Effect of Different Substituents on Uracil and its 2-Hydroxy-4-oxo Enol Tautomer – A Theoretical Study

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The uracil/2-hydroxy-4-oxo uracil tautomeric system was studied by employing the MNDO semi-empirical method for the calculations. The uracil structure was found to be energetically favourable as indicated by the calculated heat of formation, the Gibbs free energy, the HOMO and LUMO energies, and charges. The substitution by F, OH, NH_2, CH_3, and BH_2 at the carbon-6 position was found to affect the geometrical parameters of the substituted molecules. All of the substituents were found to shift the equilibrium in forward direction compared to the unsubstituted tautomeric pair as indicated by the calculated values for the equilibrium constants.

Key words: Uracil; 2-Hydroxy-4-oxo Uracil; Tautomerization; MNDO.