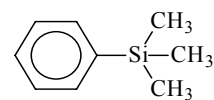


**876**      **C<sub>9</sub>H<sub>14</sub>Si**  
ED, *ab initio* and MM  
calculations

**Trimethylphenylsilane**  
(Trimethylsilyl)benzene

**C<sub>s</sub>**



$r_g$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
C(1)–C(2)	1.409(3)	C–C(1)–C	117.2(2)
C(2)–C(3)	1.398 <sup>b)</sup>	C–C(2)–C <sup>c)</sup>	121.4(2)
C(3)–C(4)	1.398 <sup>b)</sup>	C–C(3)–C <sup>c)</sup>	120.8(2)
Si–C(1)	1.877(4)	C–C(4)–C <sup>c)</sup>	118.5(4)
Si–C(m)	1.881 <sup>d)</sup>	C(1)–Si–C(m) <sup>c)</sup>	109.6(4)
C–H (ring)	1.103(3)	C(m)–Si–C(m)	109.4(4)
C(m)–H	1.109 <sup>b)</sup>	Si–C(m)–H	110.8(4)

According to molecular mechanics and *ab initio* (HF/6-31G\*, MP2(fc)/6-31G\*) calculations, a potential energy minimum corresponds to the coplanar conformation of the molecule, with one Si–C(m) bond in the plane of the benzene ring. The perpendicular conformation, with Si–C(m) bond in the plane orthogonal to the ring plane, was found to be a rotational transition state and only 0.2...0.5 kJ mol<sup>−1</sup> higher in energy. A model approximating a freely rotating Si(CH<sub>3</sub>)<sub>3</sub> group was consistent with the experimental data. It was assumed that the benzene ring has C<sub>2v</sub> symmetry and the trimethylsilyl and methyl groups have C<sub>3v</sub> symmetry and staggered conformations.

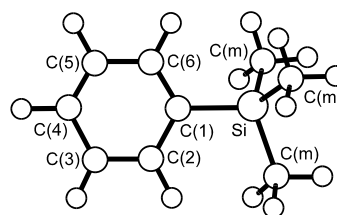
The nozzle temperature was about 305 K.

<sup>a)</sup> Estimated total errors.

<sup>b)</sup> Differences in the C–C and C–H distances were assumed at the values from MP2(fc)/6-31G\* calculations.

<sup>c)</sup> Dependent parameter.

<sup>d)</sup> Difference in the Si–C distances was assumed at the value from molecular mechanics (MM3) calculations.



Campanelli, A.R., Ramondo, F., Domenicano, A., Hargittai, I.: J. Organomet. Chem. **536-537** (1997) 309.