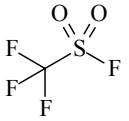
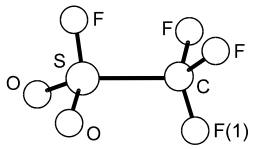
52 **CF_4O_2S** **Trifluoromethanesulfonyl fluoride** **C_s** assumed

ED, *ab initio* and DFT calculations



r_a	Å [a])	θ_a	deg [a])
S–C	1.835(5)	C–S–F	95.4(7)
S=O	1.410(3)	C–S=O	108.5(6)
S–F	1.543(3)	O=S=O	124.1(10)
C–F (mean)	1.325(2)	F–C–F	109.8(3)
		τ [b])	180 [c])

Local C_{3v} symmetry was assumed for the CF_3 group.
The nozzle was at room temperature.



[a]) Three times the estimated standard errors.
[b]) Torsional angle F–S–C–F(1).
[c]) Assumed.

Haist, R., Trautner, F., Mohtasham, J., Winter, R., Gard, G.L., Oberhammer, H.: J. Mol. Struct. **550-551** (2000) 59.