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UV-VIS SPECTRA OF SOME PHENOLIC SCHIFF BASES: EXPERIMENTAL AND THEORETICAL STUDY

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Schiff bases represents important class of synthetic compounds which was first synthesized in condensation reactions of aldehydes and aromatic amines [1]. Phenolic Schiff bases found wide application in medicine and pharmacy. These compounds exhibit good antitumor, antiviral, antifungal and antibacterial activity [2]. Due to these biological properties Schiff bases were used for the synthesis of many drugs [3]. Ten phenolic Schiff bases were put under examination of their UV-Vis properties. The solutions of all compounds were prepared in methanol, and the UV/Vis measurements were performed in the area of 200-500 nm range. The quantum-chemical interpretation of UV-Vis spectra of these compounds has become a crucial support for experimental data. The time-depend density functional theory (TDDFT) appear to be an effective tool to estimate UV-Vis absorption of medium sized π -conjugated compounds. Gaussian program package [4] was used for simulation of UV-Vis spectra of examined compounds and calculation were performed at the B3LYP/6-311+G(d,p) level of theory. To provide better understanding of distribution of electron density, natural bond orbital (NBO) analysis was used. NLMO clusters were constructed and they represent a part of a molecule characterized with eminent electron density. Synergism between the TDDFT and NBO theory helps for better understanding of electronic transitions engaged in the UV-Vis light absorption of the examined compounds. The Kohn–Sham orbitals can be replaced with NLMO clusters since they are described with specified energies and shapes. NLMO clusters provide delocalization over the definite part of molecule, while the Kohn-Sham orbitals are delocalized through the whole structure.

References:

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