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Faculty of science
Department of chemistry

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(in the field of physical chemistry)

Title:

Investigating the effect of substitution on the strength of hydrogen bond interactions in 7-formyl-8-hydroxyquinoline

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Abstract

In this research, using density function theory calculations at the theoretical level of PBEKCIS/6-311++G**, optimization of structures with Gossin 09 software package, electron charge densities with AIM2000 software, electron transfers between parts The different compounds were analyzed with NBO 3.1 software and the aromaticity of the rings in the compounds was done with Multiwfn software. The purpose of this research is to investigate the effect of H, F, Cl, OH, CH_3, CN, NO, and NO_2 substitutions, as well as the effect of two H_2O and H_2S molecules as intermolecular hydrogen bond donors with N position, on the hydrogen bond strength. Some derivatives of 7-formyl-8-hydroxyquinoline are intramolecular. In general, the aim is to investigate the effect of intramolecular hydrogen bonds on the intermolecular type. In the first step, the interaction of derivatives in closed configuration with water molecules and hydrogen sulfide is investigated. In the second step, the interaction of the open configuration of the derivatives with water and hydrogen sulfide molecules is studied, and in the third step, the formyl group is removed from the structures until the intermolecular hydrogen bond interaction of water and hydrogen sulfide molecules with them be considered. The presence of formyl group and the formation of intramolecular hydrogen bond interaction in these derivatives led to an increase in the length of the intermolecular hydrogen bond in the respective complexes and an increase in the negative charge transferred to water and hydrogen sulfide molecules in the complexes that They are formed from derivatives without formyl group, it caused an increase in binding energies and also, the amount of negative charge transferred to the hydrogen sulfide molecule was more than that of the water molecule. The changes of H_2O to H_2S did not affect the trend of electron densities, and the electron density at the critical point of the intermolecular hydrogen bond (N...H) of H_2O complexes was also greater than that of H_2S complexes, and the interaction of water molecules and hydrogen sulfide with the mentioned derivatives led to the creation of a new ring in the molecular diagram created by AIM calculations. The change of substitution leads to the change of the aromaticity of the rings of the derivatives in the closed configuration, and this, in turn, affects their binding energies. Therefore, the presence of intramolecular hydrogen bond interaction in complexes formed by derivatives in a closed configuration with water molecules leads to results for the binding energies of these complexes that are consistent with energy analysis data and is effective in their stability.

Keywords: hydrogen bond, quinoline, binding energy, aromaticity and substitution.