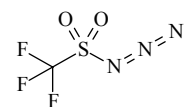


45 **CF₃N₃O₂S**
ED, *ab initio* and DFT
calculations

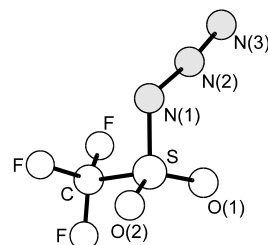
Trifluoromethanesulfonyl azide**C₁**

r_a	Å ^{a)}	θ_a	deg ^{a)}
N(2)=N(3)	1.120(6)	N-S=O (mean)	109.0(20)
N(1)=N(2)	1.252(7)	$\Delta(\text{N-S=O})$ ^{b)}	4.2 ^{c)}
C-F	1.321(3)	N-S=O(1)	111.1(22)
S=O	1.418(2)	N-S=O(2)	106.9(22)
S-N	1.668(4)	C-S=O	107.5(11)
C-S	1.849(6)	C-S-N	99.1 ^{c)}
		S-C-F	109.0(3)
		F-C-F	110.0(3)
		S-N=N	111.6(15)
		N=N=N ^{d)}	173.1(35)
		F-C-S-N	180.0 ^{e)}
		C-S-N=N	89(6)
		O(1)=S-N(1)=N(2) ^{f)}	-24(6)



Local C_{3v} symmetry and staggered position with respect to the S-N bond were assumed for the CF₃ group. Results of HF/3-21G*, HF/6-31G*, MP2/6-31G* and B3PW91/6-31G* calculations reproduced the experimental data satisfactorily except for the S-N bond length.

The nozzle was at room temperature.



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

^{b)} [N-S=O(1)] - [N-S=O(2)].

^{c)} Assumed at the value from B3PW91/6-31G* calculations.

^{d)} Bent in SNNN plane, away from O(1).

^{e)} Assumed.

^{f)} Torsional angle around the S-N bond, the negative sign indicates that the N(2) atom is rotated towards the CF₃ group from the eclipsed position.

Haist, R., Mack, H.-G., Della Védova, C.O., Cutín, E.H., Oberhammer, H.: J. Mol. Struct. Struct. **445** (1998) 197.