$Ti_3Al_2N_2$	*hP*22	(186) $P6_3mc - b^9a^2$

$Ti_3Al_2N_2$ [1]
Structural features: Close-packed Ti and Al layers in h_3c_2 stacking (sites with occ.= 0.1 ignored); N in octahedral (Ti_6 and Ti_3Al_3) voids.

Schuster J.C., Bauer J. (1984) [1]
$Al_2N_2Ti_3$
a = 0.29875, c = 2.335 nm, c/a = 7.816, V = 0.1805 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.05	0.9	
Ti2	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.1	0.1	
Ti3	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.2	0.9	
N4	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.25	0.1	
Al5	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.4		anticuboctahedron Al_9Ti_3
N6	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.55	0.1	
Ti7	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.6	0.9	
Ti8	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.7	0.1	
N9	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.75	0.9	
Ti10	2*a*	3*m*.	0	0	0.0		non-coplanar hexagon N_6
Al11	2*a*	3*m*.	0	0	0.3		non-coplanar hexagon N_6

Transformation from published data (*P*31*c*): origin shift 0 0 0.85
Experimental: powder, film, X-rays

Remarks: The description in space group (159) *P*31*c* in [1] does not take into consideration all symmetry elements (see [2]). Short interatomic distances for partly occupied site(s). The composition was later corrected to Ti_3AlN_3 and the structure refined in space group (194) $P6_3/mmc$ [3].

References: [1] Schuster J.C., Bauer J. (1984), J. Solid State Chem. 53, 260-265. [2] Cenzual K., Gelato L.M., Penzo M., Parthé E. (1991), Acta Crystallogr. B 47, 433-439. [3] Rawn C.J., Barsoum M.W., El Raghy T., Procipio A., Hoffmann C.M., Hubbard C.R. (2000), Mater. Res. Bull. 35, 1785-1796.