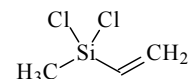


395 **C₃H₆Cl₂Si**ED, *ab initio*
calculations**Dichloro(ethenyl)methylsilane**

Dichloro(methyl)vinylsilane

C_s (*syn*)**C₁ (*gauche*)**

r_g	Å ^{a)}	θ_α	deg ^{a)}
C=C	1.341(6)	C=C-Si	123.3(17)
C(2)-Si	1.843(4)	C-Si-C	111.6(17)
Si-C(4)	1.855(4)	C(2)-Si-Cl	110.8(7)
C(2)-H	1.112 ^{b)}	Si-C(4)-H	110.7 ^{b)}
C(1)-H(8)	1.113 ^{b)}	Cl-Si-Cl	108.1(7)
C(1)-H(9)	1.104 ^{b)}	Cl-Si-C(4)	107.7(11)
Si-Cl	2.051(2)	Si-C(2)-H	118.0(17)
C(4)-H	1.140 ^{b)}	H-C(4)-H	108.2 ^{b)}
		C=C-H(8)	122.6 ^{b)}
		C=C-H(9)	121.9 ^{b)}
		C=C-H(10)	118.7 ^{b)}
		H-C(1)-H	115.5 ^{b)}
		τ_1 (C=C-Si-C)	0.0 ^{b)}
		τ_2 [H-C(4)-Si-C(2)] ^{c)}	60.0 ^{b)}



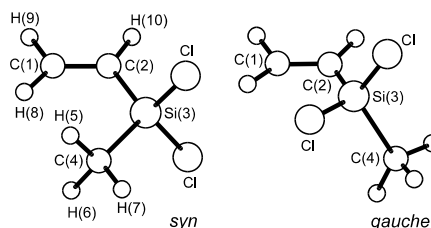
The molecule exists as a mixture of *syn* (45(64)%) and *gauche* (55(64)%) conformers. The conformational energy difference $\Delta E^\circ = E^\circ(\textit{gauche}) - E^\circ(\textit{syn})$ was estimated to be 0.3(18) kcal mol⁻¹. The structural differences between corresponding bond distances and bond angles of the two conformers were assumed at the values from HF/6-311G(d) calculations. Torsional angle τ_1 (C=C-Si-C) of the *gauche* conformer was found to be 121(16)°. The parameters are listed for the *syn* conformer.

The nozzle temperature was 297...298 K.

^{a)} Twice the estimated standard errors including a systematic error.

^{b)} Fixed in the final refinement.

^{c)} $\tau_2 = 0^\circ$ for the *syn* position.



Johansen, T.H., Hagen, K., Stølevik, R., Hassler, K.: J. Phys. Chem. A **101** (1997) 3580.

Replaces [II/25C \(3, 1247\)](#)