

## Notice for the PhD Viva Voce Examination

Ms Manju Pandey (Reg. No. 1345101), PhD scholar at the School of Sciences, CHRIST (Deemed to be University), Bengaluru will defend her PhD thesis at the public viva-voce examination on Saturday, 13 August 2022 at 10.30 am on the WebEx Meeting platform.

**Title of the Thesis** : **Spectroscopic Studies and Theoretical Analysis of some Selected Heterocycles**

**Discipline** : **Chemistry**

**External Examiner 1** : **Dr G Harichandran**  
Associate Professor  
Department of Polymer Science  
University of Madras, Chennai  
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**External Examiner 2** : **Dr Gayathri V**  
Professor  
Department of Chemistry  
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**Supervisor** : **Dr N M Nanje Gowda**  
Professor Emeritus  
Department of Chemistry  
School of Sciences  
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The faculty members of the Department and the School, interested experts and research scholars of all the branches of research are cordially invited to attend this open viva.

**Place:** Bengaluru  
**Date:** 08 August 2022



**Registrar**

## ABSTRACT

Seven derivatives of heterocycles benzimidazole, benzoxazole and benzothiazole were studied, five of which were synthesized and characterized. The molecular geometry and spectroscopic data of the compounds in the ground state were calculated using the density functional theory (DFT/B3LYP) method with the 6-311++G(d,p) basis set. A comparison between the experimental and calculated data was attempted. Molecular electrostatic potential (MEP) and global reactivity parameters were deduced using theoretical calculations.

HOMO-LUMO energy gap for each compound was determined by DFT and cyclic voltammetry. The cyclic voltammograms were recorded in acetonitrile solvent using lithium perchlorate as the supporting electrolyte. For all the compounds experimentally determined HOMO–LUMO energy gap in polar solvent was lesser than that from DFT calculated energy gap. Using the HOMO-LUMO energy gap, global reactivity parameters were calculated. The effect of solvents of varying polarity on the absorption and emission spectra of the compounds was studied. Large excitation and emission energy differences were observed for all the selected heterocycles.

The excitation and fluorescence spectra of selected heterocycles were recorded in eight solvents of different solvent polarity. It is evident from the excitation spectra that on increase of the solvent polarity, a bathochromic shift takes place for  $\pi$ - $\pi^*$  transition, and this is attributed to the high influence of solvent polarity in the excited state of heterocycle compared to its ground state.

The dipole moments in the ground and the first excited state of heterocycle derivatives were calculated using Lippert-Mataga and Kawski-Chamma-Viallet methods. Guggenheim-Debye method was adopted to calculate ground state dipole moment. The dipole moments of the compounds were also calculated using Time Dependent-Density Functional Theory (TD-DFT). The dipole moment values of the compounds suggested that the excited state has more charge separation and thus becomes more polar. This can be attributed to stronger solute solvent interaction.

Further, Light Harvesting efficiency and open circuit voltage were determined to understand the photovoltaic property. The calculated Light Harvesting Efficiency suggested that in all the heterocycles reasonably good amount of energy can be transferred to the conducting material in DSSC by photosensitization. Open-circuit voltage ( $V_{oc}$ ) results have indicated that HOMO energy level in all the heterocycles is sufficiently lower than the redox potential of I<sup>-</sup>/I<sub>3</sub><sup>-</sup> electrolyte (-4.8 eV) and LUMO energy level is above the conducting band of TiO<sub>2</sub> (-4.0 eV). This shows a good electron injection from acceptor TiO<sub>2</sub>, indicating that heterocycles may be good candidates for application in photovoltaic cells.

**Keywords:** DFT, TD-DFT, HOMO-LUMO, Dipole moment, Absorption and emission spectra, Molecular electrostatic potential, global reactivity parameters.