

$\text{Al}_7\text{C}_3\text{N}_3$	$hP26$	$(186) P6_3mc - b^7a^6$
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$\text{Al}_7\text{C}_3\text{N}_3$ [2]

Structural features: Close-packed Al layers in h_5c_2 stacking; N in tetrahedral, C in tetrahedral and octahedral voids (Al-C(t)-Al-N(t)-Al-C(o)-Al-N(t)-Al-N(t)-Al-C(t)-Al). Intergrowth of Al_4C_3 - and ZnS -type slabs in the ratio 1:3.

Jeffrey G.A., Wu V.Y. (1966) [1]

$\text{Al}_7\text{C}_3\text{N}_3$

$a = 0.3226$, $c = 3.17$ nm, $c/a = 9.826$, $V = 0.2857$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.0341		tetrahedron NC_3
N2	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.0931		tetrahedron Al_4
Al3	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.1834		non-coplanar triangle C_3
C4	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.2552		trigonal bipyramid Al_5
Al5	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.3156		tetrahedron CN_3
N6	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.4061		tetrahedron Al_4
Al7	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.4701		tetrahedron NC_3
C8	$2a$	$3m.$	0	0	0.0		octahedron Al_6
Al9	$2a$	$3m.$	0	0	0.1085		tetrahedron N_3C
C10	$2a$	$3m.$	0	0	0.1733		trigonal bipyramid Al_5
Al11	$2a$	$3m.$	0	0	0.2385		tetrahedron C_4
N12	$2a$	$3m.$	0	0	0.3314		tetrahedron Al_4
Al13	$2a$	$3m.$	0	0	0.3915		tetrahedron N_4

Transformation from published data: $-x, -y, -z$

Experimental: single crystal, photographs, X-rays, $R = 0.150$

Remarks: The same data are reported in [2]; as stated by the authors, their description in space group (36) $Cmc2_1$ does not take into consideration all symmetry elements of the proposed structure.

References: [1] Jeffrey G.A., Wu V.Y. (1966), Acta Crystallogr. 20, 538-547. [2] Jeffrey G.A., Wu V.Y. (1963), Acta Crystallogr. 16, 559-566.