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# **Electronic Supplementary Information**

Terpyridyl-imidazole based europium tris-(β-diketonate) complex as efficient molecular luminescent thermometer and single component white light emitter via synergy in energy transfer between ligand and Eu<sup>3+</sup>

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### **Experimental section**

## Materials

2-theonyltrifluoroacetone (Htta) and europium chloride or nitrate salts were purchased from Merck as their hexa- or pentahydrated forms and used as received. Solvents were dried and distilled following the standard procedure. 4'-(*p*-formylphenyl)-2,2':6',2"-terpyridine (tpy-PhCHO) and 9,10-phenanthrenedione were synthesized by following reported literature method. <sup>S1-S4</sup>

### Instruments and physical methods

UV-vis absorption spectra of the complexes were recorded with a Shimadzu UV 1800 spectrophotometer. Steady-state luminescence spectra were obtained by a Horiba Fluoromax-4 spectrofluorimeter with a photomultiplier tube (PMT). Luminescence lifetime measurements were carried out by using time–correlated single photon counting (TCSPC) as well as multi-channel scaling (MCS) setup from Horiba (Deltaflex) with a TBX Picosecond Photon Detection Module and the luminescence decay data were analyzed by using Eztime software. Spectrophotometric studies were carried out with the compounds with concentrations of ~10<sup>-5</sup> M. The Diffuse Reflectance Spectroscopic (DRS) measurements of the samples were collected from a Shimadzu-3600 UV–Vis-NIR spectrophotometer. Barium sulfate powder was used as the reflectance standard during the DRS measurements.

[Experimental uncertainties are as follows: absorption maxima,  $\pm 2$  nm; molar absorption coefficients, 10%; emission maxima,  $\pm 5$  nm; excited-state lifetimes, 10%; luminescence quantum yields, 10%.]



**Fig. S1** Change in photoluminescence intensity ratio with varying temperature from 273-343K. The dotted line indicates the best-fitted curve.



**Fig. S2** Change in lifetime values with varying temperature from 273-343K. The dotted line indicates the best-fitted curve.

Complex	Sr (%K <sup>-1</sup> )	Temp. range	Ref.
[Eu(tta) <sub>3</sub> (pyphen)]; tta=	1.68 (323 K)	283–323 K	63
thenoyltrifluoroacetone and pyphen=			
pyrazino[2,3-f][1,10]phenanthroline			
Eu(CPDK3-5) <sub>3</sub> phen; CPDK3-5 = $1-(4-(4-$	2.2% to 1.5% K <sup>-1</sup>	298-348 K	64
propylcyclohexyl)			
phenyl)octane-1,3-dione and phen=1,10-			
phenathroline			
Eu(L) <sub>3</sub> ; L= 1,3-di(thienyl)propane-1,3-diones	0.65%	100K < T < 400K	65
Eu-DT; DT= Dinaphthoylmethane (DNM) and	2.2%	298-318 K	66
trioctylphosphine oxide			
[CHOL][Eu(FOD)4]; CHOL=choline and	0.45% C -1 at 25 °C, with	298-368	67
FOD= tetrakis-1,1,1,2,2,3,3-heptafluoro-7,7-	an increase to 7.0		
dimethyloctane-4,6-dionate	% C-1 at 95 °C		

Table S1. Comparative study of some earlier reported lanthanide ( $\beta$ -diketonate) complexes.

Table S2. Solvatochromic emission spectral parameters of Eu(tta)<sub>3</sub>(tpy-HImdzphen) at RT.

Solvents	λ <sub>em</sub> , nm (Ligand-	λ <sub>em</sub> , nm (Eu <sup>3+</sup> -centered)	τ, μs (λem=614	CIE colour coordinates	
	centered)		1111)	x	у
Toluene	433	579, 593, 614, 652	561	0.35	0.17
Chloroform	447	do	381	0.20	0.12
Dichloromethane	443	do	507	0.37	0.21
Acetone	460	do	588	0.18	0.16
Ethyl acetate	444	do	306	0.18	0.10
Dimethylsulfoxide	478	do	641	0.20	0.27
Acetonitrile	465	do	581	0.35	0.26
Ethanol	460	do	318	0.17	0.20
Methanol	490	do	193	0.24	0.33

The intrinsic quantum yield ( $\Phi_{\rm ff}$ ), the energy transfer efficiency of the ligand tpy-HImzphen ( $\eta_{\rm sens}$ ), radiative ( $k_{\rm r}$ ) and non-radiative ( $k_{\rm nr}$ ) rate constants were calculated using the following equations<sup>71</sup>:

$$k_r = A_{MD,0} n^3 \left(\frac{l_{tot}}{l_{MD}}\right)$$
$$\tau_{rad} = \frac{1}{k_r}$$
$$k_{nr} = \frac{1}{\tau_{obs}} - \frac{1}{\tau_{rad}}$$
$$\tau_{obs} = \frac{1}{k_r + k_{nr}}$$
$$\Phi_{ff} = \frac{k_r}{k_r + k_{nr}} = \frac{\tau_{obs}}{\tau_{rad}}$$



Fig. S3 UV-diffuse reflectance spectra (DRS) for the LMCT state.

# **References:**

- S1. K. T. Pott, D.A. Usifer and H. D. Abruna, J. Am. Chem. Soc., 1987, 109, 3961.
- S2. F. H. Case and T. J. Kaspen, J. Am. Chem. Soc., 1956, 78, 5842.
- S3. W. Spahni and G. Helv. Calzaferri, Helv. Chim. Acta, 1984, 67, 450.
- S4. E. C. Constable, M. D. Ward and S. Corr, Inorg. Chim. Acta, 1988, 141, 201.