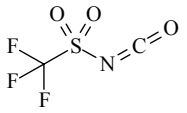
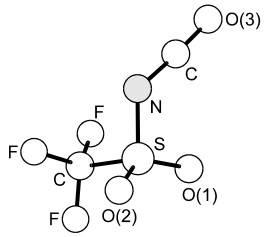
173 **$C_2F_3NO_3S$** **Trifluoromethanesulfonyl isocyanate** **C_1**

ED, *ab initio* and DFT calculations



r_a	Å [a])
C=O	1.151(8)
C=N	1.220 [b])
C–F	1.320(3)
S=O	1.416(2)
S–N	1.653(5)
C–S	1.843(5)

θ_a	deg [a])
N–S=O (mean)	110.4(16)
Δ(N–S=O) [c])	2.4 [d])
N–S=O(1)	111.6(19)
N–S=O(2)	109.2(19)
C–S=O	108.0(14)
C–S–N	97.5 [d])
S–C–F	109.1(4)
F–C–F	109.9(4)
S–N=C	126.5(15)
N=C=O [e])	174 [b])
F–C–S–N	180.0 [b])
C–S–N=C	116(8)
O(1)=S–N=C [f])	4(8)



Local C_{3v} symmetry and staggered position with respect to the S–N bond were assumed for the CF_3 group.
The nozzle was at room temperature.

[a]) Three times the estimated standard errors including a systematic error.
[b]) Assumed according to results of HF/3-21G*, HF/6-31G*, MP2/6-31G* and B3PW91/6-31G* calculations.
[c]) [N–S=O(1)] – [N–S=O(2)].
[d]) Assumed at the value from B3PW91/6-31G* calculations.
[e]) Bent in SNCO plane, away from O(1).
[f]) Torsional angle around the S–N bond, the positive sign indicates that the C atom is rotated away from the CF_3 group from the eclipsed position.

Haist, R., Mack, H.-G., Della Védova, C.O., Cutín, E.H., Oberhammer, H.: J. Mol. Struct. **445** (1998) 197.