

$\text{Gd}_{0.67}\text{Ni}_2\text{Ga}_4(\text{Ga}_{0.67}\text{Ge}_{0.33})_2$ $hP11$ $(187) P-6m2 - \text{jhgda}$ **$\text{Gd}_{0.67}\text{Ni}_2\text{Ga}_{6-x}\text{Ge}_x$ [1]**

Structural features: $\text{Gd}_2(\text{Ga}_3)$ layers (the Gd atoms and the centers of Ga_3 triangles form a triangle mesh) and slabs containing triangle-mesh Ni, Ga and (Ga,Ge) layers alternate along [001]; $\text{Gd}_2(\text{Ga}_3)$ layers in maximum stacking disorder.

Zhuravleva M.A. et al. (2002) [1]

 $\text{Ga}_{5.32}\text{Gd}_{0.58}\text{Ge}_{0.67}\text{Ni}_2$ $a = 0.41856$, $c = 0.9167$ nm, $c/a = 2.190$, $V = 0.1391$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ga1	3j	$mm2$	0.2012	0.7988	0	0.33	
M2	2i	3m.	$\frac{2}{3}$	$\frac{1}{3}$	0.2003		non-coplanar triangle Ni_3
Ni3	2h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.2455		
Ga4	2g	3m.	0	0	0.349		10-vertex polyhedron Ni_3Ga_7
Ga5	1d	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		8-vertex polyhedron Ni_2Ga_6
Gd6	1a	$-6m2$	0	0	0	0.58	

 $\text{M2} = 0.667\text{Ga} + 0.333\text{Ge}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.027$, $T = 293$ K

Remarks: Ga and Ge could not be distinguished, the refinement was performed with site Ga1 occupied by Ge and site M2 fully occupied by Ga. We assigned a Ga/Ge distribution in agreement with the refinement of $\text{Y}_{0.6}\text{Co}_2\text{Ga}_{6-x}\text{Ge}_x$ on neutron diffraction data reported in the same paper. Short interatomic distances for partly occupied site(s). A similar model was proposed for disordered RNi_3Al_9 in [2].

References: [1] Zhuravleva M.A., Chen X.Z., Wang X., Schultz A.J., Ireland J., Kannewurf C.K., Kanatzidis M.G. (2002), Chem. Mater. 14, 3066-3081. [2] Gladyshevskii R.E., Cenzual K., Flack H.D., Parthé E. (1993), Acta Crystallogr. B 49, 468-474.