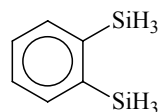


742 **C₆H₁₀Si₂**
ED, *ab initio*
calculations

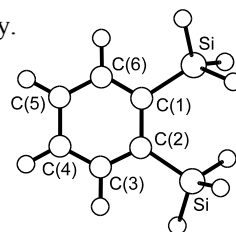
1,2-Phenylenebissilane
1,2-Disilylbenzene

C₂



r_a	Å ^{a)}	θ_a	deg ^{a)}
Si–C(2)	1.875(2)	Si–C(2)–C(1)	123.9(2)
C(1)–C(2)	1.418(3) ^{b)}	Si–C(2)–C(3)	116.2(2)
C(2)–C(3)	1.401(2) ^{b)}	C(1)–C(2)–C(3)	119.9(2)
C(3)–C(4)	1.394(2) ^{b)}	C(2)–C(3)–C(4)	120.0(3)
C(4)–C(5)	1.389(3) ^{b)}	C(3)–C(4)–C(5)	120.1(3)
Si–H	1.500(7)	C(2)–C(3)–H	119.0(10) ^{b)}
C–H	1.111(6)	C(3)–C(4)–H	120.3(10) ^{b)}
		H–Si...X ^{c)}	110.2(12) ^{b)}
		tilt(SiH ₃) ^{d)}	1.1(1)
		wag(SiH ₃) ^{e)}	–2.0(2)
		torsion(SiH ₃) ^{f)}	16.5(19)

The benzene ring was assumed to have local C_{2v} symmetry.
The nozzle temperature was 52...67 °C.



^{a)} Estimated standard errors.

^{b)} Differences in the C–C bond lengths, H–Si...X and C–C–H angles were restrained to the values from MP2/6-311G(d) calculations.

^{c)} X is the C₃ axis of the SiH₃ group.

^{d)} Tilt of the C₃ axis of the SiH₃ group from the C–Si direction in the plane perpendicular to the plane of the ring.

^{e)} Wag of the C₃ axis of SiH₃ group from the C–Si direction in the ring plane, positive if the local C₃ axes are displaced away from each other.

^{f)} Torsional angle of the SiH₃ group.

Mitzel, N.W., Brain, P.T., Hofmann, M.A., Rankin, D.W.H., Schröck, R., Schmidbauer, H.:
Z. Naturforsch. **57b** (2002) 202.