

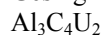
hP18

(186) $P6_3mc - b^5a^4$

$\text{U}_2\text{Al}_3\text{C}_4$ [1]

Structural features: Close-packed U and Al layers in hc_4 stacking (-Al-Al-U-U-Al-); C in octahedral and trigonal bipyramidal voids. Slabs of edge-linked CU_6 and $\text{C}(\text{U}_3\text{Al}_3)$ octahedra are interconnected via vertex-linked CAI_5 trigonal bipyramids to form a 3D-framework.

Gesing T.M., Jeitschko W. (1995) [1]



$a = 0.3422$, $c = 2.323$ nm, $c/a = 6.788$, $V = 0.2356$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.006		non-coplanar triangle C_3
C2	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.117		non-coplanar triangle Al_3
U3	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.31107		octahedron C_6
U4	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.68654		octahedron C_6
C5	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.887		non-coplanar triangle Al_3
C6	$2a$	$3m.$	0	0	0.0		trigonal bipyramid Al_5
Al7	$2a$	$3m.$	0	0	0.0861		tetrahedron C_4
C8	$2a$	$3m.$	0	0	0.249		octahedron U_6
Al9	$2a$	$3m.$	0	0	0.4129		tetrahedron C_4

Transformation from published data: $-x, -y, -z$; origin shift 0 0 0.251

Experimental: twinned crystal, diffractometer, X-rays, $R = 0.030$

Remarks: Space group (194) $P6_3/mmc$ with splitting of the Al site near Wyckoff position $2b$ was tested and rejected ($R = 0.028$).

References: [1] Gesing T.M., Jeitschko W. (1995), Z. Naturforsch. B 50, 196-200.