

1195 C₃H₅ClOED, *ab initio* calculations
(HF/6-31G*, MP2/6-31G*)**2-Chloropropionaldehyde**

2-Chloropropional

C₁H₃C–CHCl–C(O)H

r_g	Å ^a) ^b)	θ_α	deg ^a) ^b)
C(3)–H	1.115(10)	H–C(2)–Cl	108.1(39)
C(2)–H	1.097(10)	C(1)–C(2)–Cl	108.9(7)
C(1)–H	1.134(10)	C(1)–C(2)–C(3)	112.4(15)
C(1)–C(2)	1.529(4)	C(2)–C(1)=O	124.3(18)
C(2)–C(3)	1.527(4)	C(3)–C(2)–Cl	109.2(7)
C(1)=O	1.205(4)	C(2)–C(3)–H	110.4 ^c)
C(2)–Cl	1.805(6)	C(2)–C(1)–H	115.3 ^c)
		ϕ_1 ^d) ^e)	27(7)
		ϕ_2 ^d) ^f)	109(20)
		ϕ_3 ^d) ^g)	240 ^c)

The molecule exists as a mixture of the conformers with different torsional angles ϕ . For the first conformer (66(26)%) the C(2)–C(3) bond is nearly eclipsed with respect to the C(1)=O bond; for the second conformer (23(28)%) the C(2)–H bond is eclipsed with respect to the C(1)=O bond; for the third conformer (11(26)%) the C(2)–Cl bond is eclipsed with respect to the C(1)=O bond. The differences in the corresponding bond distances and valence angles between the three conformers were fixed at the *ab initio* values. Local C_{3v} symmetry was assumed for the methyl group.

The nozzle temperature was 72 °C.

^a) Twice the estimated standard errors including a systematic error.

^b) Unlabeled distances and angles are given for the first conformer.

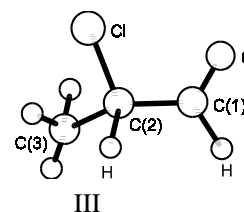
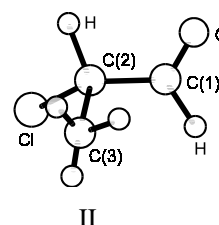
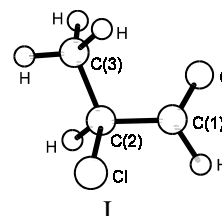
^c) Fixed at the *ab initio* value.

^d) Dihedral angle C(3)–C(2)–C(1)=O; $\phi = 0^\circ$ for the *syn* position.

^e) First conformer.

^f) Second conformer.

^g) Third conformer.



Aarset, K., Hagen, K., Frenking, G., Wehrsig, A.: J. Phys. Chem. **97** (1993) 10670.