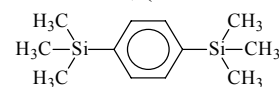


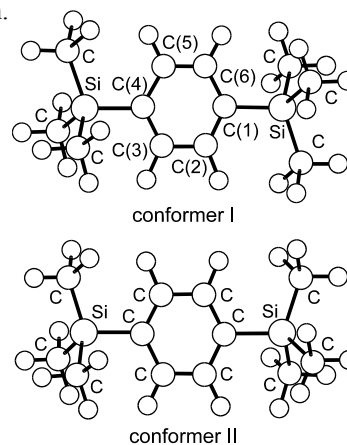
910 **C₁₂H₂₂Si₂**ED, *ab initio* and
DFT calculations**1,4-Phenylenebis(trimethylsilane)**

1,4-Bis(trimethylsilyl)benzene

C_{2h} (conformer I)**C_{2v}** (conformer II)

r_g	Å ^{a)}	θ_a	deg ^{a)}
C–C ^{b)}	1.407(3)	C(2)–C(1)–C(6)	117.2(3)
C(1)–C(2)	1.410 ^{c)}	C(3)–C(2)–H	118.7 ^{d)}
C(2)–C(3)	1.399 ^{c)}	C(ring)–Si–C(methyl)	109.3(4)
Si–C ^{b)}	1.881(4)	C(methyl)–Si–C(methyl)	109.6(4)
Si–C(ring)	1.878 ^{d)}	Si–C–H(methyl)	111.4(4)
Si–C(methyl)	1.882 ^{d)}		
C–H ^{b)}	1.108(3)		
C–H (ring)	1.104 ^{c)}		
C–H(methyl)	1.109 ^{c)}		

The ED intensities from [1] were reanalyzed using a model based on a 1:1 mixture of the two conformers. Local C_{3v} symmetry was assumed for the methyl and Si(CH₃)₃ groups. The *p*-phenylene moiety, C₆H₄, was assumed to have D_{2h} symmetry. The effective torsional angles of the Si(CH₃)₃ groups indicate nearly free rotation. The nozzle temperature was 385 K.

^{a)} Estimated total errors.^{b)} Average value.^{c)} Differences between the C(1)–C(2) and C(2)–C(3) bond lengths as well as between the C–H(ring) and C–H(methyl) bond lengths were assumed at the values from MP2(fc)/6-31G* calculations.^{d)} Assumed at the value from MP2(fc)/6-31G* calculations.Campanelli, A.R., Ramondo, F., Domenicano, A., Hargittai, I.: Struct. Chem. **10** (1999) 29.[1] Rozsondai, B., Zelei, B., Hargittai, I.: J. Mol. Struct. **95** (1982) 187.Replaces [II/25D \(3, 2824\)](#)