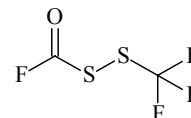


178 C₂F₄OS₂ED, vibrational spectroscopy,
ab initio and DFT calculations**Carbonyl(dithioperoxy)fluoridic acid
trifluoromethyl ester**

Fluoroformic trifluoromethanesulfenic thioanhydride

C₁ (*syn*)**C₁ (*anti*)**

r_a	Å ^{a)}	θ_a	deg ^{a)}
C(1)=O	1.176(7)	S–C(1)=O	129.9(16)
C(1)–F	1.342(2) ^{b)}	S–C(1)–F	105.7(3) ^{b)}
C(2)–F	1.329(2) ^{b)}	S–C(2)–F (mean)	110.3(3) ^{b)}
S–C(1)	1.785(5) ^{b)}	F–C–F (mean)	108.6(3)
S–C(2)	1.817(5) ^{b)}	S–S–C(1)	101.4(4) ^{b)}
S–S	2.027(4)	S–S–C(2)	100.0(4) ^{b)}
		S–S–C(1)=O ^{c)}	2.3 ^{d)}
		S–S–C(2)–F(2) ^{c)}	180.0 ^{d)}
		C–S–S–C	95.0(27)
		tilt(CF ₃) ^{c)}	4.4(9)



The molecule was found to exist as a mixture of *syn* (85(13)%) and *anti* conformers. Local C_{3v} symmetry and staggered position with respect to the S–S bond were assumed for the CF₃ group. The FC(O)S moiety was assumed to be planar. The differences in the structural parameters of the conformers were assumed at the values from MP2/6-31G* calculations. The nozzle was at room temperature. The parameters are given for the *syn* conformer.

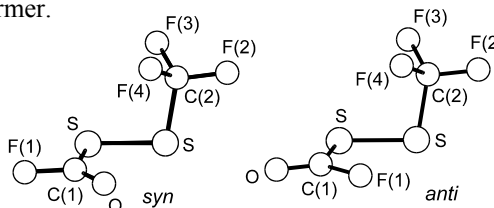
^{a)} Three times the estimated standard errors.

^{b)} Differences between the corresponding parameters for C(1) and C(2) were assumed at the values from MP2/6-31G* calculations.

^{c)} Torsional angles of the FC(O) and CF₃ groups from the *syn* position around the S–C(1) and S–C(2) bonds, respectively; positive values lead to a decrease of the O...F(2) distance.

^{d)} Assumed at the value from MP2/6-31G* calculations.

^{e)} Angle between the C₃ axis of CF₃ group and the S–C(2) bond direction, away from the S–S bond.



Hermann, A., Ulic, S.E., Della Védova, C.O., Mack, H.-G., Oberhammer, H.: J. Fluor. Chem. **112** (2001) 297.