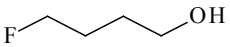
580 **C_4H_9FO** **4-Fluoro-1-butanol**

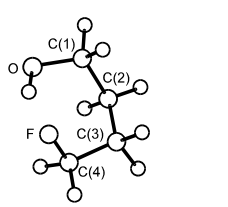
C_1 ($G^-G^+G^-g^+$)
C_1 ($G^+G^-G^-g^+$)
C_1 (G^+AG^-a)
C_1 (G^-AG^-a)
C_1 (G^-Aaa)
C_s (AAAa)

ED, *ab initio* and DFT calculations

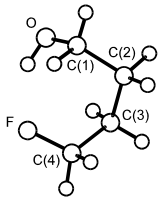
r_a	Å [a])	θ_a	deg [a])
C–O	1.428(5)	C–O–H	106.1 [b])
C(1)–C(2)	1.533(3)	C–C–O	112.5(20)
C(2)–C(3)	1.540(3)	C(1)–C(2)–C(3)	112.5(8)
C(3)–C(4)	1.520(3)	C(2)–C(1)–H	109.5(16)
C–F	1.408(6)	C–C–F	109.8(18)
O–H	0.947 [b])		
C–H	1.102(4)		



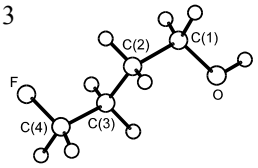
The best agreement with the experimental data was obtained with a model consisting of about equal amounts of hydrogen-bonded ($G^-G^+G^-g^+$ and $G^+G^-G^-g^+$, 48.5(140)%) and non-hydrogen-bonded (G^+AG^-a, G^-AG^-a, G^-AAa and AAAa , 51.6(140)%) conformers with the ratios of $G^-G^+G^-g^+$: $G^+G^-G^-g^+$ ≈ 3 : 1 in the hydrogen-bonded part and (G^+AG^-a + G^-AG^-a) : G^-AAa : AAAa ≈ 2 : 5 : 3 in the non-hydrogen-bonded part, where the letters A or a (*anti*) and G or g (*gauche*) indicate the torsions around the bonds in the order C(3)–C(4), C(2)–C(3), C(1)–C(2) and C(1)–O. Differences in the structural parameters of different conformers and torsional angles of all conformers were assumed at the values from HF/6-31G* calculations. The structural parameters are given for the $G^-G^+G^-g^+$ conformer. The nozzle temperature was 83 °C.



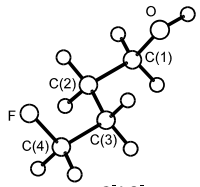
$G^-G^+G^-g^+$



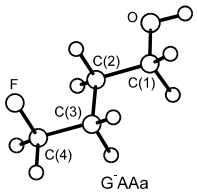
$G^+G^-G^-g^+$



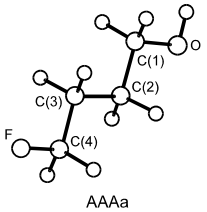
G^+AG^-a



G^-AG^-a



G^-AAa



AAAa

[a]) Twice the estimated standard errors.
[b]) Assumed.

Trætteberg, M., Richardson, A.D., Hedberg, K., Winter, R.W., Gard, G.L.: J. Phys. Chem. A **105** (2001) 9587.