

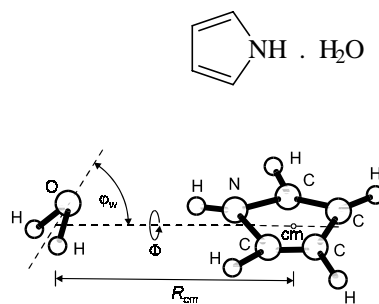
1707
MW

C₄H₇NO

Pyrrole – water (1/1)
(weakly bound complex)

C_s or C₁
(effective symmetry class)

r_0	\AA	
	crossed structure	hinged structure
R_{cm}	4.2015(18)	4.2026(55)
O...N	3.0283(37)	3.0326(116)
θ_0	deg	
	crossed structure	hinged structure
ϕ_w	37.3(46)	41.5(132)



Two likely orientations of the monomer planes: crossed ($\Phi = 0^\circ$) and hinged ($\Phi = 90^\circ$).

Tubergen, M.J., Andrews, A.M., Kuczkowski, R.L.: J. Phys. Chem. **97** (1993) 7451.