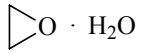
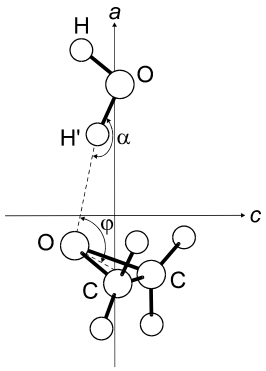
303 **$C_2H_6O_2$** **Oxirane – water (1/1)** **C_s**
MW (weakly bound complex) (effective symmetry class)
(large-amplitude motion)



r_0	Å	θ_0	deg
H'...O [a])	1.92(1)	φ [b])	103(1)
R_{cm}	2.84(2) [c])	α [b])	163(2)

Atom [d])	$\lvert a_s \rvert$ [Å]	$\lvert b_s \rvert$ [Å]	$\lvert c_s \rvert$ [Å]
O	2.152	0.0	0.162
H'	1.282	0.15	0.442
H	2.821	0.25	0.456



The water molecule lies in the plane of symmetry of the oxirane perpendicular to the ring; the water hydrogen involved in the hydrogen bond points toward the ring oxygen, while the "free" hydrogen is *entgegen* to the ring.

[a]) H' denotes the water hydrogen that is involved in the hydrogen bond and O is the oxygen of the oxirane.
[b]) See figure for the definition.
[c]) Uncertainty was not estimated in the original paper.
[d]) Atoms of the water.

Caminati, W., Moreschini, P., Rossi, I., Favero, P.G.: J. Am. Chem. Soc. **120** (1998) 11144.