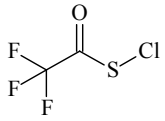
168 **C_2ClF_3OS** **Trifluoroethanethioic acid anhydrosulfide with thiohypochlorous acid** **C_1**

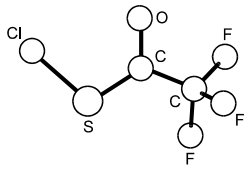
ED, *ab initio* calculations

Trifluoroacetyl thiohypochlorite



r_a	Å [a])
C=O	1.224(5)
C–F	1.340(2)
C–C	1.546(5)
C–S	1.765(5)
S–Cl	2.013(3)

θ_α	deg [a])
S–C=O	126.4(8)
S–C–C	112.5(6)
C–C=O	121.1(10)
C–S–Cl	99.4(6)
F–C–F	109.0(2)
τ_1 [b])	39.5(16)
τ_2 [c])	0.0 [d])



The experimental scattering intensities were consistent only with the existence of a *syn* conformer ($\tau_2 = 0°$). The theoretically predicted energy difference ΔE between *anti* ($\tau_2 = 180°$) and *syn* forms is 5.6 kcal mol^{-1} (HF/3-21G*) or 3.0 kcal mol^{-1} (HF/6-31G*). The molecular skeleton was assumed to be planar. Local C_{3v} symmetry and no tilt were assumed for the CF_3 group.

The nozzle was at room temperature.

[a]) Three times the estimated standard errors.

[b]) O=C–C–F torsional angle, $\tau_1 = 0°$ for the *syn* position.

[c]) O=C–S–Cl torsional angle, $\tau_2 = 0°$ for the *syn* position.

[d]) Assumed.

Gobbato, K.I., Della Védova, C.O., Mack, H.G., Oberhammer, H.: Inorg. Chem. **35** (1996) 6152.