

$\text{Sc}_3\text{Rh}_{1.59}\text{In}_4$ $hP18$ (174) $P-6 - lkjihba$ **$\text{Sc}_3\text{Rh}_{1.59}\text{In}_4$** [1]

Structural features: Infinite columns of base-linked RhIn_6Sc_3 (partial vacancies ignored) and RhSc_6In_3 tricapped trigonal prisms share atoms to form a 3D-framework; additional In in columns of hexagonal cross-section.

Lukachuk M. et al. (2004) [1]

 $\text{In}_4\text{Rh}_{1.59}\text{Sc}_3$ $a = 0.7694$, $c = 0.6841$ nm, $c/a = 0.889$, $V = 0.3507$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
In1	$6l$	1	0.25659	0.2537	0.2601		14-vertex Frank-Kasper $\text{Rh}_3\text{In}_5\text{Sc}_6$
Sc2	$3k$	$m..$	0.0353	0.4214	$\frac{1}{2}$		15-vertex Frank-Kasper $\text{Rh}_3\text{In}_8\text{Sc}_4$
Sc3	$3j$	$m..$	0.0414	0.4106	0		15-vertex Frank-Kasper $\text{Rh}_3\text{In}_8\text{Sc}_4$
In4	$2i$	$3..$	$\frac{2}{3}$	$\frac{1}{3}$	0.237		pseudo Frank-Kasper In_5Sc_6
Rh5	$2h$	$3..$	$\frac{1}{3}$	$\frac{2}{3}$	0.2505		pseudo Frank-Kasper $\text{Sc}_6\text{In}_3\text{Rh}_2$
Rh6	$1b$	$-6..$	0	0	$\frac{1}{2}$	0.412	pseudo Frank-Kasper $\text{In}_6\text{Sc}_3\text{Rh}_2$
Rh7	$1a$	$-6..$	0	0	0	0.775	pseudo Frank-Kasper $\text{In}_6\text{Sc}_3\text{Rh}_2$

Transformation from published data: y, x, z ; origin shift 0 0 $\frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.031$

References: [1] Lukachuk M., Zaremba V.I., Hoffmann R.D., Pöttgen R. (2004), Z. Naturforsch. B 59, 182-189.