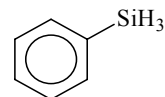


737 C₆H₅SiED, *ab initio*
calculations**Phenylsilane****C_{2v}** assumed (without
H atoms in the SiH₃ group)

r_g	Å ^{a)}	θ_a	deg ^{a)}
C(1)–C(2)	1.410(3)	C(2)–C(1)–C(6)	118.1(2)
C(2)–C(3)	1.400 ^{b)}	C(1)–C(2)–C(3)	121.1(1)
C(3)–C(4)	1.400 ^{b)}	C(2)–C(3)–C(4)	119.9(2)
Si–C	1.870(4)	C(3)–C(4)–C(5)	120.0(3)
Si–H	1.497(7)	C–Si–H	110.3 ^{c)}
C–H	1.100(4)	$\tau^d)$	15 ^{e)}



The benzene ring was assumed to have local C_{2v} symmetry and the silyl group local C_{3v}. The C–H bonds were assumed to bisect the corresponding C–C–C angle. MP2(fc)/6-31G* calculations indicated that the perpendicular conformation of the molecule, with an Si–H bond in a plane orthogonal to the benzene ring plane, corresponds to the potential energy minimum and the coplanar conformation, with an Si–H bond in a plane of the ring, corresponds to a torsional transition state. However, the energy difference for these states is only 0.13 kJ mol^{–1}, implying essentially free rotation of the SiH₃ group at room temperature. The nozzle temperature was *ca.* 301 K.

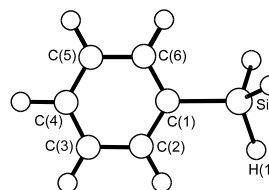
^{a)} Estimated total errors.

^{b)} The differences [C(1)–C(2)] – [C(2)–C(3)] and [C(1)–C(2)] – [C(3)–C(4)] were assumed at the values from MP2(fc)/6-31G* calculations.

^{c)} Assumed at the value from MP2(fc)/6-31G* calculations.

^{d)} Torsional angle of the SiH₃ group, H(1)–Si–C(1)–C(2), zero degree for the eclipsed position.

^{e)} Assumed effective value, corresponding to free rotation of the SiH₃ group about the Si–C bond.



Portalone, G., Ramondo, F., Domenicano, A., Hargittai, I.: J. Organomet. Chem. **560** (1998) 183.

ED, *ab initio*
calculations

r_a^0	Å ^{a)}	θ_a^0	deg ^{a)}
C(1)–C(2)	1.403(3) ^{b)}	C(2)–C(1)–C(6)	118.2(2)
C(2)–C(3)	1.396(2) ^{b)}	C(1)–C(2)–C(3)	121.1(3)
C(3)–C(4)	1.397(3) ^{b)}	C(2)–C(3)–C(4)	119.7(4)
Si–C	1.863(3)	C(3)–C(4)–C(5)	120.0(5)
Si–H	1.466(3)	Si–C(1)–C(2)	120.9(2)
C–H	1.094(4)	C–Si–H	111.7(14)
		C(1)–C(2)–H	120.2(12)

The SiH₃ groups were assumed to have local C_{3v} symmetry and modeled as freely rotating. Barrier to internal rotation of the SiH₃ group was predicted to be very low (0.11 kJ mol^{–1}) by MP2/6-31G(d) calculations.

^{a)} Estimated standard errors.

^{b)} Differences in the C–C bond lengths 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.

Replaces [II/25D \(3, 2290\)](#), ED