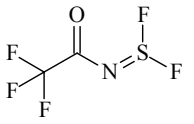
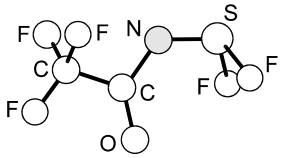
180 **C_2F_5NOS** **(Trifluoroacetyl)imidosulfurous difluoride** **C_s** assumed

ED, vibrational spectroscopy, *ab initio* and DFT calculations



r_a	Å [a])	θ_a	deg [a])
N=S	1.481(7)	S=N–C	128.2(16)
N–C	1.406(16)	N–C=O	128.4(17)
C–C	1.517(10)	N–C–C	109.6(22)
C=O	1.201(6)	F–C–F	108.7(4)
C–F	1.327(4)	N=S–F	110.4(12)
S–F	1.585(2)	F–S–F	89.3(11)

According to vibrational spectra and ED data, the molecule exists as a *syn-syn* conformer with C=O and C–N bonds in the *syn* positions with respect to the N=S bond and the F–S–F bisector, respectively. Presence of any other conformer larger than *ca*. 5% was excluded. This conclusion agrees with results of HF/6-31G*, MP2/6-31G* and B3LYP/6-31G* calculations, which predicted that the second-lowest conformer (*syn-anti*) was less stable by 2.4 kcal mol^{-1} or more. Local C_{3v} symmetry was assumed for the CF_3 group in the ED analysis. The nozzle was at room temperature.



[a]) Three times the estimated standard errors.

Mora Valdez, M.I., Cutin, E.H., Della Vedova, C.O., Mews, R., Oberhammer, H.: J. Mol. Struct. **607** (2002) 207.