

$\text{Zr}_2\text{Rh}_{12}\text{P}_7$	$hP22$	$(176) P6_3/m - h^3db$
---------------------------------------	--------	------------------------

Zr₂Rh₁₂P₇ [1]

Structural features: Infinite columns of base-linked P(Zr₂Rh₄)Rh₃ tricapped trigonal prisms share atoms to form a 3D-framework with propeller-like columns; additional P in channels of hexagonal cross-section parallel to [001] (partial disorder). See Fig. IV.56.

Pivan J.Y. et al. (1984) [1]

P₇Rh₁₂Zr₂

$a = 0.9516$, $c = 0.3773$ nm, $c/a = 0.396$, $V = 0.2959$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Rh1	6 <i>h</i>	<i>m</i> ..	0.0722	0.4539	1/4		11-vertex polyhedron P ₄ Rh ₅ Zr ₂
Rh2	6 <i>h</i>	<i>m</i> ..	0.2646	0.1515	1/4		square pyramid P ₅
P3	6 <i>h</i>	<i>m</i> ..	0.2869	0.4081	1/4		monocapped trigonal prism Rh ₇
Zr4	2 <i>d</i>	-6..	2/3	1/3	1/4		23-vertex polyhedron P ₉ Rh ₁₂ Zr ₂
P5	2 <i>b</i>	-3..	0	0	0	0.5	square prism (cube) P ₂ Rh ₆

Transformation from published data: *y*,*x*,*-z*; origin shift 0 0 1/2

Experimental: single crystal, diffractometer, X-rays, R = 0.040

References: [1] Pivan J.Y., Guérin R., Sergent M. (1984), C. R. Acad. Sci., Ser. II 299, 533-538.

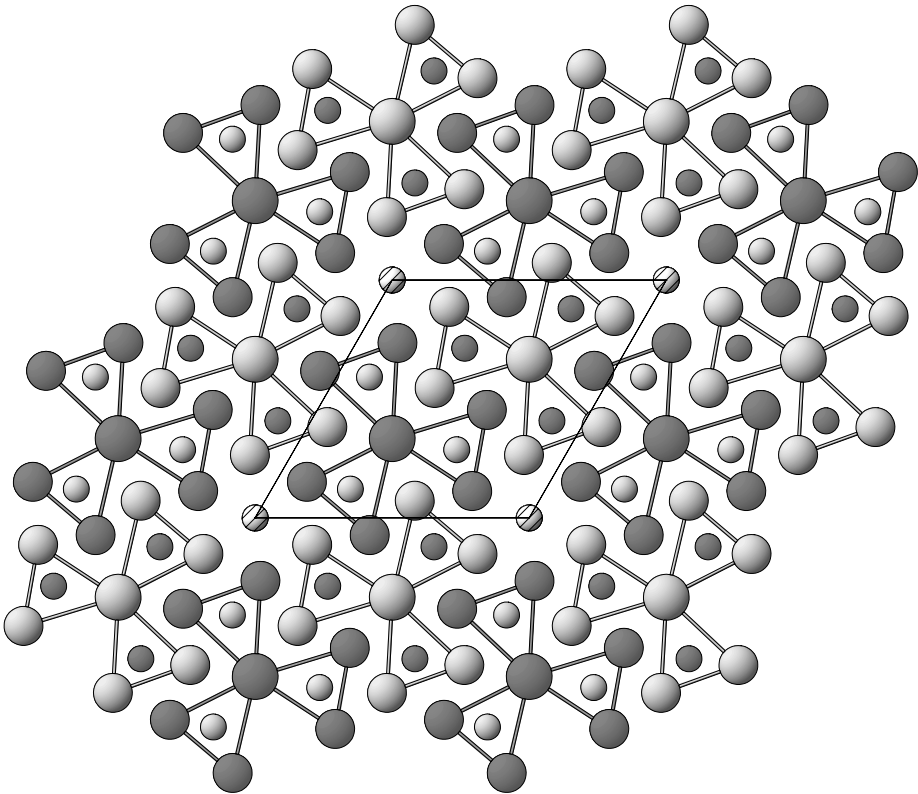


Fig. IV.56. **Zr₂Rh₁₂P₇**

Arrangement of P(Zr₂Rh₄) trigonal prisms (P atoms small, Zr atoms large, Rh atoms medium) and additional P atoms (partly occupied site) viewed along [001]. Light and dark atoms are shifted by $c/2$.