HYDRATION EFFECT ON THE STABILITY OF THE KETO-ENOL TAUTOMERS OF 5-HYDROXY-6-METHYLURACIL

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The structure and energies of six tautomeric forms of 5-hydroxy-6-methyluracil (OMU) and their 1:*n* (*n* = 1-4) complexes with water were determined by the density functional theory (PBE/3z) method. The stability series of the tautomers and changes in it depending on the number of water molecules in the nearest environment of the tautomer were found. The effect of the water solvent was also included using the continuum (B3LYP/6-311+G(*2d*,*p*), COSMO) model. Both complex formation and medium effects significantly influenced the stability series of the tautomers. Although the decrease in the energy of the diketo form on hydration was smaller than for the enol states, diketo tautomer **a** remained the most stable form of OMU in solution. Inclusion of hydration in calculations suggests that the energies of three enol tautomers **b–d** were equalized ($\Delta H \approx 5.5$ kJ/mol). This should be taken into account for the conditions that facilitate the keto-enol tautomerism of OMU.

Keywords: quantum chemical calculation, 5-hydroxy-6-methyluracil, tautomer, hydration, hydrogen bond.