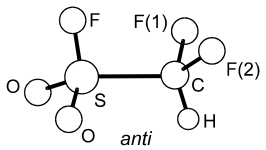
77 **CHF_3O_2S** **Difluoromethanesulfonyl fluoride** **C_1** (*gauche*)
C_s assumed (*anti*)

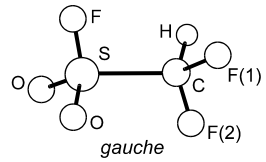
ED, *ab initio* and DFT calculations

r_a	Å [a])	θ_a	deg [a])
S–C	1.822(5)	C–S–F	95.2(14)
S=O	1.400(2)	C–S=O (mean)	109.9(8)
S–F	1.542(3)	O=S=O	123.8(17)
C–F (mean)	1.344(7)	S–C–F (mean)	107.2(6)
C–H	1.100 [b])	Δ(S–C–F) [c])	1.6 [d])
		S–C–H	109.7 [d])
		F–C–F	107.4(10)
		τ [e])	65.7(35)

The molecule was found to exist as a mixture of *gauche* (84(17)%) and *anti* (16(17)%) conformers. Local C_s symmetry was assumed for the SO_2F group. Differences between the structural parameters of these conformers were assumed at the values from B3LYP/6-31G* calculations. The parameters are listed for the *gauche* conformer.
The nozzle was at room temperature.



anti



gauche

[a]) Three times the estimated standard errors.
[b]) Assumed.
[c]) [S–C–F(2)] – [S–C–F(1)].
[d]) Assumed at the mean value from HF/6-31G* and B3LYP/6-31G* calculations.
[e]) Torsional angle F–S–C–H.

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