

Theoretical and Experimental Investigation of Vibrational (FT-IR and Raman) Spectra and Electronic Transitions of Di-p-tolylamine

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The growing interest in molecular organic materials as the basis for creating optoelectronic devices has led to an increasing interest in the structure and growth dynamics of organic molecular thin films. Molecular organic semiconductors are promising materials for organic light-emitting diodes [1, 2], thin-film transistors [3], and photovoltaic devices [4]. One of the most important molecules is di-p-tolylamine. Therefore, we report a structural and spectroscopic investigation of the di-p-tolylamine molecule. The optimized geometry of this molecule was calculated from *ab-initio* and quantum chemistry density functional theory (B3PW91 and B3LYP methods) with using 6-31+G(d) basis set on the ground state. Vibrational wavenumbers, infrared and Raman intensities and normal mode descriptions were predicted. Calculated wavenumbers and intensities were compared with the FT-IR and Raman spectra of di-p-tolylamine, thus supporting for a general assignment of the recorded spectra. In Fig. 1(a) and (b), FT-IR and Raman spectra of di-p-tolylamine are presented, representively.

Density Functional Theory (DFT) method was used to determine the minimum energy structures of di-p-tolylamine by using B3LYP and B3PW91 functional 6-31+G(d) level. Then, theoretical UV spectrum was obtained by Time-Dependent DFT (TDDFT) and compared to the experimental spectrum (Fig. 1(c)). The singlet and triplet excited states of di-p-tolylamine found by TDDFT calculations. The lowest excited triplet state of di-p-tolylamine almost entirely consists of the single HOMO→LUMO+1 configuration. The excitation energy of 3.47 eV is rather close to the difference in energies of HOMO and LUMO.

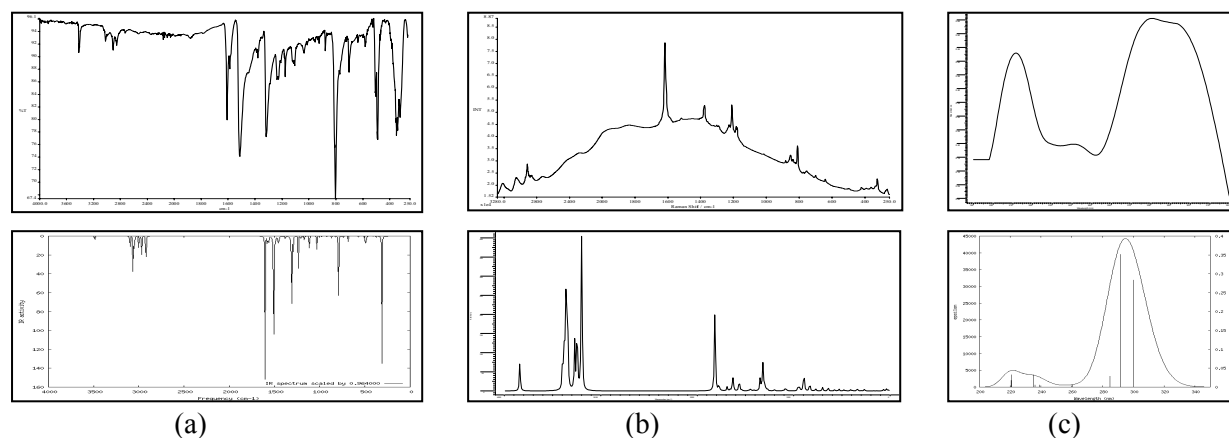


Fig. 1: Experimental and Theoretical Infrared spectra (a) Raman Spectra (b) UV spectra (c) of di-p-tolylamine

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