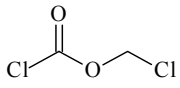
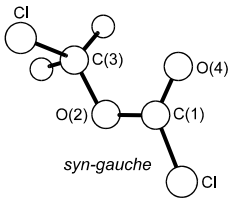
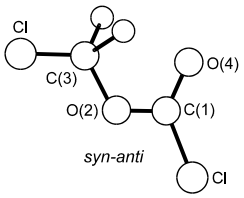
213 **$C_2H_2Cl_2O_2$** **Carbonochloridic acid chloromethyl ester** **C_1** (*syn-gauche*)
ED, *ab initio* and DFT calculations Chloromethyl chloroformate **C_s** (*syn-anti*)



r_g	Å [a])	θ_α	deg [a])
C–H [b])	1.097(14)	O–C(1)=O	126.8(3)
C(1)=O(4)	1.193(2)	O(2)–C(1)–Cl	108.9(3)
C(1)–O	1.348(3)	C(1)–O(2)–C(3)	117.8(7)
C(3)–O	1.416(4)	O–C(3)–Cl	111.4(5)
C(1)–Cl [c])	1.745(2)	O–C–H [b])	108.3(17)
C(3)–Cl [c])	1.777(2)	τ_1 [d])	83.5(19)
		τ_2 [e])	181.7 [f])

The molecule exists as a mixture of *syn-gauche* (94(6)%) and *syn-anti* conformers. This composition and entropy difference from MP2/6-31G(d) calculations correspond to the energy difference of $\Delta E° = 1.7(7)$ kcal mol^{-1}. The differences between corresponding parameters in the two conformers were assumed at the value from MP2/6-31G(d) calculations. The parameters are listed for the *syn-gauche* conformer.
The nozzle temperature was 298 K.





[a]) Twice the estimated standard errors including a systematic error.
[b]) Average value.
[c]) Difference between the C–Cl bond lengths was assumed at the value from MP2/6-31G(d) calculations.
[d]) C(1)–O(2)–C(3)–Cl torsional angle.
[e]) C(3)–O(2)–C(1)–Cl torsional angle.
[f]) Assumed at the value from MP2/6-31G(d) calculations.

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