

Sc₅Co₁₉P₁₂*hP*37(189) *P*-62*m* – k²jg²f³ec**Sc₅Co₁₉P₁₂** [1]; Zr₅Co₁₉P₁₂ [2]

Structural features: Infinite columns of base-linked P(Sc₂Co₄)Co₃ and P(Sc₄Co₂)Co₃ tricapped trigonal prisms (site splitting ignored) share atoms to form a 3D-framework (a framework of base- and edge-linked P(Sc₄Co₂) prisms with 6-fold prism columns shifted by $c/2$ in channels). Variant of Ho₅Ni₁₉P₁₂.

Jeitschko W., Reinbold E.J. (1985) [1]

Co₁₉P₁₂Sc₅ $a = 1.2124$, $c = 0.3633$ nm, $c/a = 0.300$, $V = 0.4625$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
P1	6 <i>k</i>	<i>m</i> ..	0.167	0.4845	$\frac{1}{2}$		tricapped trigonal prism Co ₇ Sc ₂
Co2	6 <i>k</i>	<i>m</i> ..	0.35489	0.48137	$\frac{1}{2}$		cuboctahedron P ₄ Co ₅ Sc ₃
Co3	6 <i>j</i>	<i>m</i> ..	0.1767	0.37392	0		cuboctahedron P ₄ Co ₅ Sc ₃
Co4	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.28329	0	$\frac{1}{2}$		cuboctahedron P ₄ Co ₆ Sc ₂
Sc5	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.8171	0	$\frac{1}{2}$		
P6	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.1759	0	0		
Co7	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.44923	0	0		13-vertex polyhedron P ₅ Co ₈
P8	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.6405	0	0		tricapped trigonal prism Co ₇ Sc ₂
Co9	2 <i>e</i>	3. <i>m</i>	0	0	0.0827	0.5	
Sc10	2 <i>c</i>	-6..	$\frac{1}{3}$	$\frac{2}{3}$	0		23-vertex polyhedron P ₉ Co ₁₂ Sc ₂

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

Experimental: single crystal, diffractometer, X-rays, R = 0.023

Remarks: Short interatomic distances for partly occupied site(s). In [1] the Wyckoff position of former Co(4) is misprinted as 2*b* instead of 2*e*.

References: [1] Jeitschko W., Reinbold E.J. (1985), Z. Naturforsch. B 40, 900-905. [2] Ghetta V., Chaudouet P., Madar R., Sénateur J.P., Lambert Andron B. (1986), J. Less-Common Met. 120, 197-201.