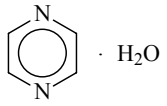
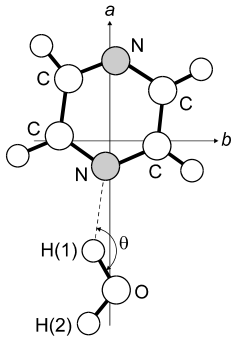
534 **$C_4H_6N_2O$** **Pyrazine – water (1/1)** **C_s**
MW (weakly bound complex) (effective symmetry class)
(large-amplitude motion)



r_0	Å	θ_0	deg
N...H(1)	1.94(2)	θ [a])	152(4)

Atom	$\lvert a_s \rvert$ [Å]	$\lvert b_s \rvert$ [Å]	$\lvert c_s \rvert$ [Å]
O	3.432	0.18	0.16
H(1)	2.526	0.25	0.27
H(2)	3.977	0.56	0.29



Each of the observed transitions is split into two components of approximately equal intensity and with a statistical weight of 5:3 depending on the parity of K_a. The geometrical structure, which is derived from the observed spectra, is consistent with one water hydrogen bound to one pyrazine nitrogen and with the oxygen lying in the plane of the aromatic molecule.

[a]) See figure for the definition.

Caminati, W., Favero, L.B., Favero, P.G., Maris, A., Melandri, S.: Angew. Chem. **110** (1998) 852; Angew. Chem., Int. Ed. Engl. **37** (1998) 792.