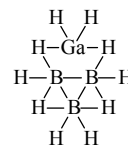


71 **B₃GaH₁₀****2-Galla-arachno-tetraborane(10)****C_s** assumedED, *ab initio*
calculations

r_a	Å ^{a)}	θ_a^0	deg ^{a)}
B(1)–B(3)	1.800(13)	B(3)–B(1)–H(1)	111.6(10)
B(1)–H(1)	1.182(8)	H(2) _{endo} –Ga(2)–H(2) _{exo}	131.0(19)
B(1)–H(1,4)	1.252(11)	H(4) _{endo} –B(4)–H(4) _{exo}	119.2(10)
B(1)–H(1,2)	1.243(11)	B(1)–B(4)–B(3)	57.8(3)
B(4)–H(1,4)	1.433(18)	B(1)–Ga–B(3)	45.3(4)
B(4)–H(4) _{endo}	1.190(8)	tilt(GaH ₂) ^{b)}	–2.5(6)
B(4)–H(4) _{exo}	1.190(8)	tilt(BH ₂) ^{c)}	0.7(7)
Ga(2)–H(1,2)	1.81(4)	ϕ ^{d)}	117.1(7)
Ga(2)–H(2) _{endo}	1.507(14)	ϕ_1 ^{e)}	10.7(10)
Ga(2)–H(2) _{exo}	1.505(14)	ϕ_2 ^{f)}	0.3(2)
B(1)–B(4)	1.841(13)		
B(1)–Ga(2)	2.310(2)		



The differences in the similar parameters were restrained flexibly by the values from MP2/6-311G** calculations.

The experimental curves were obtained in [1].

The nozzle temperature was 273 K.

^{a)} Estimated standard errors.

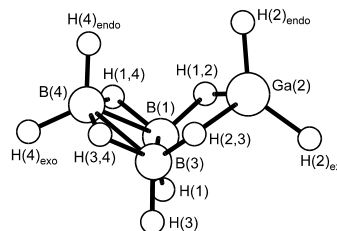
^{b)} Tilt angle between the bisector of the H(2)_{endo}–Ga(2)–H(2)_{exo} angle and the B(1)GaB(3) plane, negative value for the tilt away from the cage structure.

^{c)} Tilt angle between the bisector of the H(4)_{endo}–B(4)–H(4)_{exo} angle and the B(1)B(4)B(3) plane, positive value for the tilt into the cage structure.

^{d)} Dihedral angle between the B(1)B(3)B(4) and B(1)B(3)Ga(2) planes.

^{e)} Dihedral angle between the B(1)Ga(2)B(3) and B(1)Ga(2)H(1,2) planes, positive for elevation of H(1,2).

^{f)} Dihedral angle between the B(1)B(4)B(3) and B(1)B(4)H(1,4) planes, positive for elevation of H(1,4).



Morrison, C.A., Smart, B.A., Brain, P.T., Pulham, C.R., Rankin, D.W.H., Downs, A.J.: J. Chem. Soc., Dalton Trans. (1998) 2147.

[1] Pulham, C.R., Downs, A.J., Rankin, D.W.H., Robertson, H.E.: J. Chem. Soc., Dalton Trans. (1992) 1509.

Replaces [II/25A\(2, 132\)](#)