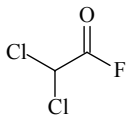
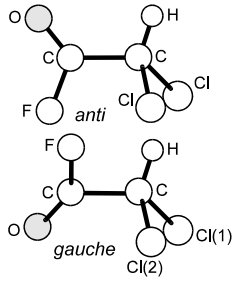
186 **C_2HCl_2FO** **Dichloroacetyl fluoride** **C_s** assumed (*anti*)
ED, *ab initio* **C_1** (*gauche*)
calculations



r_g	Å [a])		θ_α	deg [a])	
	anti	*gauche*		*anti*	*gauche*
C–C	1.534(4)	1.540 [b])	C–C=O	126.4(6)	129.9 [b])
C–Cl [c])	1.768(1)		C–C–F	111.6(5)	108.3 [b])
C–Cl(1)		1.757 [b])	C–C–Cl [c])	108.8(2)	
C–Cl(2)		1.777 [b])	C–C–Cl(1)		110.0 [b])
C=O	1.190(2)	1.191 [b])	C–C–Cl(2)		107.0 [b])
C–F	1.336(2)	1.364 [b])	Cl–C–Cl	112.1(3)	112.1 [b])
C–H	1.115 [d])	1.119 [d])	C–C–H	107.6 [d])	108.9 [d])
			τ [e])	180 [d])	39.1(34)

The molecule exists as a mixture of *anti* and *gauche* (29(5)%) conformers. The energy difference for these conformers was estimated to be 2.4 kJ mol^{-1} by MP2/6-31+G** calculations. The nozzle was at about 293 K.



[a]) Estimated standard errors.
[b]) Differences between the parameters of the *gauche* and *anti* conformers were assumed at the values from MP2/6-31+G** calculations.
[c]) Mean value.
[d]) Assumed.
[e]) H–C–C–F torsional angle, $\tau = 0°$ for the *syn* position.

Brain, P.T., Rankin, D.W.H., Robertson, H.E., Bühl, M.: J. Mol. Struct. **376** (1996) 123.