<i>m</i> ..	0.3866	0.1449	¹ / ₄		21-vertex polyhedron P ₇ Ni ₈ Tb ₆
Ni18	6 <i>h</i>	<i>m</i> ..	0.3915	0.0224	¹ / ₄		cuboctahedron P ₄ Ni ₄ Tb ₄
Tb19	6 <i>h</i>	<i>m</i> ..	0.4151	0.3196	¹ / ₄		21-vertex polyhedron Ni ₈ P ₇ Tb ₆
Tb20	6 <i>h</i>	<i>m</i> ..	0.5335	0.1167	¹ / ₄		21-vertex polyhedron P ₇ Ni ₈ Tb ₆
Tb21	6 <i>h</i>	<i>m</i> ..	0.5613	0.2948	¹ / ₄		pseudo Frank-Kasper P ₆ Ni ₆ Tb ₈
Ni22	2 <i>c</i>	-6..	¹ / ₃	² / ₃	¹ / ₄		tricapped trigonal prism P ₃ Tb ₆

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

Experimental: single crystal, diffractometer, X-rays, R = 0.044

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).