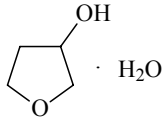
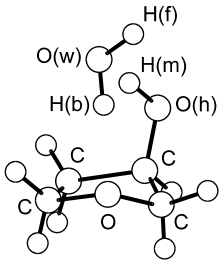
598 **$C_4H_{10}O_3$** **3-Hydroxytetrahydrofuran – water (1/1)** **C_1**
MW, *ab initio* calculations
Tetrahydro-3-furanol – water (1/1) (weakly bound complex)
(large-amplitude motion)

Atom [a])	$\lvert a_s \rvert$ [Å]	$\lvert b_s \rvert$ [Å]	$\lvert c_s \rvert$ [Å]
H(m)	0.997	1.175	0.264
H(b)	1.529	0.990	0.248
H(f)	3.0911	0.562	0.408
O(w)	2.342	0.430	0.233



The spectra are assigned to the network structure of the complex, with intermolecular hydrogen bonds from the hydroxyl group to the water oxygen atom and from water to the furanose-ring oxygen. *Ab initio* calculations at the MP2/6-31G** level indicate that this is the lowest energy structure of the complex, and it is based on the lowest-energy ring puckering conformation of 3-hydroxytetrahydrofuran monomer, C_4-endo.



[a]) For the identification of atoms, see figure.

Lavrich, R.J., Torok, C.R., Tubergen, M.J.: J. Phys. Chem. A **105** (2001) 8317.