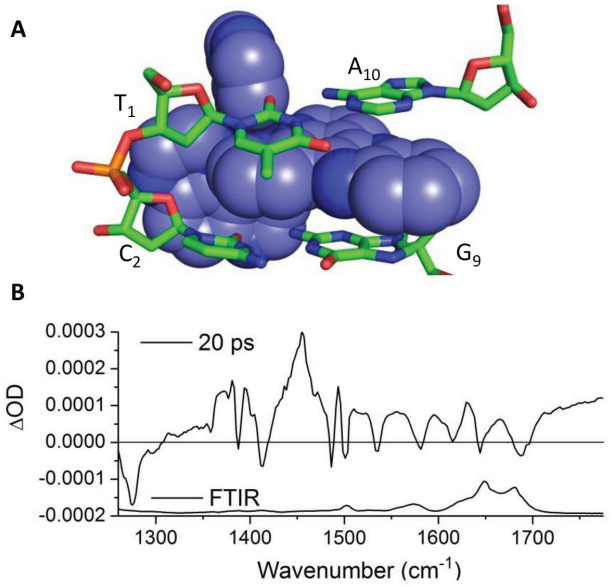

Figure 1. Λ-[Ru(TAP)$_2$(dppz)]$^{2+}$ (purple) intercalates into d(TCGGCGCCGA) at the terminal GA step in the duplex. (B) TRIR spectra were at multiple time delays, including 20ps. By fitting the data at multiple time delays, the lifetimes of different excited states can be determined.

Keywords: Photochemistry, ultrafast spectroscopy, DNA

MS38-P17 Theoretical analysis (NBO, NPA, Mulliken Population Method) and molecular orbital studies (hardness, chemical potential, electrophilicity and Fukui Function Analysis) of (E)-2-((4-hydroxy-2-methylphenylimino) methyl)-3-methoxyphenol

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The molecular structure and spectroscopic properties of (E)-2-((4-hydroxy-2-methylphenylimino) methyl)-3-methoxyphenol, were characterized by X-ray diffraction, FT-IR and UV-Vis spectroscopy. All of theoretical calculations and optimized geometric parameters have been calculated by using density functional theory (DFT) with hybrid method B3LYP by 6-31G(d,p) basis set. The title compound of $C_{15}H_{15}N_1O_3$ have been analyzed according to electronic and energetics behaviors for enol-imine and keto-amine tautomers. Both these tautomers engender six-membered ring due to intramolecular hydrogen bonded interactions. The theoretical vibrational frequencies have been found in good agreement with the corresponding experimental data. A study on the electronic and optical properties, absorption wavelengths, excitation energy, dipole moment, molecular electrostatic potential (MEP) and frontier molecular orbital energies are performed using DFT method. Additionally, geometry optimizations in solvent media were performed with the same level of theory by the polarizable continuum model (PCM). The effect of solvents on the tautomeric stability has been investigated. Mulliken population method and natural population analysis (NPA) have been studied. NBO analysis is carried out to picture the charge transfer between the localized bonds and lone pairs. The local reactivity of the molecule has been studied using the Fukui function. NLO properties related to polarizability and hyperpolarizability are also discussed.

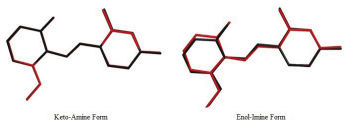

Figure 1. Superimposition of the X-ray structure (red) and calculated structure (black) of the enol-imine and keto amine forms of the title molecule.

Keywords: Natural Population Analysis (NPA), Fukui Function Analysis, Natural Bond Orbital Analysis (NBO)