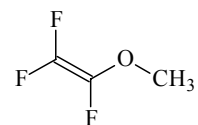


355 **C₃H₃F₃O**ED, *ab initio*
calculations**Trifluoro(methoxy)ethene**

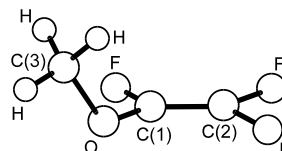
Methyl trifluorovinyl ether

C₁

r_a	Å ^{a)}	θ_a	deg ^{a)}
C–H	1.10 ^{b)}	C(2)=C(1)–O	118.2(5)
C(1)=C(2)	1.310 ^{c)}	C=C–F (mean)	123.3(6)
C–F (mean)	1.335(6)	C(2)=C(1)–F ^{d)}	120.6(9)
C(1)–F ^{c)}	1.348(9)	C(1)=C(2)–F ^{d)}	124.6(7)
C(2)–F ^{c)}	1.328(7)	C–O–C	109.3(18)
O–C (mean)	1.381(7)	H–C–H	110.5 ^{f)}
O–C(1)	1.326(13)	tilt(CH ₃) ^{g)}	3.0 ^{f)}
O–C(3)	1.436(13)	τ^h	111.1(35)

Methyl group was assumed to have local C_{3v} symmetry and staggered conformation with respect to the O–C(1) bond.

The nozzle was at room temperature.



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

^{b)} Not refined.

^{c)} Assumed at the experimental value for the F₂C=CF₂ molecule.

^{d)} Difference between the C=C–F bond angles was assumed at the mean value from HF/3-21G and MP2/6-31G* calculations.

^{e)} Difference between the C–F bond lengths was assumed at the mean value from HF/3-21G and MP2/6-31G* calculations.

^{f)} Constrained to the mean value from HF/3-21G and MP2/6-31G* calculations.

^{g)} Tilt angle between the C₃ axis of the CH₃ group and the O–C bond direction away from the O–C(1) bond.

^{h)} C=C–O–C torsional angle from the *syn* position.

Leibold, C., Reinemann, S., Minkwitz, R., Resnik, P.R., Oberhammer, H.: J. Org. Chem. **62** (1997) 6160.