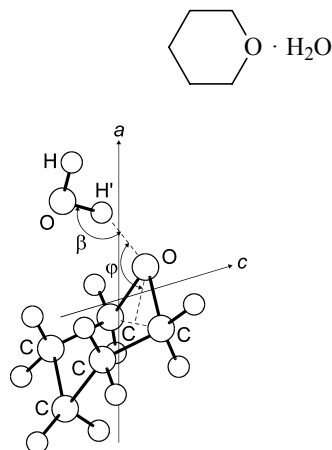


675  
MW $C_5H_{12}O_2$ Tetrahydro-2*H*-pyran – water (1/1) $C_s$ (effective symmetry class)  
(large-amplitude motion)

$r_0$	Å	$\theta_0$	deg
H...O <sup>a)</sup>	1.91(2)	$\varphi$ <sup>b)</sup>	122(2)
$R_{cm}$	3.324(4)	$\beta$ <sup>b)</sup>	176(4)
O...O	2.866(4)		

Atom	$ a_s $ [Å]	$ b_s $ [Å]	$ c_s $ [Å]
O <sup>c)</sup>	2.669	0.0	0.76

In the complex, the water molecule lies in the plane of symmetry of tetrahydropyran; the water hydrogen involved in the hydrogen bond is axial with respect to the ring, while the free hydrogen is *entgegen* to the ring. The three atoms involved in the hydrogen bonding adopt a slightly bent arrangement.



<sup>a)</sup> Hydrogen bond distance, namely the distance between the H atom of water involved in the hydrogen bonding and the O atom of tetrahydropyran.

<sup>b)</sup> See figure for the definition.

<sup>c)</sup> Water oxygen.

Spoerel, U., Stahl, W., Caminati, W., Favero, P.G.: Chem. Eur. J. **4** (1998) 1974.