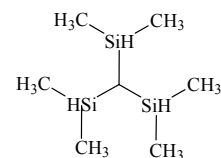


818 **C₇H₂₂Si₃**ED, *ab initio*
calculations**Methylidynetris(dimethylsilane)**

Tris(dimethylsilyl)methane

C₃ (ccc)**C₁ (all other conformers)**

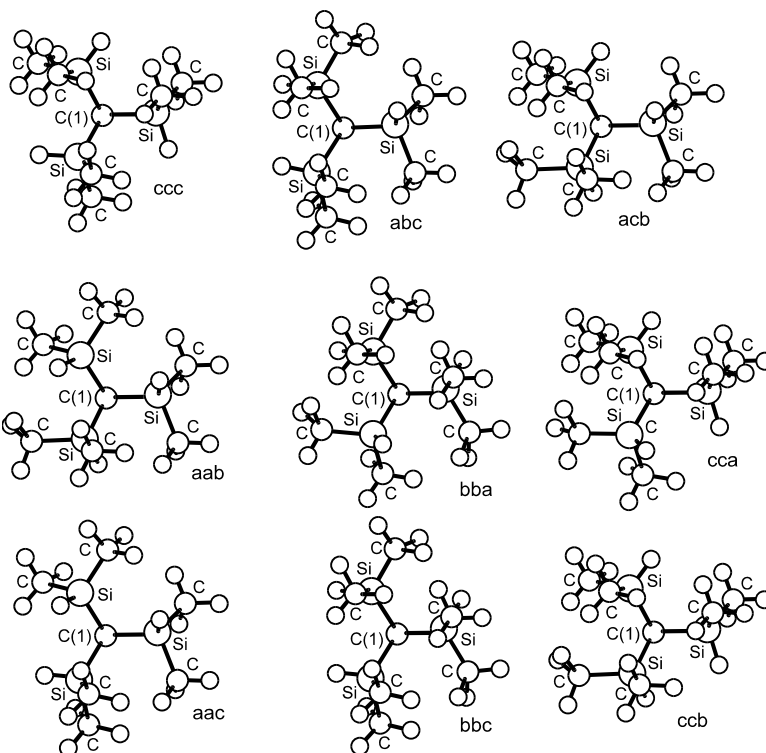
r_a	\AA^a	θ_a	deg ^{a)}
C(1)–H	1.110(4)	Si–C–Si	113.5(7) ^{b)}
C–H (methyl)	1.100(4)	τ^c (ccc)	–81.2(17)
Si–C(1)	1.880(1)	τ_c^d (cca)	–79.2(18)
Si–C(methyl)	1.878(1)	τ_c^d (cca)	–83.0(18)
Si–H	1.496(2)	τ_a^d (cca)	168.3(18)
		τ_c^d (ccb)	–82.8(18)
		τ_c^d (ccb)	–81.9(18)
		τ_b^d (ccb)	47.0(18)
		τ_b^d (bba)	46.4(18)
		τ_b^d (bba)	48.8(18)
		τ_a^d (bba)	159.2(18)
		τ_b^d (bbc)	47.8(18)
		τ_b^d (bbc)	44.8(18)
		τ_c^d (bbc)	–83.5(18)
		τ_a^d (aac)	153.1(18)
		τ_a^d (aac)	163.1(18)
		τ_c^d (aac)	–78.8(18)
		τ_a^d (aab)	163.3(18)
		τ_a^d (aab)	147.3(18)
		τ_b^d (aab)	50.3(18)
		τ_a^d (acb)	162.2(18)
		τ_c^d (acb)	–83.3(18)
		τ_b^d (acb)	49.0(18)
		τ_a^d (abc)	164.0(18)
		τ_b^d (abc)	46.1(18)
		τ_c^d (abc)	–82.1(18)



The potential energy surface was studied at the MP2/6-31G* level. The minima of 11 conformers were found to lie within a range of 8.5 kJ mol^{–1}, predicting that nine different conformers, ccc (13%), aab (8%), aac (6%), bba (14%), bbc (6%), cca (24%), ccb (11%), acb (10%) and abc (8%), may exist under conditions of the ED experiment. All conformers were described by three different branch types a, b and c with H–C(1)–Si–H torsional angles of *ca.* 160, 40 and –80°, respectively. Local C_{3v} symmetry was assumed for the methyl groups. The parameters involving hydrogen atoms and the differences in the C–H, Si–C and Si–C–Si parameters were flexibly restrained to the values from MP2/6-31G* calculations. The nozzle temperature was 343 K.

^{a)} Estimated standard errors.^{b)} Mean value.^{c)} Torsional angle H–C(1)–Si–H from the *syn* position.^{d)} τ_a , τ_b and τ_c are torsional angles H–C(1)–Si–H in the a, b and c branches, respectively.

Structure Data of Free Polyatomic Molecules



Morrison, C.A., Rankin, D.W.H., Robertson, H.E., Eaborn, C., Farook, A., Hitchcock, P.B., Smith, J.D.: J. Chem. Soc., Dalton Trans. (2000) 4312.