

Supporting Information

for

Di-functional Luminescent Sensors Based on Y³⁺ Doped Eu³⁺ and Tb³⁺ Coordination Polymers: Fast Responsive and Visible Detection of Cr³⁺, Fe³⁺ ions in aqueous solutions and Acetone

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Table S1

Complex	1-Y	1-Eu¹	1-Tb¹	1-Gd²
Crystal data	1989014	1814159	1814160	1864276
formula	[Y(C ₁₆ H ₆ O ₈) _{0.5} (C ₄ H ₉ ON) (C ₂ H ₃ O ₂)(H ₂ O)]	[Eu ₂ (C ₁₆ H ₆ O ₈)(C ₄ H ₉ ON) ₂ (C ₂ H ₃ O ₂) ₂ ·4H ₂ O	[Tb ₂ (C ₁₆ H ₆ O ₈)(C ₄ H ₉ ON)) ₂ (C ₂ H ₃ O ₂) ₂ ·4H ₂ O	[Gd(C ₁₆ H ₆ O ₈) _{0.5} (C ₄ H ₉ ON) (C ₂ H ₃ O ₂)(H ₂ O)]
<i>M_r</i>	416.2	988.5	1002.4	484.5
Temperature/K	298	298	298	298
crystal size/mm ³	0.11 × 0.14 × 0.14	0.13 × 0.16 × 0.14	0.13 × 0.12 × 0.15	0.11 × 0.15 × 0.13
Crystal system,	Monoclinic	Monoclinic	Monoclinic	Monoclinic
space group	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>n</i>
<i>a</i> (Å)	9.3026(8)	9.4453(5)	9.3676(7)	9.3992(8)
<i>b</i> (Å)	17.5625 (14)	17.7439(14)	17.6232(14)	17.6714(15)
<i>c</i> (Å)	11.3369 (9)	11.3019(8)	11.3172(9)	11.2971(9)
<i>α, β, γ</i> °	90, 94.35(1), 90	90, 94.278(1), 90	90, 94.351(2), 90	90, 94.318(3), 90
<i>V</i> /Å ³	1846.9(3)	1888.9(2)	1862.9(3)	1871.1(3)
<i>Z</i>	2	1	1	2
F(000)	836	932	972	944
Radiation type	Mo <i>Kα</i>	Mo <i>Kα</i>	Mo <i>Kα</i>	Mo <i>Kα</i>
<i>μ</i> (mm ⁻¹)	3.2	3.36	3.83	3.58
Data collection	Bruker APEXII CCD	Bruker APEXII CCD	Bruker APEXII CCD	Bruker APEXII CCD
Diffractionmeter	Multi-scan (SADABS);	Multi-scan (SADABS);	Multi-scan (SADABS);	Multi-scan (SADABS);
Absorption correction	Sheldrick, 2003)	Sheldrick, 2003)	Sheldrick, 2003)	Sheldrick, 2003)
<i>T_{min}, T_{max}</i>	0.682, 0.741	0.356, 0.610	0.659, 0.656	0.368, 0.423
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	3254, 3254, 1686	8950, 3206, 2250	8955, 3162, 2200	8879, 3296, 2207
<i>R_{int}</i>	0.060	0.0101	0.072	0.0080
(sin <i>θ</i> /λ) _{max} (Å ⁻¹)	0.595	0.595	0.595	0.595
Refinement <i>R</i> [<i>F</i> ² > 2σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.062, 0.294, 1.0	0.072, 0.196, 0.96	0.060, 0.155, 1.01	0.091, 0.258, 1.07
No. of reflections	3354	3206	3162	3296
No. of parameters	222	208	221	209
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
<i>Δρ</i> _{max} , <i>Δρ</i> _{min}	1.80, -1.00	1.42, -2.36	1.50, -1.58	2.43, -2.74

Computer programs: *CrysAlis PRO*, Agilent Technologies, *SHELXL97* (Sheldrick, 1997). *SHELXL2014* (Sheldrick, 2015),

DIAMOND (Brandenburg & Putz, 2005) and *pubCIF* (Westrip, 2010).

1-Eu, **1-Tb** and **1-Gd** have been published in our previous work.¹⁻²

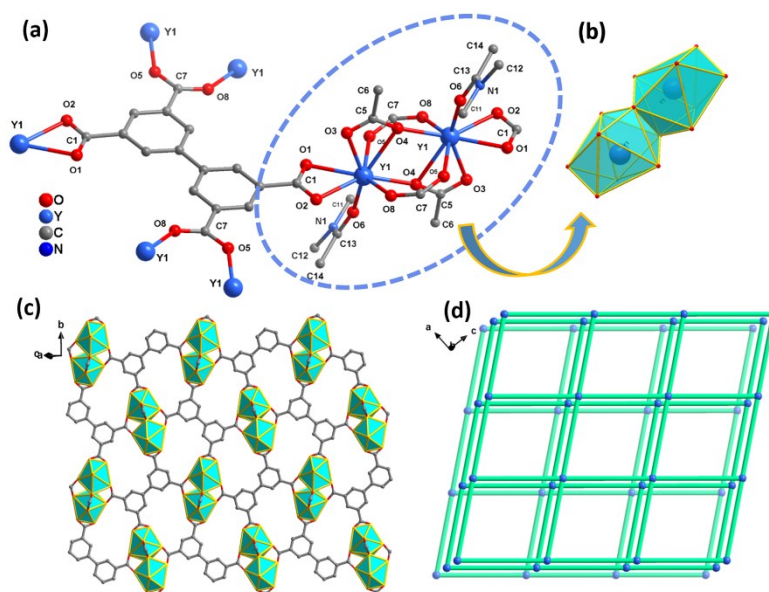


Fig.S1 View of the coordination environments of the ligand (a) and Y(III)(b) atoms. (code: C, gray ; O, red; N, dark blue; Y, blue) The hydrogen atoms are omitted for clarity. (c) The polyhedron of 3D framework viewed from b axis. (d) The simplified topology structure of **1-Y**.

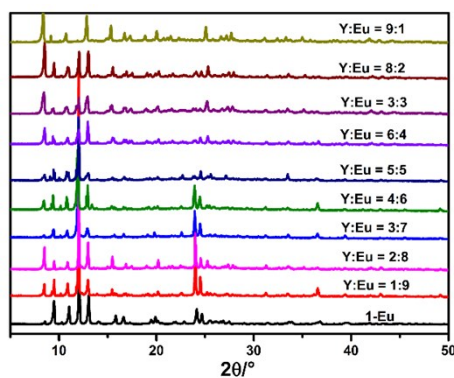


Fig. S2 PXRD patterns of $\text{Eu}_x\text{Y}_{1-x}$ ($x = 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9$).

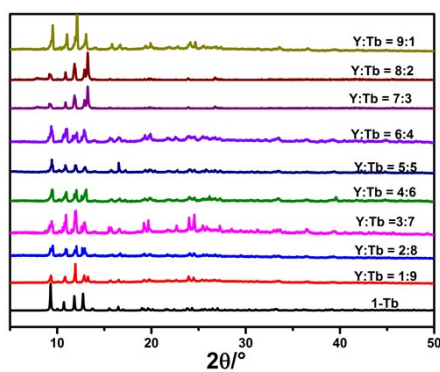


Fig.S3 PXRD patterns of Tb_xY_{1-x} ($x = 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9$).

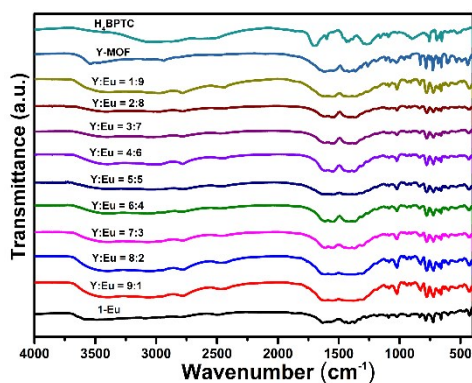


Fig.S4 IR spectra (KBr pellet, cm⁻¹) of H₄BPTC, 1-Y and Eu_xY_{1-x} ($x = 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9$).

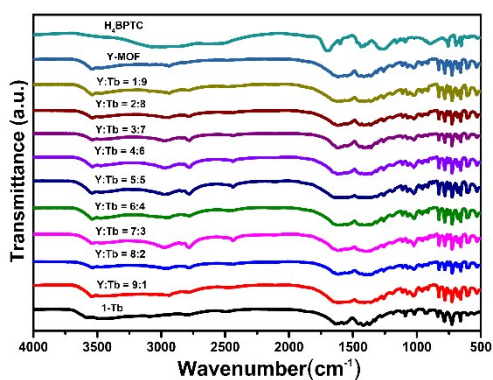


Fig.S5 IR spectra (KBr pellet, cm⁻¹) of H₄BPTC, 1-Y and Tb_xY_{1-x} ($x = 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9$).

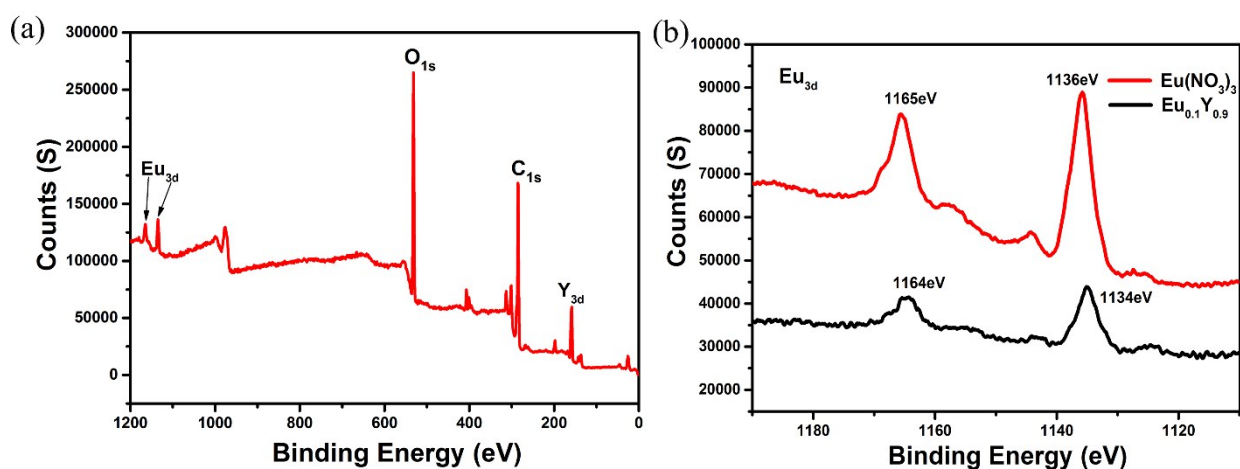


Fig. S6 XPS spectra (a) and (b) Eu_{3d} of Eu_xY_{1-x} .

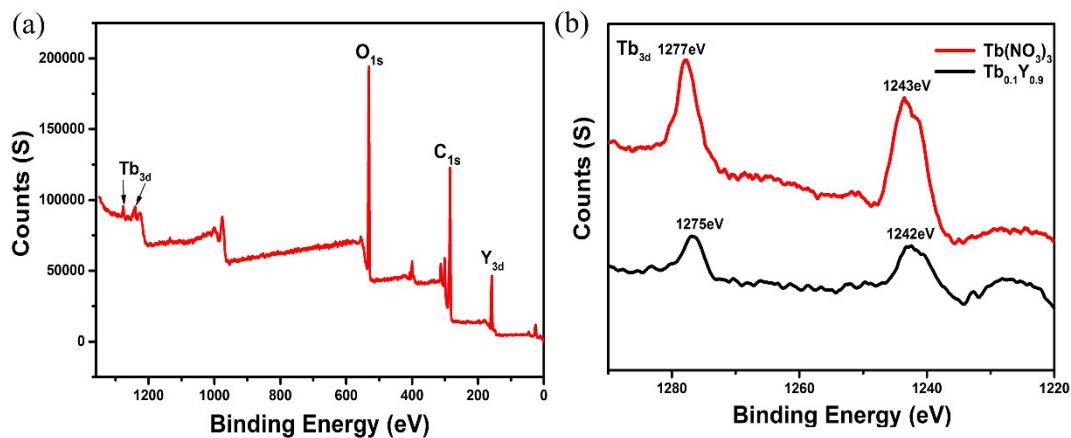


Fig. S7 XPS spectra (a) and (b) Tb_{3d} of Tb_xY_{1-x} .

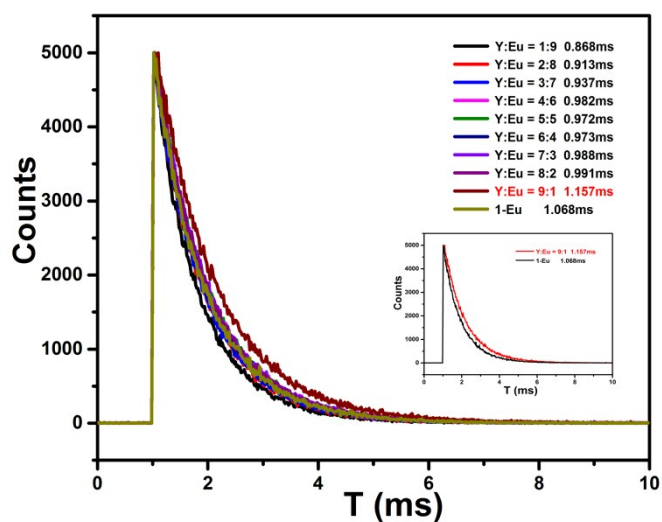


Fig.S8 The luminescence decay lifetimes of Eu_xY_{1-x} at room temperature. Insert: The luminescence decay lifetimes of 1-Eu and $Eu_{0.1}Y_{0.9}$.

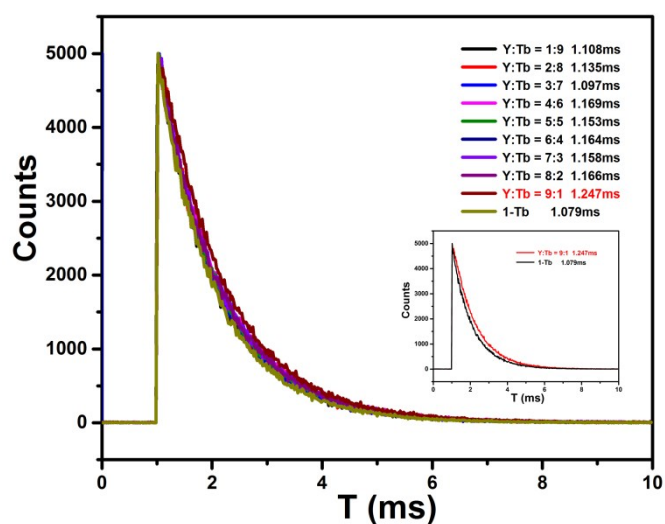


Fig.S9 The luminescence decay lifetimes of Tb_xY_{1-x} at room temperature. Insert: The luminescence decay lifetimes of **1-Tb** and $Tb_{0.1}Y_{0.9}$.

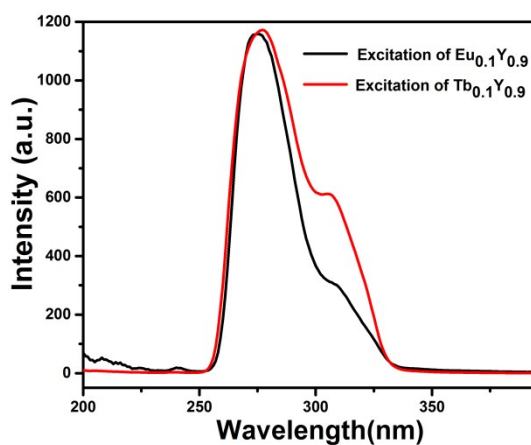


Fig. S10 The excitation spectra of $Eu_{0.1}Y_{0.9}$ and $Tb_{0.1}Y_{0.9}$.

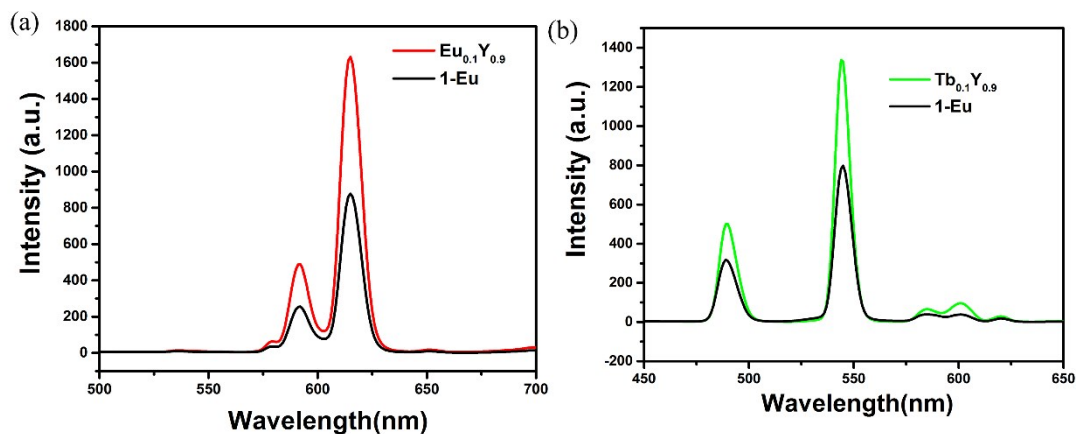


Fig.S11 Luminescent spectra of (a) $Eu_{0.1}Y_{0.9}$, **1-Eu** and (b) $Tb_{0.1}Y_{0.9}$, **1-Tb** (2mg) in DMF (2mL) when excited at 275 nm.

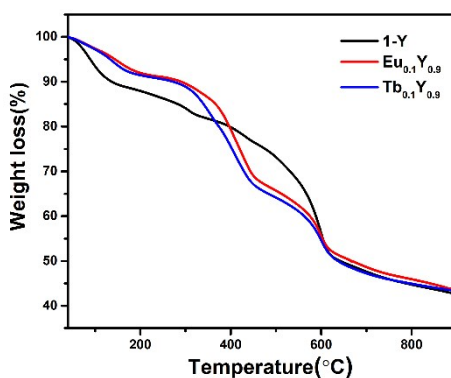


Fig.S12 TG curves of **1-Y**, $Eu_{0.1}Y_{0.9}$ and $Tb_{0.1}Y_{0.9}$.

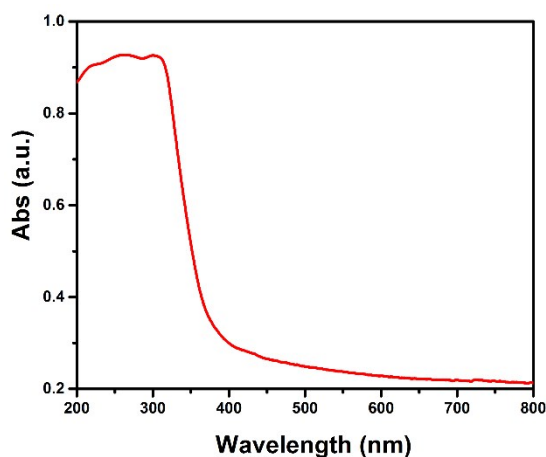


Fig.S13 UV-vis adsorption spectra of H₄BPTC in the solid state at room temperature.

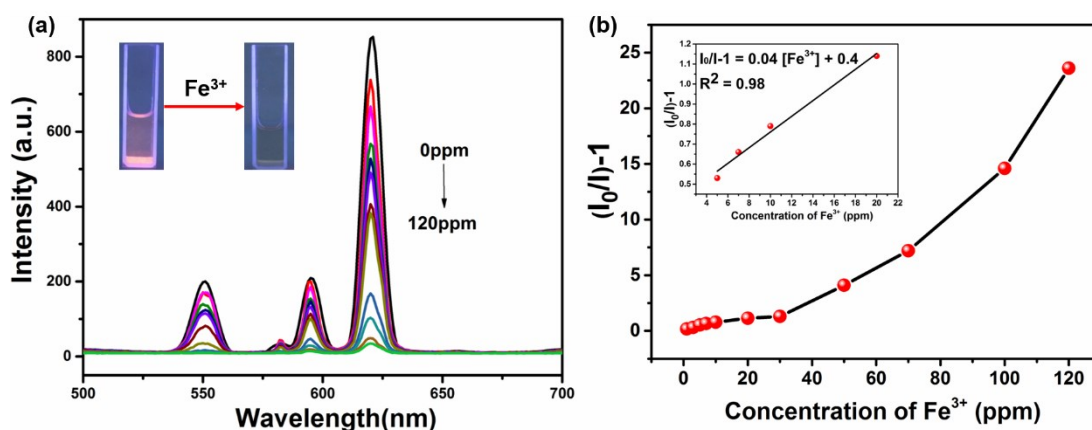


Fig.S14 (a) Luminescent spectra of Eu_{0.1}Y_{0.9} upon the addition of various Fe³⁺ concentrations in DMF when excited at 275 nm. (b) Nonlinear Stern-Volmer plot for Fe³⁺ by exponential quenching equation. Inset: linear fitting plot of the Stern-Volmer plot with 0-20 ppm of Fe³⁺.

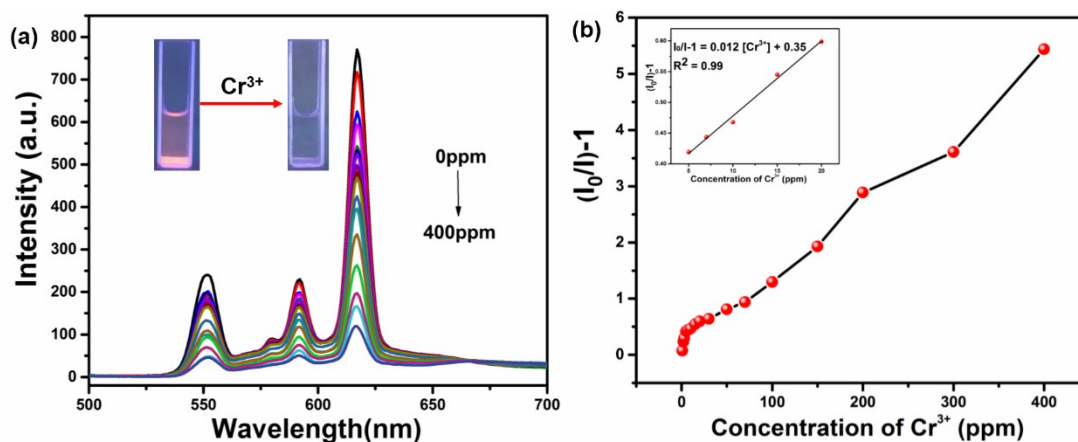


Fig.S15 (a) Luminescent spectra of Eu_{0.1}Y_{0.9} upon the addition of various Cr³⁺ concentrations in DMF when excited at 275 nm. (b) Nonlinear Stern-Volmer plot for

Cr^{3+} by exponential quenching equation. Inset: linear fitting plot of the Stern-Volmer plot with 0-20 ppm of Cr^{3+} .

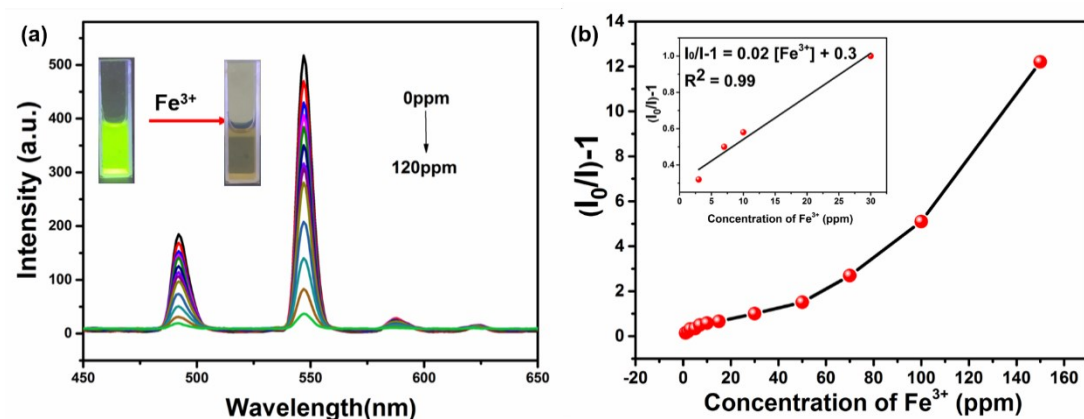


Fig.S16 (a) Luminescent spectra of $\text{Tb}_{0.1}\text{Y}_{0.9}$ upon the addition of various Fe^{3+} concentrations in DMF when excited at 275 nm. (b) Nonlinear Stern-Volmer plot for Fe^{3+} by exponential quenching equation. Inset: linear fitting plot of the Stern-Volmer plot with 0-30 ppm of Fe^{3+} .

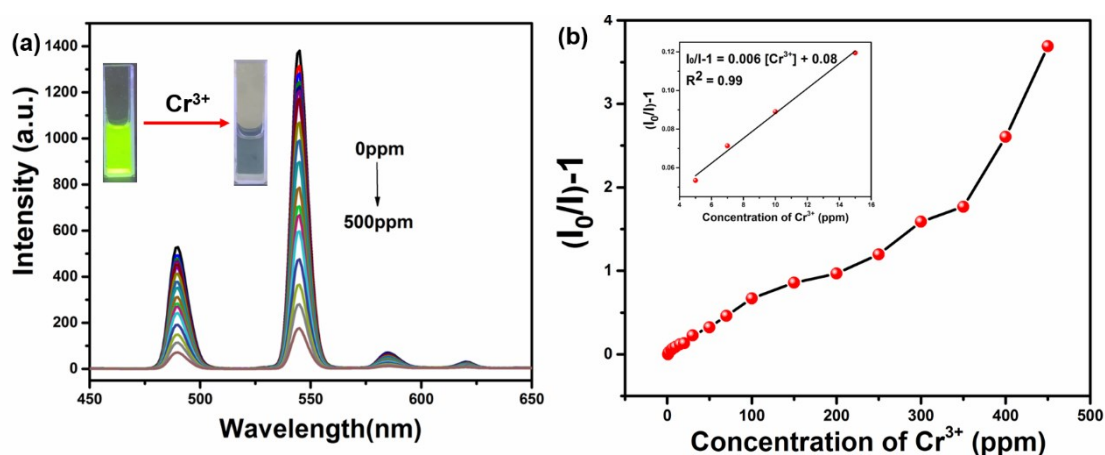


Fig.S17 (a) Luminescent spectra of $\text{Tb}_{0.1}\text{Y}_{0.9}$ upon the addition of various Cr^{3+} concentration in DMF when excited at 275 nm. (b) Nonlinear Stern-Volmer plot for Cr^{3+} by exponential quenching equation. Inset: linear fitting plot of the Stern-Volmer plot with 0-15 ppm of Cr^{3+} .

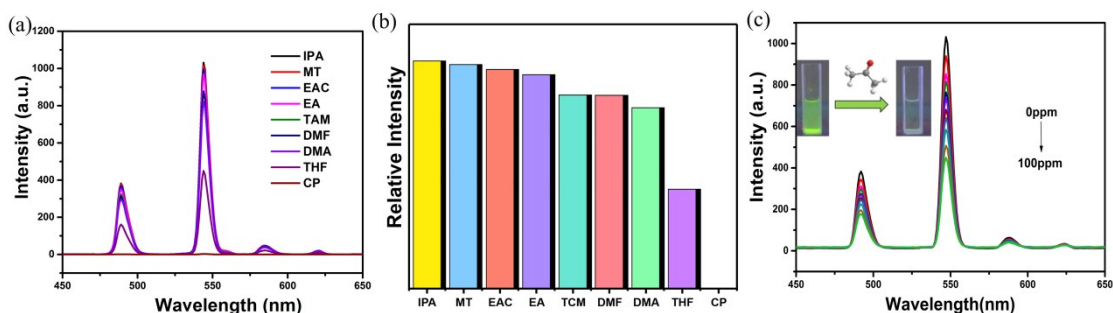


Fig.S18 (a) Luminescent spectra of $\text{Tb}_{0.1}\text{Y}_{0.9}$ dissolved in different solvents ($\lambda_{\text{ex}} = 275 \text{ nm}$). (b) Bar chart obtained for $\text{Tb}_{0.1}\text{Y}_{0.9}$ upon addition of different solvents. (c) Luminescent spectra of $\text{Tb}_{0.1}\text{Y}_{0.9}$ with the gradual addition of acetone (0-100ppm).

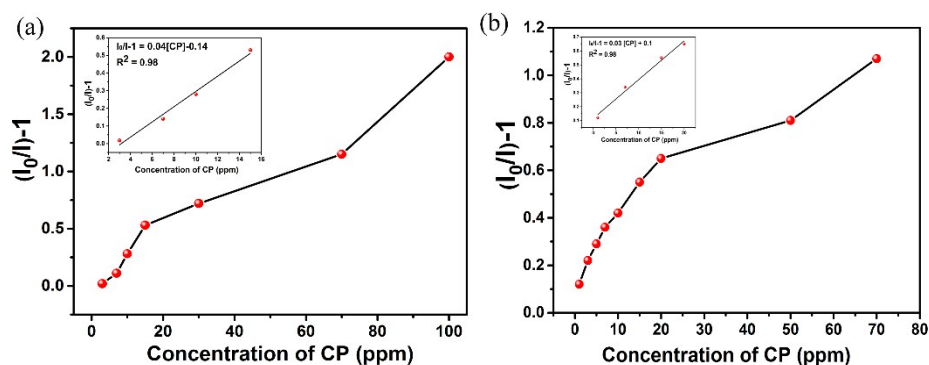


Fig.S19 (a) Nonlinear Stern-Volmer plot for acetone by exponential quenching equation for $\text{Eu}_{0.1}\text{Y}_{0.9}$. Inset: linear fitting plot of the Stern-Volmer plot with 0-15 ppm of acetone. (b) Nonlinear Stern-Volmer plot for acetone by exponential quenching equation for $\text{Tb}_{0.1}\text{Y}_{0.9}$. Inset: linear fitting plot of the Stern-Volmer plot with 0-20 ppm of acetone.

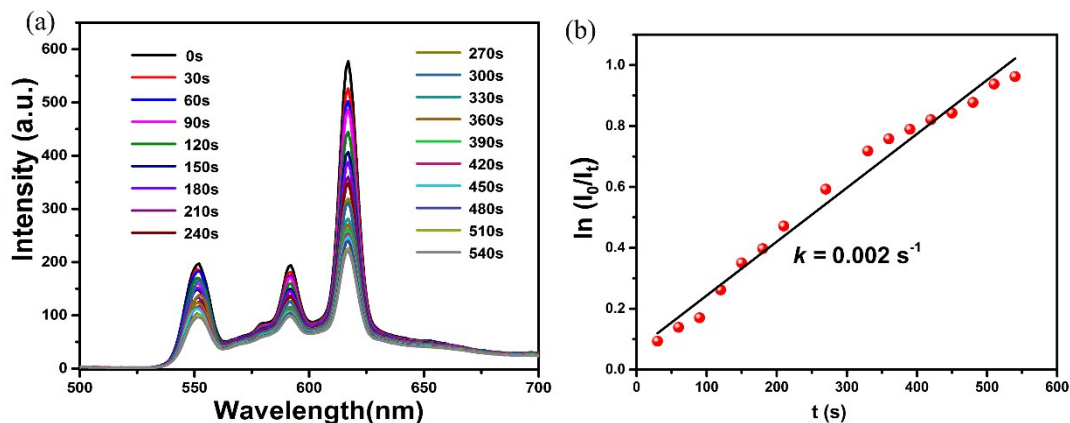


Fig.S20 (a) Time-dependent emission spectra after exposure of $\text{Eu}_{0.1}\text{Y}_{0.9}$ to Cr^{3+} ($\lambda_{\text{ex}} = 275 \text{ nm}$). (b) Plots of $\ln(I_0/I_t)$ for the luminescent intensity of $\text{Eu}_{0.1}\text{Y}_{0.9}$ at 615 nm obtained from the spectra.

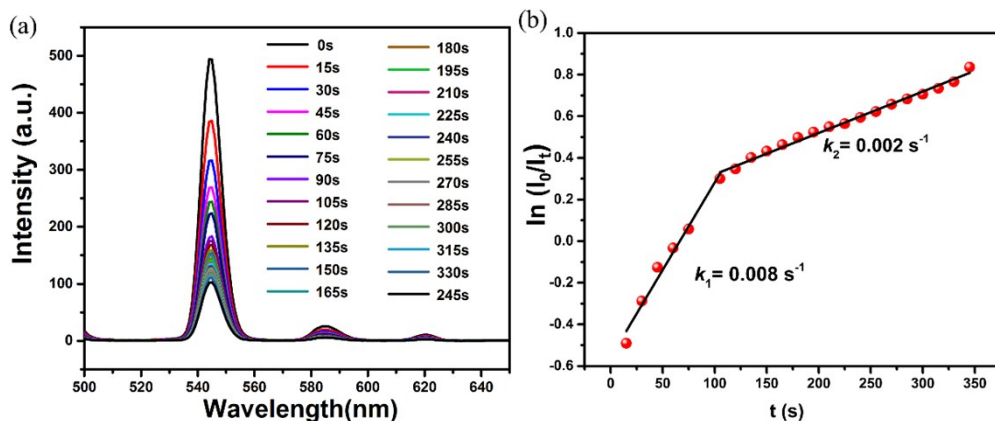


Fig.S21 (a) Time-dependent emission spectra after exposure of $\text{Tb}_{0.1}\text{Y}_{0.9}$ to Fe^{3+} ($\lambda_{\text{ex}} = 275$ nm). (b) Plots of $\ln(I_0/I_t)$ for the luminescent intensity of $\text{Tb}_{0.1}\text{Y}_{0.9}$ at 544 nm obtained from the spectra.

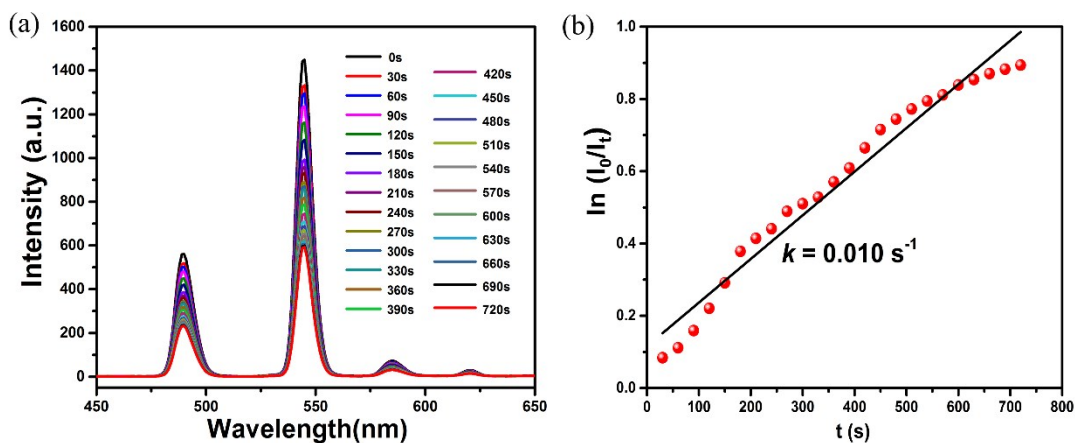


Fig.S22 (a) Time-dependent emission spectra after exposure of $\text{Tb}_{0.1}\text{Y}_{0.9}$ to Cr^{3+} ($\lambda_{\text{ex}} = 275$ nm). (b) Plots of $\ln(I_0/I_t)$ for the luminescent intensity of $\text{Tb}_{0.1}\text{Y}_{0.9}$ at 544 nm obtained from the spectra.

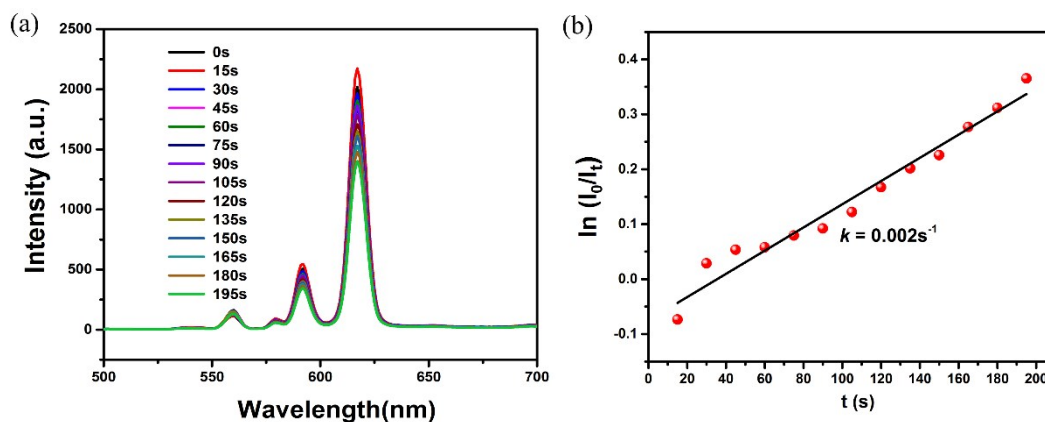


Fig.S23 (a) Time-dependent emission spectra after exposure of **1-Eu** to Fe^{3+} ($\lambda_{\text{ex}} = 275 \text{ nm}$). (b) Plots of $\ln(I_0/I_t)$ for the luminescent intensity of **1-Eu** at 615nm obtained from the spectra.

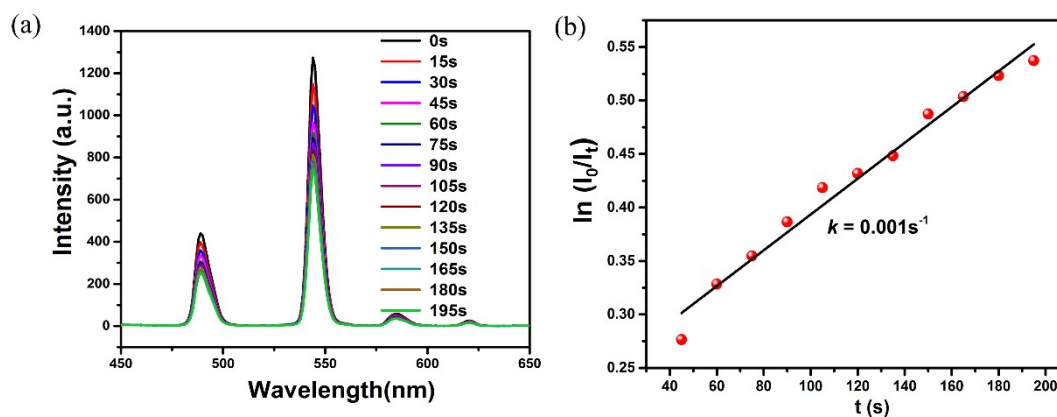


Fig.S24 (a) Time-dependent emission spectra after exposure of **1-Tb** to Fe^{3+} ($\lambda_{\text{ex}} = 275 \text{ nm}$). (b) Plots of $\ln(I_0/I_t)$ for the luminescent intensity of **1-Tb** at 544 nm obtained from the spectra.

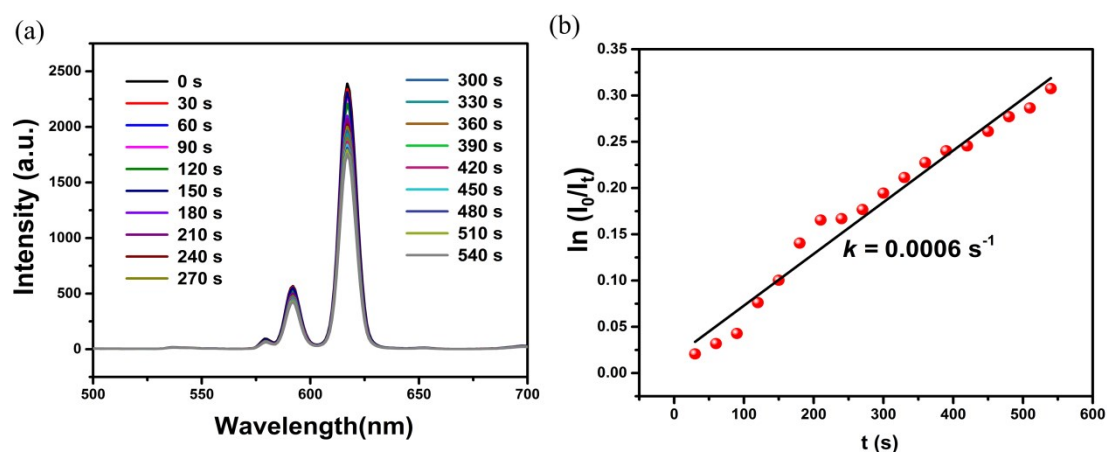


Fig.S25 (a) Time-dependent emission spectra after exposure of **1-Eu** to Cr^{3+} ($\lambda_{\text{ex}} = 275 \text{ nm}$). (b) Plots of $\ln(I_0/I_t)$ for the luminescent intensity of **1-Eu** at 615nm obtained from the spectra.

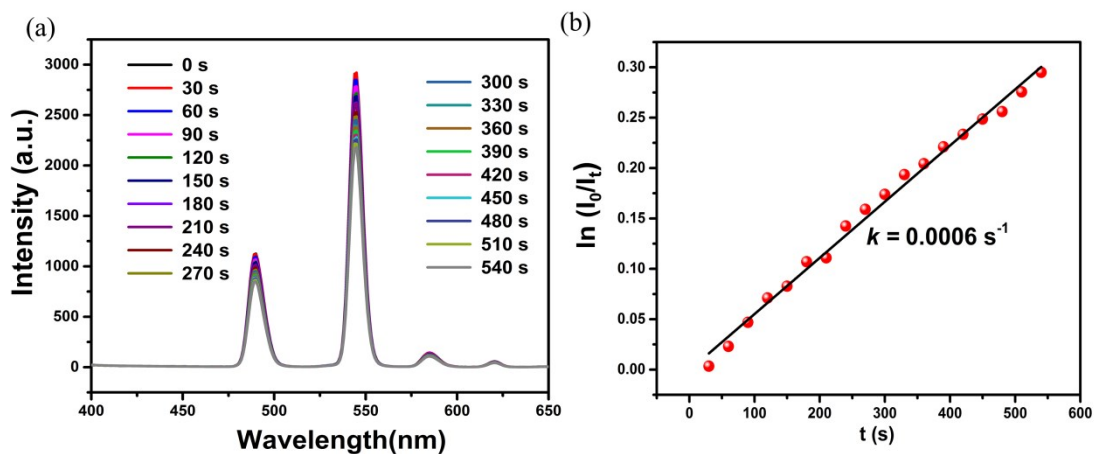


Fig.S26 (a) Time-dependent emission spectra after exposure of **1-Tb** to Cr^{3+} ($\lambda_{\text{ex}} = 275 \text{ nm}$). (b) Plots of $\ln(I_0/I_i)$ for the luminescent intensity of **1-Tb** at 544nm obtained from the spectra.

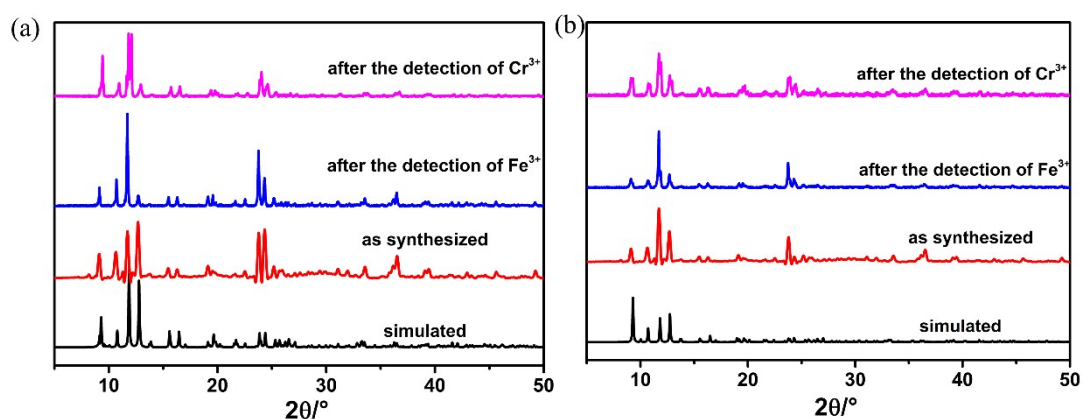


Fig.S27 The PXRD pattern of (a) $\text{Eu}_{0.1}\text{Y}_{0.9}$ and (b) $\text{Tb}_{0.1}\text{Y}_{0.9}$ before and after the detection of Fe^{3+} , Cr^{3+} and acetone.

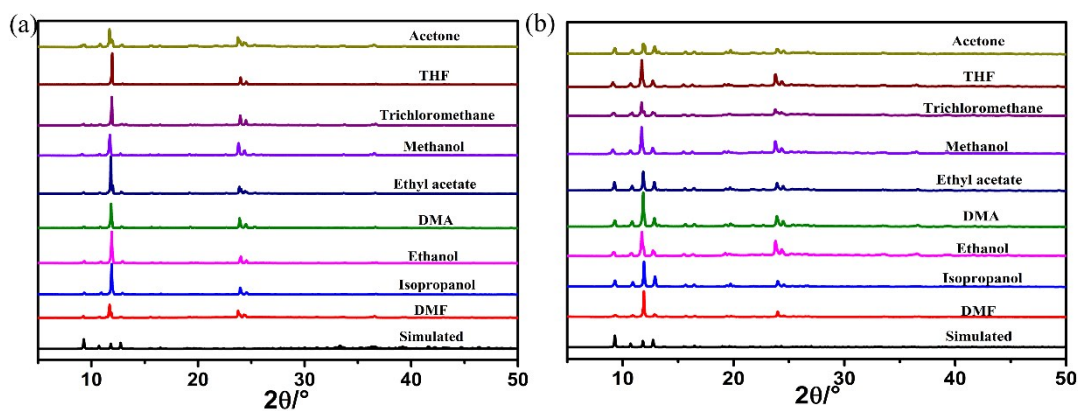


Fig.S28 PXRD patterns of (a) $\text{Eu}_{0.1}\text{Y}_{0.9}$ and (b) $\text{Tb}_{0.1}\text{Y}_{0.9}$ immersed in different organic solutions for 24 hours.

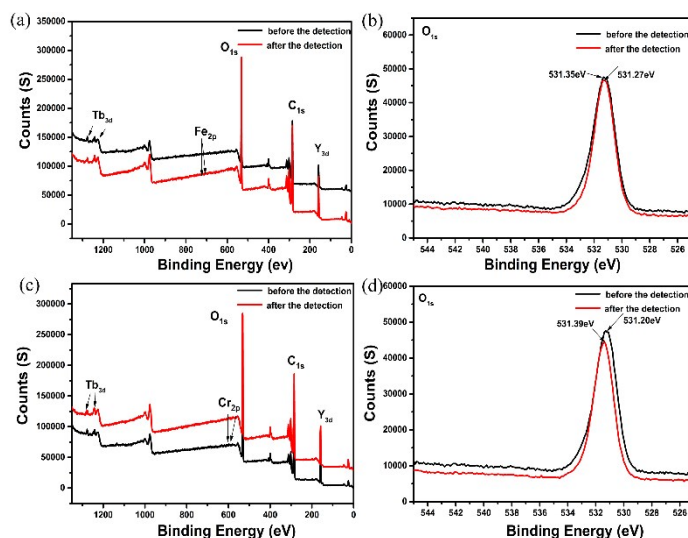


Fig.S29 The XPS spectra of $Tb_{0.1}Y_{0.9}$ before and after the detection of Fe^{3+} and Cr^{3+} .

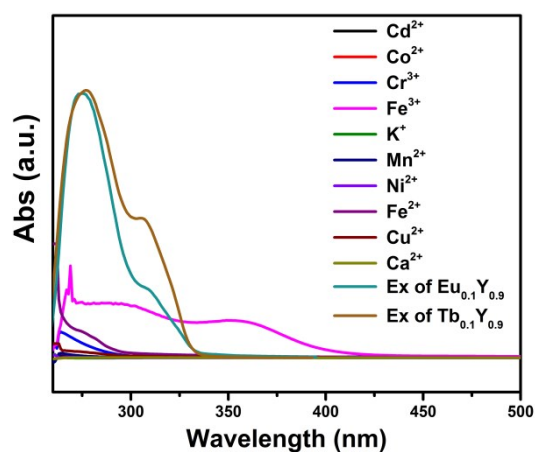


Fig.S30 Spectral overlap between the excitation spectrum of $Eu_{0.1}Y_{0.9}$, $Tb_{0.1}Y_{0.9}$ ($\lambda_{ex} = 275$ nm) and the absorption spectra of metal ions investigated in this work.

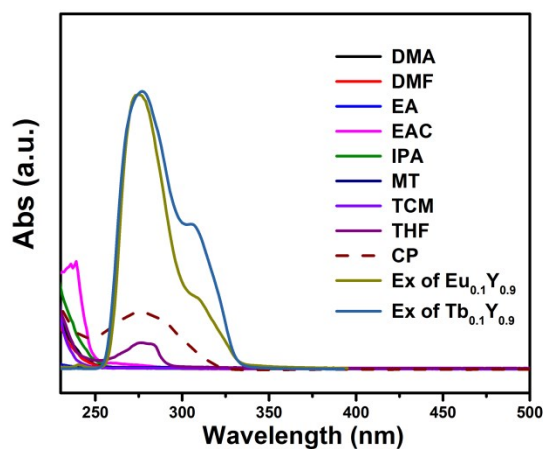


Fig.S31 Spectral overlap between the excitation spectrum of $Eu_{0.1}Y_{0.9}$, $Tb_{0.1}Y_{0.9}$ ($\lambda_{ex} = 275$ nm) and the absorption spectra of organic solutions investigated in this work.

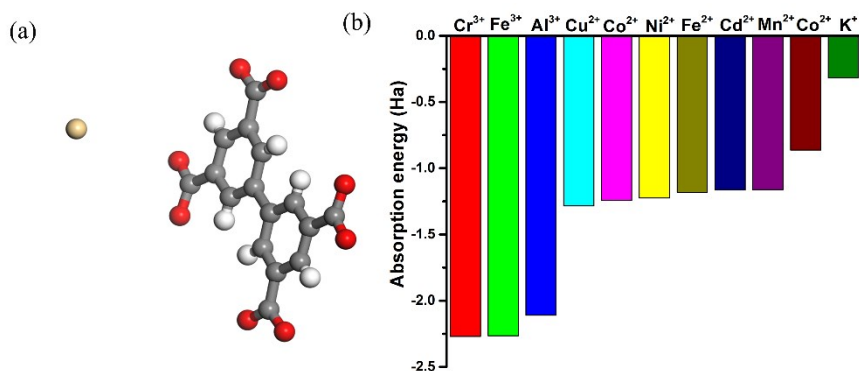


Fig. S32 (a) The proposed structural model of Mⁿ⁺ in 1-Ln. (code: C, gray; O, red; Mⁿ⁺, brown). (b) The adsorption energy results of 1-Ln treated with different metal ions calculated by DFT.

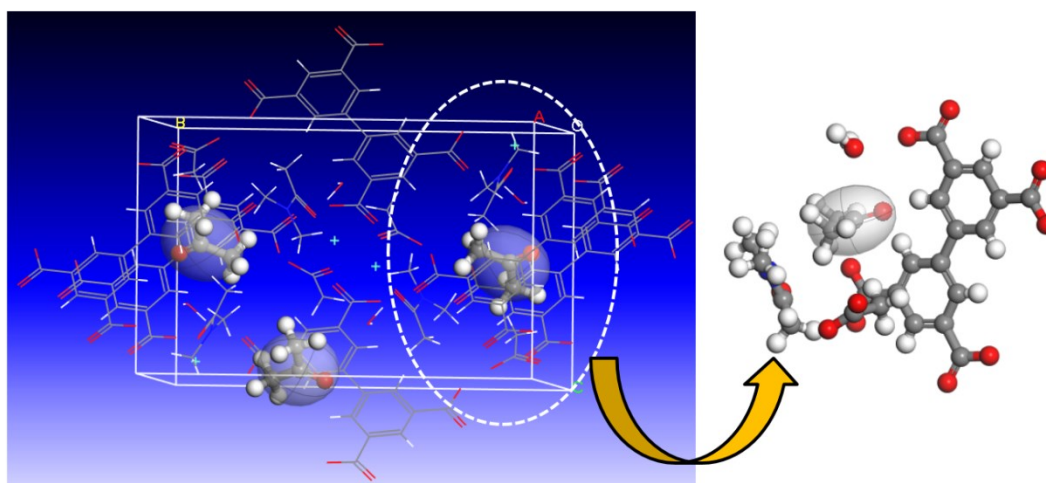


Fig.S33 The calculated adsorption locate for acetone in 1-Ln using the Sorption method.

Table S2

CP	Metal ratios from starting material preparation	Metal ratios from ICP of digested sample	X
Eu _{0.9} Y _{0.1} x = 0.9	Eu : Y = 9 : 1	Eu : Y = 0.91 : 0.09	0.91
Eu _{0.8} Y _{0.2} x = 0.8	Eu : Y = 8 : 2	Eu : Y = 0.82 : 0.18	0.82
Eu _{0.6} Y _{0.4} x = 0.6	Eu : Y = 6 : 4	Eu : Y = 0.64 : 0.36	0.64
Eu _{0.5} Y _{0.5} x = 0.5	Eu : Y = 5 : 5	Eu : Y = 0.53 : 0.57	0.53
Eu _{0.3} Y _{0.7} x = 0.3	Eu : Y = 3 : 7	Eu : Y = 0.29 : 0.71	0.29
Eu _{0.2} Y _{0.8} x = 0.2	Eu : Y = 2 : 8	Eu : Y = 0.24 : 0.76	0.24
Eu _{0.1} Y _{0.9} x = 0.1	Eu : Y = 1 : 9	Eu : Y = 0.08 : 0.92	0.08

CP	Metal ratios from starting material preparation	Metal ratios from ICP of digested sample	X

Tb_{0.8}Y_{0.2} x = 0.8	Tb : Y = 8 : 2	Tb: Y = 0.87 : 0.13	0.87
Tb_{0.6}Y_{0.4} x = 0.6	Tb : Y = 6 : 4	Tb: Y = 0.67 : 0.33	0.67
Tb_{0.4}Y_{0.6} x = 0.4	Tb : Y = 4 : 6	Tb: Y = 0.33 : 0.64	0.33
Tb_{0.2}Y_{0.8} x = 0.2	Tb: Y = 2 : 8	Tb : Y = 0.21 : 0.79	0.21
Tb_{0.1}Y_{0.9} x = 0.1	Tb : Y = 1 : 9	Tb: Y = 0.19 : 0.81	0.19

Table S3 Quantum yield of **Eu_xY_{1-x}** and **Tb_xY_{1-x}**.

Sample	Quantum yield (Φ)	Sample	Quantum yield (Φ)
Eu_{0.9}Y_{0.1}	45.35%	Tb_{0.9}Y_{0.1}	24.81%
Eu_{0.8}Y_{0.2}	59.57%	Tb_{0.8}Y_{0.2}	18.88%
Eu_{0.7}Y_{0.3}	65.66%	Tb_{0.7}Y_{0.3}	23.47%
Eu_{0.6}Y_{0.4}	70.53%	Tb_{0.6}Y_{0.4}	26.51%
Eu_{0.5}Y_{0.5}	74.47%	Tb_{0.5}Y_{0.5}	22.26%
Eu_{0.4}Y_{0.6}	73.19%	Tb_{0.4}Y_{0.6}	19.39%
Eu_{0.3}Y_{0.7}	71.41%	Tb_{0.3}Y_{0.7}	17.99%
Eu_{0.2}Y_{0.8}	66.73%	Tb_{0.2}Y_{0.8}	15.45%
Eu_{0.1}Y_{0.9}	69.04%	Tb_{0.1}Y_{0.9}	14.02%
1-Eu	62.65%	1-Tb	20.32%

Table S4 Selected bond lengths (Å) for **1-Y**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Y1	O2	2.397(8)	Y1	O3	2.397(11)
Y1	O6	2.211(13)	Y1	O1	2.457(9)
Y1	O5	2.294(9)	Y1	O4	2.561(9)
Y1	O4 ¹	2.303(9)			

Table S5 Selected bond angles (°) for **1-Y**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O6	Y1	O5	89.2(7)	O6	Y1	O1	76.5(5)
O6	Y1	O4 ¹	80.1(4)	O5	Y1	O1	78.8(3)
O5	Y1	O4	76.2(3)	O4 ¹	Y1	O1	145.8(3)
O6	Y1	O8 ¹	116.2(7)	O8 ¹	Y1	O1	135.8(3)
O5	Y1	O8 ¹	139.1(3)	O3	Y1	O1	75.2(4)
O4 ¹	Y1	O8 ¹	77.3(3)	O2	Y1	O1	53.9(3)
O6	Y1	O3	151.6(5)	O6	Y1	O4	150.5(5)
O5	Y1	O3	87.1(4)	O5	Y1	O4	70.0(3)
O4 ¹	Y1	O3	126.0(4)	O4 ¹	Y1	O4	74.8(3)
O8 ¹	Y1	O3	83.8(4)	O9	Y1	O4	85.7(3)
O6	Y1	O2	84.0(5)	O8 ¹	Y1	O4	73.2(3)
O5	Y1	O2	132.5(3)	O3	Y1	O4	51.2(3)
O4 ¹	Y1	O2	147.0(3)	O2	Y1	O4	125.5(3)

O8 ¹	Y1	O2	84.2(3)	O1	Y1	O4	117.6(3)
O3	Y1	O2	77.9(3)	O1	Y1	O4	117.6(3)
O6	Y1	O5	89.2(7)	O6	Y1	O1	76.5(5)
O6	Y1	O4 ¹	80.1(4)	O5	Y1	O1	78.8(3)

Reference

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