

$\text{Rh}_{20}\text{Si}_{13}$ $hP34$ $(176) P6_3/m - h^5cb$ **Rh₂₀Si₁₃** [1]

Structural features: Infinite columns of base-linked SiRh₆Rh monocapped and SiRh₆Rh₂ bicapped trigonal prisms share atoms to form a 3D-framework with WC-type columns (6 prisms in the triangular cross-section); additional Si in channels of hexagonal cross-section parallel to [001] (partial disorder).

Engström I. (1965) [1]

 $\text{Rh}_{20}\text{Si}_{13}$ $a = 1.1851$, $c = 0.3623$ nm, $c/a = 0.306$, $V = 0.4407$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Rh1	6h	$m..$	0.0033	0.1876	$\frac{1}{4}$		pseudo Frank-Kasper Si ₅ Rh ₈
Rh2	6h	$m..$	0.0713	0.4613	$\frac{1}{4}$		tricapped pentagonal prism Si ₅ Rh ₈
Rh3	6h	$m..$	0.2725	0.4008	$\frac{1}{4}$		tricapped pentagonal prism Si ₅ Rh ₈
Si4	6h	$m..$	0.3391	0.2333	$\frac{1}{4}$		bicapped square prism Rh ₈ Si ₂
Si5	6h	$m..$	0.5497	0.1678	$\frac{1}{4}$		pentacapped trigonal prism Rh ₇ Si ₄
Rh6	2c	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		anticuboctahedron Si ₆ Rh ₆
Si7	2b	$-3..$	0	0	0	0.5	square prism (cube) Si ₂ Rh ₆

Experimental: single crystal, Weissenberg photographs, X-rays, $R = 0.105$

Remarks: Identical to the phase called Rh_{1.5}Si in [2]. Short interatomic distances for partly occupied site(s).

References: [1] Engström I. (1965), Acta Chem. Scand. 19, 1924-1932. [2] Engström I. (1963), Acta Chem. Scand. 17, 775-784.