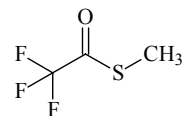


356 **C₃H₃F₃OS**ED, *ab initio*
calculations**Trifluoroethanethioic acid S-methyl ester**

S-Methyl (trifluoro)thioacetate

C₁

r_a	Å ^{a)}	θ_a	deg ^{a)}
C=O	1.206(6)	S-C=O	127.2(19)
C-F	1.335(2)	S-C-C	116.0(8)
C-C	1.527(5)	C-C=O	116.8(21)
C(1)-S	1.743(14)	C-S-C	97.5(13)
S-C(3)	1.807(16)	F-C-F	107.7(2)
C-H	1.095(13)	H-C-H	109.0 ^{b)}
		τ_1 ^{c)}	38.1(14)
		τ_2 ^{d)}	0.0 ^{b)}



The experimental scattering intensities were consistent only with the existence of a *syn* ($\tau_2 = 0^\circ$) conformer. The theoretically predicted energy difference ΔE between the *anti* ($\tau_2 = 180^\circ$) and *syn* forms is 4.2 kcal mol⁻¹ (HF/3-21G*, HF/6-31G*). The molecular skeleton was assumed to be planar. It was also assumed that the CF₃ and CH₃ groups have local C_{3v} symmetry and no tilt and the C(3)-H bonds are staggered with respect to the S-C(1) bond.

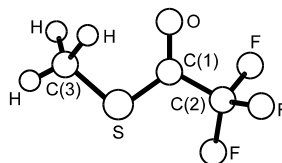
The nozzle was at room temperature.

^{a)} Three times the estimated standard errors.

^{b)} Assumed.

^{c)} O=C-C-F torsional angle, $\tau_1 = 0^\circ$ for the *syn* position.

^{d)} O=C-S-C torsional angle, $\tau_2 = 0^\circ$ for the *syn* position.



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