

$\text{Sr}_{0.5}\text{CaSc}_3\text{O}_6$ $hP22$ $(176) P6_3/m - h^3cb$ **SrCa₂Sc₆O₁₂** [1]

Structural features: Double infinite chains of edge-linked ScO_6 octahedra share vertices to form a 3D-framework; Ca in trigonal prismatic voids, Sr in channels of hexagonal cross-section parallel to [001] (partial disorder).

Müller Buschbaum H., Muschick W. (1975) [1]

 $\text{CaO}_6\text{Sc}_3\text{Sr}_{0.50}$ $a = 0.9659$, $c = 0.3136$ nm, $c/a = 0.325$, $V = 0.2534$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Sc1	$6h$	$m..$	0.003	0.349	$\frac{1}{4}$		octahedron O_6
O2	$6h$	$m..$	0.195	0.309	$\frac{1}{4}$		non-coplanar triangle Sc_3
O3	$6h$	$m..$	0.602	0.132	$\frac{1}{4}$		square pyramid Sc_3Ca_2
Ca4	$2c$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism O_6
Sr5	$2b$	$-3..$	0	0	0	0.5	

Experimental: single crystal, diffractometer, X-rays, $R = 0.044$

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Müller Buschbaum H., Muschick W. (1975), Z. Anorg. Allg. Chem. 412, 209-214.