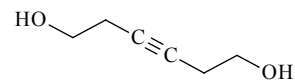


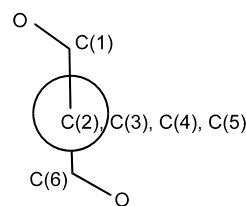
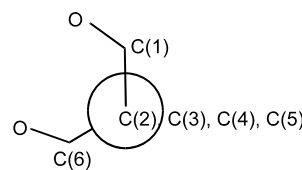
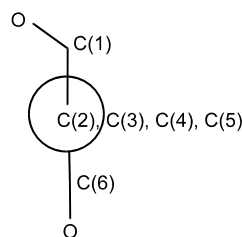
741 **C₆H₁₀O₂**ED, *ab initio*
calculations**3-Hexyne-1,6-diol****C_i (G⁺G⁻)****C₂ (G⁺G⁺)****C₁ (GA)**

r_a	Å ^{a)}
C(3)≡C(4)	1.213(3)
C(2)–C(3)	1.459(4)
C(1)–C(2)	1.548(3)
O–C	1.427(3)
O–H	0.977(17)
C–H	1.089(5)

θ_a	deg ^{a)}
C(2,5)–C≡C	185 ^{b)}
C(1)–C(2)–C(3)	107.3(7)
C(2)–C(1)–O	113.6(9)
τ_1 ^{c)}	64.8(22)



The experimental data were in accordance with a conformational mixture consisting of GG (equal amounts of G⁺G⁻ and G⁺G⁺) and GA conformers in the ratio of 62.2(103):37.8(103). G (*gauche*) and A (*anti*) describe the conformation of oxygen atoms relative to their neighboring C≡C–C group. Similar results were, however, obtained when a small contribution (up to 12%) from the high energy AA conformer was introduced. Differences between the parameters of the *gauche* and *anti* parts of the molecule were assumed at the values from MP2/6-31G* calculations. The C–C–O–H torsional angle in the *anti* part was assumed to be equal to 180°. The C–C–O–H and C–C–C–O torsional angles in the *gauche* part were assumed to be equal but of opposite signs. The distribution of the conformers with different τ_2 [C(1)–C(2)...C(5)–C(6)] angles was determined using potential energy curves from HF/6-31G* calculations. The figure shows the conformers at the values of τ_2 corresponding to the minima of these curves. The nozzle temperature was 179 °C.

G⁺G⁻ ($\tau_2 = 180^\circ$)G⁺G⁺ ($\tau_2 = -120^\circ$)GA ($\tau_2 = 180^\circ$)^{a)} Estimated standard errors.^{b)} Assumed at the value from MP2/6-31G* calculations.^{c)} Torsional angle C–C–C–O in the *gauche* part of the molecule, $\tau_1 = 180^\circ$ for the *anti* position.

Trættemberg, M., Bakken, P., Hopf, H., Mlynek, C., Mahle, A.H.: J. Mol. Struct. **554** (2000) 191.