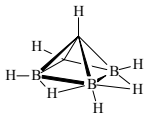
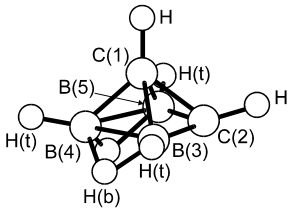
309 **$C_2H_7B_3$** ***nido*-1,2-Dicarbapentaborane(7)** **C_s**

ED, MW, *ab initio* calculations



r_α^0	Å [a])	θ_α^0	deg [a])
C(1)–C(2)	1.626(6)	B(3)–B(4)–B(5)	80.9(1)
C(1)–B(3)	1.614(3)	B(4)–C(1)–H	132.8(7) [b])
C(2)–B(3)	1.543(2)	C(1)–B(4)–H(t)	128.0(9) [b])
C(1)–B(4)	1.574(5)	C(1)–C(2)–H	118.8(6) [b])
B(3)–B(4)	1.857(3)	φ_1 [c])	61.0(6) [b])
C(2)–H	1.097(5) [d])	φ_2 [e])	2.7(6) [b])
C(1)–H	1.089(5) [d])	wag(H(t)) [f])	2.4(4) [b])
B(3)–H(t)	1.193(4) [d])	tilt(H(t)) [g])	10.8(10) [b])
B(4)–H(t)	1.192(4) [d])		
B(3)–H(b)	1.372(6) [h])		
B(4)–H(b)	1.342(7) [h])		



The nozzle temperature was 291 K.

[a]) Estimated standard errors.
[b]) Flexibly restrained by the value from CCSD(T)/TZP (employing DZP basis for H) calculations.
[c]) Angle between the extension of the B(3)B(4)B(5) plane and the B(3)B(4)H(b) plane (H(b) lies below the B(3)B(4)B(5) plane).
[d]) Difference from the mean value was assumed at the value from CCSD(T)/TZP (employing DZP basis for H) calculations.
[e]) Angle between the extension of the B(3)B(4)B(5) plane and the B(3)B(5)C(2) plane (C(2) lies below the B(3)B(4)B(5) plane).
[f]) Acute angle between the B(3)…B(5) vector and the projection of B(3)–H(t) onto the B(3)B(4)B(5) plane, positive value when H(t) moves towards C(2).
[g]) Acute angle between the B(3)–H(t) bond and the B(3)B(4)B(5) plane, positive value when H(t) moves towards C(1).
[h]) Difference from the mean value was flexibly restrained by the value from CCSD(T)/TZP (employing DZP basis for H) calculations.

Fox, M.A., Greatrex, R., Nikrahi, A., Brain, P.T., Picton, M.J., Rankin, D.W.H., Robertson, H.E., Bühl, M., Li, L., Beaudet, R.A.: Inorg. Chem. **37** (1998) 2166.