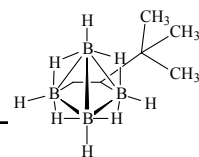


763 **C₆H₂₀B₄**ED, *ab initio*
calculations**2,4[1-(1,1-Dimethylethyl)-1,2-ethanediyl]tetraborane(10)** **C₁**2,4-(*t*-Butylethano)tetraborane(10)

r_a	Å ^{a)}	θ_a	deg ^{a)}
B(1)–B(2)	1.896(8)	B(1)–B(2)–B(3)	54.5(4) ^{b)}
B(1)–B(4)	1.884(7)	B(1)–B(4)–B(3)	54.5(4)
B(1)–B(3)	1.731(16)	C(1)–C(2)–C(<i>t</i>)	112.2(11) ^{c)}
C(2)–B(2)	1.612(8)	C(m)–C(<i>t</i>)–C(m)	110.2(8) ^{c)}
C(1)–B(4)	1.603(12)	B(1)–B(3)–H(t)	113.4(20) ^{b)}
C(1)–C(2)	1.556(6)	B(1)–B(3)–H(b)	111.7(7) ^{b)}
C(2)–C(<i>t</i>)	1.560(6)	C–C–H	108.5(7)
C(<i>t</i>)–C(m) (mean)	1.552(5)	ϕ ^{d)}	98.2(7)
B(2)–H(t)	1.203(19)	twist(CH ₃) ^{e)}	18.0(20)
B(1)–H(t)	1.194(19)	twist(<i>t</i> -butyl) ^{f)}	5.1(15)
B(1)–H(b)	1.238(19) ^{b)}	tilt(<i>t</i> -butyl) ^{g)}	0.0 ^{h)}
B(4)–H(b)	1.427(18)	τ_1 ⁱ⁾	6.6(14)
B(2)–H(b)	1.431(18)	τ_2 ^{j)}	–11.0(24) ^{c)}
C–H (mean)	1.143(6)		

The B₄H₈ fragment was assumed to have local C_s symmetry, with the mirror plane passing through B(2) and B(4). The *t*-butyl fragment was assumed to have C₃ local symmetry, with C_{3v} symmetry for each C–CH₃ group. The distortion of the B₄H₈ group from C_{2v} local symmetry was found to be insignificant.

The nozzle temperature was 348 K.

^{a)} Estimated standard errors.

^{b)} Flexibly restrained by the value from MP2/6-31G* calculations.

^{c)} Dependent parameter.

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

^{e)} Torsional angle C(2)–C(*t*)–C(m)–H, 0° for the staggered position; positive value for the counter-clockwise rotation.

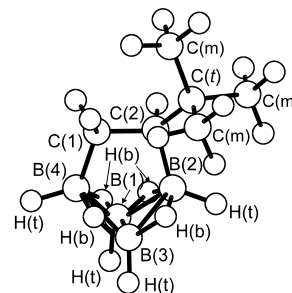
^{f)} Torsional angle C(1)–C(2)–C(*t*)–C(m), 0° for the *anti* position; positive value for the counter-clockwise rotation.

^{g)} Angle between the C₃ axis of *t*-butyl group and C(2)–C(*t*) bond.

^{h)} Refined and then fixed.

ⁱ⁾ Angle of rotation of the C(1)–C(2) bond about the *z*-axis passing through the center of the C(1)–C(2) bond and perpendicular to the B(1)–B(3) bond, bringing C(2) closer to B(1).

^{j)} B(2)–C(2)–C(1)–B(4) torsional angle.



Brain, P.T., Bühl, M., Fox, M.A., Greatrex, R., Hnyk, D., Nikrahi, A., Rankin, D.W.H., Robertson, H.E.: J. Mol. Struct. **445** (1998) 319.