

$\text{Rb}_{0.3}(\text{W}_{0.9}\text{Ga}_{0.1})\text{O}_3$ $hP13$ (183) $P6mm - ec^2a$ **Rb_{0.3}Ga_{0.1}W_{0.9}O₃** [1], HTB (hexagonal tungsten bronze)Structural features: (W,Ga)O₆ octahedra distorted towards square pyramids share vertices to form a 3D-framework; Rb in large channels of hexagonal cross-section parallel to [001].

Mattes R. et al. (1990) [1]

 $\text{Ga}_{0.20}\text{O}_3\text{Rb}_{0.09}\text{W}_{0.80}$ $a = 0.726$, $c = 0.376$ nm, $c/a = 0.518$, $V = 0.1716$ nm³, $Z = 3$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6e	.m.	0.211	0.789	0.575		non-colinear W ₂
O2	3c	2mm	$\frac{1}{2}$	0	0.009		single atom W
M3	3c	2mm	$\frac{1}{2}$	0	0.57		octahedron O ₆
Rb4	1a	6mm	0	0	0.0	0.28	non-coplanar hexagon O ₆

 $\text{M3} = 0.8\text{W} + 0.2\text{Ga}$

Transformation from published data: -x,-y,-z; origin shift 0 0 0.93

Experimental: single crystal, diffractometer, X-rays, wR = 0.035, T = 295 K

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions.

References: [1] Mattes R., Leimkühler M., Nagel A. (1990), Z. Anorg. Allg. Chem. 582, 131-142.