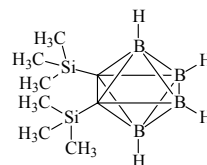


860 **C₈H₂₂B₄Si₂*****closo*-1,2-Bis(trimethylsilyl)-1,2-dicarbahexaborane(6)****C₂**ED, *ab initio*
calculations

r_a	Å ^{a)}	θ_a	deg ^{a)}
C(1)–C(2)	1.59(4)	C(1)–C(2)–Si	133.1(6)
B–C (mean)	1.587(7)	C(m)–Si–C(m)	112.5(8)
Δ (B–C) ^{b)}	0.040 ^{c)}	H–C–H	107.2(3)
B(4)–C(1)	1.613(12)	$\tau^d)$	41.3(19)
B(5)–C(1)	1.573(10)		
B–B (mean)	1.698(6)		
Δ (B–B) ^{e)}	0.050 ^{c)}		
B(3)–B(4)	1.658(16)		
B(3)–B(5)	1.708(8)		
Si–C (mean)	1.867(2)		
C–H	1.097(5)		
B–H	1.20 ^{f)}		



It was assumed that the trimethylsilyl and methyl groups have local C_{3v} symmetry and the carborane skeleton has local C_{2v} symmetry.

The Si–C(1) and Si–C(m) bond lengths were assumed to be equal.

The nozzle was at 55 °C.

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

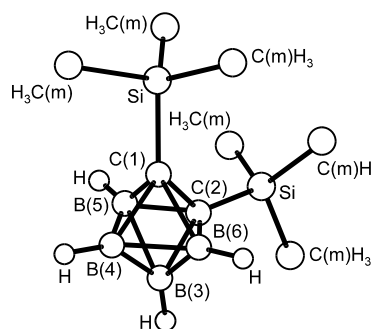
^{b)} [B(4)–C(1)] – [B(5)–C(1)].

^{c)} Constrained to the value from HF/6-31G* calculations.

^{d)} C(1)–C(2)–Si–C(m) torsional angle from the *syn* position.

^{e)} [B(3)–B(5)] – [B(3)–B(4)].

^{f)} Assumed.



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.