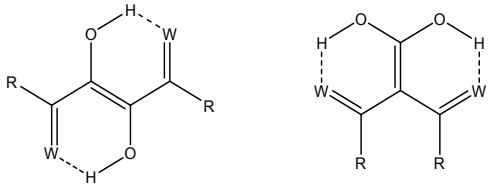
symmetrically substituted derivatives have been studied. The influence of the coexistence of two intramolecular hydrogen bonded rings in these molecular systems on the molecular structure, intramolecular hydrogen bonding and π-electron delocalization were investigated [1,2].



system A system B

Fig.1. W=O, S R= H, F, Cl, Br, CN, CH3

In the present study, all of the computations were performed by Gaussian 09 series of programs. The geometry optimizations were carried out at MP2/6-311++G(3df,3pd) level of theory. The Quantum Theory of "Atom in Molecules" (QTAIM) of Bader was also applied here to get more details about the nature of hydrogen bonds. The results of quantum chemical calculations, for A systems, show that such coexistence between the RAHB rings decreases the π-electron delocalization and it leads also to the weakening the hydrogen bond. While, the coupling between these two rings within the B systems, cause an increase of resonance effect that it leads to the increase of strength of hydrogen bond. In the present work, we also evaluated the intramolecular hydrogen bond energies by the RRM and open-close models. Moreover, the correlations between the hydrogen bond energies and different descriptors were also analyzed. It was found that topological characteristics of critical points (bond critical points and ring critical points) are also useful to estimate the strength of intramolecular hydrogen bond in two-ring RAHB systems.

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A novel view of interaction between HSA and hemin-HSA in the absence and presence of lomefloxacin: Flurescence quenchinginvestigation

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Aim: It is important to study the interaction of the drug with the proteins because protein–drug binding plays an important role in pharmacology and pharmacodynamics. Human serum albumin (HSA) is a very important transporter protein in the circulatory system. It is a multi-domain binding protein, which binds a wide variety of ligands in its multiple binding sites. Porphyrins are a class of tetrapyrroles that have extensive applications as photosensitizing drugs in medicine.In this study, we investigated the interaction between HSA and hemin-HSA in the absence and presence of lomefloxacin by flurescence spectroscopy methods. Lomefloxacin is a fluoroquinoloneantibiotic, used to treat bacterial infections including bronchitis and urinary tract infections. Methods:The synchronous fluorescence spectra at $\Delta\lambda$ = 60nm and $\Delta\lambda$ = 15nm of HSA and hemin-HSA in the absence and presence of lomefloxacin and absorption spectra were used to study protein conformation. In addition, the fluorescence spectra at λ = 280nm and λ = 295nm were applied to measure the number of binding sites 'n' and apparent binding constant 'K' by Stern–Volmer equation. The interaction of hemin-HSA with human serum albumin (HSA) as pure and heme complex in the presence of lomefloxcain shows that It acts as quencher. The interaction between hemin-HSA with HSA in the presence of lomefloxcan is consistent with static quenching and the conformational changes of HSA observed.

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DFT calculations and NBO analysis on stability of cis and trans isomers of bis(4-amino-3-penten-2-onato)nickel(II)

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The late transition metal complexes, are generally considered to be good tolerant toward polar media and thus are used as catalysts for polar monomer polymerizations [1, 2]. The aim of the present work is the modified synthesis and the improved understanding of the structural information of bis(4-amino-3-penten-2-onato)nickel(II), Ni $(APO)_2$, by means of density functional theory (DFT) studies and NBO analysis. The calculated geometrical parameters were compared with those observed experimentally. In this work, the molecular equilibrium geometry, harmonic force field, and geometrical parameters of $Ni(APO)_2$ were computed with the GAUSSIAN 03W software system [3] and NBO 5.0 [4] programs. The geometry optimization and vibrational frequencies are performed at the B3LYP6-311G* / level. The results show the trans isomer is more stable in the gas phase ($\Delta E=E_{cis}-E_{Trans}=27.45$ kJ.mol^{-1}). In solution the stability of trans is lowered ($\Delta E=13.07$ kJ.mol^{-1}) and in the solid phase, according to x-ray report[5], the cis isomer is more stable than the trans one. The charge distribution calculated by NBO, confirms existing of significant resonance in the trans isomer relative to the cis