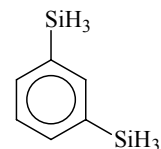


743 **C₆H₁₀Si₂**
ED, *ab initio*
calculations

1,3-Phenylenebissilane
1,3-Disilylbenzene

C_{2v} assumed (without
H atoms in the SiH₃ groups)

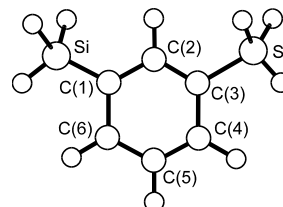
r_a	Å ^{a)}	θ_a	deg ^{a)}
Si–C	1.871(1)	H–Si–C	108.4(8) ^{b)}
C(1)–C(2)	1.404(4) ^{b)}	C(1)–C(6)–H	121.7(15)
C(1)–C(6)	1.404(4) ^{b)}	Si–C(1)–C(2)	120.1(2)
C(6)–C(5)	1.393(4) ^{b)}	Si–C(1)–C(6)	120.5(2)
Si–H	1.488(6)	C(2)–C(1)–C(6)	119.4(3)
C–H	1.092(7)	C(1)–C(2)–C(3)	120.4(4)
		C(1)–C(6)–C(5)	120.2(3)
		C(6)–C(5)–C(4)	120.4(5)



The SiH₃ groups were assumed to have local C_{3v} symmetry and modeled as freely rotating.
The nozzle temperature was 52...73 °C.

^{a)} Estimated standard errors.

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



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