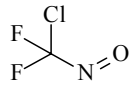
22 **$CClF_2NO$** **Chlorodifluoronitrosomethane** **C_1** (*gauche*)
ED, *ab initio* calculations **C_s** (*syn*)

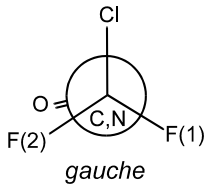


r_α	Å [a])	
	syn	*gauche*
C–N	1.567(5)	1.559(5)
N=O	1.175(3)	1.179(3)
C–Cl	1.739(2)	1.742(2)
C–F(1)	1.320(2)	1.321(2)
C–F(2)		1.310(2)

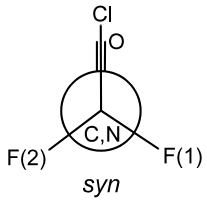
θ_α	deg [a])	
	syn	*gauche*
C–N=O	110.8(12)	110.7(12)
N–C–Cl	117.5(5)	108.9(5)
F–C–F [b])	108.0(4)	108.6(4)
N–C–F(1)	103.7(2)	104.2(2)
N–C–F(2)		111.6(2)
Cl–C–F(1) [b])	111.5(2)	111.6(2)
Cl–C–F(2) [b])		111.7(2)
φ [c])	123.6(14)	119.2(14)
		123.7(14)
τ [d])	0 [e])	104.0(10)

According to *ab initio* (MP2/TZ2P + MP2/DZP) calculations, the *gauche* conformer is more stable than the *syn* conformer by 1.1 kJ mol^{-1} and connected by a barrier of *ca*. 1.0 kJ mol^{-1}. Two equivalent *gauche* conformers are predicted to be separated by a barrier of 5…10 kJ mol^{-1}. The ED analysis was based on a dynamic model, where *syn* and *gauche* conformers are interconverted freely at ambient temperature. Differences between parameters of these conformers were assumed at the values from *ab initio* calculations.
The nozzle was at 293 K.

[a]) Estimated standard errors.
[b]) Dependent parameter.
[c]) Dihedral angle between the ClCN and CNF(1,2) planes.
[d]) Cl–C–N=O torsional angle.
[e]) Assumed.



gauche



syn

Smart, B.A., Brain, P.T., Robertson, H.E., Rankin, D.W.H.: Inorg. Chem. **37** (1998) 2687.