Tm_2NiAs_2	*hP*10	(186) $P6_3mc$ – b^3a^2

Tm_2NiAs_2 rt [1]
Structural features: As layers in hc stacking; Tm in octahedral, Ni in trigonal voids in h-stacked layers. $NiAs_3$ trigonal units share vertices to form infinite layers. Deformation derivative of Ho_2NiAs_2 with slightly puckered hexagon-mesh NiAs layers.

Jeitschko W. et al. (2001) [1]
As_2NiTm_2
a = 0.4074, c = 1.3591 nm, c/a = 3.336, V = 0.1954 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
As1	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.0157		tricapped trigonal prism Ni_3Tm_6
Tm2	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.38407		9-vertex polyhedron Ni_3As_6
Tm3	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.6486		9-vertex polyhedron As_6Ni_3
Ni4	2*a*	3*m*.	0	0	0.0		non-coplanar triangle As_3
As5	2*a*	3*m*.	0	0	0.2673		octahedron Tm_6

Transformation from published data: origin shift 0 0 0.2336
Experimental: single crystal, diffractometer, X-rays, R = 0.044

Remarks: Phase stable at room temperature. Refinement of the site occupancies showed no significant deviation from unity. Space group (194) $P6_3/mmc$ was tested and rejected (R = 0.047 for Ni in Wyckoff position 2*b*, 0.045 for Ni in Wyckoff position 4*e*).

References: [1] Jeitschko W., Terbüchte L.J., Rodewald U.C. (2001), Z. Naturforsch. B 56, 1281-1288.