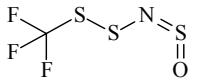
40 **CF_3NOS_3** **(*Z*)-Sulfinylamino trifluoromethyl disulfide** **C_1** (*anti*)

ED, *ab initio* and DFT calculations

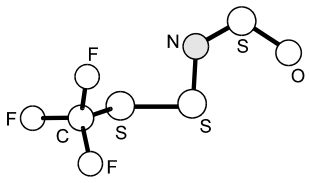
S-Trifluoromethyldisulfanyl sulfinylimine



r_a	Å [a])	θ_a	deg [a])
C–F	1.329(2)	N=S=O	116.3(17)
S=O	1.458(4)	S–N=S	125.9(13)
S=N	1.523(6)	S–S–N	97.9(14)
S–N	1.681(6)	S–S–C	103.9(12)
S–C	1.824(7)	F–C–F	108.0(4)
S–S	2.016(4)	tilt(CF_3) [b])	3.6 [c])
		C–S–S–N	81.3(94) [d])

CF_3 group was assumed to have local C_{3v} symmetry and to be in the staggered position with respect to the S–S bond. The S–S–N=S=O skeleton was found to be planar. The main conformer has the S–S–N=S unit in the *anti* position. A possible contribution of the conformer with the S–S–N=S unit in the *syn* position was estimated to be less than 10%, *i.e.*, $\Delta G° = G°(syn) - G°(anti) \geq 1.3$ kcal mol^{-1}.

The nozzle was at room temperature.



[a]) Three times the estimated standard errors.

[b]) Angle between the C_3 axis of the CF_3 group and the C–S bond direction, away from the S–S bond.

[c]) Assumed according to the results of HF/3-21G* calculations.

[d]) 0° for the *syn* position.

Romano, R.M., Della Védova, C.O., Pfeiffer, A., Mack, H.-G., Oberhammer, H.: J. Mol. Struct. **446** (1998) 127.