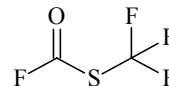


**177 C<sub>2</sub>F<sub>4</sub>OS**ED, IR, *ab initio* and DFT calculations**Carbonofluoridothioic acid *S*-(trifluoromethyl) ester***S*-Trifluoromethyl fluorothioformate**C<sub>s</sub> (*syn*)****C<sub>s</sub> (*anti*)**

$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
C=O	1.185(6)	S–C(1)=O	132.6(14)
C–F (mean)	1.334(3)	S–C(1)–F	104.7(10)
C(1)–F	1.344(5) <sup>b)</sup>	O=C(1)–F	122.7(18)
C(2)–F	1.330(4) <sup>b)</sup>	C–S–C	98.5(6)
S–C (mean)	1.798(4)	F–C–F	108.4(3)
S–C(1)	1.776(7)	tilt(CF <sub>3</sub> ) <sup>c)</sup>	3.2(7)
S–C(2)	1.821(7)		



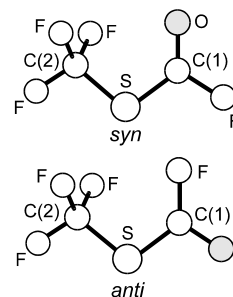
The molecule exists as a mixture of planar *syn* (90(5) %) and *anti* (10(5) %) conformers. This conformational composition corresponds to  $\Delta G^\circ = G^\circ(\text{anti}) - G^\circ(\text{syn}) = 1.3(4) \text{ kcal mol}^{-1}$ . The experimental energy difference,  $\Delta E(\text{IR}) = E(\text{anti}) - E(\text{syn}) = 1.46 \text{ kcal mol}^{-1}$ , was found to be slightly larger than theoretical predictions ( $\Delta E = 1.24 \text{ kcal mol}^{-1}$  (MP2/6-31G\*) and  $\Delta E = 1.03 \text{ kcal mol}^{-1}$  (BPW91/6-31G\*)). The differences between the bond lengths and bond angles of the two conformers were assumed in the ED analysis at the BPW91/6-31G\* values. Local C<sub>3v</sub> symmetry and the staggered position with respect to the S–C(1) bond were assumed for the CF<sub>3</sub> group. The structural parameters are listed for the *syn* conformer.

The nozzle was at room temperature.

<sup>a)</sup> Three times the estimated standard errors including a systematic error.

<sup>b)</sup> Difference between the C(1)–F and C(2)–F bond lengths was assumed at the BPW91/6-31G\* value.

<sup>c)</sup> Tilt angle of the CF<sub>3</sub> 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.