

Supporting information

FOR

A new TPE-based tetrapodal ligand and its Ln(III) complexes: Multi-stimuli responsive AIE (aggregation-induced emission)/ILCT (intraligand charge transfer)-Bifunctional Photoluminescence and NIR emission sensitization

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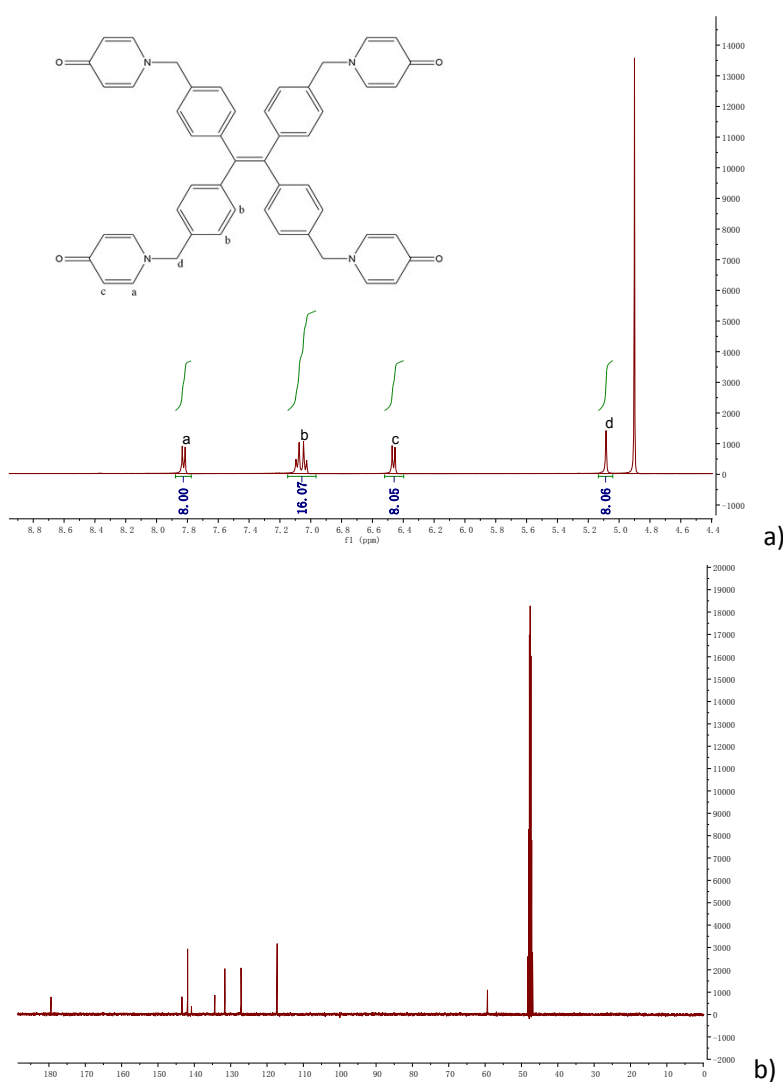


Fig. S1 (a) ¹H NMR (400 MHz, CD₃OD, 25 °C) and (b) ¹³C NMR (101 MHz, CD₃OD, 25 °C) of TPE-4PO ligand.

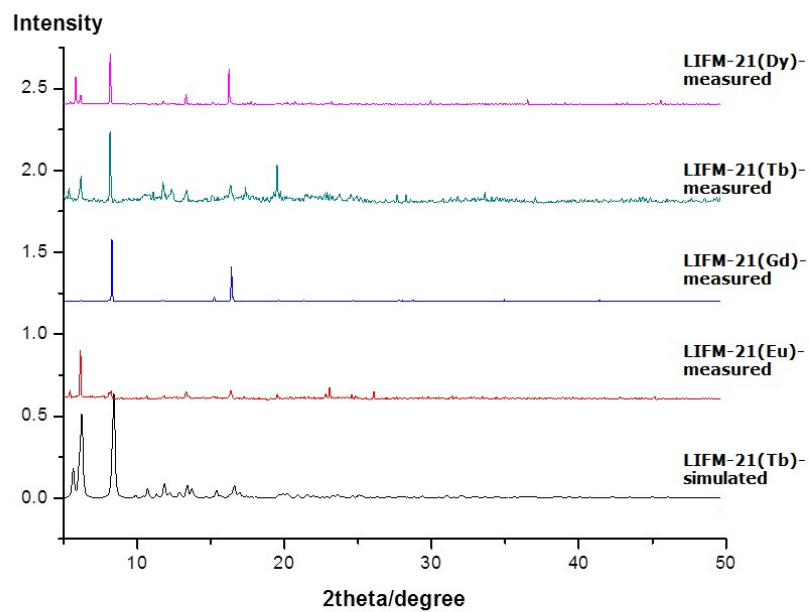


Fig. S2 The measured powder XRD patterns of complexes LIFM-21(Ln) series (Ln = Eu, Gd, Tb, Dy) in comparison to the simulated pattern of single-crystal LIFM-21(Tb).

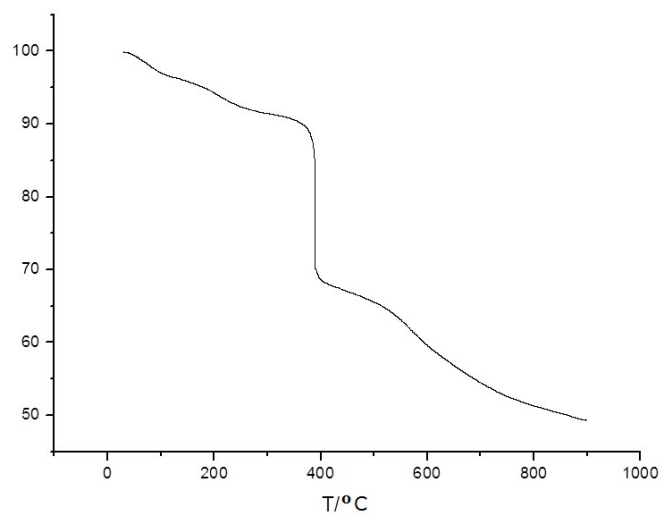


Fig. S3 TG curve of complex LIFM-21(Tb).

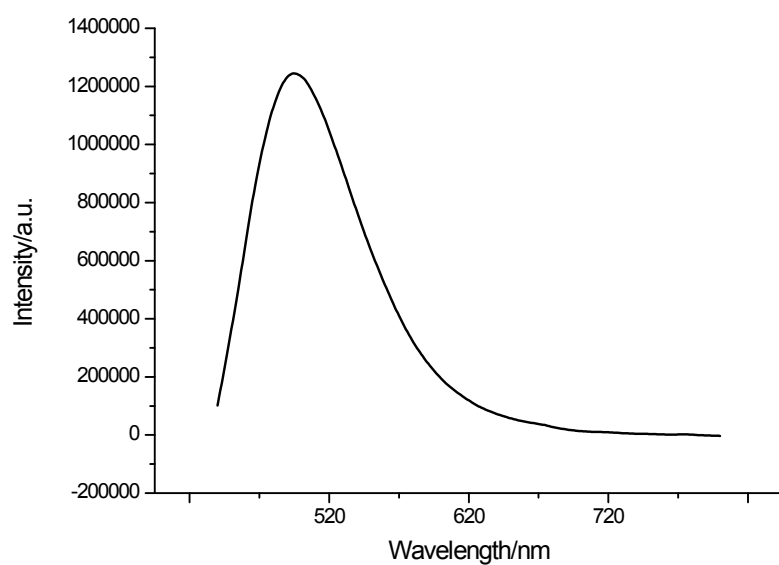


Fig. S4 Solid-state phosphorescence spectra of complex LIFM-21(Gd) measured at 77 K.

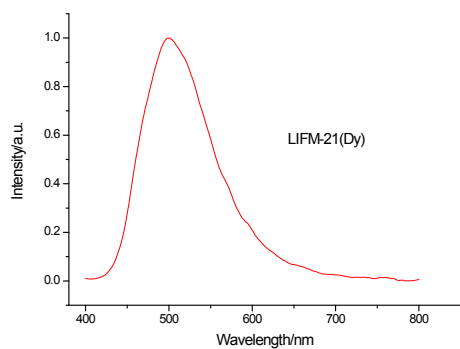
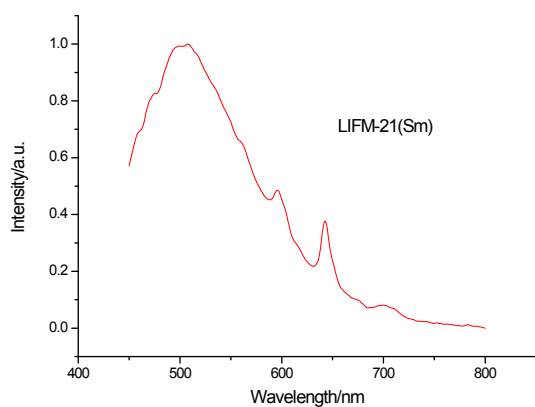


Fig. S5 Solid state visible emission of complex LIFM-21(Sm) and LIFM-21(Dy) measured at room temperature ($\lambda_{\text{ex}} = 395 \text{ nm}$).

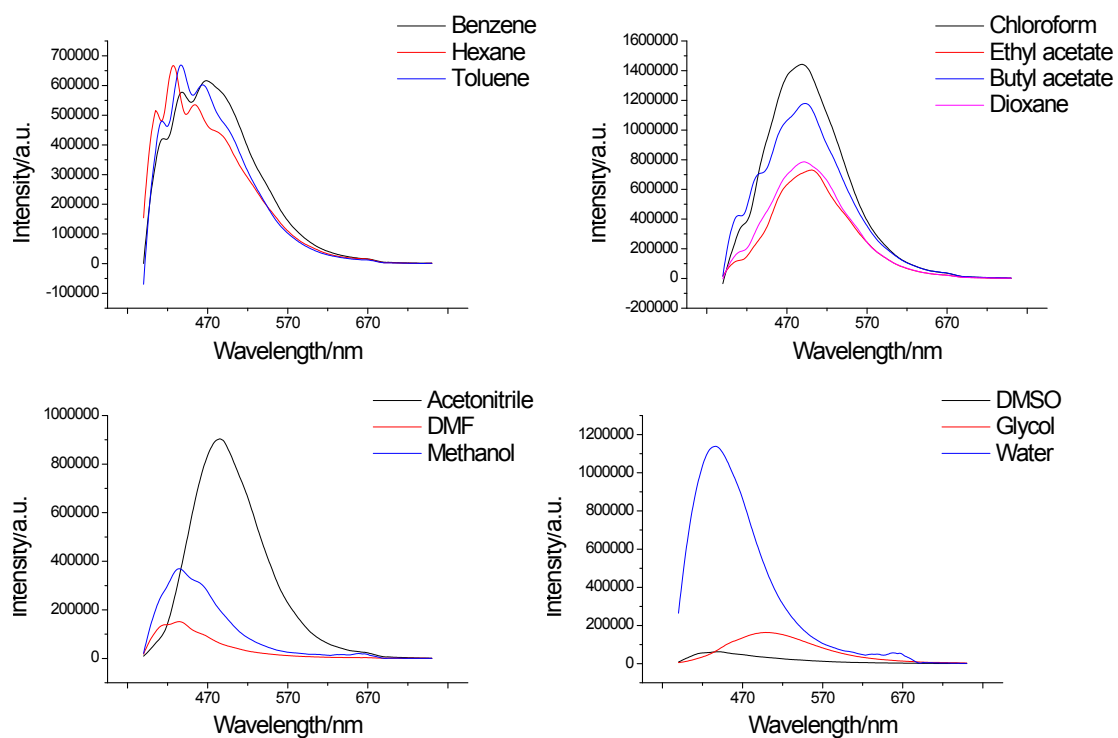


Fig. S6 Emission spectra of LIFM-21(Tb) dispersed in different solvents.

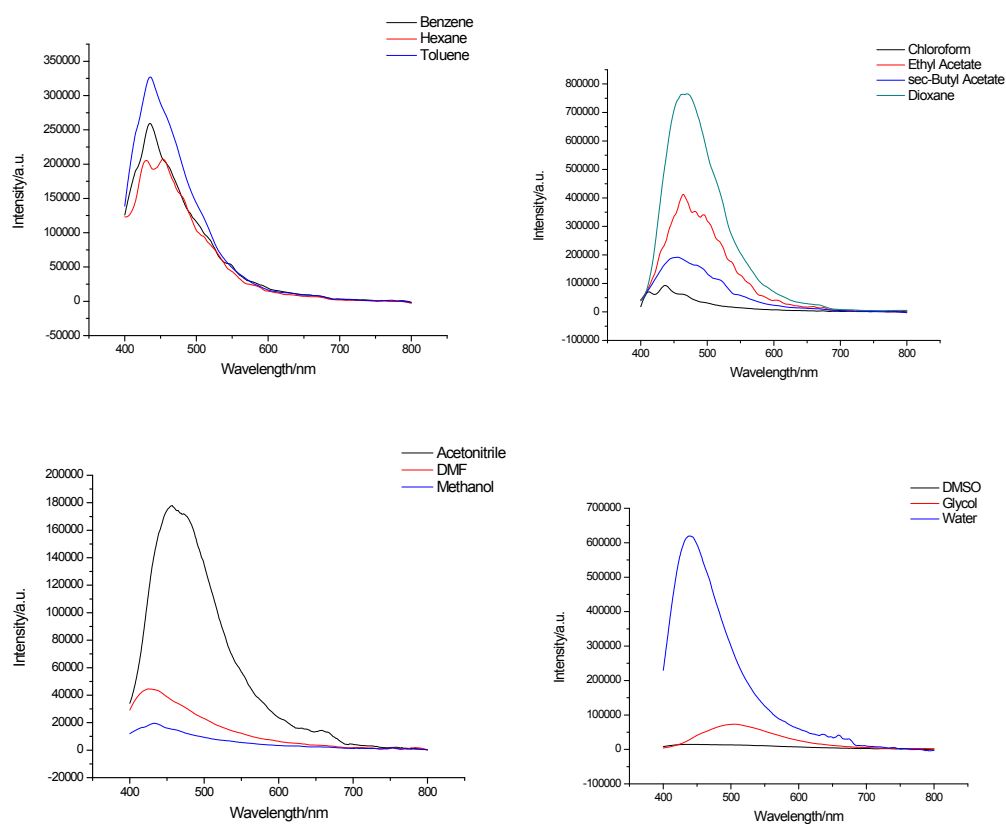


Fig. S7 Emission spectra of TPE-4PO dispersed in different solvents.

Table S1 Crystallographic data for complex LIFM-21(Tb).

LIFM-21(Tb)	
Formula	C ₅₀ H ₄₀ N ₆ O ₁₁ Tb
F.w.	1059.80
<i>T</i> (K)	173(2)
Crystal system	monoclinic
Space group	<i>P</i> 2 ₁ /c
<i>a</i> (Å)	28.363(2)
<i>b</i> (Å)	17.009(3)
<i>c</i> (Å)	15.655(9)
α (°)	90
β (°)	90
γ (°)	90
<i>V</i> (Å ³)	7552.4 (4)
<i>Z</i>	4
<i>D</i> _c (g cm ⁻³)	0.932
μ (mm ⁻¹)	4.958
<i>F</i> (000)	2140
<i>R</i> ₁ (>2 σ)	0.0831
<i>wR</i> ₂ (all data)	0.2464
GOF	0.946

Table S2 Selected bond lengths (Å) and angles (°) for complex LIFM-21(Tb).

LIFM-21(Tb)			
Bond	Å	Angle	°
O6-Tb1	2.488(15)	O1#4-Tb1-O1 #2	138.4(7)
O2-Tb1	2.266(6)	O1-Tb1-O2 #4	82.9(4)
O1-Tb1 #2	2.261(10)	O1-Tb1-O2 #2	90.0(3)
Tb1-O1 #4	2.261(10)	O1#4-Tb1-O2#3	90.0(3)
Tb1-O1 #2	2.261(10)	O1#2-Tb1-O2#3	82.9(4)
Tb1-O2 #3	2.266(6)	O2-Tb1-O2#3	160.0(4)
Tb1-O3	2.410(9)	O1-Tb1-O3 #4	78.0(5)
Tb1-O3 #3	2.410(9)	O1-Tb1-O3 #2	138.4(4)
Tb1-O6 #3	2.488(16)	O2-Tb1-O3	119.6(3)
Tb1-O5	2.586(7)	O2-Tb1-O3 #3	76.7(3)
Tb1 O5 #3	2.586(7)	O1 #4-Tb1-O3 #3	138.4(4)
Tb1-N3	2.853(13)	O1#2- Tb1-O3 #3	78.0(5)
Tb1-N3 #3	2.853(13)	O2-Tb1-O3 #3	76.7(3)

'x, y, z'; '-x+1/2, -y+1/2, z'; 'x, -y+1/2, -z'; '-x+1/2, y, -z'; '-x, -y, -z'; 'x-1/2, y-1/2, -z'; '-x, y-1/2, z'; 'x-1/2, -y, z'