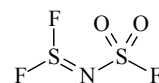


**189**      **F<sub>3</sub>NO<sub>2</sub>S<sub>2</sub>**ED, *ab initio* and DFT  
calculations**[N-(Fluorosulfonyl)imido]sulfurous difluoride**

Sulfur difluoride fluorosulfonylimide

**C<sub>1</sub>**

$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
S=O	1.407(2)	S(1)–N=S(2)	129.9(8)
N=S(2)	1.487(5)	N–S(1)–F(1)	95.5(24)
S–F (mean)	1.568(2)	N–S(1)=O (mean)	110.6(13)
$\Delta$ (S–F) <sup>b)</sup>	0.022(5) <sup>c)</sup>	$\Delta$ (N–S=O) <sup>d)</sup>	4.0(20) <sup>c)</sup>
S(1)–F	1.553(4)	N–S(1)=O(1)	112.6(17)
S(2)–F	1.575(3)	N–S(1)=O(2)	108.6(17)
N–S(1)	1.638(5)	F(1)–S(1)=O	107.4(21)
		N=S(2)–F	109.7(8)
		F–S(2)–F	92.2(9)
		$\tau^e$	113(7)



The S(2)F<sub>2</sub> group was found to be *syn* with respect to the N–S(1) bond. Barrier to internal rotation of the FSO<sub>2</sub> group around the S(1)–N bond was estimated to be *ca.* 0.6 kcal mol<sup>–1</sup> by the MP2 and B3LYP methods.

The nozzle was at room temperature.

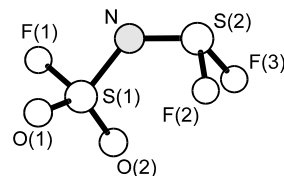
<sup>a)</sup> Three times the estimated standard errors including a systematic error.

<sup>b)</sup> [S(2)–F] – [S(1)–F].

<sup>c)</sup> Estimated according to the results of B3LYP/6-31G\* and MP2/6-31G\* calculations and varied within the estimated uncertainty.

<sup>d)</sup> [N–S=O(1)] – [N–S=O(2)].

<sup>e)</sup> 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.