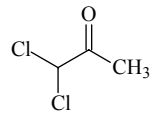
369 **$C_3H_4Cl_2O$** **1,1-Dichloro-2-propanone** **C_s** (*sp*)
ED, *ab initio* calculations 1,1-Dichloroacetone **C_1** (*ac*)

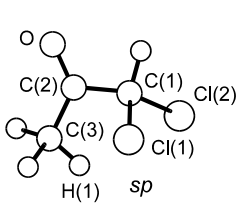


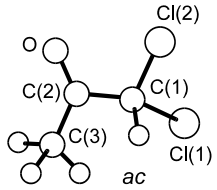
r_g	Å [a])
C–H [b])	1.093(14)
C=O	1.196(6)
C–C(1) [c])	1.524(4)
C–C(3) [c])	1.496(4)
C–Cl [b]) [c])	1.775(2)

θ_α	deg [a])
C(1)–C(2)=O [c])	119.6(5)
C(3)–C(2)=O [c])	125.2(5)
H–C–Cl	107.8(6)
C(2)–C(1)–Cl [b])	110.6(5)
C(3)–C(2)–C(1) [d])	115.2(5)
H–C(1)–C(2)=O	2(8)
H(1)–C(3)–C(2)=O	25.6 [e])

The molecule was found to exist predominantly as the *sp* conformer, where the C(1)–H bond is eclipsed with respect to the C(2)=O bond. However, a small amount (up to 15%) of the *ac* conformer could not be ruled out. According to results of MP2/6-311+G(d) calculations, the *sp* conformer is more stable by 2.25 kcal mol^{-1}.
The nozzle temperature was 60 °C.

[a]) Twice the estimated standard errors.
[b]) Average value.
[c]) Differences in the C–C, C–Cl and C–C=O parameters were assumed at the values from MP2/6-311+G(d) calculations.
[d]) Dependent parameter.
[e]) Assumed at the value from MP2/6-311+G(d) calculations.





Hagen, K., Shen, Q., Carter, R., Marion, M.: J. Phys. Chem. A **106** (2002) 4263.