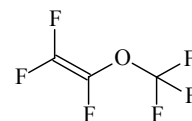


335 C₃F₆OED, *ab initio*
calculations**Trifluoro(trifluoromethoxy)ethene**

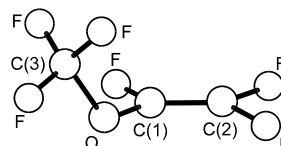
Trifluoromethyl trifluorovinyl ether

C₁

r_a	\AA^a	θ_a	deg^a
C(1)=C(2)	1.310 ^b	C(2)=C(1)-O	117.5(18)
C-F (mean)	1.322(3)	C=C-F (mean)	123.9(12)
C(3)-F ^c	1.326(4)	C(2)=C(1)-F ^d	123.1(13)
C(1)-F ^c	1.331(7)	C(1)=C(2)-F ^d	124.3(13)
C(2)-F ^c	1.316(7)	C-O-C	118.9(19)
O-C (mean)	1.373(14)	F-C(3)-F	108.9(3)
		tilt(CF ₃) ^e	4.2(28)
		τ^f	103.7(19)

Local C_{3v} symmetry and the staggered conformation with respect to the O-C(1) bond were assumed for the CF₃ group.

The nozzle was at room temperature.



- ^a) Three times the estimated standard errors including a systematic error.
- ^b) Assumed at the experimental value for the F₂C=CF₂ molecule.
- ^c) Differences between the C-F bond lengths were assumed at the mean values from HF/3-21G and MP2/6-31G* calculations. Two inequivalent C(2)-F bond lengths were essentially equal.
- ^d) Difference between the C=C-F bond angles was assumed at the mean value from HF/3-21G and MP2/6-31G* calculations. Two inequivalent C(1)=C(2)-F bond angles were essentially equal.
- ^e) Tilt angle between the C₃ axis of the CF₃ group and the O-C bond direction away from the O-C(1) bond.
- ^f) 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.