CHRIST
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Notice for the PhD Viva Voce Examination

Mr Suman G R (Reg. No. 1445206), PhD scholar at CHRIST (Deemed to be University), will defend his PhD thesis at the public viva voce examination on Friday, 12 June 2020 at 3.00 pm. The defense will be conducted online on the Webex platform.

Title of the Thesis	:	**Synthesis, Spectroscopic and DFT Studies of some Benzimidazole and Benzothiazole Derivatives**
Discipline	:	**Physics**
External Examiner (Outside Karnataka)	:	**Dr M Umadevi** Associate Professor Department of Physics Mother Teresa Women's University Kodaikanal - 624102 Tamil Nadu
External Examiner (Within Karnataka)	:	**Dr Suresh Kumar H M** Professor and HOD Department of Physics Siddaganga Institute of Technology Tumakuru-572 103 Karnataka
Supervisor	:	**Dr Bubbly S G** Professor Department of Physics CHRIST (Deemed to be University) Bengaluru – 560029

Since it is an open viva, faculty members and research scholars of all branches of research are cordially invited to attend.

Registrar

Place: Bengaluru
Date: 3 June 2020

ABSTRACT

Benzimidazole, benzothiazole and benzoxazole compounds and their derivatives having azole moieties are biologically active and are extensively used in pharmaceutical industry. Benzimidazoles/benzothiazoles scaffolds have also been widely used as π−spacers and donor/acceptor units. The lone pair electrons and conjugated structures of these heterocyclic molecules assist in tuning of electronic properties enabling their use in devices like dye sensitized solar cells, organic light emitting diodes etc. However, the design and synthesis of organic ligands for these applications is still a challenging task. Though we have made an effort in this direction fabricating a dye sensitized solar cell with benzimidazole based sensitizer, the moderate Stokes shift and efficiency prompted us to tune these molecules and improve their electronic properties. Considering that some of the benzimidazole/benzothiazole fluorophores possessing metal-ion chelating properties and having hydrogen donor-acceptor sites in close proximity play vital role in sensor and bioimaging applications, we have designed and synthesized novel fluorophores for metal ion sensing applications. Since most of the available literature shows studies on fluorophores with single excited state intramolecular proton transfer sites or dual proton transfer sites with symmetrical structures, we have considered investigating fluorophores having asymmetrical structures and proton donating sites. In this perspective, we have synthesized and conducted spectroscopic and density functional theory studies on some novel fluorophores based on benzimidazole/benzothiazole Schiff bases and the details are presented in this thesis.

Chapter 1 gives an introduction to the benzimidazole/benzothiazole heterocycles and the different photophysical and chemical phenomena involved. A brief literature survey in support of our studies is presented in Chapter 2. Chapter 3 gives a brief description of the experimental methods and techniques used in our work. Chapter 4 reports the synthesis of a benzimidazole Schiff base fluorophore 2-[(3′-N-salicylidenephenyl)benzimidazole] (Spbzl) and its characterization using FT-IR, FT-Raman, 1H NMR and single crystal XRD techniques. Energy level analysis using cyclic voltammetry and computational studies using density functional theory are also presented. Chapter 5 describes the synthesis and characterization of four novel fluorophores, (E)-2-(1Hbenzimidazol-2-yl)-4-(2hydroxybenzylideneamino)phenol(HBZS), (E)-1-((3-(1Hbenzo[d]imidazol-2-yl)-4-hydroxyphenylimino)methyl) naphthalen-2-ol (HBZNP), (E)-2(benzothiazol-2-yl)-4-(2-hydroxybenzylideneamino) phenol (HBTS) and (E)-1-((3(benzo[d]thiazol-2-yl)-4-hydroxyphenylimino)methyl)naphthalen-2-ol (HBTNP), with dual excited state intra-molecular proton transfer sites. Solvatochromic studies, fluorescence life-time measurements, aggregation induced emission studies, metal-ion sensing studies and computational

studies performed on these fluorophores are discussed in this chapter. Synthesis of ESIPT-ICT coupled novel fluorophores (E)-2-(1H-benzo[d]imidazol-2-yl)-4-(4-(diethylamino)-2hydroxybenzylideneamino) phenol (HBZA) and (E)-2-(benzo[d]thiazol-2-yl)-4-(4(diethylamino)-2-hydroxybenzylideneamino) phenol (HBTA) and their characterization using 1H NMR and LC-MS is reported in Chapter 6. Discussion on fluorescence studies in different solvent environments, fluorescence life time measurements, aggregation induced emission studies, metal ion sensing studies and computational studies for understanding the sensing mechanism in these two fluorophores are included in this chapter. Chapter 7 gives the summary of the research work along with the scope for future work.

Keywords: ESIPT, AIE, Schiff, Benzimidazole, DFT