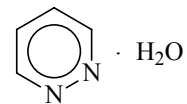


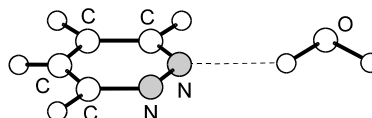
532  
MW $\text{C}_4\text{H}_6\text{N}_2\text{O}$ **Pyridazine – water (1/1)**  
(weakly bound complex) $\text{C}_s$   
(effective symmetry class)  
(large-amplitude motion)

| $r_0$           | Å                     |
|-----------------|-----------------------|
| N...O           | 2.966(3)              |
| $R_{\text{cm}}$ | 4.08(1) <sup>a)</sup> |

| $\theta_0$ | deg         |
|------------|-------------|
| N–N...O    | 153.8(3)    |
| N...H–O    | 180 – 10(2) |



| Atom | $ a_s $ [Å] | $ b_s $ [Å] | $ c_s $ [Å] |
|------|-------------|-------------|-------------|
| O    | 3.385       | 0.12        | 0.06        |



The derived moments of inertia are consistent with a 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.

<sup>a)</sup> Uncertainty was not estimated in the original paper.

Caminati, W., Moreschini, P., Favero, P.G.: J. Phys. Chem. A **102** (1998) 8097.