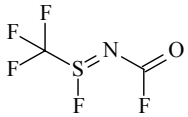
181 **C_2F_5NOS** **1,1,1-Trifluoro-*N*-(fluorocarbonyl)methanesulfinimidoyl fluoride** **C_1**

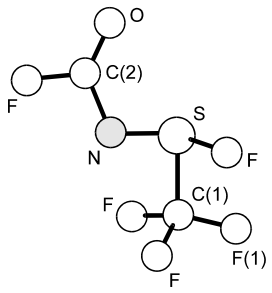
ED, IR, *ab initio* and DFT calculations



r_a	Å [a])	θ_a	deg [a])
N=S	1.549(5)	S=N–C	112.4(11)
N–C	1.391(8)	N=S–F	108.8(33)
S–F	1.599(4)	N=S–C	97.4(12)
S–C	1.852(6)	F–C(1)–F	109.7(4)
C=O	1.186(5)	F–S–C	90.3(14)
C–F (mean)	1.323(1)	N–C=O	129.9(12)
Δ(C–F) [b])	0.010 [c])	N–C–F	108.2(12)
C(1)–F [d])	1.321(1)	tilt(CF_3) [e])	2.8 [c])
C(2)–F [d])	1.331(1)	τ_1 [f])	158(8)
		τ_2 [g])	–110(9)
		τ_3 [h])	166 [c])
		τ_4 [i])	169(5)

Two isomers, *trans* (79(12) %) and *cis* (21(12) %), were found to be present in the vapor. "*Trans"* and "*cis"* describe the orientations of the FCO group around the S=N double bond relative to the sulfur substituents. Each isomer exists as a *syn* conformer, *i.e.*, the C=O bond is *syn* with respect to the S=N bond. Differences in the corresponding bond lengths and angles between these isomers were assumed at the values from B3LYP/6-31G* calculations. Planarity of the FCO group and local C_{3v} symmetry of the CF_3 group were assumed. The parameters are listed for the *syn* conformer of the *trans* isomer. The nozzle was at room temperature.

[a]) Unidentified, possibly the estimated standard errors.
[b]) [C(1)–F] – [C(2)–F].
[c]) Assumed at the value from B3LYP/6-31G* calculations.
[d]) Dependent parameter.
[e]) Tilt angle between the C_3 axis of the CF_3 group and the S–C bond, away from the N=S bond.
[f]) Torsional angle C–N=S–C from the *syn* position.
[g]) Torsional angle C–N=S–F from the *syn* position.
[h]) Torsional angle S=N–C–F from the *syn* position.
[i]) Torsional angle N=S–C(1)–F(1) from the *syn* position.



Trautner, F., Cutin, E.H., Della Vedova, C.O., Mews, R., Oberhammer, H.: Inorg. Chem. **39** (2000) 4833.