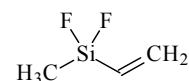


399 **C₃H₆F₂Si**ED, *ab initio*
calculations**Ethenyldifluoro(methyl)silane**

Difluoro(methyl)vinylsilane

C_s (*syn*)**C₁ (*gauche*)**

r_g	Å ^{a)}	θ_α	deg ^{a)}
C=C	1.344(5)	C=C-Si	123.3(8)
C(2)-Si	1.846(3)	C-Si-C	113.4(11)
Si-C(4)	1.851(3)	C(2)-Si-F	112.8(5)
C(2)-H	1.114 ^{b)}	Si-C(4)-H	111.6(34)
C(1)-H(8)	1.119 ^{b)}	F-Si-F	106.0(6)
C(1)-H(9)	1.109 ^{b)}	F-Si-C(4)	105.6(8)
Si-F	1.592(2)	Si-C(2)-H	118.8(8)
C(4)-H	1.140 ^{b)}	H-C(4)-H	107.2(37)
		C=C-H(8)	122.5 ^{b)}
		C=C-H(9)	122.1 ^{b)}
		C=C-H(10)	117.9 ^{b)}
		H-C(1)-H	115.4 ^{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* (35(41)%) and *gauche* (65(41)%) conformers.

The conformational energy difference $\Delta E^\circ = E^\circ(\textit{gauche}) - E^\circ(\textit{syn})$ was estimated to be 0.0(12) 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)

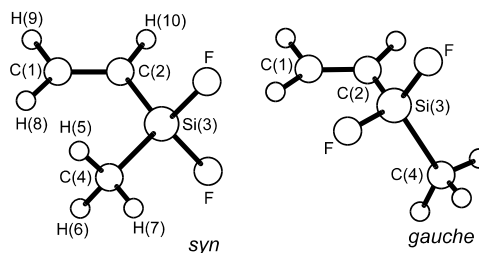
of the *gauche* conformer was found to be 117(14)°. The parameters are listed for the *syn* conformer.

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.