

Gd₃Ru₂C₅*hP50*(176) *P6₃/m – h⁷fe***Gd₃Ru₂C₅** [1]

Structural features: Ru₃C₁₀ units (a Ru₃ triangle with a C=C pair bonded to each Ru and single C capping all edges and one side of the triangle in statistical disorder; all atoms coplanar except the latter C); additional Ru in channels parallel to [001] (partial disorder).

Pohlkamp M.W. et al. (2001) [1]

C_{4.86}Gd₃Ru_{1.85} $a = 1.147$, $c = 0.5047$ nm, $c/a = 0.440$, $V = 0.5750$ nm³, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
C1	6 <i>h</i>	<i>m</i> ..	0.0686	0.3218	¹ / ₄		single atom C
C2	6 <i>h</i>	<i>m</i> ..	0.1199	0.6116	¹ / ₄		non-colinear Ru ₂
Ru3	6 <i>h</i>	<i>m</i> ..	0.2056	0.5028	¹ / ₄		trigonal bipyramid C ₅
C4	6 <i>h</i>	<i>m</i> ..	0.2074	0.0188	¹ / ₄		single atom C
Gd5	6 <i>h</i>	<i>m</i> ..	0.2182	0.22	¹ / ₄	0.247	
Gd6	6 <i>h</i>	<i>m</i> ..	0.2597	0.2599	¹ / ₄	0.753	
Gd7	6 <i>h</i>	<i>m</i> ..	0.507	0.1233	¹ / ₄		pentagonal pyramid C ₆
C8	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.0014	0.36	non-coplanar triangle Ru ₃
Ru9	4 <i>e</i>	3..	0	0	0.0654	0.351	

Experimental: single crystal, diffractometer, X-rays, R = 0.052

Remarks: Refinement of the site occupancies showed no significant deviation from unity except for sites Gd5, Gd6, C8 and Ru9. Short interatomic distances for partly occupied site(s).

References: [1] Pohlkamp M.W., Hoffmann R.D., Kotzyba G., Jeitschko W. (2001), J. Solid State Chem. 160, 77-87.