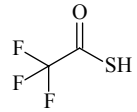
188 **C_2HF_3OS** **Trifluoroethanethioic acid** **C_1**

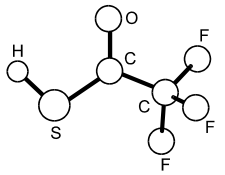
ED, *ab initio* and DFT calculations

(Trifluoro)thioacetic *S*-acid



r_a	Å [a])
C=O	1.217(5)
C–F	1.340(2)
C–C	1.524(4)
C–S	1.738(4)
S–H	1.335 [b])

θ_α	deg [a])
S–C=O	127.6(10)
S–C–C	115.7(9)
C–C=O	116.7(14)
C–S–H	96.5 [b])
F–C–F	107.4(2)
τ_1 [c])	29.5(12)
τ_2 [d])	0.0 [e])



The conformational properties could not be determined unambiguously in the experiment. According to results of HF/3-21G*, HF/6-31G*, MP2/6-31G*, LDFT and NLDFT calculations, the energy difference ΔE between *anti* ($\tau_2 = 180°$) and *syn* ($\tau_2 = 0°$) conformers is 0.9…2.2 kcal mol^{-1}. Therefore only a *syn* conformer was considered in the experimental structure analysis. 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]) Assumed at the value for CH_3SH molecule from the literature.
[c]) O=C–C–F torsional angle, $\tau_1 = 0°$ for the *syn* position.
[d]) O=C–S–H torsional angle, $\tau_2 = 0°$ for the *syn* position.
[e]) Assumed.

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