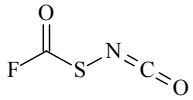
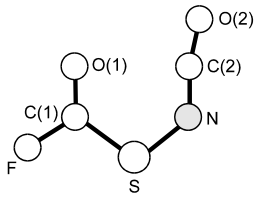
172 **C_2FNO_2S** **(Isocyanatothio)formyl fluoride** **C_s** (*syn-syn*)
ED, *ab initio* and DFT calculations
(Fluorocarbonyl)sulfenyl isocyanate



r_a	Å [a])
C=O (mean)	1.177(4)
C(1)=O(1) [b])	1.187(5)
C(2)=O(2) [b])	1.167(5)
N=C(2)	1.208(8)
C(1)–F	1.333(4)
S–C(1)	1.748(5)
S–N	1.669(3)

θ_α	deg [a])
S–C(1)=O(1)	129.5(8)
S–C(1)–F	107.3(5)
F–C(1)=O(1)	123.2(10)
C(1)–S–N	101.6(20)
S–N=C(2)	127.8(14)
N=C(2)=O(2)	165.9(32)
τ_1 [c])	17(6) [d])
τ_2 [e])	0.0 [f])



Only the *syn-syn* conformer was compatible with the experimental intensities. Several theoretical calculations (HF/3-21G*, HF/6-31G*, MP2/6-31G*, BPW91/6-31G* and B3PW91/6-31G*) confirmed that this conformer has the most stable structure.
The nozzle was at room temperature.

[a]) Three times the estimated standard errors including a systematic error.
[b]) Difference between the C(1)=O(1) and C(2)=O(2) bond lengths was constrained to the theoretical value.
[c]) Effective C(1)–S–N=C(2) torsional angle from the *syn* position.
[d]) Deviation from a planar equilibrium structure is due to a large-amplitude torsional vibration.
[e]) O(1)=C(1)–S–N torsional angle, $\tau_2 = 0°$ for the *syn* position.
[f]) Assumed at the value from the theoretical calculations.

Gobbato, K.I., Ulic, S.E., Della Védova, C.O., Mack, H.-G., Oberhammer, H.: Chem. Phys. Lett. **266** (1997) 527.