

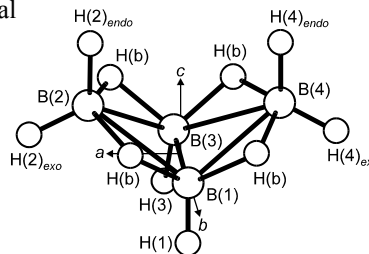
73 **B₄H₁₀**
ED, MW, *ab initio*
calculations

arachno-Tetraborane(10)

C_{2v} assumed
B₄H₁₀

r_{α}^0	Å ^{a)}	θ_{α}^0	deg ^{a)}
B–B (average)	1.840(2)	H(2) _{exo} –B(2)–H(2) _{endo}	119.6(13)
B–H (average)	1.273(3)	H(1)–B(1)–B(3)	115.0(16)
B(1)–B(2) ^{b)}	1.866(2)	B(1)–B(2)–B(3) ^{b)}	55.5(2)
B(1)–B(3) ^{b)}	1.737(5)	φ ^{c)}	117.2(4)
B(1)–H(b) ^{b)}	1.230(15)	dip(H(b)) ^{d)}	6.2(5)
B(2)–H(b) ^{b)}	1.417(8)	tilt(BH ₂) ^{e)}	1.2(12)
B(1)–H(1) ^{b)}	1.198(8)		
B(2)–H(2) _{endo} ^{b)}	1.210(8)		
B(2)–H(2) _{exo} ^{b)}	1.205(8)		

The ED data from [1] were reanalyzed. The rotational constants were taken from the literature (see [II/25A\(2, 140\)](#), MW). The structural parameters were obtained by supplementing experimental data with restraints based on the results of CCSD(T)/TZP calculations. The nozzle was at room temperature.



^{a)} Estimated standard errors.

^{b)} Dependent parameter.

^{c)} Dihedral angle between the two BBB planes.

^{d)} Dihedral angle describing the elevation of the bridging-hydrogen atoms from the BBB planes, *i.e.*, the angle between the B(1)B(2)B(3) and B(1)B(2)H(b) planes.

^{e)} Tilt angle of the BH₂ groups in the B(2)B(4)H_{endo}H_{exo} plane, *i.e.*, the angle between the bisector of the H_{endo}–B–H_{exo} angle and the BBB plane, a positive angle representing an *endo* tilt.

Brain, P.T., Morrison, C.A., Parsons, S., Rankin, D.W.H.: J. Chem. Soc., Dalton Trans. (1996) 4589.

[1] Dain, C.J., Downs, A.J., Laurenson, G.S., Rankin, D.W.H.: J. Chem. Soc., Dalton Trans. (1981) 472.

Replaces II/25A(2, 140), ED