

$\text{Zr}_3\text{Al}_3\text{C}_5$ $hP22$ $(186) P6_3mc - b^7a^4$ **Zr₃Al₃C₅** [1]

Structural features: Close-packed Zr and Al layers in hc_5 stacking (-Al-Al-Zr-Zr-Zr-Al-); C in octahedral and trigonal bipyramidal voids. Quadruple slabs of edge-linked CZr_6 and $\text{C}(\text{Zr}_3\text{Al}_3)$ octahedra are interconnected via vertex-linked CAl_5 trigonal bipyramids to form a 3D-framework.

Gesing T.M., Jeitschko W. (1998) [1]

 $\text{Al}_3\text{C}_5\text{Zr}_3$ $a = 0.3343$, $c = 2.7609$ nm, $c/a = 8.259$, $V = 0.2672$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.0236		tetrahedron C ₄
C2	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.0961		trigonal bipyramid Al ₅
Al3	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.1696		tetrahedron C ₄
C4	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.2962		octahedron Zr ₆
Zr5	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.44216		octahedron C ₆
Zr6	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.75169		octahedron C ₆
C7	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.8962		octahedron Zr ₆
C8	$2a$	$3m.$	0	0	0.0		non-coplanar triangle Al ₃
Al9	$2a$	$3m.$	0	0	0.1024		non-coplanar triangle C ₃
C10	$2a$	$3m.$	0	0	0.1964		non-coplanar triangle Al ₃
Zr11	$2a$	$3m.$	0	0	0.3472		octahedron C ₆

Transformation from published data: $-x, -y, -z$; origin shift 0 0 0.1528Experimental: single crystal, diffractometer, X-rays, $R = 0.024$ Remarks: Identical to the phase called ZrAlC_{2-x} in [2].

References: [1] Gesing T.M., Jeitschko W. (1998), J. Solid State Chem. 140, 396-401. [2] Mikhaleiko S.I., Kuz'ma Y.B., Popov V.E., Gurin V.N., Nechitailov A.P. (1979), Inorg. Mater. 15, 1532-1535 (Izv. Akad. Nauk SSSR, Neorg. Mater. 15, 1948-1951).