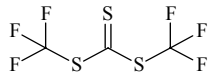
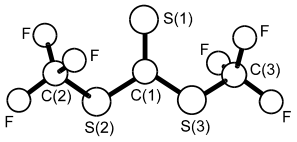
337 **$C_3F_6S_3$** **Carbonotrithioic acid bis(trifluoromethyl) ester** **C_2** assumed (*syn-syn*)
ED, *ab initio* and DFT calculations Bis(trifluoromethyl) carbonotrithioate essentially **C_s** (*syn-anti*)

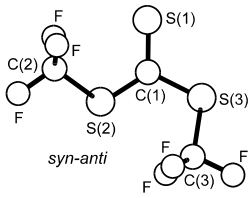


r_a	Å [a])	θ_a	deg [a])
C=S	1.605(8)	S(1)=C–S	128.1(3)
C(1)–S	1.784(3) [b])	C–S–C	102.7(7)
S–C(2,3)	1.820(3) [b])	F–C–F (mean)	108.4(2)
C–F (mean)	1.329(2)	tilt (CF_3) [c])	5.7(4)
		$\tau_{1,2}$ [d])	31.8(33)
		τ (CF_3) [e])	–0.2(25)
		τ_1 [f])	8.6 [g])
		τ_2 [h])	–167.7 [g])

The molecule was found to exist as a mixture of *syn-syn* (84(12)%) and *syn-anti* (16(12)%) conformers. Local C_{3v} symmetry was assumed for the CF_3 groups. Differences between the corresponding bond lengths and bond angles of these conformers were assumed at the values from MP2/6-31G* calculations. The bond lengths and bond angles are listed for the *syn-syn* conformer .
The nozzle was at room temperature.



syn-syn



syn-anti

[a]) Three times the estimated standard errors.
[b]) Difference between the S–C bond lengths was assumed at the value from MP2/6-31G* calculations.
[c]) Tilt angle between the C_3 axis of the CF_3 group and the S–C direction, away from the C(1)=S(1) bond.
[d]) Torsional angle S(1)=C–S–C(2,3) of *syn-syn* conformer; $\tau_{1,2} = 0°$ for planar *syn* position.
[e]) Torsional angle of CF_3 group from the staggered conformation.
[f]) Torsional angle S(1)=C–S(2)–C(2) of *syn-anti* conformer; $\tau_1 = 0°$ for planar *syn* position.
[g]) Assumed at the value from MP2/6-31G* calculations.
[h]) Torsional angle S(1)=C–S(3)–C(3) of *syn-anti* conformer; $\tau_2 = 0°$ for planar *syn* position.

Hermann, A., Ulic, S.E., Della Védova, C.O., Lieb, M., Mack, H.-G., Oberhammer, H.:
J. Mol. Struct. **556** (2000) 217.