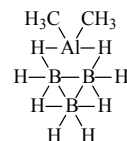


322  $C_2H_{14}AlB_3$ 2-Dimethyl-2-alumina-*arachno*-tetraborane(10) $C_s$ ED, *ab initio*  
calculations

$r_a$	$\text{\AA}^a$	$\theta_a^0$	$\text{deg}^a$
B(1)–B(3)	1.787(12)	B(3)–B(1)–H(1)	112.3(12)
B(1)–H(1)	1.218(10)	H(4) <sub>endo</sub> –B(4)–H(4) <sub>exo</sub>	118.5(13)
B(1)–H(1,4)	1.282(11)	C(2) <sub>endo</sub> –Al(2)–C(2) <sub>exo</sub>	132.0(23)
B(1)–H(1,2)	1.261(12)	H–C–Al(2)	111.0(15)
B(4)–H(1,4)	1.439(11)	$\phi^b$	123.8(20)
B(4)–H(4) <sub>endo</sub>	1.221(10)	tilt(AlC <sub>2</sub> ) <sup>c</sup> <sup>d</sup>	–7.1(4)
B(4)–H(4) <sub>exo</sub>	1.223(10)	tilt(BH <sub>2</sub> ) <sup>d</sup> <sup>e</sup>	0.7(13)
Al(2)–C(2) <sub>endo</sub>	1.948(5)	dip[H(1,2)] <sup>f</sup>	13.4(13)
Al(2)–C(2) <sub>exo</sub>	1.945(5)	dip[H(1,4)] <sup>g</sup>	1.5(16)
Al(2)–H(2,1)	1.830(13)		
C–H(methyl)	1.087(4)		
B(1)–B(4)	1.852(10)		
B(1)–Al(2)	2.316(7)		



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 273 K.

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

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

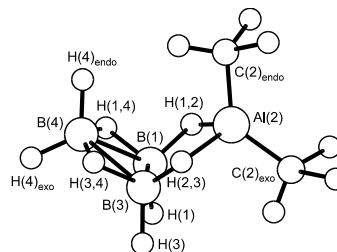
<sup>c</sup>) Tilt angle between the bisector of the C(2)<sub>endo</sub>–Al(2)–C(2)<sub>exo</sub> angle and the B(1)Al(2)B(3) plane.

<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)Al(2)B(3) plane, *i.e.*, the dihedral angle between the B(1)H(1,2)Al(2) and B(1)Al(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\(3, 973\)](#)