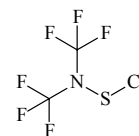
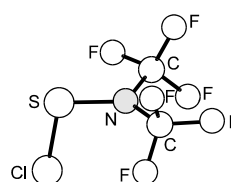


169 **C₂ClF₆NS**ED, *ab initio* and DFT
calculations**Bis(trifluoromethyl)amidosulfenyl chloride****C₁**

r_a	Å ^{a)}	θ_a	deg ^{a)}
C–F	1.331(2)	C–N–C	116.4(18)
C–N	1.453(5)	C–N–S	121.5(6)
S–N	1.667(7)	N–S–Cl	98.2(13)
S–Cl	2.090(8)	F–C–F	108.4(6)
		φ ^{b)}	7.8(38)
		τ_1 ^{c)}	0.6(19)
		τ_2 ^{c)}	45.5(38)
		tilt(CF ₃) ^{d)}	3.7(13)
		$\Sigma\alpha(N)$ ^{e)}	359.4(4)



Local C_{3v} symmetry for the CF₃ groups and local C_s symmetry for the C₂NSCl skeleton were assumed. The experimental analysis was supported by HF/3-21G* and B3PW91/6-311G* calculations. The nozzle was at room temperature.



^{a)} Three times the estimated standard errors.

^{b)} Angle between the S–N bond and the CNC plane; the deviation from planarity is such, that the molecule possesses an *anti* conformation.

^{c)} Torsional angle of the CF₃ group around the C–N bond, $\tau_{1,2} = 0^\circ$ for the staggered position of the CF₃ group with respect to the opposite N–C bond.

^{d)} Tilt angle between the C₃ axis of the CF₃ group and the N–C bond direction in the CNC plane away from the opposite CF₃ group.

^{e)} Sum of the bond angles around the nitrogen atom.

Korn, M., Mack, H.-G., Meckstroth, W., Minkwitz, R., Oberhammer, H.: J. Mol. Struct. **471** (1998) 79.