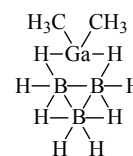
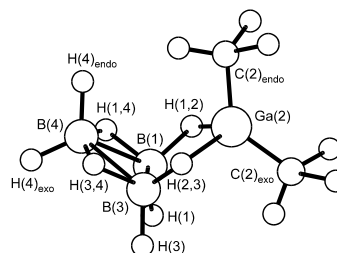


**323**      **C<sub>2</sub>H<sub>14</sub>B<sub>3</sub>Ga**ED, *ab initio*  
calculations**2-Dimethyl-2-galla-arachno-tetraborane(10)**Dimethyl[ $\eta^2$ -octahydrotriborato]gallium**C<sub>s</sub>**

$r_a$	Å <sup>a)</sup>	$\theta_\alpha^0$	deg <sup>a)</sup>
B(1)–B(3)	1.794(23)	B(3)–B(1)–H(1)	111.6(13)
B(1)–H(1)	1.185(17)	H(4) <sub>endo</sub> –B(4)–H(4) <sub>exo</sub>	118.5(13)
B(1)–H(1,4)	1.245(18)	C(2) <sub>endo</sub> –Ga(2)–C(2) <sub>exo</sub>	132.5(15)
B(1)–H(1,2)	1.237(19)	H–C–Ga(2)	108.6(10)
B(4)–H(1,4)	1.40(3)	$\varphi^b$	119.8(13)
B(4)–H(4) <sub>endo</sub>	1.194(17)	tilt(GaC <sub>2</sub> ) <sup>c)</sup> <sup>d)</sup>	–4.7(23)
B(4)–H(4) <sub>exo</sub>	1.187(17)	tilt(BH <sub>2</sub> ) <sup>d)</sup> <sup>e)</sup>	0.5(21)
Ga(2)–C(2) <sub>endo</sub>	1.941(4)	dip[H(1,2)] <sup>f)</sup>	14.3(16)
Ga(2)–C(2) <sub>exo</sub>	1.939(4)	dip[H(1,4)] <sup>g)</sup>	–0.2(16)
Ga(2)–H(2,1)	1.86(6)		
C–H(methyl)	1.124(9)		
B(1)–B(4)	1.85(23)		
B(1)–Ga(2)	2.344(8)		

The experimental curves from [1] were reanalyzed. Some structural parameters and differences in the similar parameters were restrained flexibly by the values from MP2/6-311G\*\* calculations.

The sample temperature was 297 K.



<sup>a)</sup> Estimated standard errors.

<sup>b)</sup> Dihedral angle between the B(1)B(3)B(4) and Ga(2)B(1)B(3) angles.

<sup>c)</sup> Tilt angle between the bisector of the C(2)<sub>endo</sub>–Ga(2)–C(2)<sub>exo</sub> angle and the B(1)Ga(2)B(3) plane.

<sup>d)</sup> Positive value for the tilt into the heavy atom cage.

<sup>e)</sup> Tilt angle between the bisector of the H(4)<sub>endo</sub>–B(4)–H(4)<sub>exo</sub> angle and the B(1)B(4)B(3) plane.

<sup>f)</sup> Elevation of the H(1,2) bridging atom above the B(1)Ga(2)B(3) plane, *i.e.*, the dihedral angle between the B(1)H(1,2)Ga(2) and B(1)Ga(2)B(3) planes.

<sup>g)</sup> Elevation of the H(1,4) bridging atom above the B(1)B(4)B(3) plane, *i.e.*, the dihedral angle between the B(1)H(1,4)B(4) and B(1)B(4)B(3) planes.

Morrison, C.A., Smart, B.A., Brain, P.T., Rankin, D.W.H., Downs, A.: J. Chem. Soc., Dalton Trans. (1998) 2155.

[1] Dain, C.J., Downs, A.J., Rankin, D.W.H.: J. Chem. Soc., Dalton Trans. (1981) 2465.

Replaces [II/25B\(3, 974\)](#)