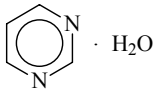
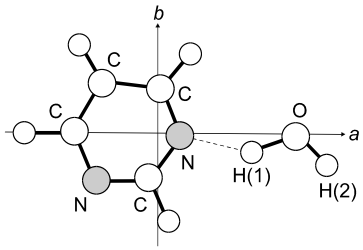
533 **$C_4H_6N_2O$** **Pyrimidine – water (1/1)** **C_s**
MW (weakly bound complex) (effective symmetry class)
(large-amplitude motion)



Atom	$\lvert a_s \rvert$ [Å]	$\lvert b_s \rvert$ [Å]	$\lvert c_s \rvert$ [Å]
O	3.40	0.09	0.06
H(1) [a])	2.48	0.41	0.13
H(2) [b])	3.95	0.54	0.31

The derived moments of inertia are consistent with a planar (or nearly planar) structure of the adduct in which one hydrogen of the water molecule is bound to the nitrogen of the aromatic ring, and the "free" water hydrogen is *entgegen* to the ring. The hydrogen bond stretching force constant is 13.8 N m^{-1}.



[a]) Water hydrogen that is involved in hydrogen bonding.
[b]) Water hydrogen that is not involved in hydrogen bonding.

Melandri, S., Sanz, M.E., Caminati, W., Favero, P.G., Kisiel, Z.: J. Am. Chem. Soc. **120** (1998) 11504.