

Tm₁₃Ni₂₅As₁₉ [1]

Structural features: AsTm₆Ni₃, As(Tm₄Ni₂)Ni₃ and As(Tm₂Ni₄)(TmNi₂) tricapped trigonal prisms share atoms to form a 3D-framework with AlB₂-type (BaLiSi) columns (13 and 7 prisms in the dented triangular cross-sections).

Jeitschko W. et al. (2001) [1]

As₁₉Ni_{25.22}Tm_{12.57}

$a = 1.6219$, $c = 0.38778$ nm, $c/a = 0.239$, $V = 0.8834$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Tm1	3 <i>k</i>	<i>m</i> ..	0.0362	0.29789	1/2	0.931	22-vertex polyhedron As ₈ Ni ₁₀ Tm ₄
Tm2	3 <i>k</i>	<i>m</i> ..	0.15262	0.13241	1/2		21-vertex polyhedron As ₇ Ni ₈ Tm ₆
Ni3	3 <i>k</i>	<i>m</i> ..	0.15582	0.53237	1/2		cuboctahedron As ₄ Ni ₃ Tm ₅
Ni4	3 <i>k</i>	<i>m</i> ..	0.24946	0.34985	1/2		cuboctahedron As ₄ Ni ₄ Tm ₄
As5	3 <i>k</i>	<i>m</i> ..	0.29327	0.51566	1/2		tricapped trigonal prism Ni ₅ Tm ₄
Ni6	3 <i>k</i>	<i>m</i> ..	0.37426	0.19191	1/2		cuboctahedron As ₄ Ni ₄ Tm ₄
As7	3 <i>k</i>	<i>m</i> ..	0.40278	0.3509	1/2		tricapped trigonal prism Ni ₅ Tm ₄
Ni8	3 <i>k</i>	<i>m</i> ..	0.49048	0.03448	1/2		cuboctahedron As ₄ Ni ₃ Tm ₅
As9	3 <i>k</i>	<i>m</i> ..	0.52104	0.19492	1/2		tricapped trigonal prism Ni ₅ Tm ₄
Ni10	3 <i>j</i>	<i>m</i> ..	0.01647	0.14883	0		tricapped trigonal prism As ₃ Tm ₆
As11	3 <i>j</i>	<i>m</i> ..	0.05027	0.43628	0		tricapped trigonal prism Ni ₆ Tm ₃
As12	3 <i>j</i>	<i>m</i> ..	0.16547	0.27603	0		bicapped square antiprism Ni ₅ Tm ₅
Ni13	3 <i>j</i>	<i>m</i> ..	0.19584	0.43976	0		cuboctahedron As ₄ Ni ₄ Tm ₄
As14	3 <i>j</i>	<i>m</i> ..	0.28097	0.11199	0		tricapped trigonal prism Ni ₅ Tm ₄
Ni15	3 <i>j</i>	<i>m</i> ..	0.31005	0.26834	0		cuboctahedron As ₄ Ni ₄ Tm ₄
M16	3 <i>j</i>	<i>m</i> ..	0.38368	0.46488	0		pseudo Frank-Kasper As ₆ Ni ₈ Tm ₄
Ni17	3 <i>j</i>	<i>m</i> ..	0.42947	0.11183	0		cuboctahedron As ₄ Ni ₄ Tm ₄
Tm18	3 <i>j</i>	<i>m</i> ..	0.53048	0.34101	0		22-vertex polyhedron As ₈ Ni ₉ Tm ₅
Ni19	1 <i>f</i>	-6..	2/3	1/3	1/2		tricapped trigonal prism As ₃ Tm ₆
Tm20	1 <i>c</i>	-6..	1/3	2/3	0		23-vertex polyhedron As ₉ Ni ₉ Tm ₅
As21	1 <i>a</i>	-6..	0	0	0		tricapped trigonal prism Ni ₃ Tm ₆

M16 = 0.856Tm + 0.144Ni

Experimental: single crystal, diffractometer, X-rays, R = 0.025

References: [1] Jeitschko W., Terbüchte L.J., Rodewald U.C. (2001), Z. Anorg. Allg. Chem. 627, 2095-2099.