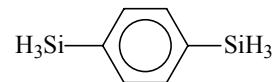


744 **C₆H₁₀Si₂**
ED, *ab initio*
calculations

1,4-Phenylenebissilane
1,4-Disilylbenzene

D_{2h} (without H atoms
in the SiH₃ groups)

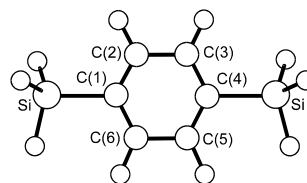
r_a	Å ^{a)}	θ_a	deg ^{a)}
Si–C	1.870(2)	H–Si–C	108.9(9)
C(1)–C(2)	1.405(2) ^{b)}	C(1)–C(2)–H	117.9(12)
C(2)–C(3)	1.397(3) ^{b)}	Si–C(1)–C(2)	120.5(1)
Si–H	1.497(6)	C(6)–C(1)–C(2)	119.0(2)
C–H	1.104(6)	C(1)–C(2)–C(3)	120.5(1)



The SiH₃ groups were assumed to have local C_{3v} symmetry and modeled as freely rotating.
The nozzle temperature was 53...69 °C.

^{a)} Estimated standard errors.

^{b)} Difference in the C–C bond lengths was restrained to the value 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.