TaN	*hP*6	(189) *P*-62*m* – fda

TaN ε [2]
Structural features: NTa_5 square pyramids share edges and vertices to form a 3D-framework. Filled-up derivative of ω-Ti.

Petrunin V.F., Sorokin N.I. (1982) [1]
NTa
$a = 0.517$, $c = 0.289$ nm, $c/a = 0.559$, $V = 0.0669$ nm^3, $Z = 3$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
N1	3*f*	*m*2*m*	0.393	0	0		square pyramid Ta_5
Ta2	2*d*	-6..	$^1/_3$	$^2/_3$	$^1/_2$		trigonal prism N_6
Ta3	1*a*	-62*m*	0	0	0		coplanar triangle N_3

Experimental: powder, diffractometer, neutrons, $R_B = 0.030$

Remarks: Phase stable at T < ~2273 K. The same data are quoted in [6]. A structure proposal in space group (191) *P*6/*mmm* with N in octahedral voids ([3]; [4]; [7]) is superseded (see [2]). In [5] the Hermann-Mauguin symbol for the space group (quoted from [2]) is misprinted as *P*-6, and in [6] as *P*6/*mmm* instead of *P*-62*m*.

References: [1] Petrunin V.F., Sorokin N.I. (1982), Inorg. Mater. 18, 1733-1736 (Izv. Akad. Nauk SSSR, Neorg. Mater. 18, 2005-2208). [2] Christensen A.N., Lebech B. (1978), Acta Crystallogr. B 34, 261-263. [3] Brauer G., Zapp K.H. (1953), Naturwissenschaften 40, 604. [4] Schönberg N. (1954), Acta Chem. Scand. 8, 199-203. [5] Brauer G., Kiliani W. (1979), Z. Anorg. Allg. Chem. 452, 17-26. [6] Ogawa T. (1994), J. Alloys Compd. 203, 221-227. [7] Brauer G., Zapp K.H. (1954), Z. Anorg. Allg. Chem. 277, 129-139.