

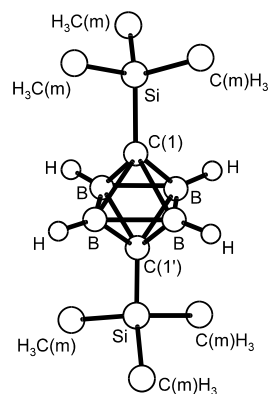
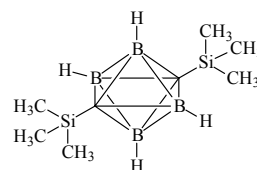
861 **C₈H₂₂B₄Si₂**ED, *ab initio*
calculations***closo*-1,6-Bis(trimethylsilyl)-1,6-
dicarbahexaborane(6)****C_{2h} assumed**

r_a	Å ^{a)}	θ_a	deg ^{a)}
B–B (mean)	1.699(8)	C(m)–Si–C(m)	110.9(10)
B–C	1.636(3)	C(1)–Si–C(m)	108.0(10)
Si–C (mean)	1.867(2)	H–C–H	107.7(7)
$\Delta(\text{Si–C})$ ^{b)}	0.005(14)		
Si–C(1)	1.863(11)		
Si–C(m)	1.868(4)		
C–H	1.102(5)		
B–H	1.212(26)		

Local D_{4h} symmetry was assumed for the carborane skeleton. Local C_{3v} symmetry was assumed for the trimethylsilyl and methyl groups. ED and *ab initio* (HF/6-31G*) methods gave very similar bond lengths for the carborane cage. The internal rotation of the SiMe₃ groups was expected to be essentially free, but no clear experimental evidence could be obtained. The nozzle was at 45 °C.

^{a)} Three times the estimated standard errors.

^{b)} [Si–C(m)] – [Si–C(1)].



Maguire, J.A., Lu, K.-J., Thomas, C.J., Gray, T.G., Wang, Y., Eintracht, J.F., Hosmane, N.S., Binder, H., Wanitschek, M., Borrmann, H., Simon, A., Oberhammer, H.: Chem. Eur. J. **3** (1997) 1059.