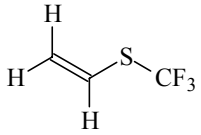
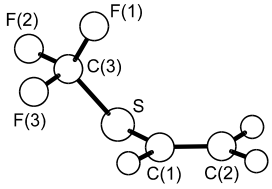
357 **$C_3H_3F_3S$** **[(Trifluoromethyl)thio]ethene** **C_1**
ED, *ab initio* calculations
Trifluoromethyl vinyl sulfide



r_a	Å [a])	θ_α	deg [a])
C–F	1.337(3)	C=C–S	120.9(24)
C=C	1.336 [b])	C–S–C	100.4(14)
S–C (mean)	1.784(2)	F–C–F	107.9(3)
S–C(1)	1.755(6)	C=C–H	121.5 [b])
S–C(3)	1.813(6)	τ [c])	129.4(39)
C–H	1.084(14)	tilt(CF_3) [d])	2.4(18)
		π(CF_3) [e])	3.4(38)

According to the experimental data and the results of HF/3-21G* and MP2/6-31G* calculations, the molecule exists as a single conformer.
The nozzle was at room temperature.



[a]) Three times the estimated standard errors including a systematic error.
[b]) Assumed at the MP2/6-31G* value.
[c]) C=C–S–C torsional angle from the *syn* position.
[d]) Tilt angle between the C_3 axis of the CF_3 group and S–C(3) bond direction, away from the S–C(1) bond.
[e]) Torsional angle of the CF_3 group, $\tau = 0°$ corresponds to the staggered orientation and positive value leads to an increase in the C(1)...F(3) distance.

Lieb, M., Oberhammer, H.: Chem. Ber. Rec. **130** (1997) 131.