

597  
MW $\text{C}_4\text{H}_{10}\text{O}_3$ **1,4-Dioxane – water (1/1)**  
(weakly bound complex) $\text{C}_s$   
(effective symmetry class)  
(large-amplitude motion)

$r_0$	$\text{\AA}$	$\theta_0$	deg
O...H' <sup>a)</sup>	1.90(3)	$\varphi$ <sup>b)</sup>	128(3)
$R_{\text{cm}}$	3.34(4)	$\beta$ <sup>b)</sup>	163(6)

Atom <sup>c)</sup>	$ a_s $ [ $\text{\AA}$ ]	$ b_s $ [ $\text{\AA}$ ]	$ c_s $ [ $\text{\AA}$ ]
O	2.669	0.0	0.76
H'	1.97	0.14(18)	0.28
H	3.40	0.17(17)	0.65

The water molecule lies in the plane of symmetry of 1,4-dioxane; 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 bond adopt a bent arrangement.

<sup>a)</sup> Distance of the hydrogen bond between O in the ring to H' of the water.

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

<sup>c)</sup> Atoms in the water; H' is involved in the hydrogen bond.

Caminati, W., Dell'Erba, A., Melandri, S., Favero, P.G.: J. Am. Chem. Soc. **120** (1998) 5555.

