

ScAl₃C₃ [1]

Structural features: Close-packed Sc and Al layers in hc₃ stacking (Sc forming the central c-stacked layer); C in octahedral and trigonal bipyramidal voids. Double slabs of edge-linked C(Sc₃Al₃) octahedra are interconnected via vertex-linked CAl₅ trigonal bipyramids to form a 3D-framework. See Fig. IV.20.

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

Al₃C₃Sc

$a = 0.3352$, $c = 1.6778$ nm, $c/a = 5.005$, $V = 0.1633$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Al1	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.1294		tetrahedron C ₄
C2	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.2496		trigonal bipyramid Al ₅
Al3	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.3703		tetrahedron C ₄
C4	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.5897		7-vertex polyhedron Al ₄ Sc ₃
Al5	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.7418		non-coplanar triangle C ₃
C6	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.9152		octahedron Al ₃ Sc ₃
Sc7	2 <i>a</i>	3 <i>m</i> .	0	0	0.0		octahedron C ₆

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.031$

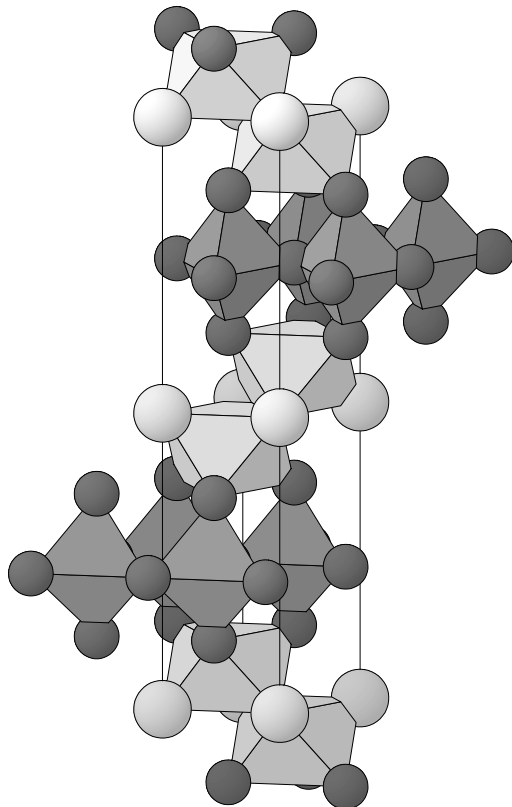


Fig. IV.20. **ScAl₃C₃**

Arrangement of CAl₅ trigonal bipyramids (dark) and C(Sc₃Al₃) octahedra (light) (Sc atoms large, Al atoms small).

References: [1] Gesing T.M., Jeitschko W. (1998), J. Solid State Chem. 140, 396-401.