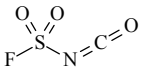
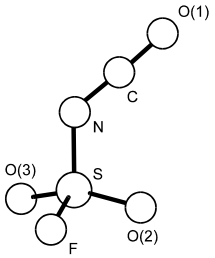
31 **$CFNO_3S$** **Sulfuryl fluoride isocyanate** **C_1**

ED, *ab initio* calculations

Fluorosulfonyl isocyanate



r_a	Å [a])	θ_α	deg [a])
C=O	1.175(8)	O=S=O	129.5(31)
N=C	1.22 [b])	F–S–N	96.5 [c])
S=O	1.409(3)	N–S=O [d])	108.2(12)
S–F	1.568(12)	S–N=C	123.0(11)
S–N	1.613(6)	N=C=O [e])	173 [c])
		τ(F–S–N=C) [f])	101(10)
		τ(O(2)–S–N=C) [g])	8(10)



HF/3-21G*, HF/6-31G* and MP2/6-31G* calculations predicted the overall minimum for the conformer with C_1 symmetry (τ(F–S–N=C) = 106.7…117.3°). The *anti* form (τ(F–S–N=C) = 180°) represents a transition state with ΔE = 0.6…1.2 kcal mol^{-1}. According to HF/3-21G* calculations, an additional unstable conformer (ΔE = 1.6 kcal mol^{-1}) has *syn* form (τ(F–S–N=C) = 0°). Only one conformer with C_1 symmetry was found in the ED analysis.

The nozzle was at room temperature.

[a]) Three times the estimated standard errors including a systematic error.
[b]) Assumed.
[c]) Assumed at the value from MP2/6-31G* calculations.
[d]) N–S=O(2) and N–S=O(3) angles were assumed to be equal.
[e]) O(1) atom is bent away from the S=O(2) bond in the S–N=C plane.
[f]) τ = 0° for the *syn* position.
[g]) Dependent parameter.

Della Védova, C.O., Cutín, E.H., Mack, H.-G., Oberhammer, H.: J. Mol. Struct. **380** (1996) 167.