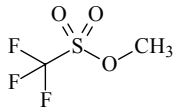
244 **$C_2H_3F_3O_3S$** **Trifluoromethanesulfonic acid methyl ester** **C_1**

ED, *ab initio* and DFT calculations

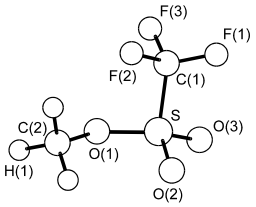
Methyl trifluoromethanesulfonate



r_a	Å [a])
S=O(2,3)	1.413(3)
S–O(1)	1.555(4)
S–C	1.838(5)
O–C	1.451(22)
C–F	1.323(2)
C–H	1.100 [c])

θ_a	deg [a])
C–S–O(1)	99.1 [b])
C–S=O(2,3)	106.6(9)
O–S=O(2,3)	108.1(6)
O(2)=S=O(3)	125.3(23)
S–O(1)–C	124.5(21)
F–C–F	109.9(9)
H–C–H	111.5 [d])
O(1)–S–C(l)–F(1) [e])	182.0 [d])
S–O(1)–C(2)–H(1) [e])	166.2 [d])
C(2)–O(1)–S–C(1) [e])	89(7)
tilt(CF_3)	0.8 [d]) [f])
tilt(CH_3)	3.5 [d]) [g])

The molecule was found to exist as a *gauche* conformer. Local C_{3v} symmetry was assumed for the CF_3 and CH_3 groups.
The nozzle was at room temperature.



[a]) Three times the estimated standard errors.
[b]) Constrained to the mean value from HF/3-21G* and B3LYP/6-31G* calculations.
[c]) Assumed.
[d]) Assumed at the mean value from HF/3-21G* and B3LYP/6-31G* calculations.
[e]) Torsional angle, zero degree for the *syn* position.
[f]) A positive value means that the C_3 axis is bent towards the O(1) atom.
[g]) A positive value means that the C_3 axis is bent away from the S atom.

Trautner, F., Ben Altabef, A., Fernandez, L.E., Varetti, E.L., Oberhammer, H.: Inorg. Chem. **38** (1999) 3051.