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Structure and properties of aromatic and aliphatic aromatic azomethine

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Abstract

The review of works on studying the reaction of Schiff bases, as well as peculiarities of their structure and properties which were carried out at the Department of Organic and Biological Chemistry of Ivanovo State University is presented. With use of quantum chemical methods it is shown that there are two stages in azomethines formation, semiaminal being an intermediate product. Accounting the solvent effect in the simulated system leads to lowering the energy profile of the reaction. Peculiarities of structure of Schiff bases with substituents of different nature and position in the benzene ring are discussed. ^{1}H NMR spectra proved the existence of imine-enamine tautomerism in a solution with the predominance of enamine form, both tautomers being stable. Conformation analysis for the molecules of aromatic Schiff bases at temperatures of existence of different phases and phase transitions showed that the phase transitions are accompanied by changes of conformation and length of the molecule, which is determined by the possibility of rotation of the benzene rings and alkyl groups mobility. It is shown that the catalysts on the base on carbon nanomaterials are considerably more active in hydrogenation of the Schiff bases in comparison with analogs on activated carbon. A number of computer models are developed with the use of special algorithms of analysis of multi-parameter data and the selected molecular descriptors. Biochemical activity of the Schiff bases and corresponding secondary amines is predicted.