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SUPPLEMENTARY INFORMATION

A Smart luminescent Molecular Europium complex and their versatile

applications

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General Information for synthesis:

All the reaction was done in the inert atmosphere. Solvent THF is dried and distilled by using Na Metal. All the commercially available reagents (Sigma Aldrich and Alpha Ezar) were used without further refinement unless otherwise needed. The progress of all the reactions was checked by thin-layer chromatography (TLC) with silica gel 60 F254 Aluminium plates (Merck) at a regular interval of time. Further purification of crud, the reaction mass was carried out by the column chromatography using silica gel (Sigma-Aldrich).

Measurements:

For recording the ¹H and ¹³C-NMR spectra the AV 400 Advance-III 400MHz Fourier transform nuclear magnetic resonance (FT-NMR) Spectrometer Bruker Biospin International, Switzerland was used. All the ¹H and ¹³C-NMR spectra were recorded in deuterated chloroform/dimethyl sulfoxide solution and tetramethylsilane (TMS) was used as a standard reference for chemical shift measurement. The Fourier transform infrared spectroscopy (FTIR) was executed by PerkinElmer Spectrum Version 10.4.00, in the spectrum range of 400 – 4000 cm⁻¹ making KBr pellets and elemental analysis was measure by Elementar Analysen Systeme, Germany/Vario EL spectrometer. The PL emission and excitation spectra in the solution and solid were recorded by using the Edinburg spectrofluorometric FS- 5 instruments associated with SC - 10 modules and SC - 5 modules respectively. The photoluminescence (excitation and emission) spectra, lifetime and quantum yield were monitored by using Edinburg Spectrofluorometer FS-5 instruments with attaching SC - 10 modules and SC - 30 integrating sphere module. The CIE color coordinate for all emission spectra is calculated by MATLAB software. The absorption spectra of all the synthesized compounds in solution form were utilizing UV-Visible spectrometer (Shimadzu Corporation, Japan or UV-2450 Perkin Elmer, USA/Lamda 25 and Lamda Perkin Elmer). The electrochemical properties of the ligands and their respective complex were estimated by utilizing cyclic voltammetry (CV), AUTOLAB

302N Modular potentiostat at RT in Dimethylformamide (DMF). The CV analysis is the set-up of mainly three electrode, the working (glass-carbon rod), auxiliary (counter, Pt wire) and reference (Ag/Agcl wire) electrodes. DMF containing 0.1 M Bu₄NClO₄ was used as an electrolyte and the sweep rate was kept 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. A UV-Visible spectrum of the molecule is obtained by exciting molecule vertically after conformation of ground state geometry of the ligand. The vertical singlet and triplet transitions were calculated by using TD-DFT method with the polarized continuum model (PCM) using the optimized ground state geometry. Further, to the depiction of PL emission and excitation mechanism of the Eu(III) complex, triplet energized condition of the ligand is additionally accessed by utilizing the same procedure specified previously. 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). The optimization study of ligand is effectively accomplished by the G09W program.

Materials:

The synthesis of Eu(III) chloride(EuCl₃.6H₂O) from europium(III) oxide is done by the wellknown process.¹The resultant product (EuCl₃.6H₂O) was then treated with an alcoholic solution of DBM (3 eq.) in the presence of 1 N sodium hydroxide solution (3.1 eq.) to get $Eu(DBM)_3(H_2O)_2$ were synthesized with little modification as reported in the literature.² 1, 10-Phenanthroline-5,6-dione was synthesized from 1,10-phenanthroline by a previously reported procedure.^{3,4} All the ligands were successfully synthesized by a well-reported procedure ⁴⁻⁶

General synthesis of ligands:

3-(2-(3-(trifluoromethyl)phenyl)-1H-imidazo[4,5-f][1,10]phenanthrolin-1-

yl)benzonitrile (Ligand 1): 1, 10-phenanthroline-5,6-dione (phen-dione) (1.0 g, 4.762 mmol) solution in acetic acid is poured in two neck round bottom flask and vigorously stirrer for 15 min. After obtaining the clear solution, we added 3-aminobenzonitrile (0.618 g, 5.238 mmol) and 3-(trifluoromethyl) benzaldehyde (0.910 g, 5.238 mmol) followed by ammonium acetate(3.66g, 47.61 mmol). The whole reaction mixture is stirred at 110°C under inert condition. The progress of the reaction is monitored by TLC (MeOH: DCM = 1 : 9) at a regular interval of time. After completion of the reaction, the reaction mass was neutralized with ammonia solution to pH~7 and extracted with DCM (Dichloromethane) followed by drying with sodium sulphate. It was concentrated by evaporating and further the obtained crude purification is done by column chromatography using silica bed (100–200 mesh) with 5% MeOH in DCM (dichloromethane) as the eluent. 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 product was pale-yellow color solid was formed is 150 mg (Yield: 68%). ¹H-NMR Data (400 MHz, CDCl₃): 1H(d)=9.25(J = 6),2H(dd)=9.151(J =13.2),1H(m)=8.057-8.031,2H(dd)=7.88(J=6),2H(m)=7.839-7.808,2H(m)=7.729-

7.679,1H(d)=7.53(J=7.6),2H(m)=7.439-7.28. ¹³C-NMR (100 MHz, CDCl₃, TMS, δ ppm): 148.62, 134.17, 133.34, 132.06, 131.82, 130.68, 129.33, 123.89, 77.33, 77.01, 76.70, Calculated m/z ratio = 465.43 found m/z ratio = 466.61

3-(2-(4-(trifluoromethyl)phenyl)-1H-imidazo[4,5-f][1,10]phenanthrolin-1-yl)benzonitrile (Ligand 2): Same procedure is followed as above for synthesis of ligand 2; 1,10phenanthroline-5,6-dione (phen-dione) (1.0 g, 4.762 mmol), 3-aminobenzonitrile (0.618 g, 5.238 mmol) and 4-(trifluoromethyl)benzaldehyde (0.910 g, 5.238 mmol). The product was pale-yellow color solid was formed is 140 mg (Yield: 63%). 1H-NMR Data (400 MHz, **CDCl₃**): 1H(dd)=9.25(J=4), 2H(m)=9.15-9.13, 1H(m)8.06-8.03, 3H(m)=7.90-7.87, 1H(m)=7.83-7.80, 4H(m)=7.69-7.64, 2H(m)=7.39-7.38. ¹³C-NMR (100 MHz, CDCl₃, TMS, δ ppm):_149.65, 148.62, 138.78, 134.78, 134.22, 133.35, 132.08, 131.85, 130.67, 129.67, 127.44, 125.72, 123.88, 123.73, 122.42, 116.76, .33, 77.01, 76.70, Calculated m/z ratio = 465.43 found m/z = 466.39

3-(2-(p-tolyl)-1H-imidazo[4,5-f][1,10]phenanthrolin-1-yl)benzonitrile (Ligand 3): Same procedure is followed as above for synthesis of ligand 3; 1,10-phenanthroline-5,6-dione (phendione) (1.0 g, 4.762 mmol), 3-aminobenzonitrile (0.618 g, 5.238 mmol) and 4-methylbenzaldehyde (0.629 g, 5.238 mmol). The product was pale-yellow color solid was formed is 140 mg (Yield: 72%).1H-NMR Data (400 MHz, CDCl₃): 1H(s) =9.23, 2H(dd)=9.14(J=20), 1H(s)=7.98, 4H(m)=7.84-7.82, 4H(m)=7.40-7.38, 2H(d)=7.18(J=8), 3H(s)=2.39. ¹³C-NMR (100 MHz, CDCl₃, TMS, δ ppm):131.50, 129.46, 129.32, 127.41, 77.34, 77.02, 76.71, 29.71, Calculated m/z ratio = 411.46 found m/z =412.58

3-(2-(naphthalen-1-yl)-1H-imidazo[4,5-f][1,10]phenanthrolin-1-yl)benzonitrile (Ligand **4)**: Same procedure is followed as above for synthesis of ligand 4; 1, 10-phenanthroline-5,6-dione (phen-dione) (1.0 g, 4.762 mmol), 3-aminobenzonitrile (0.618 g, 5.238 mmol) and 1-naphthaldehyde (0.818 g, 5.238 mmol). The product was pale-yellow color solid was formed is 150 mg (Yield: 70%). **1H-NMR Data (400 MHz, CDCl_3):** 1H(dd)=9.265(J=4), 2H(dd)=9.17(J=12), 3H(m)=7.95-7.86, 1H(m)=7.83-7.80, 2H(m)=7.76-7.72, 1H(dd)=7.66(J=8), 3H(m)=7.57-7.53, 4H(m)=7.50-7.40.¹³C-NMR (100 MHz, CDCl_3, TMS, **5 ppm):** 149.49, 148.52, 133.41, 132.71, 131.50130.97, 130.78, 129.49, 128.55, 127.67, 127.44, 126.69, 125.18, 124.61, 123.85, 122.38, 77.34, 77.02, 76.71, Calculated m/z = 447.49 found m/z ratio = 448.69

3-(2-(naphthalen-2-yl)-1H-imidazo[4,5-f][1,10]phenanthrolin-1-yl)benzonitrile (Ligand
5): Same procedure is followed as above for synthesis of ligand 5; 1,10-phenanthroline-5,6-

dione (phen-dione) (1.0 g, 4.762 mmol), 3-aminobenzonitrile (0.618 g, 5.238 mmol) and 2naphthaldehyde (0.818 g, 5.238 mmol). The product was pale-yellow color solid was formed is 140 mg (**Yield: 66%**). **1H-NMR Data (400 MHz, CDCl₃):** 1H(dd)=9.25(J=4), 1H(dd)=9.2(J=8), 1H(dd)=9.13(J=4), 2H(m)=8.02-7.99, 1H(s)=7.93, 6H(m)=7.90-7.77, 3H(m)=7.60-7.54, 2H(m)=7.46-7.38. ¹³C-NMR (100 MHz, CDCl₃, TMS, δ ppm): 149.48, 148.35, 133.88, 133.58, 132.28, 131.62, 130.72, 129.77, 128.53, 127.77, 127.47, 126.94, 125.85, 123.81, 122.36 Calculated m/z ratio = 447.49 found m/z = 448.69

C1; The solution of Eu(DBM)₃(H₂O)₂ (0.150 g, 0.175mmol) in dry THF (15 mL) was taken in round bottom flask and stirrer constantly, after 20 minutes a mixture of ligand1(0.0810g, 0.174) in dry THF was added slowly drop by drop. The reaction mixture was then stirred for 6 hours at 60°C under N₂ environment. The completion of the reaction is monitored by TLC. The resulting product was dissolved in a minimum amount of THF and an excess of hexane was added to get a solid product that is a pale yellow color with 160 mg (71%). Eu(TTA) **ESI-MS:** m/z = 1290.16, found: m/z = 1313.28 [M + Na] ⁺. Elemental analysis: Anal. Calc. for C₆₄H₄₆EuF₃N₃O₆: C, 67.19; H, 3.68; N, 5.44. Found: C, 67.11; H, 3.82; N, 5.4 %.

C2; The complex was synthesized by previously described procedure using **ligand3** as the ligand instead of ligand1. The resulting product was dissolved in a minimum amount of THF and an excess of hexane was added to get a solid product that is a pale yellow color with 150 mg (66%). **ESI-MS:** $\mathbf{m/z} = 1290.16$, found: $\mathbf{m/z} = 1313.28$ [M + Na]⁺. **Elemental analysis:** Anal. Calc. for C₆₄H₄₆EuF₃N₃O₆: C, 67.19; H, 3.68; N, 5.44. Found: C, 67.21; H, 3.67; N, 5.36 %.

C3; The complex was synthesized by previously described procedure using **ligand3** as the ligand instead of ligand1. The resulting product was dissolved in a minimum amount of THF and an excess of hexane was added to get a solid product that is a pale yellow color with 150 mg (70%). **ESI-MS:** m/z = 1236.19, found: m/z = 1237.32 [M + H]⁺. Elemental analysis:

Anal. Calc. for C₆₄H₄₆EuF₃N₃O₆: C, 70.13; H, 4.09; N, 5.68. Found: C, 69.87; H, 4.18; N, 5.52 %.

C4; The complex was synthesized by previously described procedure using ligand4 as the ligand instead of ligand1. The resulting product was dissolved in a minimum amount of THF and an excess of hexane was added to get a solid product that is a pale yellow color with 150 mg (65%). ESI-MS: m/z = 1272.31, found: m/z = 1273.32 [M + H]⁺. Elemental analysis: Anal. Calc. for C₆₄H₄₆EuF₃N₃O₆: C, 70.97; H, 3.97; N, 5.52. Found: C, 70.88; H, 4.13; N, 5.61%.

C5; The complex was synthesized by previously described procedure using **ligand5** as the ligand instead of ligand1. The resulting product was dissolved in a minimum amount of THF and an excess of hexane was added to get a solid product that is a pale yellow color with 160 mg (72%). **ESI-MS:** m/z = 1272.31, found: m/z = 1273.32 [M + H]⁺. **Elemental analysis:** Anal. Calc. for C₆₄H₄₆EuF₃N₃O₆: C, 70.97; H, 3.97; N, 5.52. Found: C, 70.90; H, 4.12; N, 5.46%.

1. NMR Spectroscopy:



Figure S1. ¹H NMR spectroscopy of Ligand 1 in CDCl₃



Figure S2. ¹H NMR spectroscopy of Ligand 2 in CDCl₃



Figure S3. ¹H NMR spectroscopy of Ligand 3 in CDCl₃



Figure S4. ¹H NMR spectroscopy of Ligand 4 in CDCl₃



Figure S5. ¹H NMR spectroscopy of Ligand 5 in CDCl₃



Figure S6. ¹³C NMR spectroscopy of Ligand 1 in CDCl₃



Figure S7. ¹³C NMR spectroscopy of Ligand 2 in CDCl₃



Figure S8. ¹³C NMR spectroscopy of Ligand 3 in CDCl₃



Figure S9. ¹³C NMR spectroscopy of Ligand 4 in CDCl₃



Figure S10¹³C NMR spectroscopy of Ligand 5 in CDCl₃



Fig. S11 ¹H-NMR spectroscopy of Eu(DBM)₃.2H₂O in CDCl₃

Mass spectral analysis:







Figure S13. Mass spectral data of Ligand 2





Figure S14. Mass spectral data of Ligand3

Figure S15. Mass spectral data of Ligand 4





Figure S16. Mass spectral data of Ligand5

Figure S17. Mass spectral data of complex C1



Figure S18. Mass spectral data of complex C2



Figure S19. Mass spectral data of complex C3



Figure S20. Mass spectral data of complex C4



Figure S21. Mass spectral data of complex C5

UV-Vis spectra (DFT studies):



Figure S22a. UV-Vis spectra of the ligands in DCM solution $(1x10^{-5} \text{ m})$.



Figure S22b. Theoretical UV spectra of the ligands in gas phase and DCM solution.



Figure S22c. UV absorption spectrum of DBM in CHCl₃(1x10⁻⁵M conc.)



Figure S23. Absorption spectra, for the Visible titration of ligands $(1x10^{-5}M)$ with Eu(DBM)_{3.}2H₂O in methanol at 298 K.

PL Spectral studies of ligand diluted with KBr



Figure 24a. PL Excitation ($\lambda_{em} = 450 \text{ nm}$) and emission ($\lambda_{ex} = 368 \text{ nm}$) spectrum of ligand 1



Figure 24b. PL Excitation ($\lambda em = 445 \text{ nm}$) and emission ($\lambda ex = 344 \text{ nm}$) spectrum of ligand

2



Figure 24c. PL Excitation ($\lambda_{em} = 462 \text{ nm}$) and emission ($\lambda_{ex} = 330 \text{ nm}$) spectrum of ligand 3



Figure 24d. PL Excitation (λ_{em} = 440 nm) and emission (λ_{ex} = 330 nm) spectrum of ligand 4



Figure 24e. PL Excitation ($\lambda_{em} = 454 \text{ nm}$) and emission ($\lambda_{ex} = 355 \text{ nm}$) spectrum of ligand 5



FigS24f. Excitation and emission spectrum of pure DBM in CHCl₃

PL spectra: Solvatochromism study of ligands:





Figure S25a. Solvatochromism PL excitation and emission spectra of the all ligands

Stokes shift:

The Lippert–Mataga equation (eq 1a and 1b) describes the solvatochromic Stokes shift $\Delta v \Box$ (expressed in wavenumbers) as a function of the change of the dipole moment $\Delta \mu ge = \mu e - \mu g$ of the dye upon excitation. The validity of equation 1a can be checked by using various solvents with different dielectric constants (ε) and refractive indices (n) and by plotting $\Delta v \Box$ as a function of $\Delta f.^{7,8}$

$$\Delta v = \frac{2}{4\pi \varepsilon ohca^3} (\mu e - \mu g) + constant \quad (1a)$$

$$F(\varepsilon) = \frac{f(\varepsilon - 1)}{f(2\varepsilon + 1)} \text{ and } f(n^2) = \frac{(n^2 - 1)}{(2n^2 - 1)}$$
(1b)

 $\Delta v \Box = \Delta v \Box_{abs} - \Delta v \Box_{em}$ is the solvatochromic shift (in cm⁻¹) between the maxima of absorption and fluorescence emission [$\Delta v \Box abs = 1/\lambda abs$ (max), $\Delta v \Box em = 1/\lambda em$ (max)]. $\epsilon 0$ is the permittivity of vacuum, represents the radius of the cavity in which the solute resides. h is Planck's constant, c is the velocity of light, μe , μg are dipolemoments in the excited and ground states. Figure S25represents the Lippert–Mataga plot for all the ligands in the solvents listed in Table S1-Table ST5. As is evident from Figure S25, there is close to linear relationship of the Stoke's shift plotting $\Delta v \Box$ verses Δf for the 10 solvents.





Figure S25b.Stokes shift of all ligands Δv versus the Lippert solvent parameter $\Delta f = f(\varepsilon) - f(n2)$ (The numbers refer to the solvents in Table S1-5). The straight line represents the linear fit to the 10 data points.

S.No.	Solvent	λ_{abs} (max) in nm	λem (max) in	Stokes shift ($\Delta v \Box$)
			nm	in cm-1
1	DMF	350	402	3771
2	ACN	338	399	3569
3	МеОН	327	408	6081
4	DMSO	353	406	3728
5	Acetone	338	398	4585
6	Toluene	335	389	4150
7	EtOAc	337	393	4273
8	THF	349	393	3253
9	CHCl ₃	392	392	3569
10	DCM	350	395	3170

Table ST1: PL spectra	l data of liga	and1 in va	arious so	lvents
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S.No.	Solvent	λ_{abs} (max) in	λ em (max) in	Stokes shift
		nm	nm	$(\Delta v \Box)$ in cm-1
1	DMF	359	400	2855
2	ACN	341	398	4225
3	МеОН	335	408	5350
4	DMSO	344	407	4569
5	Acetone	349	397	3553
6	Toluene	352	387	2609
7	EtOAc	350	391	3071
8	THF	358	391	2432
9	CHCl ₃	349	391	3153
10	DCM	362	391	2124

 Table ST2: PL spectral data of ligand2 in various solvents

Table ST3: PL spectral data of ligand3 in various solvents

S.No.	Solvent	λ_{abs} (max) in	λ em (max) in	Stokes shift
		nm	nm	$(\Delta v \Box)$ in cm-1
1	DMF	330	421	6603
2	ACN	329	416	6395
3	МеОН	333	428	6670
4	DMSO	329	423	6795
5	Acetone	342	413	5039
6	Toluene	329	401	5495
7	EtOAc	342	407	4739
8	THF	344	410	4769
9	CHCl ₃	332	408	5620
10	DCM	329	408	5895

S.No.	Solvent	λ_{abs} (max) in	λ em (max) in	Stokes shift
		nm	nm	$(\Delta v \Box)$ in cm ⁻¹
1	DMF	338	407	5085
2	ACN	326	399	5674
3	МеОН	314	416	7847
4	DMSO	328	409	6047
5	Acetone	339	402	4698
6	Toluene	337	401	4773
7	EtoAc	325	401	5869
8	THF	338	399	4585
9	CHCl3	345	400	3985
10	DCM	336	401	1954

Table ST4: PL spectral data of ligand4 in various solvents

Table ST5: PL spectral data of ligand5 in various solvents

S.No.	Solvent	λ_{abs} (max) in	λ em (max) in	Stokes shift
		nm	nm	$(\Delta v \Box)$ in cm ⁻¹
1	DMF	355	407	3598
2	ACN	371	406	2323
3	МеОН	368	416	3135
4	DMSO	365	409	2947
5	Acetone	368	402	2298
6	Toluene	370	392	1516
7	EtOAc	370	398	1901
8	THF	368	395	1857
9	CHCl ₃	372	400	1881
10	DCM	371	400	1954



Solvatochromism study of Eu(III) complexes:

Figure S26. The emission intensity ratio of the ligand and Eu(III) ion in bar graph for all Eu(III) complex(C1, C2, C3, C4and C5) in solvatochromism study.



Figure S27. Digital image of C1 complexes in in different solvent.



Figure S28. Digital image of C2 complexes in in different solvent.



Figure S29. Digital image of C3 complexes in in different solvent.



Figure S30. Digital image of C4 complexes in in different solvent.



Figure S31. Digital image of C5 complexes in in different solvent.



Figure S32a. Different excitation spectral wavelength analysis of the C1 complex in CHCl₃.b. CIE for the different excitation spectral wavelength analysis of the C1 complex in CHCl₃.



Figure 33a. Different excitation spectral wavelength analysis of the C2 complex in CHCl₃.b. CIE for the different excitation spectral wavelength analysis of the C2 complex in CHCl₃.











CIE for the different excitation spectral wavelength analysis of the C4 complex in CHCl3.





SOLVENT	C1		C2		C3		C4		C5	
	(x, y)	AR	(x, y)	AR	(x, y)	AR	(x, y)	AR	x y	AR
DCM	(0.298, 0.172)	4.68	(0.212, 0.132)	4.85	(0.371, 0.236)	4.52	(0.293, 0.208)	4.27	(0.253, 0.175)	4.23
DMF	(0.411, 0.251)	11.22	(0.430, 0.237)	14.88	(0.348, 0.231)	9.16	(0.253, 0.251)	3.56	(0.255, 0.178)	7.12
DMSO	(0.491, 0.278)	10.83	(0.374, 0.215)	8.93	(0.287, 0.223)	6.22	(0.356, 0.256)	6.27	(0.242, 0.175)	5.51
TOLUENE	(0.467, 0.254)	8.49	(0.366, 0.177)	4.51	(0.355, 0.228)	7.22	(0.237, 0.188)	4.61	(0.278, 0.167)	5.75
МеОН	(0.201, 0.184)	3.50	(0.228, 0.173)	3.63	(0.292, 0.316)	3.39	(0.284, 0.300)	3.19	(0.286, 0.297)	2.89
CHCl ₃	(0.397, 0.232)	4.9	(0.313, 0.255)	4.01	(0.259, 0.272)	2.52	(0.354,0.274)	4.03	(0.348, 0.230)	4.67
ACN	(0.480, 0.298)	9.98	(0.512, 0.275)	7.84	(0.543, 0.310)	5.39	(0.336, 0.304)	4.47	(0.465, 0.283)	5.92
ACETONE	(0.563, 0.300)	14.02	(0.407, 0.224)	6.81	(0.286, 0.224)	5.37	(0.266, 0.269)	3.02	(0.395, 0.246)	6.03
THF	(0.618, 0.315)	13.95	(0.185, 0.097)	5.99	(0.500, 0.282)	6.59	(0.311, 0.248)	4.28	(0.425, 0.250)	6.50
EtOAc	(0.511, 0.277)	4.83	(0.434, 0.230)	4.48	(0.577, 0.310)	4.24	(0.270, 0.207)	4.82	(0.390, 0.237)	4.99

Table ST6. The calculated CIE from the PL emission data of Eu(III) complexes in different

solvents and corresponding asymmetric ratio.



Figure S37. Emission ($\lambda ex = 280$ nm) spectra of a) Ligand (1×10^{-5} mol/L conc.) in the absence (black line) and presence (Red line) of Eu(III) ions and b) emissiom of complex in the absence (black line) and presence (Red line) of Ligand1.

Judd-Ofelt (J –O) analysis:

Judd–Ofelt theory is an important tool for studying f-f electronic transitions of Ln(III) ion and also used to examine the symmetry and chemical environment around the europium ion, which can be calculated by using emission spectra of Eu(III) complex, with the help of following eqn 3.

$$\Omega_{\lambda} = \frac{3hC^{3}A_{o-\lambda}}{4e^{2}\omega^{3}\chi < 5D_{0}\|U(\lambda)\|^{7}FJ > 2}....(3)$$

Where A_{0J} represent the coefficient of spontaneous emission for the ${}^{5}D_{0} \rightarrow {}^{7}F_{J}$ transition, C is for Lorentz local-field correction term given by $C = n(n^2 + 2)^2/9$, n is the refractive index of the medium(in this case n = 1.5), and $\langle 5D_0 || U(\lambda) ||^7 FJ \rangle^2$ are the square reduced matrix element whose values 0.0032, 0.0023 and 0.0002 for λ = 2, 4, and 6 respectively. The Judd–Ofelt (J–O) parameters Ω_{λ} ($\lambda = 2, 4, \text{ and } 6$) prove to be important in calculating the interaction parameters of the ligand fields. In all the J-O parameters, Ω_2 intensity parameter is more important for ligand field sequence and symmetry while $\Omega_4 ({}^5D_0 \rightarrow {}^7F_2)$ is less sensitive compared to Ω_2 for coordination sphere. The $\Omega_4 ({}^5D_0 \rightarrow$ ⁷F₂) show the rigidity of Eu(III) ion chemical environment. The intensity parameter Ω_{2} , Ω_4 values for all the Eu(III) complexes are tabulated in Table ST7. The Ω_6 (⁵D₀ \rightarrow ⁷F₆) cannot be calculated experimentally because of the absence $({}^{5}D_{0} \rightarrow {}^{7}F_{6})$ transition. The radiative properties (A_{rad}), radiative lifetime (τ_{rad}) and branching ratio (β_{1-3}) of the Eu(III) complexes were calculated by help of the J-O intensity parameter according to the reported method.⁹ The fluorescence branching ratio (β) was calculated to represent the transitions starting from the ${}^{5}D_{0}$ level. All the value of radiative properties and branching ratio were tabulated in the Table ST7 and Table ST8.

Complexes	$\mathbf{A}_{\mathrm{rad}}(\mathrm{s}^{-1})$	$\tau_{\rm rad}$	Anr	η_{Ln}	η _{sen} (%)	η	β1	β ₂	β4
		(ms)	(ms)	(%)		overall			
C1	606.593	1.648	1.28	31.06	12.87	4.0	8.242	77.827	13.929
C2	507.327	1.971	5.37	8.62	58.70	5.06	9.855	80.585	9.558
C3	432.240	2.313	1.01	29.65	9.00	2.67	11.567	66.514	21.917
C4	345.377	2.895	5.53	5.80	98.96	5.74	14.476	67.428	18.0950
C5	453.089	2.207	3.01	13.04	17.79	2.32	11.035	66.805	22.159

Table ST7. Radiative Properties and Branching Ratios of the Complexes

Table ST8. Calculated luminescence lifetimes τ_{obs} and intensity parameters of ligands and corresponding Eu(III) complexes.

	Inte	nsity	A ₀₋₁ in S ⁻¹	A ₀₋₂ in S ⁻¹	A ₀₋₄ in S ⁻¹	τ / ms for Eu(III)
Compound	paran	neters				complexes and; τ / ns
	(10^{-20} cm^2)					for all the ligands
	Ω_2	Ω_4				Toluene
C1	5.6743	2.104	50	472.0972	84.4966	0.512
C2	4.8901	1.212	50	408.8324	48.4949	0.170
C3	3.5067	2.349	50	287.5027	94.7378	0.686
C4	2.8267	1.543	50	232.8812	62.4962	0.175
C5	3.6790	2.479	50	302.6890	100.4006	0.288
Ligand 1						3.76
Ligand 2						5.83
Ligand 3						6.92
Ligand 4						3.69

Ligand 5	•••	 	 	3.44

Photoluminescence quantum efficiency (PLQY):

The absolute PLQYs of the Eu(III) complexes in solid form were performed ($\lambda_{ex} = 384$ nm). The absolute QY was calculated by using the expression 1 and 2:

Where, $L_0(\lambda)$ is the integrated excitation profile when the sample is directly excited by the incident beam, and $L_i(\lambda)$ is the integrated excitation profile obtained from the empty integrated sphere. $E_0(\lambda)$ is represents the integrated luminescence of solid induced by the direct excitation and $E_i(\lambda)$ is refers the indirect illumination from the sphere, respectively. The PLQY of all the Eu(III) complexes were given in the Table ST7. These obtained quantum yields suggest that the energy transfer occurs from the ligand to the Eu(III) ion, however, the QYs are poor, as mentioned earlier that the inefficient energy transfer between the ligand and Eu(III) metal ion could be one of the plausible reasons. The currently obtained QYs are compared with the reported similar Eu-complexes in Table ST9.

Table ST9	. OY	comparison	with the	reported	complexes
14010 017	· ~ +	companioon		reported	comprenes

			LED data				Reference	
S.No.	Compound name	Quantum Yield	Cl	E	CRI	ССТ	LER	
		(in solid/Solution)	Х	у	(%)	(K)	(lm/W)	
1	Eu ₂ (TTA) ₆ L1	0.7	0.33	0.33	95	5457	266,282	10
	Eu ₃ (TTA) ₉ L2	10.2	0.58	0.31				
2	Eu(DBM) ₃ L-pCH ₃	4.32	0.33	0.33	51	4978		11
3	1Eu	1.4/6.3						12
	2Eu	0.42/6.6						-
	2Eu	0.42/0.0	0.00	0.00				-
	<u>3Eu</u>	0.1/3.8	0.30	0.33				
4	Complex 3	7		-				13
5	Eu.6	10.5		-				14
6	EuL_1	7.5		-				15
7	Eu-51	2.5	0.33	0.24				16
8	complex 3	11.9		-				17
9	Hybrid film of	16.9	0.322	0.332				18
	$(HNEt_3)_2[Eu_2L_4]$							

Polymethyl methacrylate (PMMA) film of Ligands and their respective Eu(III) complexes Optical properties of the ligand and their complexes were executed in film form by doping the same in the PMMA matrix in different concentration ratio (2.5, 7.5 and 10%). In general, the PMMA is an easily available and cheap polymer with attractive optical properties and it shows good transparency in the visible range. The PL emission spectra of all ligands as well as Eu(III) complexes in thin film and their corresponding digital photographs in different concentration ratio are displayed in Figure S38 inset (Figure S39 and 40, respectively). The enhancement of the europium emission was observed, when the concentration of the complexes increased in the PMMA matrix (Figure S40). The asymmetric ratio, FWHM and CIE color coordinates of all the Eu(III) complex in the PMMA matrix are tabulated in Table ST11. The FWHM of Eu(III) doped PMMA matrix is increasing with the enhancing the concentration of Eu(III) complex, which indicates that the PMMA doping is responsible for the FWHM increment. In addition, with enhancing of the concentration of Eu(III) complex in the PMMA matric is also responsible for variation in the CIE color coordinate. As shown in the Figure 40 (Figure S42) the color is changing from red to nearly white through pinkish color due to presence of ligand emission along with Eu(III) metal ion peak in the emission spectra. The present study indicates that all the Eu(III) complexes showing the ligand peak along with Eu(III) peak in PL spectra with variating the Eu(III) concentration in PMMA matrix except the complex C1.





Figure S38. PL emission spectra of the Ligand1, Ligand2, Ligand3, Ligand4 and



Ligand5 in thin films using a PMMA matrix.

Figure S39. PL emission spectra of the complexes C1 in thin films using a PMMA matrix.



Figure S40. PL emission spectra of the complexes C2, C3, C4 and C5 in thin films using a PMMA matrix.

Correlation color temperature (CCT) calculation

The definition of color temperature is appearance of color of white LED and the unit of colour correlated temperature is Kelvin. The CCT value of warm white light is 2700K, the neutral white light at around 4000K and the cool white light is at around 5000K or >5000K. The correlation color temperature (CCT) was calculated through the McCamy empirical formula

$$CCT = -449n^3 + 3525n^2 - 6823n + 5520.33....(5)$$

In the above equation, $n = (x - x_e)/(y - y_e)$ is the inverse slope line, $x_e = 0.332$ and $y_e = 0.186$ and the x and y is the CIE values which are observed from the PMMA emission spectrum. The calculated CCT values are tabulated in Table ST11. It is also worth to note that the CCT value can be tuned from 1700 to 7000K. Among all complex, the complex C2 (2.5%) and C3 (10%) shows cool white light, while the complex C3 (2.5%) exhibits the warm white light emission.

Table ST10. Intensity ratios as well as CIE Color Coordinates for the Eu(III) Complexes in

 different concentration ratio doped PMMA

%	C1			C2	C2		C3			C4		C5			
	I_2/I_1	CIE		I_2/I_1	CIE		I_2/I_1	CIE		I_2/I_1	CIE		I_2/I_1	CIE	
		X	У		X	у		X	у		X	у		х	У
2.5	28.7	0.65	0.32	4.57	0.290	0.333	4.07	0.337	0.228	4.20	0.404	0.26	4.13	0.371	0.232
	5	3	9									4			
7.5	30.2	0.66	0.33	4.99	0.412	0.318	5.27	0.509	0.292	4.33	0.412	0.25	4.23	0.399	0.238
	3	6	0									7			
10	30.7	0.66	0.33	5.06	0.358	0.328	5.34	0.310	0.247	4.42	0.437	0.26	5.30	0.403	0.264
	9	7	0									6			

 Table ST11. CCT calculation for the Eu(III) Complexes in different concentration ratio doped

PMMA

%	C1(K)	C2(K)	C3(K)	C4(K)	C5(K)
2.5	3309	7778	4754	1912	2028
7.5	3514	2587	2062	1734	1719
10	3533	4380	8469	1726	1929

Fabrication of LED with Eu(III) complexes:





Figure S43. The emission spectra of the Eu(III) (C2, C3, C4 and C5) complexes with n-UV under a 20 mA forward bias current. The insets are the fabricated LED devices.

 Table ST12. CIE Color Coordinates for the Eu(III) Complexes in Different Concentration

 Ratio coated with LED

CIE	C1	C2	C3	C4	C5
1:10(x, y)	(0.628, 0.363)	(0.577, 0.403)	(0.650, 0.343)	(0.655, 0.342)	(0.651, 0.344)
1:50(x, y)	(0.610, 0.379)	(0.567, 0.413)	(0.601, 0.383)	(0.645, 0.349)	(0.641, 0.353)

Thermal Study:

The thermal stability of Eu(III) complexes plays an vital role in optoelectronic device fabrication. Thermal stability of ligands and their respective Eu(III) complexes can be determined by, thermal gravimetric analysis (TGA) measurement from ambient temperature to 1000°C under nitrogen atmosphere at heating rate of 10°C/min. As shown in Figure S44, all the complexes are shown thermal- decomposition (T_d) for 5% weight loss in the range of 160-180°C; C1(180°C), C2(170°C), C3(175°C), C4(162°C) and C5(160°C). The thermal decomposition of all the Eu(III) complexes is appeared in three stages in the field of ~ 180-450

 $^{\circ}$ C (first stage, major), ~ 450-580 $^{\circ}$ C (second stage), and > 580 $^{\circ}$ C (third stage). The major thermal decomposition in the Eu(III) complexes is due to presence of auxiliary ligand. The second decomposition was observed due the presence of DBM in the Eu(III) complexes. The minor decomposition is due to the loss of water molecule from the complexes. Here all the Eu(III) complexes showing the thermal decomposition more than 175 $^{\circ}$ C, which indicate that all the synthesized complexes are potential candidate. All the ligands shown the high thermal stability compare to that of Eu(III) complexes because of presence of more C-C bond, as it is already known that the C-C bond is stronger bond so more thermal energy is needed to break the bond and TGA curve also presenting the same.



Figure S44. TGA curve of ligands (top) and their respective complexes (bottom) recorded under N₂ atmosphere.



Recyclable on-off-on vapoluminescence sensor (FT-IR):

Figure S45. FTIR spectra of DBM, ligand1 and C1 complex with and without HCl and NEt₃

vapours

Temperature dependent PL emission study of Eu(III) complex:





Figure S46. Temperature dependent PL emission spectra of Eu(III) complexes (C1, C2, C3,

C4 and C5) in ACN solvent and their CIE respectively







Figure S47. Phosphorescence emission spectrum of ligands, Gd(III) complex with Ligand1,

ligand 2, ligand 3, ligand4 and ligand 5 at 77 K.



Figure S48. Energy transfer process from the ligand as well as from DBM to Eu(III) metal ion through its singlet and triplet excited states (which is calculated with 77 K value).DFT Analysis:



Figure S49. HOMO–LUMO energy gap diagram of the all the ligand by DFT calculation.

Table ST13.The	Table ST13. The HOMO-LUMO and HOMO-1, LUMO+1 energy levels of the ligand.								
Luminophore	НОМО	LUMO	HOMO-1	LUMO+1					
Ligand 1									
Ligand 2									
Ligand 3									
Ligand 4									
Ligand 5									

Table ST14. The computed vertical transitions and their oscillator strengths (f) andconfiguration of the ligands.

Luminophores	State	Energy	$\lambda_{max} nm$	f	Configuration
		(eV)			
Ligand 1	Gas	3.151	393.42	0.0018	HOMO→LUMO (70.60%)
Singlet					
		3.550	349.2	0.0487	HOMO→LUMO+1 (56.54%)
					HOMO→LUMO+2 (37.17%)
		3.751	330.5	0.247	HOMO→LUMO+1 (50.63%)
		3.475	354.5	0.002	HOMO→LUMO (69.33%)
	DCM	3.660	337.2	0.471	HOMO→LUMO+2 (58.77%)
	Dem				HOMO→LUMO+3 (33.13%)
		3.718	332.0	0.177	HOMO→LUMO+3 (58.30%)
Triplet	Gas	2.755	449.9	0	HOMO-2→LUMO+2 (11.31%)
					HOMO→LUMO+1(53.85%)
					HOMO→LUMO+4 (19.75%)
		3.195	387.9	0	HOMO-2→LUMO+3 (15.86%)
					HOMO-1→LUMO+1 (14.36%)
					HOMO-1→LUMO+3 (26.33%)
					HOMO→LUMO+4 (38.58%)
		3.270	379.0	0	HOMO→LUMO (67.08%)
	DCM	2.854	350.6	0	HOMO→LUMO (69.33%)
		3.085	337.3	0	HOMO→LUMO+2 (58.77%)
					HOMO→LUMO+3 (32.73%)
		3.175	330.5	0	HOMO→LUMO+3 (57.34%)

Ligand 2	Gas	3.177	390.1	0.002	HOMO→LUMO (70.59%)
Singlet		3.562	347.9	0.113	HOMO→LUMO+1 (56.54%)
					HOMO→LUMO+2 (41.46%)
		3.714	333.7	0.309	HOMO→LUMO+2 (52.97%)
	DCM	3.486	355.6	0.002	HOMO→LUMO (70.33%)
		3.664	338.3	0.471	HOMO→LUMO+2 (59.77%)
					HOMO→LUMO+3 (33.73%)
		3.728	332.5	0.177	HOMO→LUMO+3 (59.34%)
Triplet	Gas	2.724	455.1	0	HOMO→LUMO+1 (59.30%)
					HOMO→LUMO+4 (19.17%)
		3.180	389.7	0	HOMO-2→LUMO+3 (11.62%)
					HOMO→LUMO (61.11%)
		3.200	387.4	0	HOMO-2→LUMO+2 (14.37%)
					HOMO→LUMO (28.90%)
					HOMO→LUMO+2 (21.11%)
					HOMO→LUMO+4(35.62%)
	DCM	2.772	447.1	0	HOMO-1→LUMO+2 (10.43%)
					HOMO-1→LUMO+3 (13.11%)
					HOMO→LUMO+2(60.46%)
					HOMO→LUMO+4(15.67%)
		3.180	389.7	0	HOMO-4→LUMO+5 (11.32%)
					HOMO-1→LUMO+3 (27.66%)
					HOMO→LUMO+4(42.65%)
		3.241	382.5	0	HOMO→LUMO+3 (58.26%)
					HOMO→LUMO+4 (15.22%)

Ligand 3	Gas	3.059	405.2	0.001	HOMO→LUMO (66.82%)
Singlet					HOMO→LUMO+1 (20.83%)
		3.481	356.1	0.027	HOMO→LUMO+1 (58.84%)
					HOMO→LUMO+3 (24.98%)
		3.706	334.5	0.102	HOMO→LUMO+1 (12.94%)
					HOMO→LUMO+2 (66.34%)
					HOMO→LUMO+3 (12.66%)
	DCM	3.354	369.6	0.0005	HOMO→LUMO (70.52%)
		3.584	345.9	0.048	HOMO→LUMO+1 (67.34%)
		3.744	331.1	0.381	HOMO-1→LUMO+1 (13.48%)
					HOMO→LUMO+1 (14.63%)
					HOMO→LUMO+2 (66.15%)
Triplet	Gas	2.765	448.4	0	HOMO-1→LUMO+1 (40.45%)
		3.030	409.0	0	HOMO→LUMO (68.78%)
		3.216	385.4	0	HOMO-1→LUMO+3 (12.14%)
					HOMO→LUMO+1 (10.92%)
					HOMO→LUMO+2 (46.58%)
					HOMO→LUMO+4 (28.91%)
	DCM	2.799	442.8	0	HOMO→LUMO+1 (17.85%)
					HOMO→LUMO+2 (58.74%)
					HOMO→LUMO+3 (15.72%)
		3.144	394.2	0	HOMO→LUMO (26.97%)
					HOMO→LUMO+1 (59.49%)

		3.233	383.4	0	HOMO-3→LUMO+1 (10.95%)
					HOMO-3→LUMO+2 (14.20%)
					HOMO→LUMO+2 (12.53%)
					HOMO→LUMO+4 (44.23%)
Ligand 4	Gas	3.172	390.76	0.008	HOMO→LUMO (70.53%)
Singlet		3.554	348.7	0.108	HOMO→LUMO (62.74%)
					HOMO→LUMO+1 (30.17%)
		3.682	336.6	0.189	HOMO→LUMO+2 (60.82%)
					HOMO→LUMO+3 (11.35%)
	DCM	3.419	362.6	0.018	HOMO→LUMO (70.39%)
		3.629	341.5	0.142	HOMO→LUMO+1 (48.01%)
					HOMO→LUMO+2 (47.93%)
		3.68	336.5	0.297	HOMO→LUMO+1 (49.88%)
Triplet	Gas	2.596	477.44	0	HOMO-1→LUMO+1 (26.36%)
					HOMO→LUMO (13.99%)
					HOMO→LUMO+1 (44.57%)
					HOMO→LUMO+3 (12.16%)
		2.895	428.2	0	HOMO-2→LUMO+3 (10.42%)
					HOMO-1→LUMO+1 (23.35%)
					HOMO→LUMO (10.92%)
					HOMO→LUMO+3 (12.59%)
					HOMO→LUMO+4 (42.14%)
		3.144	394.2	0	HOMO→LUMO (65.27%)
					HOMO→LUMO+2 (14.73%)

					HOMO \rightarrow LUMO (17.39%)
					HOMO→LUMO+1 (47.26%)
		2.916	425.1	0	HOMO-1→LUMO+1 (24.80%)
					HOMO→LUMO+1 (23.54%)
					HOMO→LUMO+3 (39.93%)
		3.207	386.5	0	HOMO-1→LUMO+2 (23.34%)
					HOMO→LUMO+1 (26.10%)
					HOMO→LUMO+2 (50.31%)
Ligand 5	Gas	3.009	411.9	0.017	HOMO→LUMO (70.33%)
Singlet		3.566	347.6	0.094	HOMO→LUMO+1 (52.11%)
					HOMO→LUMO+2 (44.59%)
		3.635	341.0	0.0003	HOMO→LUMO (69.72%)
	DCM	3.281	377.8	0.050	HOMO→LUMO (69.90%)
		3.567	347.5	0.282	HOMO→LUMO+1 (63.25%)
		3.739	331.5	0.341	HOMO-2→LUMO+1 (12.16%)
					HOMO→LUMO+1 (26.32%)
					HOMO→LUMO+2 (62.70%)
Triplet	Gas	2.523	491.25	0	HOMO-1→LUMO (10.46%)
					HOMO→LUMO (29.61%)
					HOMO→LUMO+1 (45.63%)
					HOMO→LUMO+3 (11.90%)
		2.896	432.0	0	HOMO-1→LUMO (16.45%)
					HOMO-1→LUMO+1 (25.80%)
					HOMO-1→LUMO+2 (12.48%)
					HOMO→LUMO+4 (41.55%)

	3.022	410.2	0	HOMO→LUMO (58.77%)
				HOMO→LUMO+4 (13.40%)
DCM	2.557	484.86	0	HOMO-1→LUMO (10.29%)
				HOMO→LUMO (30.19%)
				HOMO→LUMO+1 (39.00%)
				HOMO→LUMO+2 (20.27%)
	2.893	428.4	0	HOMO-1→LUMO (17.18%)
				HOMO-1→LUMO+1 (20.46%)
				HOMO-1→LUMO+2 (17.06%)
				HOMO→LUMO+3 (42.66%)
	3.142	394.28	0	HOMO-1→LUMO+1 (13.05%)
				HOMO→LUMO+2 (44.74%)

Table ST15. Cartesian coordinates for optimized geometry of Ligand 1

6	-2.4384590	-4.1343910	-1.7745460
6	-1.1831950	-4.2847000	-1.2249350
6	-0.6428900	-3.2582390	-0.4232500
6	-1.4384250	-2.0799570	-0.2444590
6	-3.1440280	-2.9506490	-1.5177490
6	0.6436320	-3.2728510	0.2164720
6	-0.9351170	-0.9407250	0.5375460
6	0.3583520	-0.9951370	1.1131110

6	1.1337370	-2.1853780	0.9263680
6	0.8191760	0.1134770	1.8439490
1	1.8063320	0.0795560	2.2886180
6	-0.0059220	1.2091070	1.9742270
6	-1.2747760	1.1674970	1.3690670
1	-2.8732900	-4.9106880	-2.3927810
1	-0.6196890	-5.1856300	-1.4175030
1	-4.1393350	-2.8041610	-1.9298370
1	0.3045820	2.0864740	2.5292150
1	-1.9467860	2.0176850	1.4584220
6	2.7032140	-3.6450990	1.0060540
7	2.3961040	-2.4271640	1.3942710
7	1.6630840	-4.2275910	0.2788340
6	1.6887310	-5.5045340	-0.3672790
6	2.4387570	-5.6776850	-1.5301810
6	0.9706650	-6.5670670	0.1751880
6	2.4737350	-6.9232130	-2.1529850
1	2.9891140	-4.8384970	-1.9371210
6	1.0034530	-7.8156340	-0.4582640
1	0.3909900	-6.4252450	1.0785870

6	1.7602340	-7.9928370	-1.6261670
6	4.0029860	-4.2671400	1.3087790
6	4.1868090	-5.6378910	1.5327030
6	5.1086540	-3.4111430	1.4304210
6	5.4463210	-6.1405970	1.8490300
1	3.3490270	-6.3189960	1.4839470
6	6.3614060	-3.9209780	1.7447650
1	4.9687540	-2.3503320	1.2767050
6	6.5401800	-5.2905190	1.9519080
1	5.5701450	-7.2028690	2.0229750
1	7.5223160	-5.6801380	2.1878350
6	7.5338630	-2.9913580	1.9115820
9	7.3597770	-1.8235170	1.2600920
9	8.6789460	-3.5428530	1.4494360
9	7.7480780	-2.6888480	3.2125890
7	-2.6630080	-1.9600510	-0.7879220
7	-1.7304200	0.1387880	0.6755880
6	0.2680760	-8.9135580	0.0924770
7	-0.3224050	-9.8018230	0.5346890
1	3.0582310	-7.0577280	-3.0548940

1 1.7814380 -8.9625080 -2.1070470

Table ST16. Cartesian coordinates for optimized geometry of Ligand 2

6	-2.4523440	-4.4677900	-1.7766390
6	-1.2065130	-4.4615510	-1.1865890
6	-0.6386360	-3.2419830	-0.7641030
6	-1.3974950	-2.0499060	-1.0009410
6	-3.1208650	-3.2468480	-1.9417770
6	0.6429290	-3.0781140	-0.1352200
6	-0.8640810	-0.7295450	-0.6331100
6	0.4223170	-0.6248160	-0.0488020
6	1.1614380	-1.8302500	0.1834010
6	0.9118910	0.6508870	0.2804500
1	1.8933270	0.7399960	0.7301400
6	0.1215140	1.7497310	0.0233310
6	-1.1427390	1.5438490	-0.5571800
1	-2.9078510	-5.3933060	-2.1080930
1	-0.6715500	-5.3907090	-1.0575900
1	-4.1076980	-3.2182130	-2.3969970
1	0.4551240	2.7529740	0.2608690
1	-1.7878350	2.3933220	-0.7684480

6	2.6853010	-3.2236570	0.7662790
7	2.4121500	-1.9374670	0.7247820
7	1.6316440	-3.9851350	0.2557530
6	1.6171690	-5.4042260	0.0673010
6	2.3506350	-5.9726820	-0.9735990
6	0.8737910	-6.2064880	0.9289240
6	2.3433980	-7.3542260	-1.1519010
1	2.9205060	-5.3311830	-1.6342730
6	0.8641590	-7.5943310	0.7415470
1	0.3073910	-5.7578750	1.7352530
6	1.6043000	-8.1687150	-0.3026810
6	3.9652700	-3.7414110	1.2761700
6	4.1183270	-4.9826570	1.9096130
6	5.0870530	-2.9024390	1.1647100
6	5.3585300	-5.3829420	2.3942550
1	3.2705110	-5.6364060	2.0543400
6	6.3234400	-3.3014580	1.6476490
1	4.9648230	-1.9328810	0.7009250
6	6.4650440	-4.5482320	2.2596760
1	5.4603500	-6.3379790	2.8934190

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- 6 7.8196720 -5.0032450 2.7268230
- 9 8.5718390 -3.9756260 3.1755160
- 9 8.5203140 -5.5883700 1.7254780
- 9 7.7380980 -5.9090340 3.7245530
- 7 -2.6134930 -2.0835380 -1.5748170
- 7 -1.6253750 0.3557200 -0.8768210
- 6 0.1009340 -8.4268680 1.6212550
- 7 -0.5132620 -9.1015110 2.3289340
- 1 2.9153680 -7.7957640 -1.9587500
- 1 1.5931330 -9.2427830 -0.4375010
- 1 7.1791120 -2.6442800 1.5566770

Table ST17. Cartesian coordinates for optimized geometry of Ligand 3

- 6 -2.4726130 -4.4655720 -1.7488200
- 6 -1.2243380 -4.4587690 -1.1640070
- 6 -0.6508210 -3.2381810 -0.7512840
- 6 -1.4089310 -2.0456070 -0.9922060
- 6 -3.1389920 -3.2441790 -1.9193960
- 6 0.6340150 -3.0742130 -0.1303870
- 6 -0.8709490 -0.7253860 -0.6335270
- 6 0.4183520 -0.6218710 -0.0545490

6	1.1563740	-1.8269110	0.1799860
6	0.9131990	0.6540990	0.2663640
1	1.8969300	0.7405640	0.7115590
6	0.1257450	1.7542930	0.0065820
6	-1.1414880	1.5496640	-0.5682780
1	-2.9316290	-5.3922560	-2.0723990
1	-0.6913020	-5.3886470	-1.0310700
1	-4.1274300	-3.2161080	-2.3713590
1	0.4635570	2.7577360	0.2376410
1	-1.7844020	2.4004500	-0.7815640
6	2.6851250	-3.2180670	0.7590960
7	2.4107380	-1.9322580	0.7160460
7	1.6266400	-3.9806070	0.2566840
6	1.6163330	-5.3986340	0.0689270
6	2.3591250	-5.9656010	-0.9662030
6	0.8710090	-6.2042190	0.9258710
6	2.3597330	-7.3471020	-1.1435210
1	2.9314240	-5.3214410	-1.6219640
6	0.8689480	-7.5922350	0.7397490
1	0.2983730	-5.7571260	1.7286280

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6	1.618905	-8.1643710	-0.2986390
6	3.9657800	-3.7434030	1.2579730
6	4.1119470	-4.9658460	1.9251740
6	5.1035110	-2.9332340	1.1049800
6	5.3557940	-5.3681180	2.4041180
1	3.2561340	-5.6025120	2.1022900
6	6.3376860	-3.3442290	1.5841980
1	4.9949480	-1.9753960	0.6128250
6	6.4916000	-4.5733800	2.2389850
1	5.4380430	-6.3151450	2.9272040
6	7.8425850	-5.0179810	2.7414210
7	-2.6274330	-2.0799770	-1.5613890
7	-1.6295450	0.3617770	-0.8799010
6	0.1049990	-8.4282240	1.6155150
7	-0.5088410	-9.1066350	2.3200500
1	2.9389770	-7.7866760	-1.9463350
1	1.6138210	-9.2386900	-0.4321310
1	7.1999390	-2.6986270	1.4503200
1	8.3374510	-4.2224320	3.3052880
1	8.5034900	-5.2839800	1.9096150

1 7.7594020 -5.8912770 3.3910960

Table ST18. Cartesian coordinates for optimized geometry of Ligand 4

6	-3.8786520	2.4918710	1.1635130
6	-2.6367440	1.9865980	0.8431240
6	-2.5216530	0.6666990	0.3608120
6	-3.7276830	-0.1000060	0.2582190
6	-4.9998650	1.6665680	0.9992950
6	-1.3008590	0.0071770	-0.0123430
6	-3.6935980	-1.5028350	-0.1803110
6	-2.4538410	-2.1163910	-0.4894500
6	-1.2624270	-1.3278760	-0.3873920
6	-2.4493210	-3.4643920	-0.8883310
1	-1.5059500	-3.9395450	-1.1288210
6	-3.6499080	-4.1357460	-0.9658780
6	-4.8285190	-3.4396300	-0.6428830
1	-3.9901320	3.5033440	1.5357400
1	-1.7589540	2.6029120	0.9709210
1	-5.9943160	2.0382140	1.2338010
1	-3.6968590	-5.1747640	-1.2702100
1	-5.7898790	-3.9448500	-0.6988600

6	0.7848060	-0.6907480	-0.4310560
7	0.0224340	-1.7410210	-0.6306890
7	0.0320670	0.4244840	-0.0508330
6	0.5581840	1.7114950	0.2851340
6	1.2819710	1.8782010	1.4655910
6	0.3568690	2.7869140	-0.5757470
6	1.8055400	3.1280360	1.7874140
1	1.4311100	1.0294110	2.1211540
6	0.8775050	4.0436650	-0.2438530
1	-0.2022350	2.6508080	-1.4928170
6	1.6056910	4.2130260	0.9428750
7	-4.9290300	0.4189420	0.5709410
7	-4.8598760	-2.1741090	-0.2634720
6	2.2514150	-0.6559520	-0.6086520
6	3.0945340	-1.6057120	0.0609510
6	2.8158650	0.2858460	-1.4481640
6	2.5986570	-2.6051990	0.9405720
6	4.5099220	-1.5335210	-0.1542030
6	4.2084230	0.3439100	-1.6590930
1	2.1774290	0.9827250	-1.9765720

6	3.4521310	-3.4796010	1.5695340	
1	1.5314740	-2.6886560	1.0904310	
6	5.3600320	-2.4560010	0.5101780	
6	5.0373960	-0.5447100	-1.0232110	
1	4.6142390	1.0901530	-2.3321000	
6	4.8464190	-3.4082210	1.3541550	
1	3.0510570	-4.2365130	2.2341510	
1	6.4290650	-2.3930570	0.3362440	
1	6.1102000	-0.5066350	-1.1800720	
1	5.5060290	-4.1078100	1.8548920	
1	2.3699380	3.2551660	2.7030790	
1	2.0076420	5.1876260	1.1888900	
6	0.6721190	5.1544300	-1.1232760	
7	0.5092180	6.0522910	-1.8309480	

Table ST19. Cartesian coordinates for optimized geometry of Ligand 5

- 6 -4.3330760 2.6462310 0.1101860
- 6 -3.0696390 2.1072350 -0.0066200
- 6 -2.9069890 0.7069280 -0.0461460
- 6 -4.0909820 -0.0923020 0.0705790
- 6 -5.4285080 1.7749050 0.1873630

6	-1.6598530	0.0038200	-0.1615550
6	-4.0092580	-1.5598110	0.1001210
6	-2.7454970	-2.1980140	0.0347140
6	-1.5765890	-1.3793540	-0.0897530
6	-2.6956860	-3.6019050	0.0854000
1	-1.7335820	-4.0970460	0.0341270
6	-3.8767820	-4.3028940	0.1932530
6	-5.0819980	-3.5798990	0.2463460
1	-4.4805300	3.7191590	0.1463130
1	-2.2114730	2.7610610	-0.0574190
1	-6.4386490	2.1683220	0.2706920
1	-3.8888280	-5.3857460	0.2342380
1	-6.0288220	-4.1085730	0.3278590
6	0.4548390	-0.7203840	-0.2977640
7	-0.2781230	-1.8045240	-0.1669970
7	-0.3366220	0.4315800	-0.3079680
6	0.1299170	1.7811830	-0.3864500
6	0.7797130	2.3488650	0.7040600
6	-0.0581430	2.5160550	-1.5592200
6	1.2494250	3.6663010	0.6178120

1	0.9224210	1.7743240	1.6098160
6	0.4032010	3.8269430	-1.6375410
1	-0.5638900	2.0548910	-2.3990410
6	1.0583390	4.4069210	-0.5565080
1	0.2561180	4.3967130	-2.5470310
1	1.4231070	5.4246670	-0.6122070
7	-5.3138260	0.4589180	0.1747270
7	-5.1561660	-2.2611510	0.2029550
6	2.5950090	-1.7336600	0.3114680
6	4.0017570	-1.8619750	0.2456370
6	1.9236390	-0.7508820	-0.3935270
6	4.7019230	-2.8602420	0.9746740
6	4.7452830	-0.9581740	-0.5768110
6	2.6706310	0.1356760	-1.2195440
6	6.0688490	-2.9588010	0.8930000
1	4.1365970	-3.5448220	1.5979140
6	6.1560740	-1.0879920	-0.6397160
6	4.0353840	0.0301620	-1.3053450
1	2.1605560	0.8848480	-1.8093710
6	6.8030440	-2.0644490	0.0781110

- 1 6.5931370 -3.7242380 1.4537060
- 1 6.7181540 -0.4020580 -1.2647550
- 1 4.5899470 0.7054340 -1.9483670
- 1 7.8820410 -2.1541630 0.0234560
- 1 2.0251330 -2.4232850 0.9222130
- 6 1.9214390 4.2580360 1.7347870
- 7 2.4627030 4.7408000 2.6332550

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