

ZrRhGa	<i>hP10</i>	(189) <i>P-62m</i> – gfd
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ZrRhGa [1]

Structural features: Infinite columns of base-linked RhZr₆ trigonal prisms share edges to form a 3D-framework; single columns of base-linked RhGa₆ trigonal prisms in channels parallel to [001] (split Rh site). Variant of ZrNiAl.

Zumdick M.F. et al. (2002) [1]

GaRhZr

$a = 0.7214$, $c = 0.3367$ nm, $c/a = 0.467$, $V = 0.1517$ nm³, $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ga1	3 <i>g</i>	<i>m2m</i>	0.2704	0	$\frac{1}{2}$		
Zr2	3 <i>f</i>	<i>m2m</i>	0.6048	0	0		
Rh3	2 <i>e</i>	3. <i>m</i>	0	0	0.0573	0.5	
Rh4	2 <i>d</i>	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		tricapped trigonal prism Ga ₃ Zr ₆

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

Experimental: single crystal, diffractometer, X-rays, R = 0.020

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Zumdick M.F., Pöttgen R., Zaremba V.I., Hoffmann R.D. (2002), J. Solid State Chem. 166, 305-310.