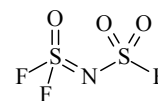


190 **F₃NO₃S₂**ED, *ab initio* and DFT
calculations***N*-(Fluorosulfonyl)imidosulfonyl fluoride**

Sulfinyl difluoride fluorosulfonylimide

C₁

r_a	Å ^{a)}	θ_a	deg ^{a)}
S=O (mean)	1.400(3)	S(1)–N=S(2)	125.9(8)
Δ (S=O) ^{b)}	0.012(5) ^{c)}	N–S(1)=O (mean)	110.5(12)
S(1)=O	1.404(5)	Δ (N–S(1)=O) ^{d)}	4.8(20) ^{c)}
S(2)=O	1.392(5)	N–S(1)=O(1)	112.9(16)
N=S(2)	1.475(5)	N–S(1)=O(2)	108.1(16)
S–F (mean)	1.535(2)	F(1)–S(1)=O	105.6(11)
Δ (S–F) ^{c)}	0.019(5) ^{c)}	N=S(2)=O(3)	116.8(22)
S(1)–F	1.548(4)	N=S(2)–F	111.1(8)
S(2)–F	1.529(3)	N–S(1)–F(1)	97.5 ^{f)}
N–S(1)	1.631(6)	F–S(2)–F	95.3(21)
		F–S(2)=O(3)	110.2(14)
		τ ^{g)}	107(4)



The S(2)F₂ group was found to be *syn* with respect to the N–S(1) bond.
The nozzle was at room temperature.

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

^{b)} [S(1)=O] – [S(2)=O].

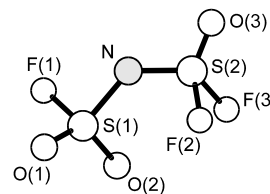
^{c)} Estimated according to the results of B3LYP/6-31G* and MP2/6-31G* calculations and varied within the estimated uncertainty.

^{d)} [N–S=O(1)] – [N–S=O(2)].

^{e)} [S(1)–F] – [S(2)–F].

^{f)} Assumed at the value from MP2/6-31G* calculations.

^{g)} Torsional angle F(1)–S(1)–N=S(2) from the *syn* position.



Haist, R., Alvaréz, R.S.M., Cutin, E.H., Della Vedova, C.O., Oberhammer, H.: J. Mol. Struct. **484** (1999) 249.