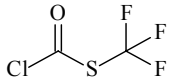
167 **C_2ClF_3OS** **Carbonochloridothioic acid *S*-(trifluoromethyl) ester** **C_s** (*syn*)

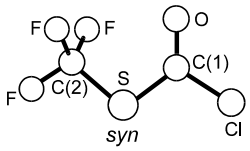
ED, IR, *ab initio* and DFT calculations

S-Trifluoromethyl chlorothioformate



r_a	Å [a])	θ_α	deg [a])
C=O	1.177(4)	S–C=O	129.1(14)
C–F	1.327(3)	S–C–Cl	108.0(4)
C–Cl	1.756(17)	O=C–Cl	122.9(20)
S–C (mean)	1.799(8)	C–S–C	98.9(7)
S–C(1)	1.770(12)	F–C–F	108.8(3)
S–C(2)	1.827(12)	tilt(CF_3) [b])	4.8(5)

The molecule exists as a single *syn* conformer. Local C_{3v} symmetry and staggered conformation with respect to the S–C(1) bond were assumed for the CF_3 group.
The nozzle was at room temperature.



[a]) Three times the estimated standard errors.
[b]) Tilt angle of the CF_3 group away from the S–C(1) bond.

Gobbato, K.I., Mack, H-G., Oberhammer, H., Ulic, S.E., Della Védova, C.O., Willner, H.: J. Phys. Chem. A **101** (1997) 2173.