

$\text{Mg}_{0.94}\text{Yb}_{1.06}\text{Ga}_4$ $hP6$ (187) $P-6m2 - ihba$ **Mg_{1-x}Yb_{1+x}Ga₄** [1]

Structural features: 3D-framework of fused Ga(Mg₃Yb₃) trigonal prisms (partial substitution ignored); Ga is displaced from the prism centers to form a tetrahedral framework. Ordering variant of ScAuSi, both substitution derivatives of CaIn₂.

Fedorchuk A. et al. (2003) [1]

 $\text{Ga}_4\text{Mg}_{0.94}\text{Yb}_{1.06}$ $a = 0.43979$, $c = 0.69671$ nm, $c/a = 1.584$, $V = 0.1167$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ga1	$2i$	$3m.$	$\frac{2}{3}$	$\frac{1}{3}$	0.2		fourcapped trigonal prism Ga ₄ Mg ₃ Yb ₃
Ga2	$2h$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.2855		fourcapped trigonal prism Ga ₄ Yb ₃ Mg ₃
Yb3	$1b$	$-6m2$	0	0	$\frac{1}{2}$		bicapped hexagonal prism Ga ₁₂ Mg ₂
M4	$1a$	$-6m2$	0	0	0		bicapped hexagonal prism Ga ₁₂ Yb ₂

 $\text{M4} = 0.942\text{Mg} + 0.058\text{Yb}$ Transformation from published data: $-x, -y, -z$; origin shift $0\ 0\ \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $wR = 0.018$

References: [1] Fedorchuk A., Prots' Y., Schmidt M., Schnelle W., Burkhardt U., Schwarz U., Grin Y. (2003), Z. Anorg. Allg. Chem. 629, 2470-2478.