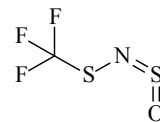


39 **CF₃NOS₂**ED, *ab initio*
calculations, Ra**(Z)-1,1,1-Trifluoro-N-sulfinylmethanesulfenamide**

(Z)-(Trifluoromethyl)sulfanyl sulfinylimine

C_s

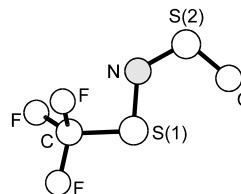
r_a	Å ^{a)}	θ_a	deg ^{a)}
C–F ^{b)}	1.328(2)	F–C–F ^{b)}	108.7(2)
S–C	1.831(4)	C–S–N	94.6(8)
S(1)–N	1.684(5)	S(1)–N=S(2)	120.6(6)
N=S(2)	1.538(6)	N=S=O	116.5(8)
S=O	1.453(6)	tilt(CF ₃) ^{c)}	5.0(7)

Local C_{3v} symmetry was assumed for the CF₃ group.

The molecule was found to exist only as *anti* form (*anti* position of the C–S(1) bond relative to the N=S(2) bond) of the Z-isomer, and the S(1)–N bond is eclipsed with respect to the S(2)=O bond. The CF₃ group is in the staggered position relative to the S(1)–N bond.

The nozzle was at room temperature.

According to HF/3-21G* and HF/6-31+G* calculations, the *anti* conformation of the Z-isomer corresponds to the global minimum on the energy surface. An analysis of the resonance

**Raman**

spectra revealed that planarity of the molecular skeleton is retained upon excitation to 2.20×10^4 and 2.35×10^4 cm⁻¹, assigned to $n \rightarrow \pi$ transition.

^{a)} Three times the estimated standard errors including a systematic error.^{b)} Average value.^{c)} Tilt angle between the C₃ axis of the CF₃ group and the C–S(1) bond, away from the S(1)–N bond.

Romano, R.M., Della Védova, C.O., Mack, H.-G., Oberhammer, H.: J. Mol. Struct. **440** (1998) 43.