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Topic of Research : **Photoluminescence, 4f-4f Absorption and NMR Studies of Ternary Lanthanide Enolates**

### *Findings*

The research work in the thesis entitled “**Photoluminescence, 4f-4f Absorption and NMR Studies of Ternary Lanthanide Enolates**” is based on the synthesis, characterization, photoluminescence, and optical absorption studies of trivalent lanthanide complexes. The thesis consists of five chapters. **Chapter I** deals with brief introduction explaining various aspects of the work. It delves into a thorough examination of literature focusing on lanthanide complexes derived from  $\beta$ -diketones and heterocyclic amines. The primary focus of this literature review is to offer a comprehensive understanding of the absorption and photoluminescence properties of lanthanide complexes. The chapter concludes by outlining the research objectives. **Chapter II** deals with design and synthesis of four Eu(III) complexes with 6,6,7,7,8,8,8,-heptafluoro-2,2-dimethyl-3,5-octadione (Hfod) and various ancillary ligands. These complexes were thoroughly characterized by NMR, FTIR, Single crystal XRD and elemental analysis. The complex's geometry was analyzed utilizing SHAPE software. Their photoluminescence properties were investigated in solid state, solution, and in PMMA based thin films. The findings indicated outstanding luminescent features, indicating promising potential for application as red components in OLEDs. Furthermore, absolute quantum yields of the complexes in solid state were measured and compared with the literature values. Additionally, the band gap of the complexes was determined from absorption spectra using Tauc's equation. The effect of solvents on the luminescence properties of europium complexes were analyzed and thoroughly discussed. **Chapter III** reports four heteroleptic samarium complexes [Sm(fod)<sub>3</sub>(bzi)] (**1**), [Sm(fod)<sub>3</sub>(bath)] (**2**), [Sm(fod)<sub>3</sub>(py-im)] (**3**), and [Sm(fod)<sub>3</sub>(terpy)] (**4**) (fod is the anion of 6,6,7,7,8,8,8- heptafluoro-2,2-dimethyl-3,5-octanedione (Hfod), bzi is benzimidazole, bath is 4,7-diphenyl-1,10-phenanthroline, py-im is 2-(2-pyridyl) benzimidazole and terpy is 2,2':6',2''-terpyridine. These complexes were thoroughly

characterized by NMR, FTIR, and elemental analysis. Furthermore, the crystal structures of complexes **2** and **4** were obtained, and their shapes were determined using SHAPE software. Photoluminescence properties were explored in both the visible and near-infrared regions, revealing robust luminescence indicative of efficient energy transfer from ligand to metal ion. Absolute photoluminescence quantum yields (PLQY) were determined in the solid state, demonstrating good quantum yield for these complexes. Additionally, the chapter delves into the temperature-dependent photoluminescence of complex **2**, to investigate the effect of temperature on the luminescence of [Sm(fod)<sub>3</sub>(bath)] complex. The results divulge the potential application of this complex as a temperature sensor in the range of 60 K to 350 K. **Chapter IV** reports four terbium complexes using fluorinated β-diketone (fod) as main chromophore along with the different heterocyclic amines as ancillary ligands. These complexes were thoroughly characterized by FTIR and CHN analysis. Single X-ray crystallography of complex **1** and **2** was analyzed to elucidate their molecular structure. The photoluminescence properties of these complexes were further investigated in different phases. The photoluminescence studies showed that efficient energy transfer takes place from ligands to metal center. The optical band gap of these complexes was determined and showed that these values lie in semiconductor region. **Chapter V** present four novel Neodymium based complexes using different ancillary ligands and these complexes were thoroughly characterized by <sup>1</sup>H NMR, FTIR, CHN analysis and TGA. Single X-ray crystallography of complex **2** was analyzed to elucidate their molecular structure. Upon the excitation in the ultraviolet region of the spectrum, the neodymium ion of the complexes emits in near IR region with the maxima at 1060 nm. These complexes show good luminescence properties. It has been shown that ancillary ligands are efficient in enhancing luminescence in the complexes and the C-H vibrational quenching of the excited state of Nd<sup>3+</sup> can effectively be reduced by using fluorinated ligands in the coordination sphere. Moreover, the oscillator strength and effect of solvents on the band shape of the 4f-4f absorption were investigated and discussed. The change in the band shape was correlated with asymmetry of the complexes.