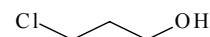


413 **C₃H₇ClO**ED, *ab initio*
calculations**3-Chloro-1-propanol**C₁ (aGG)C₁ (aGA)C₁ (gGA)

r_g	Å ^{a) b)}	θ_α	deg ^{a) b)}
C–C ^{c)}	1.527(5)	C–C–Cl	111.6(11)
C(1)–C(2)	1.547(12)	C–C–C, C–C–O ^{c)}	110.3(11)
C(2)–C(3)	1.497(12)	Δ ^{d)}	3.7 ^{e)}
C–H ^{c)}	1.099(9)	C–C–H	112.7(30)
C–O	1.424(6)	C–O–H	107.3 ^{e)}
C–Cl	1.803(4)	τ_1 ^{f)}	61.5(87)
		τ_2 ^{g)}	67.8(61)



The molecule was found to exist as a mixture of 13 conformers. The most abundant conformers at 115 °C are GG (50(14)%) and GA (35(15)%), symbols G (*gauche*) and A (*anti*) designating heavy atom (O or Cl) conformations. The fractions of the hydrogen-bonded species, gG[−]G and gGG[−] (lower case letters denoting the orientation of the H atom), that form O–H...Cl hydrogen bonds were found to be 4(14)% and 5(24)% at 115 and 367 °C, respectively. These values agree with the *ab initio* (HF/6-31G*) prediction of 1.7% but differ from 20(2)% reported in [1]. The differences in the bond lengths and angles between the aGG and each of other 12 conformers were assumed at the values from HF/6-31G* calculations.

The experimental data were obtained at nozzle temperatures of 115 and 367 °C.

The data are presented here for 115 °C.

^{a)} Twice the estimated standard errors.

^{b)} Averages over all conformers weighted by the mole fractions.

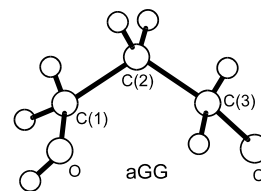
^{c)} Average value.

^{d)} [C–C–C] – [C–C–O].

^{e)} Assumed at the HF/6-31G* value.

^{f)} Weighted absolute value of the *gauche* torsional angle O–C–C–C, 0° for the *syn* position.

^{g)} Weighted absolute value of the *gauche* torsional angle C–C–C–Cl, 0° for the *syn* position.



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[1] Bastiansen, O., Brunvoll, J., Hargittai, I.: "Molecular Structure and Vibrations", Ed.:

S.J. Cyvin, Elsevier, Amsterdam, London, New York, **1972**, chapter 18/II, p.330.

Replaces [II/25C \(3, 1302\)](#), ED