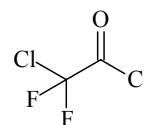


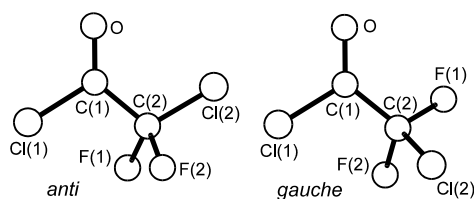
170
ED**C₂Cl₂F₂O****Chlorodifluoroacetyl chloride****C₁ (*gauche*)
C_s (*anti*)**

<i>r_a</i>	Å ^{a)}	<i>θ_α</i>	deg ^{a)}
C=O	1.179(4)	C(2)–C(1)=O	128.0(18)
C–C	1.519(8)	C–C–Cl (mean)	111.1(4)
C–F (mean)	1.325(3)	C(2)–C(1)–Cl(1)	112.9(7) ^{b)}
C–Cl (mean)	1.746(2)	C(1)–C(2)–Cl(2)	109.3(7) ^{b)}
C(1)–Cl(1)	1.736(6) ^{b)}	Cl(1)–C(1)=O	119.2(17)
C(2)–Cl(2)	1.756(6) ^{b)}	C–C–F (mean)	109.2(6)
		C–C–F(1)	110.4(8) ^{b)}
		C–C–F(2)	108.0(8) ^{b)}
		Cl(2)–C(2)–F (mean)	110.9(7)
		F–C–F	107.1(14)
		<i>τ</i> ^{c)}	75.4(10)



The molecule exists as a mixture of *gauche* (93(3)%) and *anti* conformers.
The nozzle was at room temperature.

- ^{a)} Three times the estimated standard errors including a systematic error.
^{b)} Differences between the corresponding parameters were assumed at the MP2/6-31G* values from the literature.



- ^{c)} Cl–C–C–Cl torsional angle for the *gauche* conformer; *τ* = 0° for the *syn* position, *τ* = 180° for the *anti* conformer.

Gobbato, K.I., Leibold, C., Centeno, S., Della Védova, C.O., Mack, H.-G., Oberhammer, H.:
J. Mol. Struct. **380** (1996) 55.