

$\text{Sc}_3\text{Co}_{15}\text{Si}_{9.5}$ $hP62$ $(176) P6_3/m - h^{10}a$ **Sc₆Co₃₀Si₁₉** [1]

Structural features: Infinite columns of base-linked $\text{Si}(\text{Sc}_2\text{Co}_4)\text{Co}_2$ bicapped and $\text{Si}(\text{Sc}_2\text{Co}_4)\text{Co}_3$ tricapped trigonal prisms share atoms to form a 3D-framework with triple propeller-like columns; additional Si (partial disorder, splitting of neighboring Co site) in channels of hexagonal cross-section parallel to [001]. Filled-up derivative of UCo_5Si_3 .

Kotur B.Y., Sikiritsa M. (1991) [1]

 $\text{Co}_{15}\text{Sc}_3\text{Si}_{9.51}$ $a = 1.4776$, $c = 0.3613$ nm, $c/a = 0.245$, $V = 0.6831$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Co1	6h	m..	0.0533	0.27357	$\frac{1}{4}$		
Si2	6h	m..	0.0591	0.4299	$\frac{1}{4}$		tricapped trigonal prism Co_7Sc_2
Co3	6h	m..	0.1032	0.126	$\frac{1}{4}$	0.467	
Co4	6h	m..	0.1326	0.1611	$\frac{1}{4}$	0.534	
Co5	6h	m..	0.22473	0.57278	$\frac{1}{4}$		square pyramid Si_5
Si6	6h	m..	0.2587	0.1161	$\frac{1}{4}$		
Sc7	6h	m..	0.29829	0.39791	$\frac{1}{4}$		sixcapped hexagonal prism $\text{Si}_6\text{Co}_{12}$
Co8	6h	m..	0.41673	0.26569	$\frac{1}{4}$		11-vertex polyhedron $\text{Si}_4\text{Co}_5\text{Sc}_2$
Co9	6h	m..	0.53956	0.07439	$\frac{1}{4}$		cuboctahedron $\text{Si}_4\text{Co}_5\text{Sc}_3$
Si10	6h	m..	0.5541	0.2358	$\frac{1}{4}$		10-vertex polyhedron $\text{Co}_6\text{Si}_2\text{Sc}_2$
Si11	2a	-6..	0	0	$\frac{1}{4}$	0.51	trigonal bipyramid Co_3Si_2

Experimental: single crystal, diffractometer, X-rays, $R = 0.034$

Remarks: Identical to the phase called ScCo_7Si_4 in [2]. Short interatomic distances for partly occupied site(s).

References: [1] Kotur B.Y., Sikiritsa M. (1991), Sov. Phys. Crystallogr. 36, 666-669 (Kristallografiya 36, 666-669). [2] Kotur B.Y., Bodak O.I., Gladyshevskii E.I. (1977), Dopov. Akad. Nauk Ukr. RSR, Ser. A 1977, 664-666.