

Ba ₅ Ga ₆	<i>hP</i> 24	(188) <i>P</i> -6 <i>c</i> 2 – lkha
---------------------------------	--------------	-------------------------------------

"Ba₅Ga₆" [1]

Structural features: Ga₆ octahedral clusters inside fused Ba₁₂ cuboctahedra (one split Ba site).

Fornasini M.L., Pani M. (1994) [1]

Ba_{4.96}Ga₆

$a = 0.7771$, $c = 1.4376$ nm, $c/a = 1.850$, $V = 0.7518$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ga1	12 <i>l</i>	1	0.46513	0.33077	0.078		non-coplanar square Ga ₄
Ba2	6 <i>k</i>	<i>m</i> ..	0.02663	0.33457	¹ / ₄		non-coplanar square Ga ₄
Ba3	4 <i>h</i>	3..	¹ / ₃	² / ₃	0.0284	0.48	
Ba4	2 <i>a</i>	3.2	0	0	0		octahedron Ga ₆

Transformation from published data: -*x*, -*y*, -*z*; origin shift ²/₃ ¹/₃ ¹/₂

Experimental: single crystal, diffractometer, X-rays, R = 0.076

Remarks: Identical to the phase called BaGa in [3]. Short interatomic distances for partly occupied site(s). The authors of [2] state that composition Ba₅Ga₆H₂ would be in agreement with valence electron rules; the existence of Ba₅Ga₆H₂ was confirmed and its (fully ordered) structure refined in space group (158) *P*3*c*1 in [4].

References: [1] Fornasini M.L., Pani M. (1994), J. Alloys Compd. 205, 179-181. [2] Liu Q., Hoffmann R., Corbett J.D. (1994), J. Phys. Chem. 98, 9360-9364. [3] Bruzzone G. (1966), Boll. Sci. Fac. Chim. Ind. Bologna 24, 113-132. [4] Henning R.W., Leon Escamilla E.A., Zhao J.T., Corbett J.D. (1997), Inorg. Chem. 36, 1282-1285.