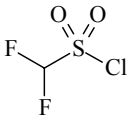
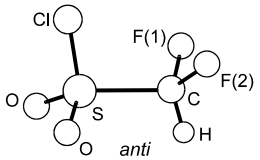
70 **$CHClF_2O_2S$** **Difluoromethanesulfonyl chloride** **C_s** assumed (*anti*)
C_1 (*gauche*)

ED, *ab initio* and DFT calculations

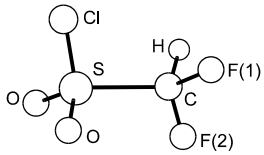


r_a	Å [a])	θ_a	deg [a])
S–C	1.846(5)	C–S–Cl	102.2(6)
S=O	1.417(1)	C–S=O (mean)	107.9(6)
S–Cl	2.013(2)	O=S=O	120.4(9)
C–F (mean)	1.330(3)	S–C–F	107.8(5)
C–H	1.100 [b])	S–C–H	106.7 [c])
		F–C–F	110.5(6)
		τ [d])	180 [b])

The molecule was found to exist as a mixture of *anti* (69(9)%) and *gauche* (31(9)%) conformers. Differences between the structural parameters of these conformers were assumed at the values from B3LYP/6-31G* calculations; torsional angle Cl–S–C–H for the *gauche* conformer was assumed to be 59°.
The parameters are listed for the *anti* conformer.
The nozzle was at room temperature.



anti



gauche

[a]) Three times the estimated standard errors.
[b]) Assumed.
[c]) Assumed at the mean value from HF/6-31G* and B3LYP/6-31G* calculations.
[d]) Torsional angle Cl–S–C–H.

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