

SUPPLEMENTARY INFORMATION

White emissive europium complex with CRI 95%: Butterfly Vs triangle structure

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Synthesis:

Every reaction was executed under inert (nitrogen / argon) condition. Solvents (tetrahydrofuran, ethanol, dimethyl sulfoxide, hexane, acetic acid, etc.,) were precisely dried and purify from relevant drying agents before use. 1,10-phenanthroline, triphenylamine, 4,4,4-Trifluoro-1-(2-thienyl)-1,3-butanedione (TTA), europium(III) chloride hexahydrate (99.99%) and tetrabutylammonium perchlorate ($\text{nBu}_4\text{NClO}_4$) electrolyte were used without further purification, were purchased from Sigma-Aldrich chemicals company. All the reactions progress (silica gel 60 F₂₅₄ Aluminium plates, Merk) was observe by thin-layer chromatography (TLC). Column chromatography was performed with the help of silica gel from Aldrich (100-200 mesh).

Measurements:

AV 400 Advance-III 400MHz Fourier Transform nuclear magnetic resonance (FT-NMR) Spectrometer Bruker Biospin International, Switzerland is used for recording ¹H- and ¹³C-NMR spectra, in deuterated chloroform/dimethyl sulfoxide solution. Chemical shifts were cited with respect to tetramethylsilane (TMS, standard reference). The Fourier transform infrared spectroscopy (FTIR) was executed in the spectrum of 400 – 4000 cm⁻¹ making KBr pellets by PerkinElmer Spectrum Version 10.4.00. The PL emission and excitation spectra were supervised by the help of Edinburg Spectrofluorometer FS-5 instruments connected with SC – 10 modules. The corresponding photoluminescence quantum yield was estimated with horiba Jobin Yvon, HR 320 and the total fluorescence quantum yield was estimated with Edinburgh Instruments, spectrofluorometer, FS5, Integrating Sphere SC-30. The calculation of CIE color coordinate obtained from spectral emission data of the phosphors done by MATLAB software and Elementar Analysen Systeme, Germany/Vario EL spectrometer was used to calculate elemental analysis. The absorption spectrum in solution, and thin film were estimated by utilizing UV-Visible spectrometer (Shimadzu Corporation, Japan or UV-2450

Perkin Elmer, USA/Lamda 25 and Lamda Perkin Elmer). The electrochemical properties of the complex and ligand were estimated by utilizing cyclic voltammetry (CV), AUTOLAB 302N Modular potentiostat at RT in dichloromethane. The working (glass-carbon rod), auxiliary (counter, Pt wire) and reference (Ag/AgCl wire) electrodes are the setups of three electrodes were utilized for CV analysis. The dimethylformamide (DMF) which contains 0.1 M Bu_4NClO_4 was utilized as the supporting electrolyte, and the sweep rate was kept up as 100 mV s^{-1} . The ligand sub-atomic structures were optimized within density functional theory (DFT) frame work utilizing B3LYP/6-31G (d, p) level of theory.¹ A UV-visible spectrum of the molecule is obtained by exciting molecule vertically after conformation of ground state geometry for the ligand. Further, to the depiction of PL emission and excitation mechanism of the Eu(III) complex, triplet energized condition of the ligand is additionally accesses by utilizing the same procedure specified previously. The optimization study of ligand is effectively accomplished by the G09W program. The Lifetime of the Eu(III) complex, as well as the ligand, were measured at 298 K with Edinburgh Instruments FLS 980 based on the time-correlated single photon counting technology upon the excitation at 380 nm. A pulsed xenon lamp was used as the excitation source, and the signals were detected with a photomultiplier. All the measurements were carried out at room temperature (RT).

Materials

The TPA-3CHO, as well as Flu- NH_2 were synthesized by the previously reported procedure² and the metal complex tris(thenoyltrifluoroacetone)europium (III) ($\text{Eu}(\text{TTA})_3 \cdot 2\text{H}_2\text{O}$) was synthesized by using the well familiar method.³

General synthesis of ligand:

L₁: TPA-3CHO (1 gram, 1 eq) with glacial acetic acid (50 mL) was taken in round bottom flask at room temperature (RT). To same reaction mixture, later ammonium acetate (18gm, 40eq) and Phen-fl- NH_2 (2.304gm, 3.1eq), after 10 minutes 1, 10-phenanthroline-5, 6-dione

(2.039g, 3.1eq) were added. The subsequent mixture was stirred for overnight at 120°C in inert atmospheric condition. The reaction was checked by thin layer chromatography (TLC) (MeOH: DCM = 1:9) for the completion. After finishing of the reaction, the obtained reaction mass was poured into a minimum amount of ice water and then neutralized by addition of ammonium hydroxide (NH₃OH) solution to the same. The obtained solid was dissolved in dichloromethane (DCM) and dried with anhydrous sodium sulphate (Na₂SO₄). The crude compound 0.3 gm is obtained after evaporation. Further to purify the crude product column chromatography is performed by using (100-200 mesh) silica gel, eluent with 10% methanol in chloroform solvent. The obtained product was dissolved in minimum amount of THF solution added excess of hexane solvent, the pale-yellow color solid was formed is 150 mg.

Yield: 68%. IR m (KBr): ν (C=N) 1598, (C-N) 1293. **¹H-NMR Data (400 MHz, CDCl₃):** δ 9.21 (dd, J = 1.6 Hz, 1H), 9.16 (dd, J =2 Hz, 1H), 9.046 (dd, J = 1.6 Hz, 1H), 7.966 (d, 1H), 7.87-7.85 (m, 1H), 7.78 (dd, J =4 Hz, 1H), 7.61-7.42 (m, 8H), 7.41-7.17 (m, 2H), 7.17- 6.93 (m, 1H), 6.91 (d, J = 1.6 Hz, 2H). **¹³C-NMR (100 MHz, CDCl₃, TMS, δ ppm):** 150.1, 147.90, 139.82, 130.18, 130.13, 129.51, 128.53, 128.53, 128.18, 127.45, 123.61, 123.19, 123.10, 122.98, 122.18, 121.42, 120.53, 77.35, 77.24, 77.03, 76.71, 56.74, 32.86, 32.69, 8.46 . ESI-MS (m/z): 1139.42(M + Na)⁺.

L₂: Same procedure followed as above, only some equivalent is different TPA-2CHO (0.35gm, 1 eq), 1, 10-phenone-dione (0.53gm, 2.2eq), Phen-fl-NH₂ (0.60gm, 2.2eq), NH₄OAc (2.23gm, 25 eq), acetic acid (25 ml) **Yield: 65%. IR ν (KBr):** ν (C=N)1599, (C-N) 1291 **¹H-NMR (400 MHz, CDCl₃, TMS, δ ppm):** 9.12 (d, J =1.6 Hz, 3H), 9.05 (d, J =1.6 Hz, 3H), 8.95 (d, J =1.6 Hz, 3H). 7.84 (d, J =7.6 Hz, 3H), 7.69 (d, J =1.6 Hz, 3H), 7.47-7.31 (m, 27H), 7.14 (d, J =4.4 Hz, 3H), 6.79 (d, J =1.6 Hz, 6H), 1.93-1.77 (m, 4H), 0.33-0.29 (m, 9H), 0.14-0.10 (m, 9H). **¹³C-NMR (100 MHz, CDCl₃, TMS, δ ppm):** 152.54, 151.58, 150.15, 148.98,

147.95, 147.28, 144.80, 144.33, 143.76, 139.79, 136.38, 136.04, 130.51, 130.22, 130.09, 128.52, 128.03, 127.44, 127.39, 127.01, 124.84, 123.89, 123.80, 123.53, 123.17, 123.09, 122.01, 121.39, 120.56, 119.85, 56.69, 32.68, 8.46. ESI-MS (m/z): 1162(M)⁺.

Synthesis of Eu(TTA)₃L1: Taken a 25 mL two neck round bottom flask with nitrogen balloon with adaptor and poured Eu(TTA)₃.2H₂O (0.152 g, 0.178 mmol, 2 eq) dissolved in dry tetrahydrofuran (THF) (10 mL). The mixture of ligand (L1) (0.100 g, 0.089 mmol, 1eq) in THF (5 mL) was added to the reaction mixture (RM) then stirred for 6 h at 60 °C. The resulting product was concentrated and dissolved in a minimum amount of THF. Then added the excess of hexane to get the solid product which is pale yellow, yield 0.112 g (70.2%). **IR v (KBr):** v (C=O) 1675, (C=N) 1537, (C-N) 1296, (C-F) 1300. Anal. Calcd. for C₁₂₆H₈₃Eu₂F₁₈N₉O₁₂S₆: C, 54.96; H, 3.04; N, 4.58; ; Found: C, 54.08; H, 3.39; N, 4.19;

Synthesis of Eu(TTA)₃L2 : Taken a 25 mL two neck round bottom flask with nitrogen balloon with adaptor and poured Eu(TTA)₃.2H₂O (0.163 g, 0.192 mmol, 3 eq) dissolved in dry tetrahydrofuran (THF) (10 mL). The mixture of ligand (L2) (0.100 g, 0.0641 mmol, 1eq) in THF (5 mL) was added to the reaction mixture (RM) then stirred for 6 h at 60 °C. The resulting product was concentrated and dissolved in a minimum amount of THF. Then added the excess of hexane to get the solid product which is pale yellow, yield 0.112 g (70.2%) **IR v (KBr):** v (C=O) 1695, (C=N) 1542, (C-N) 1290, (C-F) 1305. Anal. Calcd. for C₁₈₂H₁₁₇Eu₃F₂₇N₁₃O₁₈S₉: C, 53.95; H, 2.94; N, 4.54; Found: C, 52.19; H, 2.90; N, 5.10

1. NMR Spectroscopy:

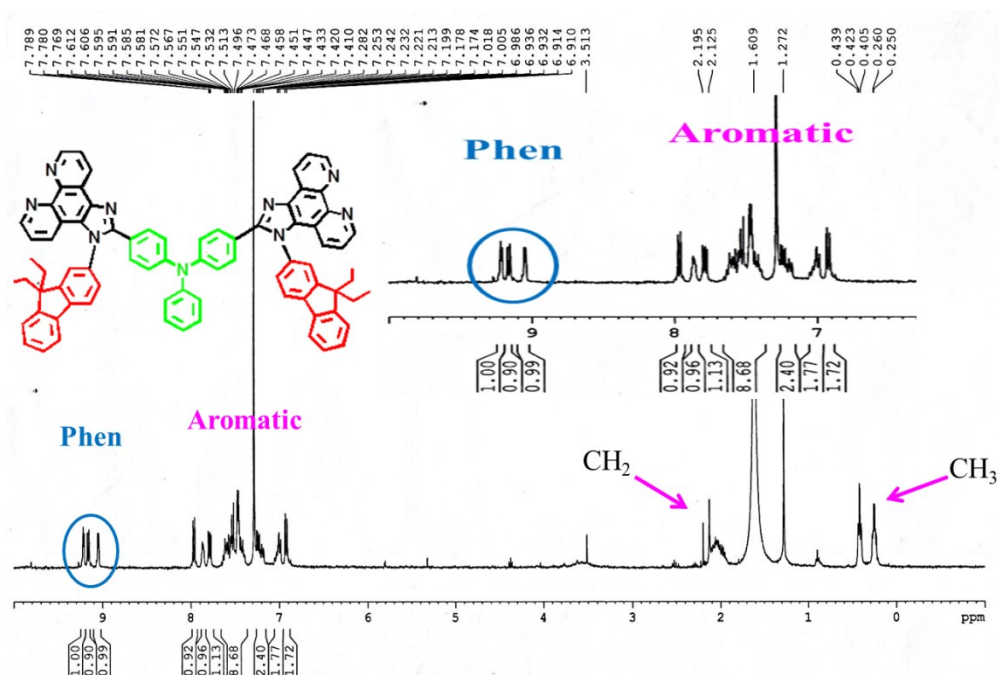


Fig. S1 ^1H -NMR spectra (full) of L1.

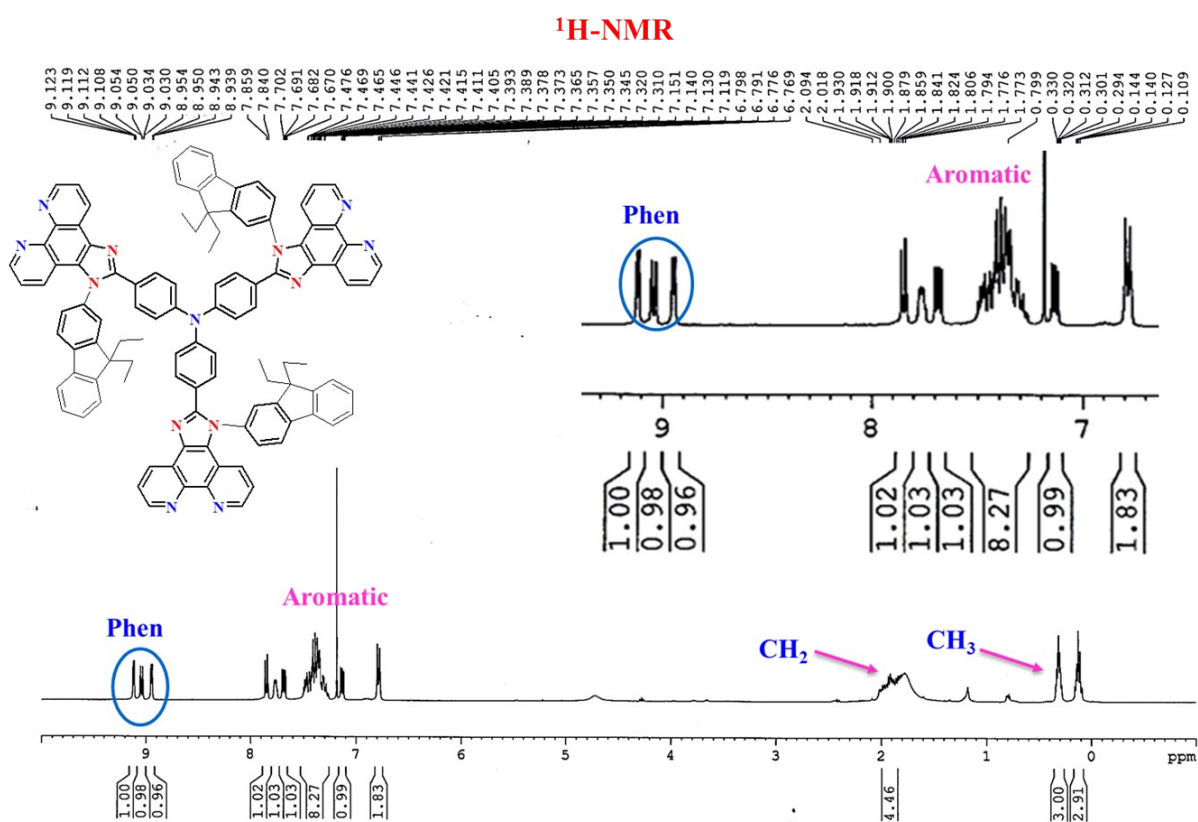


Fig. S2 ^1H -NMR spectra (Full) of L2.

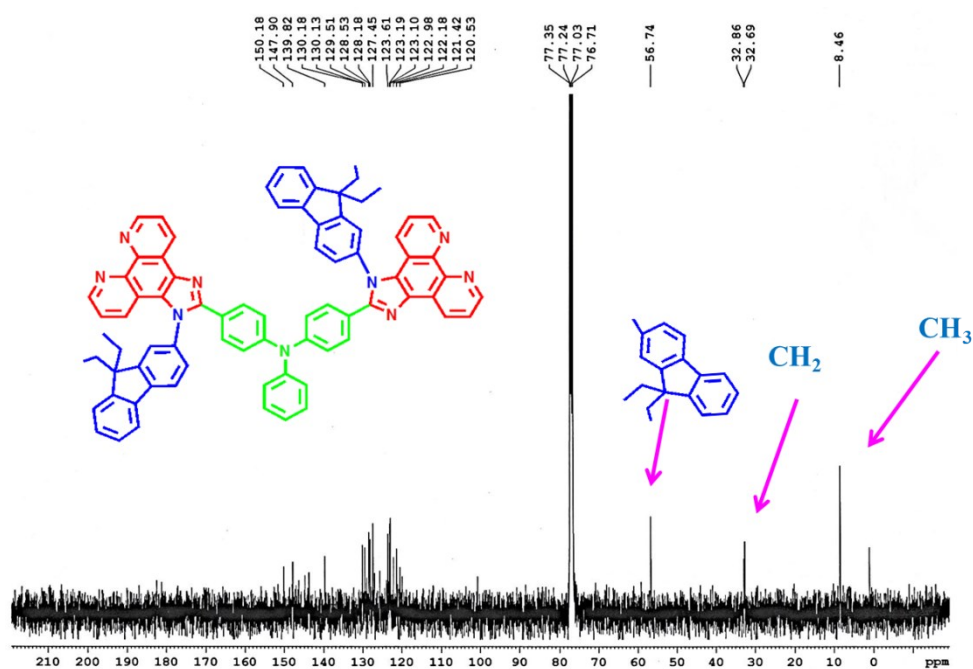


Fig. S3 ^{13}C -NMR spectra of L1.

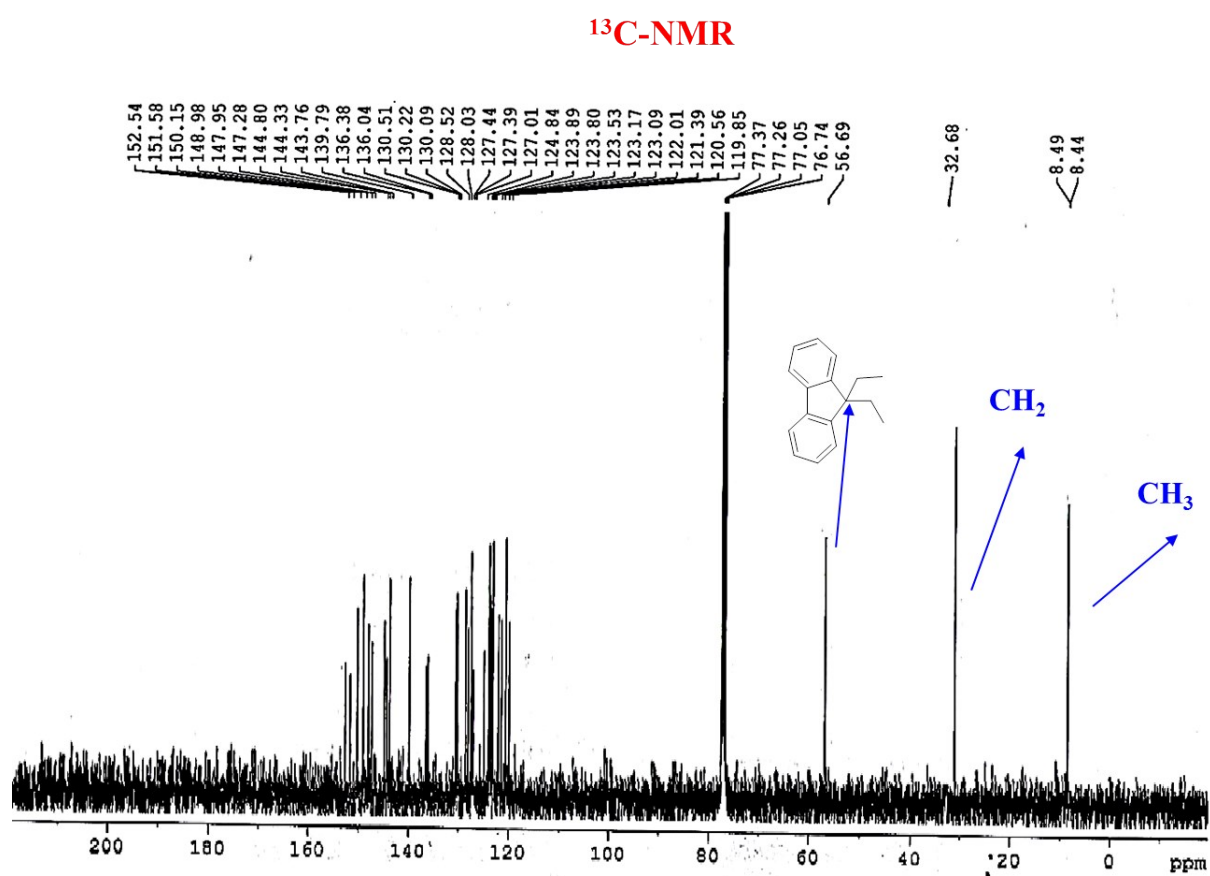


Fig. S4 ^{13}C -NMR spectra of L2.

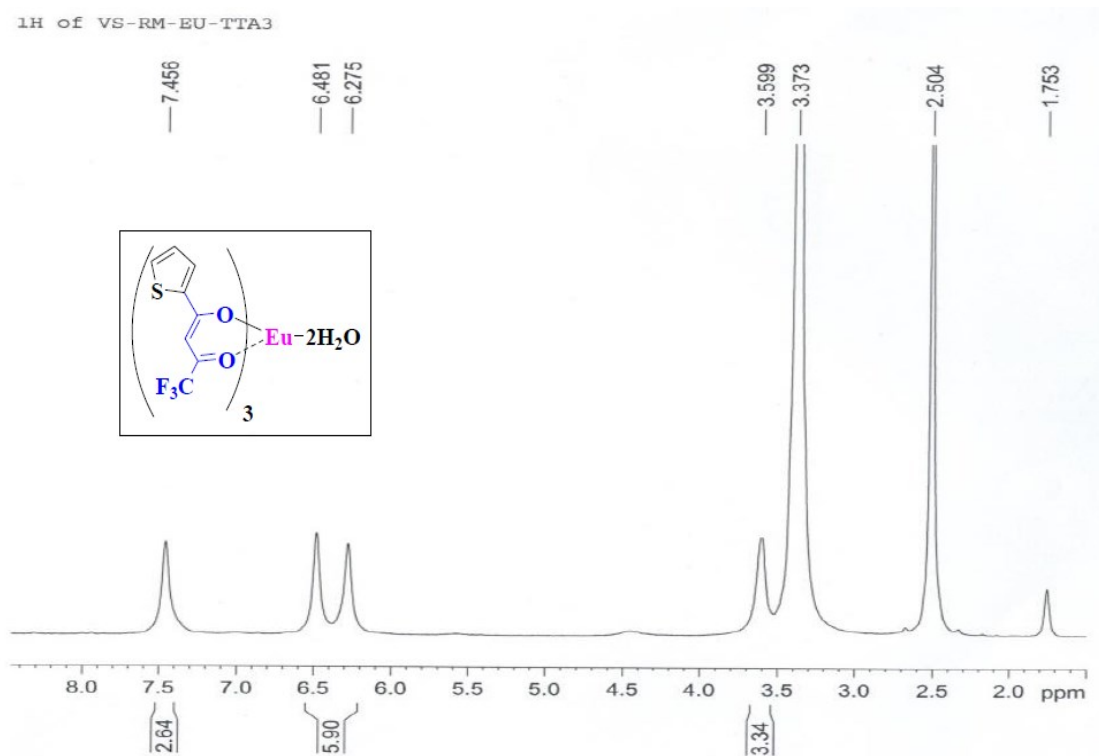


Fig. S5 The ¹H-NMR spectra of the $\text{Eu}(\text{TTA})_3 \cdot 2\text{H}_2\text{O}$

2. Mass spectral analysis:

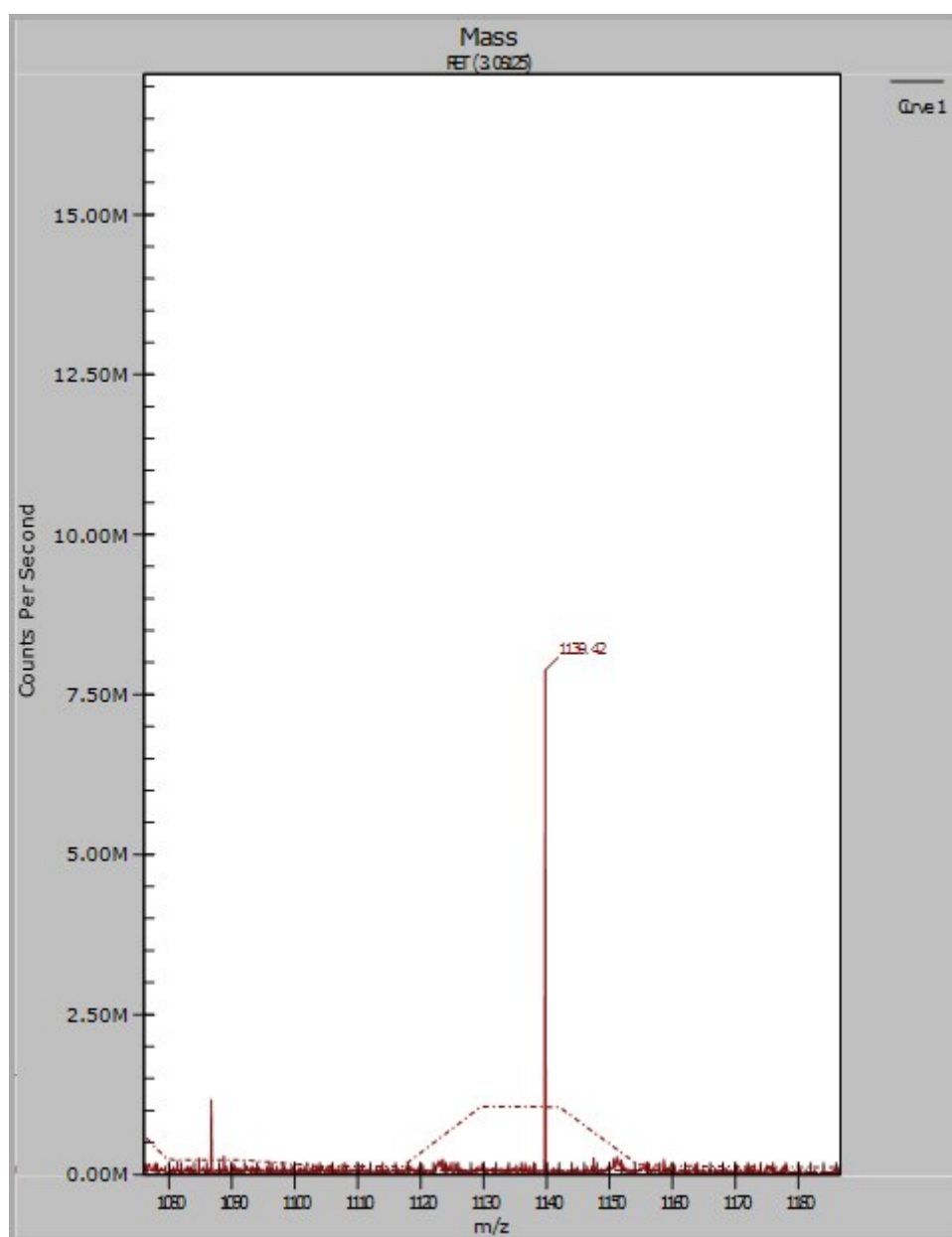


Fig. S6 Mass spectral data of L1

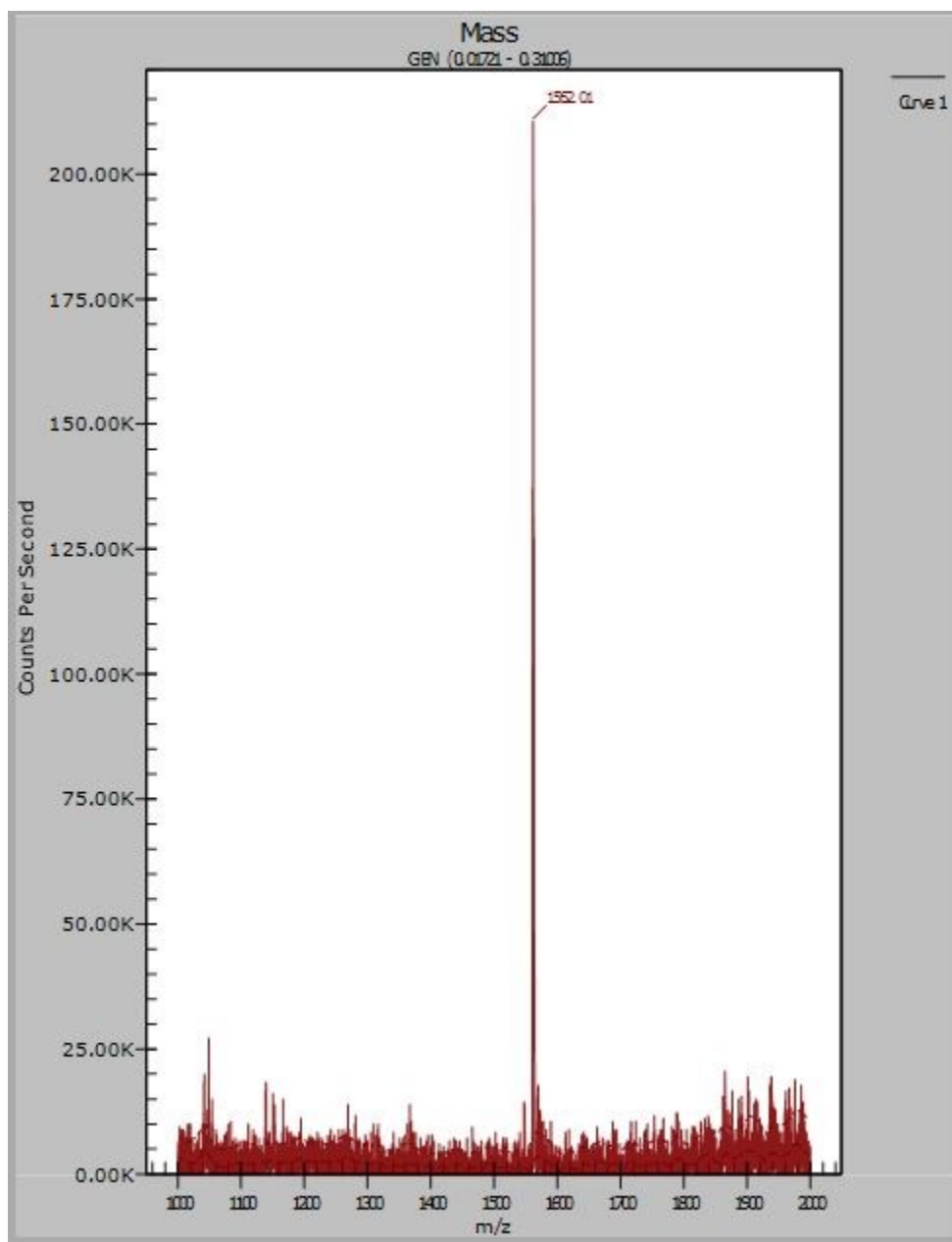


Fig. S7 Mass spectral data of L2.

Table ST1. The calculated CIE from the PL emission data of Eu(III) complexes in different solvents and corresponding asymmetric ratio.

Solvent	Eu ₂ (TTA) ₆ L1			Eu ₃ (TTA) ₉ L2		
	Asym. ratio	CIE		Asym. ratio	CIE	
		x	y		x	y
Acetone	10.15	0.26279	0.18716	23.809	0.53995	0.27127
DMSO	6.07	0.25188	0.18906	8.560	0.25689	0.16031
DMF	7.47	0.18780	0.13477	15.9494	0.29671	0.1614

MeOH	7.26	0.4326	0.26706	15.59	0.58771	0.30324
EtOAc	3.38	0.20956	0.12821	20.339	0.54692	0.2689
CHCl ₃	5.537	0.20067	0.10690	20.111	0.55774	0.27477
DCM	-	0.16456	0.09540	23.52	0.57994	0.29085
THF	7.36	0.21567	0.11168	24.2442	0.38908	0.17941
ACN	10.47	0.3009	0.2001	25.653	0.56714	0.28796
Ethanol	5.31	0.23532	0.12775	13.499	0.22513	0.09904

Judd–Ofelt analyses:

The Judd-Ofelt parameter (J-O) is the powerful tool to analyze the chemical environment around europium ion, which is determined from the emission spectrum. The J–O intensity parameters, Ω_J ($J = 2, 4$) provide an insight into the local structure and bonding in the vicinity of rare earth ions. So the Judd–Ofelt analysis can be used for calculating the parity-forbidden electric-dipole radiative transition rates between the various levels of the rare earth ions. In the standard Judd-Ofelt hypothesis of 4f-4f intensities, Ω_λ intensity parameters contain the involvement of the electric dipole and the dynamic coupling mechanism. The $^5D_0 \rightarrow ^7F_1$ transition is used as a reference for the estimation of the J–O intensity parameters. The experimental intensity parameters (Ω_2 and Ω_4) for the typical Eu(III) complex were determined for the $^5D_0 \rightarrow ^7F_2$ and $^5D_0 \rightarrow ^7F_4$ electronic transitions. The Ω_2 and Ω_4 values are $3.2 \times 10^{-20} \text{ cm}^2$, $6.5 \times 10^{-21} \text{ cm}^2$ for the complex 1 and $19 \times 10^{-20} \text{ cm}^2$ and $9.5 \times 10^{-21} \text{ cm}^2$ for the complex 2, respectively. The observed higher value of Ω_2 is responsible for asymmetric and covalent nature of ligand field environment around Eu(III) ion. The $^5D_0 \rightarrow ^7F_6$ transition is not observed experimentally; thus, the experimental Ω_6 parameter cannot be determined. The spontaneous emission probabilities $A_{0\lambda}$ ($\lambda = 2, 4$) of the transitions were related to their dipole strength to afford Equation (3).

$$A_{o\lambda} = 64\pi^4\nu^3/3h(2J + 1) \frac{n(n^2 + 2)^2}{9} S(ed) + S(md) \dots\dots\dots(3)$$

Here, $A_{o\lambda}$ is the coefficient of spontaneous emission for the $^5D_0 \rightarrow ^7F_J$ transition, ν is the average transition energy in cm^{-1} , h is the Planck constant, $2J + 1$ is the degeneracy of the initial state, and $S(ED)$ and $S(MD)$ are the ED and MD strengths, respectively. In this way, keeping in mind the end goal to examine the possible structural changes around the Eu^{III} ion, the powers parameters Ω_2 and Ω_4 were figured from the emission spectra (Fig. 3) utilizing the $^5D_0 \rightarrow ^7F_2$ and $^5D_0 \rightarrow ^7F_4$ as per equation. The Ω_2 and Ω_4 intensity parameters for both complexes were shown in Table 3, which can be calculated by the following equation (4).

$$\Omega_\lambda = \frac{3hc^3 A_{o-\lambda}}{4e^2 \omega^3 \chi < ^5D_0 || U(\lambda) || ^7F_J >^2} \dots\dots\dots(4)$$

Here, e is the electronic charge, $^7F_J || U^\lambda || ^5D_0^2$ ($\lambda = 2, 4$) are the square reduced matrix elements with values of 0.0032, 0.0023 for $J = 2$ and 4, respectively, and χ is the Lorentz local-field correction term given by $\chi = n(n^2 + 2)^2/9$; n is the refractive index of the medium ($n = 1.5$). Table ST3. shows Radiative and non-radiative properties, internal quantum efficiency, and branching ratios of the complexes

Table ST2. Radiative and non-radiative Properties, Internal Quantum Efficiency, and Branching Ratios of the Complexes

Complexes	A_{rad} (s^{-1})	τ_{rad} (ms)	A_{nr} (ms)	η_{Ln} (%)	$\eta_{\text{sen}}(\%$)	η overall	β_1	β_2	β_4
Eu₂(TTA)₆L1	344.033	2.90669	0.7871	94.0	78.4	0.7%	14.533	77.890	7.576
Eu₃(TTA)₉L2	1219.68	0.81989	0.885	70.6	50.7	10.2%	4.099	92.810	3.089

Table ST3. Intensity Ratios as Well as CIE Color Coordinates for the Eu(III) Complexes in Different Concentration Ratio Doped PMMA

Characterization	I_2/I_1 (% of Eu ^{III})	CIE	
		x	y
Eu₂(TTA)₆L₁	10.76 (Pure)	0.571 (Pure)	0.348 (Pure)
	14.19 (0.1)	0.490 (0.1)	0.286 (0.1)
	11.64 (0.5)	0.586 (0.5)	0.333 (0.5)
	13.95 (1)	0.534 (1)	0.313 (1)
	14.23 (5)	0.575 (5)	0.333 (5)
Eu₃(TTA)₉L₂	22.07 (Pure)	0.632 (Pure)	0.333 (Pure)
	24.15 (0.1)	0.662 (0.1)	0.333 (0.1)
	25.39 (0.5)	0.618 (0.5)	0.318 (0.5)
	25.49 (1)	0.630 (1)	0.323 (1)
	23.09 (5)	0.499 (5)	0.279 (5)

DFT Analysis:

Table ST4. The computed vertical transitions and there oscillator strengths (*f*) and configuration of the L1 and L2 ligand.

Luminophores	State	Energy (eV)	$\lambda_{\max}$ nm	<i>f</i>	Configuration
L1 Singlet	Gas	3.044	407.2	0.5024	HOMO→LUMO (60.16%) HOMO→LUMO+1 (25.56%)
		3.0976	400.2	0.042	HOMO-1→LUMO (63.57%)
		3.149	393.6	0.5102	HOMO→LUMO (20.35%) HOMO→LUMO+1(12.83%) HOMO→LUMO+1(65.00%)

Triplet	Gas	2.491	497.6	0	HOMO-1→LUMO+3 (12.83%) HOMO-1→LUMO+5(15.62%) HOMO→LUMO+2(51.05%)
		2.669	464.3	0	HOMO-1→LUMO+2 (27.20%) HOMO-1→LUMO+5 (11.10%) HOMO→LUMO+4 (29.20%) HOMO→LUMO+5 (35.44%) HOMO→LUMO+9 (11.81%)
		2.9413	421.5	0	HOMO-2→LUMO (10.75%) HOMO-1→LUMO+3 (23.83%) HOMO-1→LUMO+5 (10.92%) HOMO-1→LUMO+7 (10.92%) HOMO→LUMO+6 (21.43%) HOMO→LUMO+8 (29.23%)
L2 Singlet	Gas	2.882	430.1	0.048	HOMO-2→LUMO (10.99%) HOMO-1→LUMO+3 (68.92%)
		2.932	422.8	0.0254	HOMO-1→LUMO+3 (68.64%)
		3.006	412.4	0.763	HOMO-2→LUMO (59.05%) HOMO→LUMO+2 (13.11%)
Triplet	Gas	2.44	506.7	0	HOMO-1→LUMO+3 (14.92%) HOMO-1→LUMO+3 (50.21%)
		2.52	490.8	0	HOMO-1→LUMO+4 (12.02%) HOMO-1→LUMO+8(10.03%) HOMO→LUMO+8(40.81%)
		2.72	455.4	0	HOMO-2→LUMO (11.45%) HOMO-2→LUMO+3 (24.87%) HOMO-1→LUMO+4 (15.61%) HOMO→LUMO (10.33%) HOMO→LUMO+7(12.49%) HOMO→LUMO+5 (30.96%)

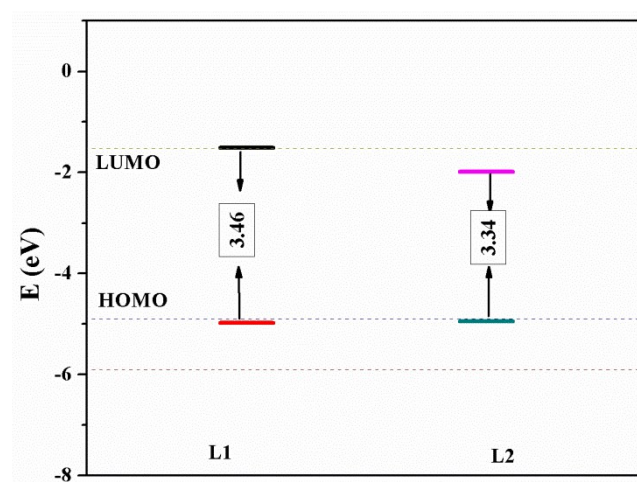


Fig. S8 Band gap calculation by HOMO-LUMO of L1 and L2 by TD-DFT calculation.

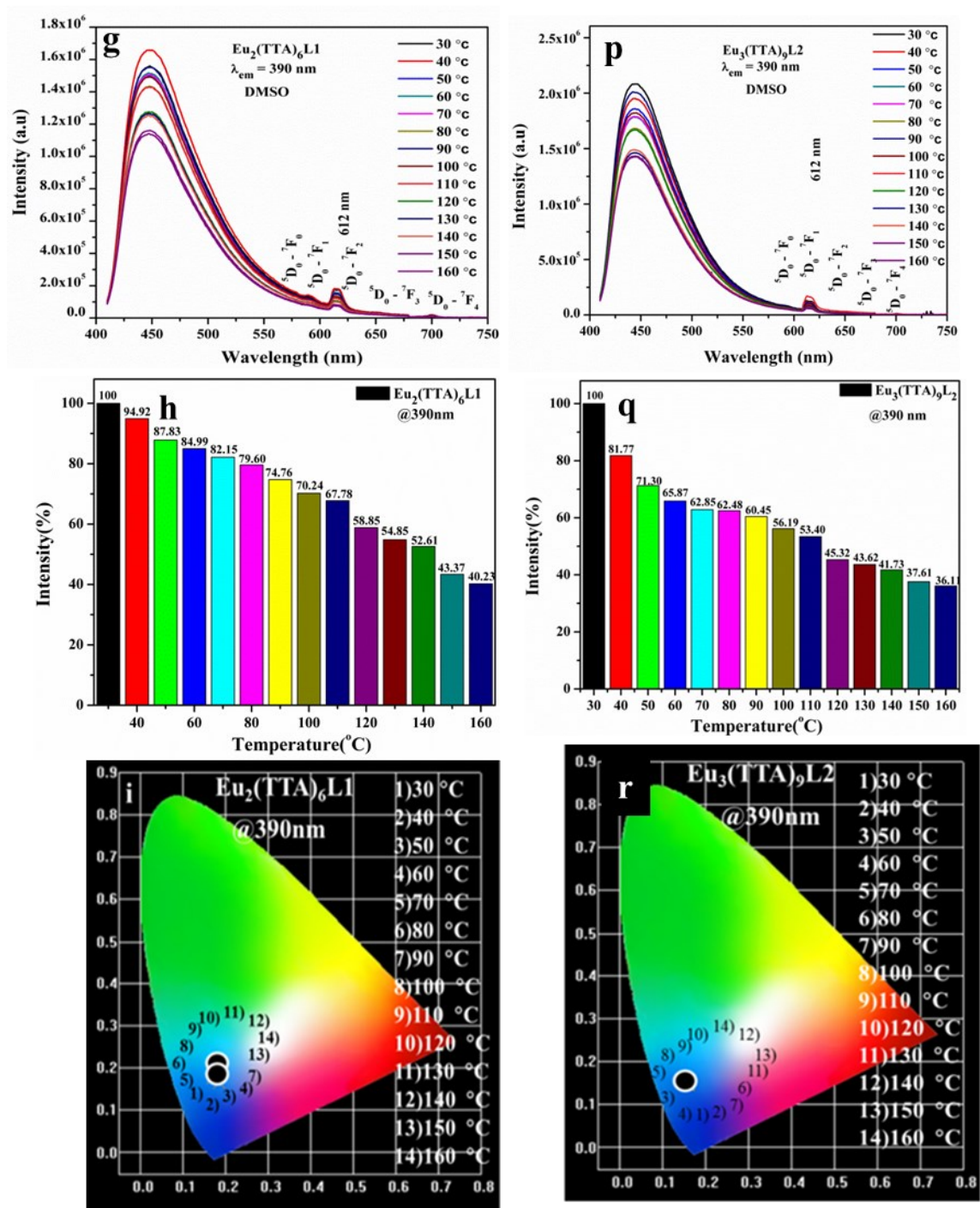


Fig. S9 Temperature dependent emission spectra of $\text{Eu}_2(\text{TTA})_6\text{L1}$ and $\text{Eu}_3(\text{TTA})_9\text{L2}$ in DMSO solvent (at 390nm) and bar graph as well as their CIE respectively

Table ST5. Cartesian coordinates for optimized geometry of L1

6	3.7620080	-3.2065650	-0.0577220
6	2.5647780	-3.8740900	0.1479160
6	1.5983040	-3.3546100	1.0263800

6	1.8788680	-2.1509760	1.6895750
6	3.0803040	-1.4812780	1.4782410
6	4.0495110	-1.9901160	0.5950270
1	4.5017010	-3.6111440	-0.7384480
1	2.3659120	-4.8025320	-0.3766670
1	1.1551110	-1.7468370	2.3893500
1	3.2635190	-0.5748310	2.0384650
6	-0.6324980	-7.61859400	1.0151300
6	0.3637540	-8.2367860	1.7732550
6	1.3629050	-7.4543380	2.3550290
6	1.3647510	-6.0706140	2.1924180
6	0.3689840	-5.4480060	1.4232720
6	-0.6290170	-6.2376240	0.8305370
1	-1.4121160	-8.2152190	0.5502470
1	0.3615230	-9.3138350	1.9085100
1	2.1408750	-7.9201520	2.9529550
1	2.1353000	-5.4660590	2.6585480
1	-1.3967530	-5.7638590	0.2281410
6	-0.8425690	-3.3077640	1.2961650
6	-1.8210910	-3.6041940	2.2605930
6	-3.0141110	-2.8961300	2.2949920
6	-3.2793580	-1.8665990	1.3730730
6	-2.2903320	-1.5638070	0.4225860
6	-1.0955270	-2.2740520	0.3804820
1	-1.6375400	-4.3934700	2.9814850
1	-3.7580020	-3.1184310	3.0517620
1	-2.4469340	-0.7652800	-0.2919130
1	-0.3477630	-2.0278250	-0.3655680
7	0.3733680	-4.0357210	1.2455670
6	-8.1217690	0.4813070	5.5794770

6	-7.1385130	-0.0095910	4.7441540
6	-7.2594150	0.2029430	3.3579230
6	-8.3910430	0.9112860	2.8734080
6	-9.2034740	1.1762230	5.0043650
6	-6.2877350	-0.2570620	2.4091850
6	-8.5550440	1.1305360	1.4280300
6	-7.5738230	0.6527950	0.4956920
6	-6.4258300	-0.0132010	1.0469970
6	-7.8350270	0.8547100	-0.8775490
1	-7.1449560	0.4848040	-1.6240860
6	-8.9848740	1.5146010	-1.2649550
6	-9.8664720	1.9675040	-0.2702980
1	-8.0709250	0.3426120	6.6549480
1	-6.2760870	-0.5499540	5.1204900
1	-9.9904380	1.5766180	5.6425380
1	-9.2072670	1.6780830	-2.3148050
1	-10.7768390	2.4986230	-0.5453240
7	-5.2870640	-0.5759070	0.4653030
7	-5.1388230	-0.9516970	2.6772200
7	-9.6667100	1.7793970	1.0250020
7	-9.3439930	1.3884590	3.7044270
6	-4.5487610	-1.1364550	1.5093020
6	-3.7243330	-1.0615110	-7.4039910
6	-3.2270580	0.2364840	-7.5611320
6	-3.1517630	1.1084390	-6.4687910
6	-3.5789400	0.6689200	-5.2200190
6	-4.0787670	-0.6392010	-5.0647210
6	-4.1540290	-1.5098530	-6.1537790
1	-3.7762120	-1.7254770	-8.2616660
1	-2.8965580	0.5708310	-8.5400740

1	-2.7637210	2.1147000	-6.6032000
1	-4.5392860	-2.5187990	-6.0361820
6	-3.5885280	1.4231030	-3.8907950
6	-4.1856730	0.3677410	-2.9590190
6	-4.4554010	0.4589260	-1.5993080
6	-4.9916150	-0.6562480	-0.9367060
6	-5.2494530	-1.8453400	-1.6263250
6	-4.9800380	-1.9369980	-2.9925880
6	-4.4513000	-0.8292860	-3.6575430
1	-4.2645820	1.3689770	-1.0375450
1	-5.6648280	-2.6892310	-1.0857460
1	-5.1847150	-2.8618280	-3.5235050
6	-2.1497570	1.8268070	-3.4488710
1	-2.2238910	2.3190700	-2.4704080
6	-4.4550250	2.7141130	-3.9527790
1	-4.4240210	3.1900540	-2.9641980
6	10.2898720	-2.8986620	-2.0053220
6	9.0258840	-2.7310590	-1.4763940
6	8.6691460	-1.4711030	-0.9603960
6	9.6243560	-0.4213380	-1.0047590
6	11.1674380	-1.7970630	-2.0038480
6	7.3826550	-1.1952560	-0.3900330
6	9.2788550	0.9081520	-0.4777420
6	7.9852370	1.1616440	0.0910370
6	7.0641080	0.0583000	0.1209500
6	7.7313670	2.4699900	0.5601380
1	6.7727080	2.7190400	0.9947310
6	8.7162400	3.4336400	0.4648000
6	9.9506790	3.0789080	-0.1022480
1	10.6098620	-3.8521140	-2.4139650

1	8.3007100	-3.5375770	-1.4444550
1	12.1707830	-1.9035850	-2.4147620
1	8.5429690	4.4446970	0.8198790
1	10.7468930	3.8172490	-0.1882780
7	5.7520200	-0.0668910	0.5830410
7	6.3342790	-2.0623750	-0.2655590
7	10.2245030	1.8663640	-0.5580450
7	10.8583600	-0.6010420	-1.5256730
6	5.3593480	-1.3808050	0.3154050
6	1.4172110	5.8495750	3.8658000
6	0.7265980	6.2178760	2.7063810
6	0.9535200	5.5491050	1.4979110
6	1.8768160	4.5094460	1.4616840
6	2.5714980	4.1413450	2.6310740
6	2.3461010	4.8079390	3.8370720
1	1.2286320	6.3781810	4.7953560
1	0.0070660	7.0303600	2.7445800
1	0.4109080	5.8444080	0.6036990
1	2.8803010	4.5250690	4.7397720
6	2.2901190	3.6354450	0.2781900
6	3.3256150	2.7243040	0.9341530
6	4.0726200	1.7039690	0.3588470
6	4.9648660	0.9824980	1.1630490
6	5.1113400	1.2805110	2.5235630
6	4.3654580	2.3087440	3.1003570
6	3.4721170	3.0293430	2.3034720
1	3.9826660	1.4510340	-0.6932820
1	5.8121570	0.7028430	3.1174480
1	4.4830730	2.5373970	4.1553480
6	1.0880330	2.8227220	-0.2893040

1	1.4596980	2.2126230	-1.1229570
6	2.9023710	4.4730510	-0.8827250
1	3.1853280	3.7802710	-1.6857340
1	0.3819220	3.5388160	-0.7293570
1	2.1035820	5.1024890	-1.2954870
6	4.1037600	5.3493810	-0.5185980
1	4.9468630	4.7492320	-0.1633060
1	4.4437660	5.9095140	-1.3952080
1	3.8503940	6.0716640	0.2627220
6	0.3509200	1.9274400	0.7099870
1	-0.0627830	2.5068830	1.5403240
1	-0.4791020	1.4103270	0.2184680
1	1.0107970	1.1613160	1.1271520
1	-3.9610120	3.4135230	-4.6391630
1	-1.7891770	2.5939180	-4.1459290
6	-5.9115790	2.5272580	-4.3843490
1	-6.4557870	1.8785850	-3.6916280
1	-6.4265090	3.4926250	-4.4067920
1	-5.9805580	2.0867790	-5.3831230
6	-1.1261300	0.6903530	-3.3746250
1	-0.9730490	0.2240140	-4.3519180
1	-0.1594360	1.0724400	-3.0317240
1	-1.4416200	-0.0929560	-2.6785430

Table ST6. Cartesian coordinates for optimized geometry of L2

6	-1.1717330	2.7341640	1.1627400
6	-1.3336540	1.3577480	1.0940480
6	-0.6045340	0.5969720	0.1626180
6	0.2872690	1.264570	-0.6921560
6	0.4602210	2.6408970	-0.6047070
6	-0.2613200	3.4058910	0.3264640

1	-1.7435500	3.3139660	1.8786920
1	-2.0255250	0.8614920	1.7656020
1	0.8377820	0.7009390	-1.4370920
1	1.1375080	3.1222200	-1.2987310
7	-0.7720810	-0.8081100	0.0828510
6	-2.0621210	-1.3826300	0.2439420
6	-2.2326210	-2.5595240	0.9922630
6	-3.1904790	-0.7956230	-0.3462630
6	-3.4904970	-3.1238130	1.1406410
1	-1.3718300	-3.0259420	1.4592270
6	-4.4528950	-1.3571180	-0.1838090
1	-3.0756560	0.1016860	-0.9447010
6	-4.6327670	-2.5327290	0.5650070
1	-3.6157020	-4.0340840	1.7153480
1	-5.2921890	-0.8843360	-0.6759640
6	0.3389250	-1.6477890	-0.1936980
6	0.2151330	-2.7392400	-1.0708680
6	1.5877530	-1.4115740	0.3981470
6	1.3012740	-3.5569140	-1.3381350
1	-0.7390980	-2.9394970	-1.5459200
6	2.6804910	-2.2256940	0.1158260
1	1.7050130	-0.5808230	1.0854670
6	2.5654490	-3.3226800	-0.7572450
1	1.1977320	-4.3933810	-2.0186320
1	3.6185790	-1.9958630	0.5994710
6	9.3263930	-5.6861920	-0.7719270
6	8.0673180	-5.1236560	-0.6934460
6	6.9797100	-5.7504540	-1.3419810
6	7.2572240	-6.9541570	-2.0736530
6	9.4868890	-6.8749180	-1.5017000

6	5.6183290	-5.2895620	-1.3479860
6	6.1900970	-7.6571000	-2.8029110
6	4.8662980	-7.1435500	-2.7906170
6	4.6098650	-5.9453750	-2.0451790
6	3.8675940	-7.8334140	-3.5030300
1	2.8537880	-7.4467870	-3.4970320
6	4.2122470	-8.9827660	-4.1855070
6	5.5521680	-9.4138650	-4.1364620
1	10.1764430	-5.2205590	-0.2830630
1	7.9199750	-4.2035910	-0.1440150
1	10.4671100	-7.3439270	-1.5769470
1	3.4761290	-9.5483050	-4.7482240
1	5.8494730	-10.3186280	-4.6654820
6	3.6424530	-4.2575060	-1.1238520
7	3.4131600	-5.3045680	-1.9018140
6	-11.7531490	-2.7833420	1.1319630
6	-10.3910720	-2.6056010	0.9874560
6	-9.5250270	-3.7150210	1.1065520
6	-10.1220870	-4.9858380	1.4041060
6	-12.2373590	-4.0747120	1.3958910
6	-8.0933780	-3.6853620	0.9816160
6	-9.2898420	-6.1835850	1.5974040
6	-7.8761550	-6.0861160	1.5037730
6	-7.3020200	-4.8084400	1.1968900
6	-7.1041280	-7.2448290	1.7094560
1	-6.0235070	-7.1770180	1.6385680
6	-7.7500130	-8.4317690	1.9914480
6	-9.1567920	-8.4285620	2.0595290
1	-12.4371080	-1.9446900	1.0473900
1	-9.9907170	-1.6193350	0.7946020

1	-13.3072290	-4.2468920	1.5063750
1	-7.1967750	-9.3510680	2.1564090
1	-9.6902650	-9.3530110	2.2778550
6	-5.9151880	-3.2256100	0.7618990
7	-5.9739290	-4.5120970	1.0649710
6	3.3122270	9.5805660	0.2103640
6	2.7319040	8.3273740	0.1971970
6	1.3488390	8.1950070	0.4504500
6	0.6145320	9.3953850	0.7330800
6	2.4997720	10.6938720	0.4795850
6	0.6093730	6.9629820	0.4679760
6	-0.8224300	9.3443170	1.0432170
6	-1.4955610	8.0941300	1.0759440
6	-0.7430240	6.9085340	0.7871050
6	-2.8683330	8.0742620	1.3863680
1	-3.3880190	7.1220400	1.4115830
6	-3.5079800	9.2696410	1.6458030
6	-2.7550710	10.4585700	1.5862930
1	4.3735140	9.7060230	0.0198960
1	3.3367020	7.4519410	0.0014300
1	2.9285160	11.6951070	0.4911970
1	-4.5653530	9.3040820	1.8892590
1	-3.2371120	11.4151720	1.7848970
6	-0.1737200	4.8688390	0.4377560
7	-1.2082010	5.6205970	0.7706770
6	2.3022680	5.1428390	-0.0066390
6	2.8286480	5.1509530	-1.3072050
6	3.05557400	4.6639440	1.0702540
6	4.1156380	4.6704940	-1.5143870
1	2.2202180	5.5286320	-2.1240320

6	4.3511440	4.1883910	0.8646610
1	2.6189980	4.6711890	2.0633890
6	4.8921900	4.5451420	-2.8249090
6	4.8792490	4.1947720	-0.4274170
1	4.9317120	3.8190020	1.7046400
6	6.2115220	3.9544790	-2.3288900
6	6.1862860	3.7592600	-0.9337870
6	7.3451940	3.6138550	-3.0602190
6	7.2940490	3.2336300	-0.2650720
6	8.4545790	3.0830490	-2.3922490
1	7.3779360	3.7566260	-4.1370720
6	8.4297430	2.8974740	-1.0053980
1	7.2785780	3.0939000	0.8123320
1	9.3447530	2.8171070	-2.9544310
1	9.3045450	2.4961250	-0.5017780
6	-7.5259450	-1.2958950	0.4002560
6	-7.9583230	-0.9517180	-0.8899570
6	-7.4267270	-0.3304060	1.4071620
6	-8.28918800	0.3705230	-1.1573330
1	-8.0258640	-1.7236550	-1.6511100
6	-7.7576040	0.9986880	1.1384700
1	-7.09204800	-0.6300240	2.3947030
6	-8.7728360	0.9907110	-2.4679460
6	-8.1896320	1.3467800	-0.1428190
1	-7.6782290	1.7451290	1.9230860
6	-8.9412010	2.4525910	-2.0555920
6	-8.5964290	2.6414400	-0.7024880
6	-9.3652790	3.5320280	-2.8237750
6	-8.6724200	3.9055190	-0.1143240
6	-9.4420000	4.7995520	-2.2350290

1	-9.6348000	3.4013070	-3.8684940
6	-9.0980160	4.9839200	-0.8916630
1	-8.4053230	4.0530320	0.9283180
1	-9.7712800	5.6484110	-2.8269390
1	-9.1622380	5.9741690	-0.4507660
6	5.6234500	-3.2474350	0.1182830
6	5.7115720	-3.52437500	1.4900440
6	6.1620420	-2.0718280	-0.4166660
6	6.3446310	-2.6082420	2.3202270
1	5.28372500	-4.4457800	1.8737180
6	6.7989480	-1.1504730	0.4159790
1	6.0752940	-1.8894010	-1.4826600
6	6.5631750	-2.6777820	3.8307780
6	6.8908720	-1.4228620	1.7833180
1	7.2096300	-0.2364470	-0.0028260
6	7.3111300	-1.3684760	4.0786420
6	7.4966370	-0.6546960	2.8779930
6	7.7930400	-0.8525400	5.2773590
6	8.1697430	0.5687280	2.8706300
6	8.4630430	0.3763690	5.2716230
1	7.6563570	-1.3913590	6.2111900
6	8.6516210	1.0796760	4.0771500
1	8.3235030	1.1120870	1.9426080
1	8.8429530	0.7862340	6.2027210
1	9.1788780	2.0290210	4.0893140
7	-7.1904850	-2.6606940	0.6903880
7	4.9880790	-4.1962310	-0.7499680
7	0.9750160	5.6356930	0.2302850
6	7.4118850	-3.9177240	4.2417780
6	5.2177090	-2.7375070	4.6133330

6	-10.1130660	0.3632660	-2.9533510
6	-7.7232070	0.8261070	-3.6074320
6	4.1707730	3.5920340	-3.8252140
6	5.0947770	5.9196440	-3.5266440
1	5.6619760	5.7404150	-4.4487200
1	4.1104980	6.2856820	-3.8457550
1	4.7648440	3.5624050	-4.7473820
1	3.2138520	4.0550550	-4.0981910
1	7.5364430	-3.8860970	5.3315720
1	5.4584710	-2.7643770	5.6836280
1	-10.3919710	0.8623340	-3.8899170
1	-9.9207710	-0.6849280	-3.2160590
1	-7.6268630	-0.2455150	-3.8240370
1	-8.1431390	1.2798700	-4.5141160
6	3.9278010	2.1621100	-3.3348040
6	5.7993030	7.0000780	-2.7022840
6	-6.3386780	1.4219810	-3.3401660
6	-11.2854580	0.4365980	-1.9719400
1	-11.5293100	1.4712810	-1.7139450
1	-12.1776220	-0.0178640	-2.4138040
1	-11.0670180	-0.1001500	-1.0440400
1	-6.3915230	2.5020800	-3.1770870
1	-5.8688880	0.9743270	-2.4590160
1	-5.6782110	1.2438670	-4.1944330
1	5.9102700	7.9143740	-3.2933640
1	5.2314590	7.2560810	-1.8027220
1	6.7977350	6.6800050	-2.3903730
1	4.8690900	1.6461940	-3.1247870
1	3.3277170	2.1435310	-2.4197800
1	3.3939060	1.5854830	-4.0964200

6	4.2276560	-1.6010410	4.3453920
1	3.9106700	-1.5815360	3.2983530
1	3.3306050	-1.7293600	4.9590170
1	4.6601690	-0.6254550	4.5862880
6	8.7851590	-4.0484620	3.5779590
1	9.3081350	-4.9289460	3.9637670
1	8.6993630	-4.1659490	2.4936570
1	9.4118630	-3.1738630	3.7752860
1	6.8186020	-4.8170370	4.0327120
1	4.7389620	-3.6990830	4.3882270
7	-9.9077990	-7.3535420	1.8724240
7	-11.4562750	-5.1349830	1.5335690
7	-1.4632160	10.5066750	1.2978790
7	1.2035320	10.6087960	0.7357760
7	6.5119190	-8.7844460	-3.4751320
7	8.4953860	-7.4854610	-2.1319390

Thermal Study:

The thermal stability and thermal decomposition of europium (III) complexes are examined by the thermogravimetric (TG) and differential thermogravimetric (DTG) curves. The TG (thermogravimetric) and DTG (differential thermogravimetric) are executed under the inert condition of argon gas with a heating rate of 10 °C/min from ambient temperature to 1000 °C temperatures. A similar trend of decomposition curves are observed in both the complexes. Decomposition Pattern in complexes $\text{Eu}_2(\text{TTA})_6\text{L1}$ and $\text{Eu}_3(\text{TTA})_9\text{L2}$ respectively are exhibited in Fig. S11. The TG curve shows the basic loss of water molecule up to 140 °C and 135 °C, which is trailed by main decay from 140 to 800 °C, 135 to 750 °C temperatures for $\text{Eu}_2(\text{TTA})_6\text{L1}$ and $\text{Eu}_3(\text{TTA})_9\text{L2}$ complexes respectively. The loss of weight percentage (83.05%) in this temperature range is mainly due to the removal of three fundamental ligands and one auxiliary ligand. At last, the residual product (14.58%) due to the oxide of europium.

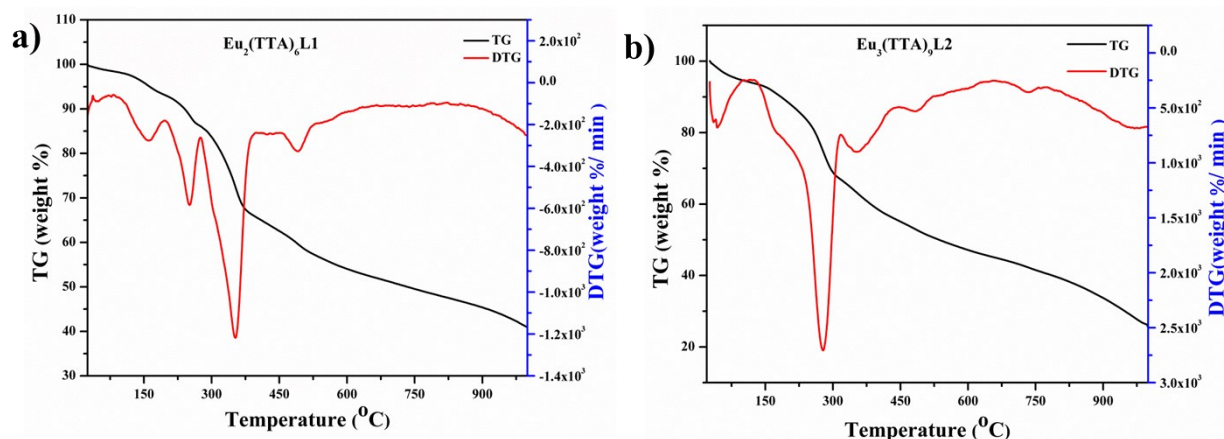


Fig. S11 TG/DTG curve of $\text{Eu}_2(\text{TTA})_6\text{L1}$ (left) and $\text{Eu}_3(\text{TTA})_9\text{L2}$ (right) complexes recorded under argon atmosphere.

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