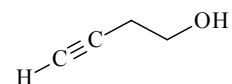


537 C₄H₆O**3-Butyn-1-ol****C₁ (*gauche*)**ED, *ab initio*
calculations**C_s (*anti*)**

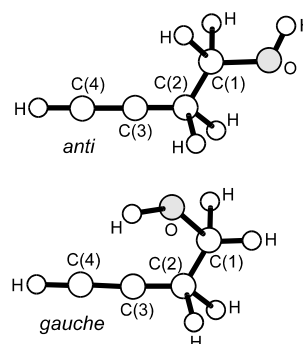
r_a	Å ^{a)}	θ_a	deg ^{a)}
C(3)≡C(4)	1.217(1)	C(1)–C(2)–C(3)	111.6(6)
C(2)–C(3)	1.469(1)	C(2)–C(1)–O	113.9(6)
C(1)–C(2)	1.536(2)	C–C–H (average)	111.3(8)
C(1)–O	1.414(1)	C–O–H	106.4 ^{b)}
O–H	0.992 ^{c)}	C(4)≡C(3)–C(2)	175.6 ^{b) d)}
C(4)–H	1.092 ^{c)}	C(3)≡C(4)–H	177.2 ^{b)}
C(1,2)–H	1.114(2)	τ_1 ^{e)}	60.2(16)
		τ_2 ^{f)}	–60.0 ^{b)}



The molecule exists as a mixture of *gauche* (85(10)%) and *anti* (15(10)%) conformers. The differences between the corresponding parameters of these conformers were taken from MP2/6-31G** calculations. The energy difference $\Delta E = E(\text{anti}) - E(\text{gauche})$ was estimated to be 1.63 kcal mol^{–1} by the *ab initio* (MP2/6-31G**) method.

The parameters are given here for the *gauche* conformer.

The temperature of the measurements was 51 °C.



^{a)} Estimated standard errors.

^{b)} Assumed at the value from MP2/6-31G** calculations.

^{c)} Assumed.

^{d)} Deviation is in the direction that brings the lobes of the π electrons closer to the OH group.

^{e)} O–C(1)–C(2)–C(3) torsional angle, $\tau_1 = 0^\circ$ for the *syn* position.

^{f)} C(2)–C(1)–O–H torsional angle, $\tau_2 = 0^\circ$ for the *syn* position.

Bakken, P., Hopf, H., Mahle, A.H., Trætteberg, M.: J. Mol. Struct. **376** (1996) 115.