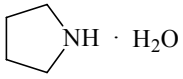
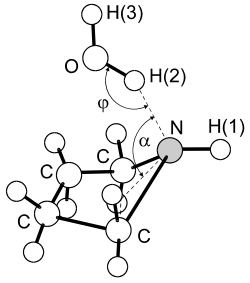
601 **$C_4H_{11}NO$** **Pyrrolidine – water (1/1)** **C_s**
MW (weakly bound complex) (effective symmetry class)
(large-amplitude motion)



r_0	Å	θ_0	deg
H(2)...N [a])	1.89(1)	α [b])	118.8(8)
R_{cm}	3.128(5) [c])	φ [b])	163.5(25)



Atom	$\lvert a_s \rvert$ [Å]	$\lvert b_s \rvert$ [Å]	$\lvert c_s \rvert$ [Å]
O	2.4857	0.0	0.3110
H(2) [a])	1.679	0.0	0.294
H(3) [d])	3.1354	0.334	0.3175
H(1)	0.246	0.31	2.120

Although only the rotational spectrum of axial-pyrrolidine has been previously reported, an adduct is formed with equatorial-pyrrolidine. The water molecule lies in the plane of symmetry of pyrrolidine; 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.

[a]) The water hydrogen that is involved in the hydrogen bonding.
[b]) See figure for the definition.
[c]) Uncertainty was not estimated in the original paper.
[d]) The water hydrogen that is not involved in the hydrogen bonding.

Caminati, W., Dell'Erba, A., Maccaferri, G., Favero, P.G.: J. Am. Chem. Soc. **120** (1998) 2616.