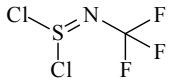
26 **CCl_2F_3NS** **[(Trifluoromethyl)imido]sulfurous dichloride** **C_s**

ED, *ab initio* and DFT calculations

Sulfur dichloride trifluoromethylimide

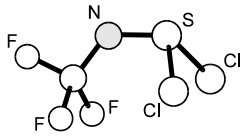


r_a	Å [a])
C–F	1.337(4)
N–C	1.417(13)
S=N	1.513(6)
S–Cl	2.077(7)

θ_a	deg [a])
C–N=S	130.8(21)
N=S–Cl	109.0(11)
Cl–S–Cl	95.6(11)
F–C–F	107.5(8)
tilt(CF_3) [b])	5.2(22)

Local C_{3v} symmetry for the CF_3 group and local C_{2v} symmetry for the SCl_2 group were assumed. The CF_3 group was found to be in the staggered position with respect to the N=S bond. The barrier to internal rotation of the CF_3 group was determined to be 0.4(3) kcal mol^{-1}. The nozzle was at room temperature.

[a]) Three times the estimated standard errors.
[b]) Tilt angle between the C_3 axis of the CF_3 group and the N–C bond direction, away from the N=S bond.



Haist, R., Cutin, E.H., Della Vedova, C.O., Oberhammer, H.: J. Mol. Struct. **475** (1999) 273.