Tautomeric Transformations and Reactivity of Polyfunctional Hydroxypyrimidines: III.[1] Tautomerism of 5-Acyl Derivatives of Hydroxypyrimidines and Formation of H-bonded Complexes with Solvents

V. I. Slesarev and A. S. Popov

St. Petersburg State Medical Academy, St. Petersburg, Russia

Received June 14, 2000

Abstract - Tautomerism of 5-formyl- and 5-acetyl derivatives of pyrimidine-2,4,6-trione, 2-thioxopyrimidine-4,6-dione, and 4,6-dihidroxy-2-methylthiopyrimidine was studied by NMR, UV, and IR spectroscopy, as well as by quantum chemistry. An equilibrium mixture of *exo*- and *endo*-enols in the neutral state and the presence of the same tautomers in monoanions were found. The energies of intramolecular hydrogen bonds in the gas phase and their changes in going to solutions in water, DMSO, and chloroform were calculated. The energies of intra- and intermolecular hydrogen bonds are close to each other. This fact suggests existence in solutions of two forms: tautomers with intramolecular H bond and H-bonded complexes with the solvents studied, whose formation involves cleavage of the intramolecular H bond. Characteristics of intermolecular hydrogen bonds are determined by the relative proton-donor and proton-acceptor powers of polyhydroxypyrimidines and solvents and are almost independent of the polarity of the medium.