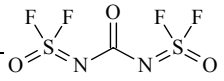
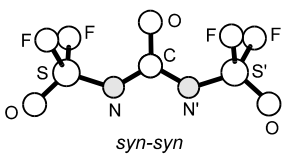
49 **$CF_4N_2O_3S_2$** **Carbonylbis(imidosulfinyl difluoride)** **C_{2v}** assumed (*syn-syn*)
ED, *ab initio* and DFT calculations **C_s** assumed (*syn-anti*)



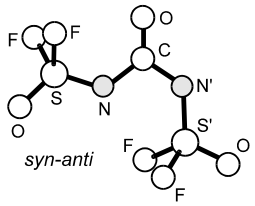
r_a	Å [a])		θ_a	deg [a])	
	syn-syn	*syn-anti*		*syn-syn*	*syn-anti*
C=O	1.193(9)	1.184	N–C=O	125.1(6)	124.8
C–N	1.365(9)	1.371	Δ(N–C=O) [b])		5.2 [c])
S=N	1.466(5)	1.463	C–N=S	125.3(10)	126.1
S=O	1.413(4)	1.414	Δ(C–N=S) [d])		5.8 [c])
S–F	1.540(2)	1.541	N=S=O	119.2(11)	119.8
			N=S–F	111.7(6)	111.8
			F–S–F	97.7(13)	97.7

The molecule was found to exist as a mixture of *syn-syn* (76(12)%) and *syn-anti* (24(12)%) conformers ($\Delta H° = H°(syn\text{-}syn) - H°(syn\text{-}anti) = 1.11(32)$ kcal mol^{-1}). Differences between parameters of the *syn-syn* and *syn-anti* conformers were constrained to the values from B3LYP/6-31G* calculations.
The nozzle was at room temperature.

[a]) Three times the estimated standard errors.
[b]) (N–C=O) – (N'–C=O).
[c]) Assumed at the value from B3LYP/6-31G* calculations.
[d]) (C–N'=S) – (C–N=S).



syn-syn



syn-anti

Trautner, F., Cutin, E.H., Della Vedova, C.O., Oberhammer, H.: J. Mol. Struct. **510** (1999) 53.