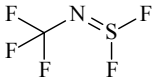
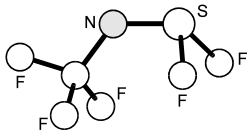
53 **CF_5NS** **(Trifluoromethyl)imidosulfurous difluoride** **C_s**

ED, MW, *ab initio* and DFT calculations



r_g	Å [a])	θ_α^0	deg [a])
S=N	1.477(6)	C–N=S	127.2(11)
S–F	1.594(2)	N=S–F	112.7(10)
N–C	1.409(8)	F–S–F	92.8(4)
C–F	1.331(3)	F–C–F	108.1(4)
		tilt(CF_3) [b])	4.0(8)

Local C_{3v} symmetry was assumed for the CF_3 group. Barrier to internal rotation of the CF_3 group around the C–N bond was determined to be 0.60(24) kcal mol^{-1}. Some structural parameters differ appreciably from those reported in [1].
The nozzle was at room temperature.



[a]) Twice the estimated standard errors.
[b]) Tilt angle between the C_3 axis of the CF_3 group and the N–C bond, positive value towards the nitrogen lone pair.

Trautner, F., Christen, D., Mews, R., Oberhammer, H.: J. Mol. Struct. **525** (2000) 135.
[1] Karl, R.R., Bauer, S.H.: Inorg. Chem. **14** (1975) 1859.

Replaces II/25B(**3**, 119)