

$\text{Al}_5\text{C}_3\text{N}$	$hP18$	$(186) P6_3mc - b^5a^4$
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$\text{Al}_5\text{C}_3\text{N}$  [1], Strukturbericht notation E9<sub>4</sub>

Structural features: Close-packed Al layers in h<sub>3</sub>c<sub>2</sub> stacking; N in tetrahedral, C in tetrahedral and octahedral voids (sandwiches consisting of nine sublayers Al-C(t)-Al-N(t)-Al-C(o)-Al-C(t)-Al). Intergrowth of Al<sub>4</sub>C<sub>3</sub>- and ZnS-type slabs in the ratio 1:1.

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

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$a = 0.3281$ ,  $c = 2.158$  nm,  $c/a = 6.577$ ,  $V = 0.2012$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Al1	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.045		tetrahedron C <sub>4</sub>
C2	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.133		tetrahedron Al <sub>4</sub>
Al3	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.239		non-coplanar triangle C <sub>3</sub>
N4	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.363		tetrahedron Al <sub>4</sub>
Al5	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.455		tetrahedron NC <sub>3</sub>
C6	$2a$	$3m.$	0	0	0.0		octahedron Al <sub>6</sub>
Al7	$2a$	$3m.$	0	0	0.155		tetrahedron C <sub>4</sub>
C8	$2a$	$3m.$	0	0	0.252		trigonal bipyramid Al <sub>5</sub>
Al9	$2a$	$3m.$	0	0	0.345		tetrahedron N <sub>3</sub> C

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

Experimental: single crystal, photographs, X-rays,  $R = 0.130$

Remarks: Supersedes a structure proposal with N in site C8 [2]. Strukturbericht notation E9<sub>4</sub> was defined on the superseded structure proposal.

References: [1] Jeffrey G.A., Wu V.Y. (1966), Acta Crystallogr. 20, 538-547. [2] Von Stackelberg M., Spiess K.F. (1936), Z. Phys. Chem., Abt. A 175, 140-153.