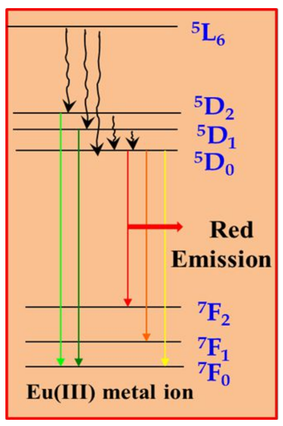
Experimental and Theoretical Investigation of Bi and Tri Nuclear Eu^{III} Complexes for Red/White Emitting LEDs

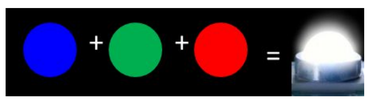
Rachna Devi, B. Rajamouli and V. Sivakumar*

Optoelectronics laboratory, Department of Chemistry
National Institute of Technology - Rourkela. Email: vsiva@nitrkl.ac.in Tel: 0661-242654, India.

Lanthanide (Ln) coordination chemistry for white-light-emitting materials have gained intense attention in recent years due to their widespread applications in optoelectronic devices such as full color displays and the back-light of portable smart display devices, organic light emitting diodes (OLEDs/LEDs) and sensors.1 Among the Lns, europium (Eu) complexes capable to give red emission and it is attractive due to their line like emission characteristics, large Stokes shifts, long luminescence life time, phosphorescent emission. In order to produce the white emission requires primary RGB colors. Generally, the Eu(III) can produce red emission and need to choose to blue and green emitting antenna in the complex to realize white emission. Since, the choosing antenna can balance the RGB colors to generate the white light via incomplete energy transfer. We have recently reported incomplete energy transfer process from ligand to Eu(III) metal ion, which leads to white light in both solution and LED. In the present study, to produce the white light we have chosen triphenylamine core moiety functionalized novel class of bipolar ligands (L1 and L2) and coordinated β-diketonate to synthesize the Eu(III) complexes. Bis (Eu2(TTA)6L1) and tris (Eu3(TTA)9L2) Eu(III) complexes are characterized by using different spectroscopic techniques. Here, the blue emitting ligand was chosen to produce the partial energy transfer to Eu(III) metal ion and confirmed by the theoretical calculations (DFT abd TD-DFT). Photophysical properties (UV-absorption and photoluminescence (PL)), lifetime analysis were measured for the synthesized Eu(III) complexes. In addition, the Judd-Ofelt calculation, electrochemical analysis, DFT calculations, temperature dependent emission behaviour for thermal sensors and finally light emitting diodes (LEDs) were measured.

WHY EUROPIUM

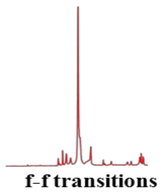


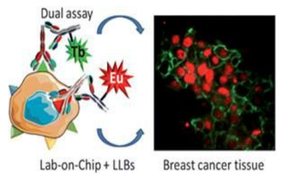


Introduction

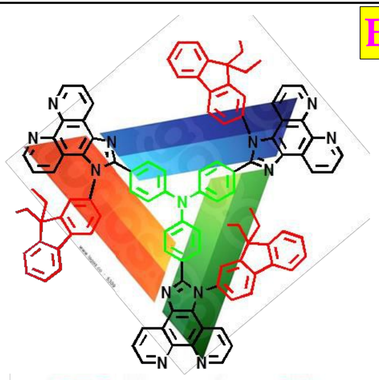
24800 cm^{-1}
21200 cm^{-1}
19000 cm^{-1}
17500 cm^{-1}

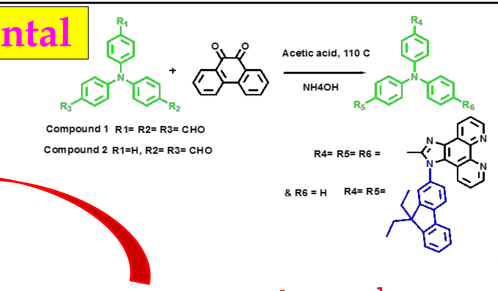
- Ln(III) ion complexes - depends on the emission wavelength.
- Visible range - television screens, liquid crystals, fluoroimmunoassays & bio physical applications.
- Near-IR – laser, telecommunications and optical amplifiers.

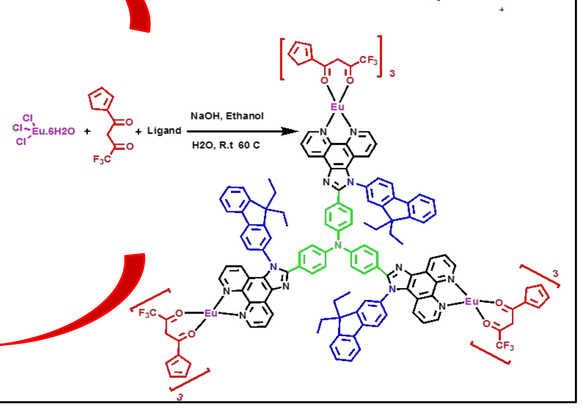


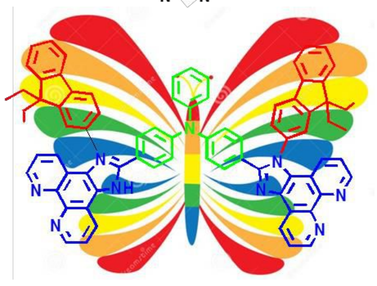


Experimental

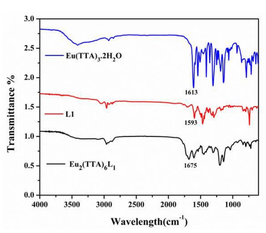


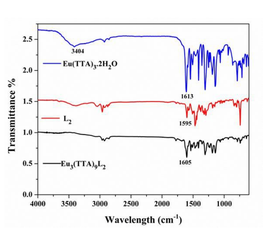


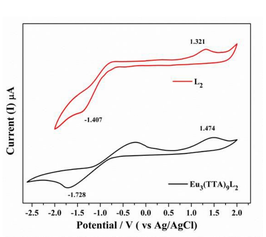


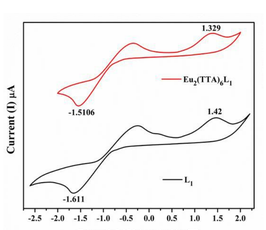


FTIR and CV Study

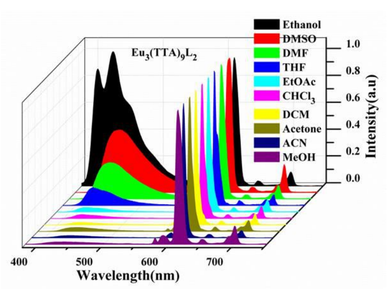


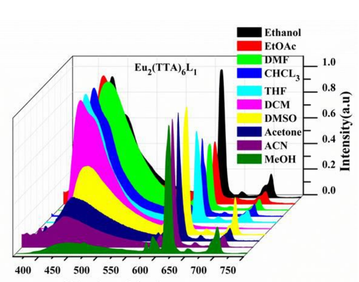




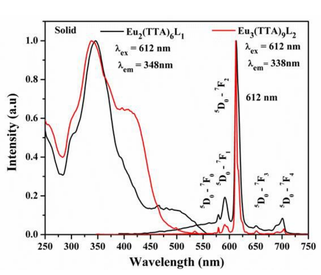


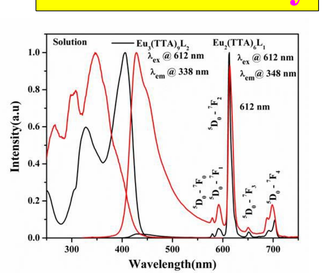
Solvatochromism Study

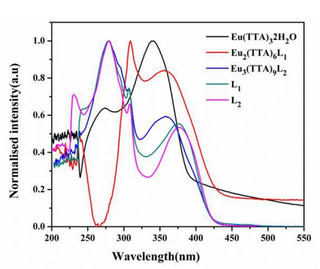




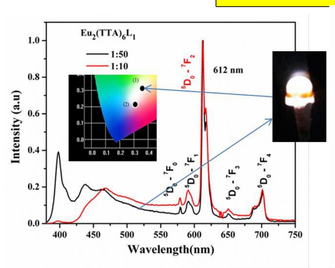
PL & UV study

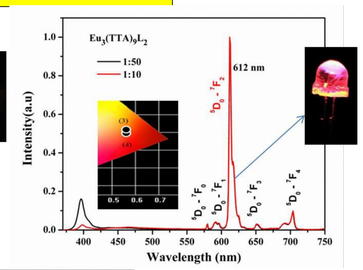


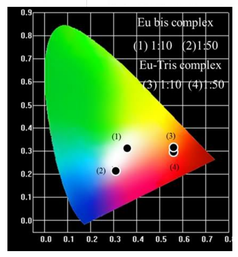




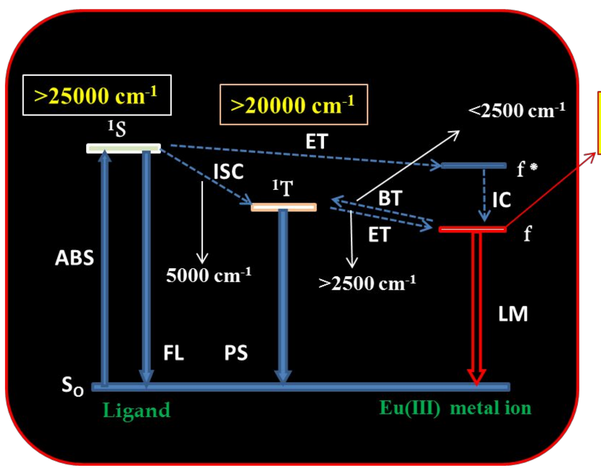
LED emission



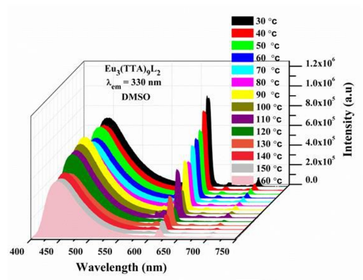


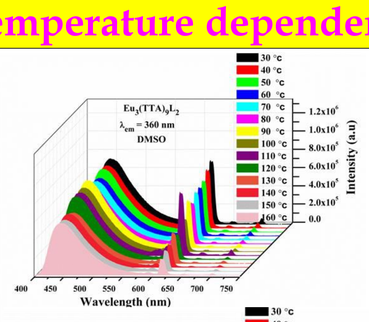


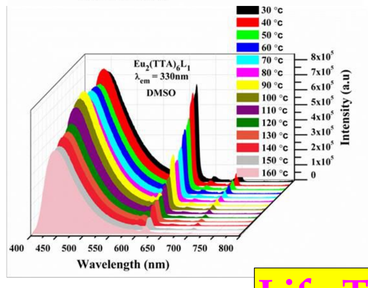
Energy transfer

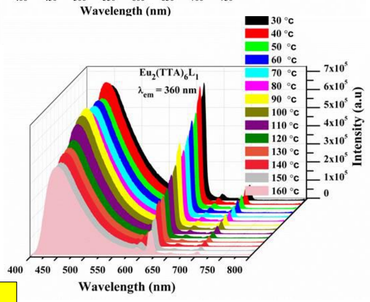


Temperature dependent PL

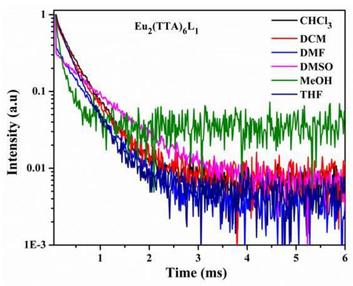


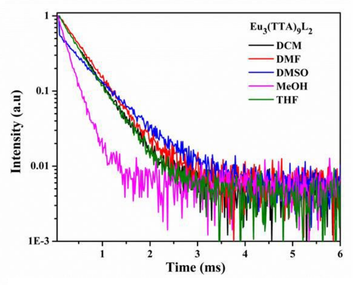




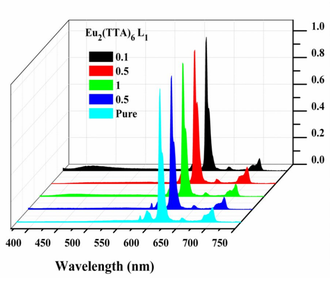


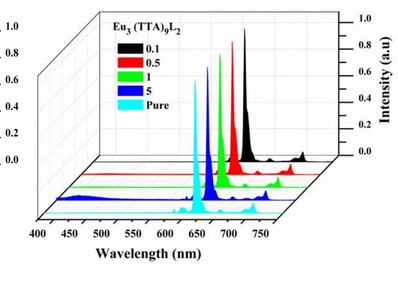
Life Time

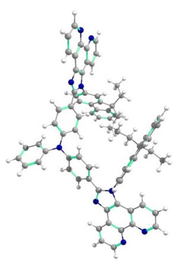


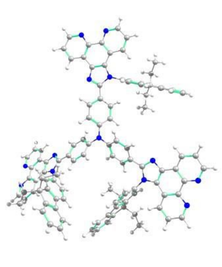


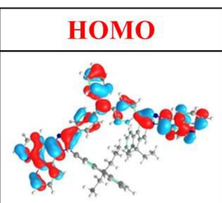
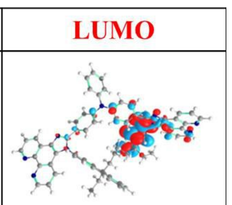
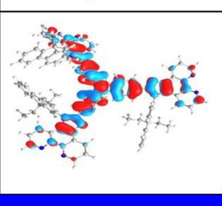
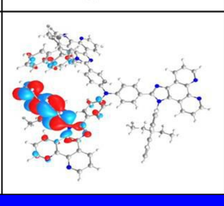
Thin film PL study









	HOMO	LUMO
L_1		
L_2		

Acknowledgements

Conclusions:

- Successfully Designed, Synthesized & characterized the triplet-dopants based on Eu(III) molecular complexes.
- Novel Eu(III) complex with tris-β-diketones have been studied in several solvents. Eu(III) complex acting as a single component white-light-emitting with tunable emission colors by changing the solvent.

References

- Wang, Q.; Ma, D. Management of charges and excitons for highperformance white organic light-emitting diodes. Chem. Soc. Rev. 2010, 39, 2387−2398.
- Rajamouli, B.; Sood, P.; Giri, S.; Krishnan, V.; Sivakumar, V. A dy. Eur. J. Inorg. Chem. 2016,, 3900− 3911