Layer-structured coordination polymers based on 5-(1H-tetrazol-5-yl)isophthalic acid: structure, sensitization of lanthanide(III) cations and small-molecule sensing

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Supporting Information

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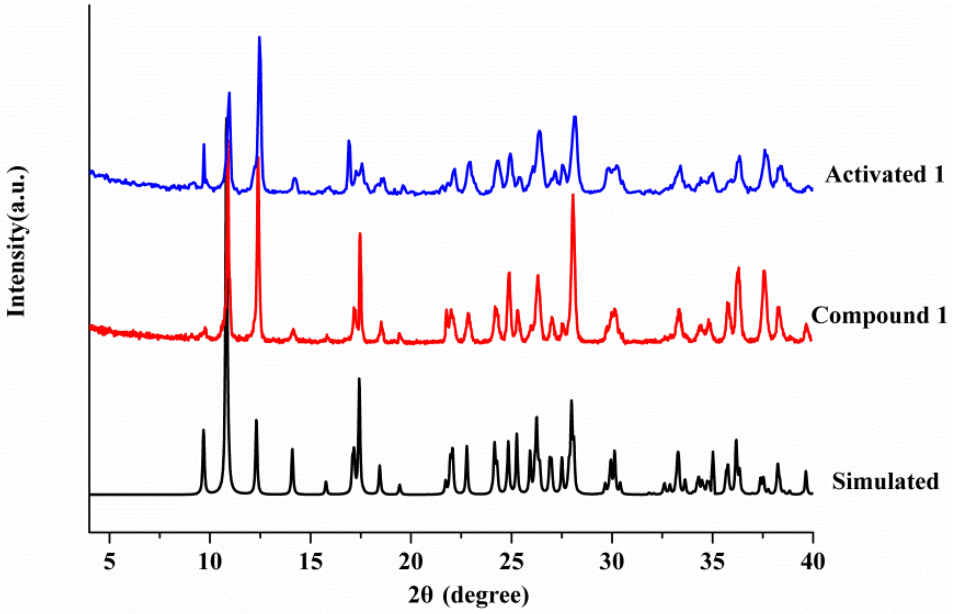


Fig. S1 PXRD patterns for **1** and activated **1**.

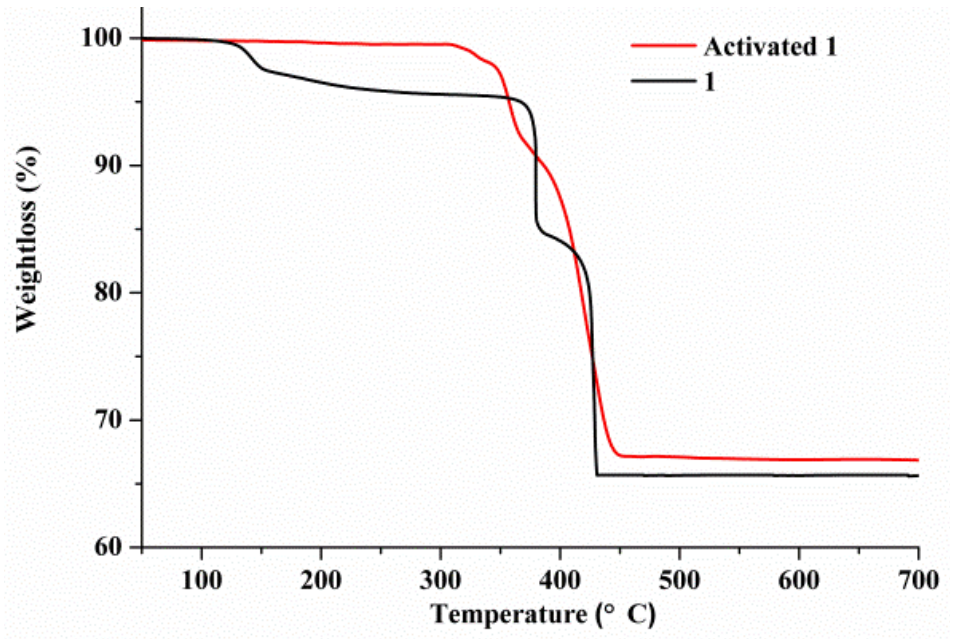


Fig. S2 TGA curve of **1** and activated **1** measured in air atmosphere.

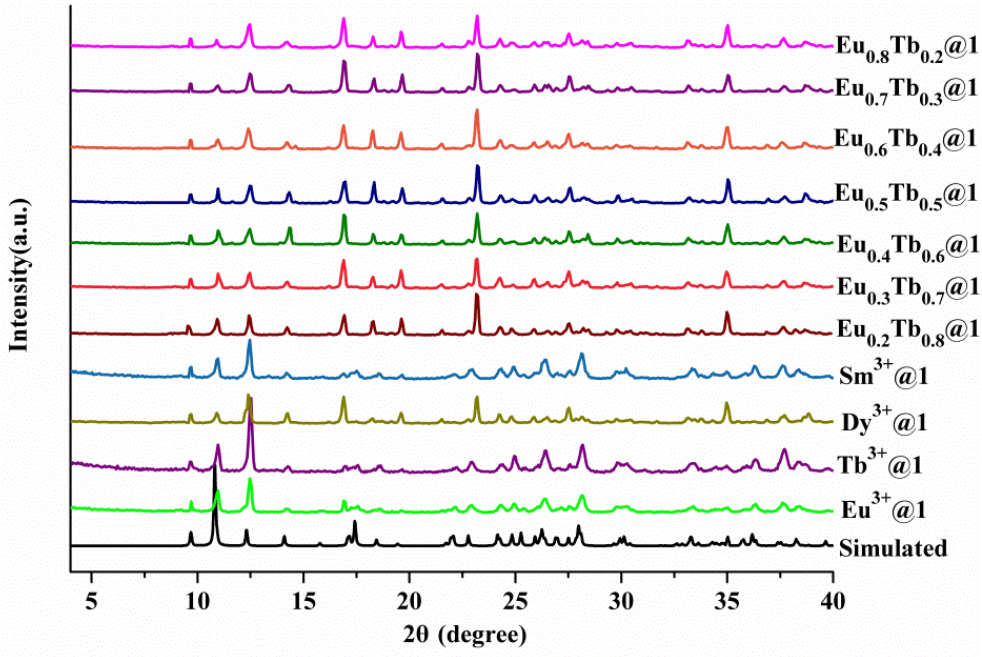


Fig.S3 Simulated and experimental X-ray diffraction patterns of Ln^{3+}@l.

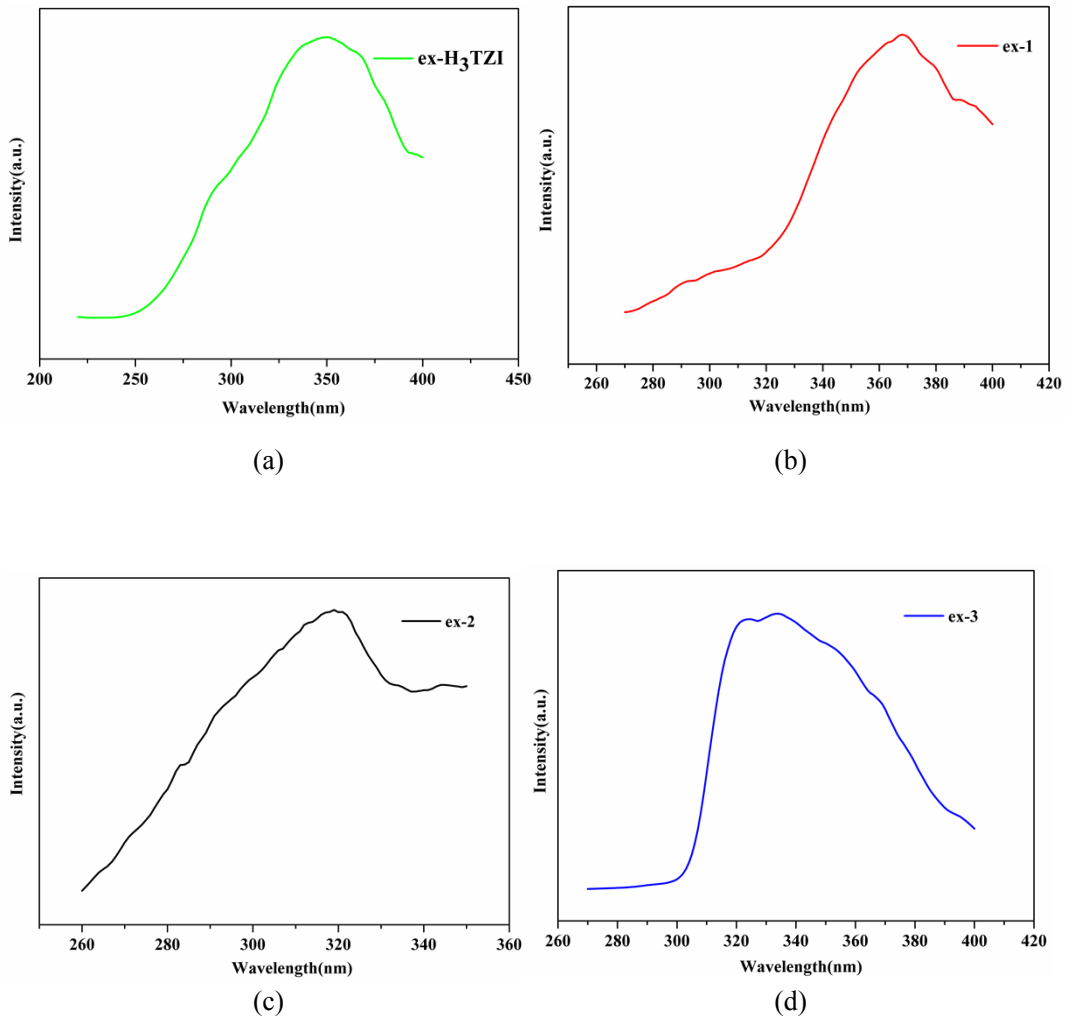


Fig. S4 Solid-state excitation spectra of (a) H_3TZI ligand, (b) compound **1**, (c) compound **2** and (d) compound **3** at room temperature.

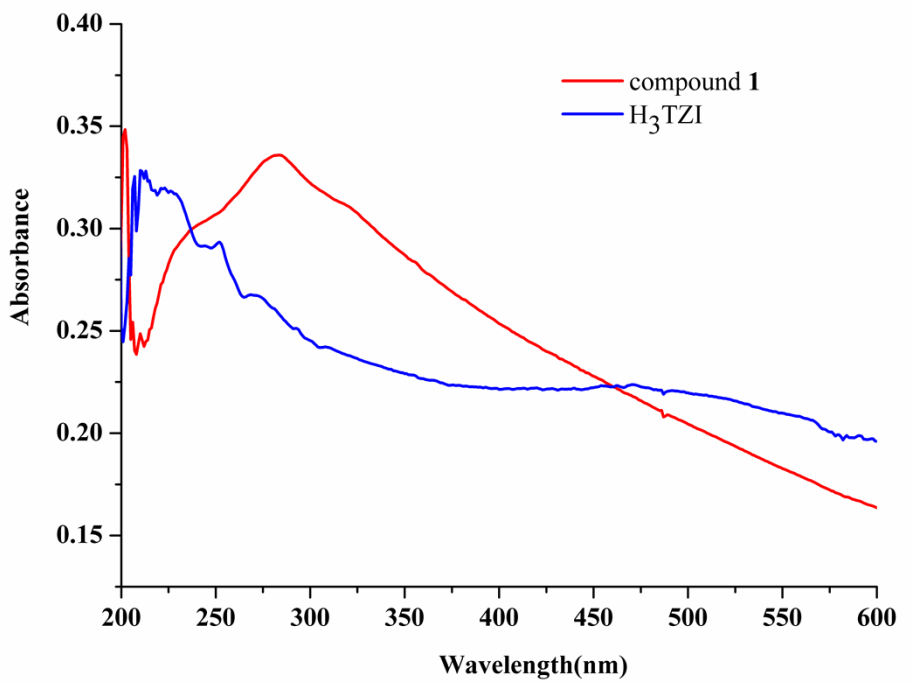


Fig. S5 UV-vis absorption spectra for compound **1** and H_3TZI ligand at room temperature.

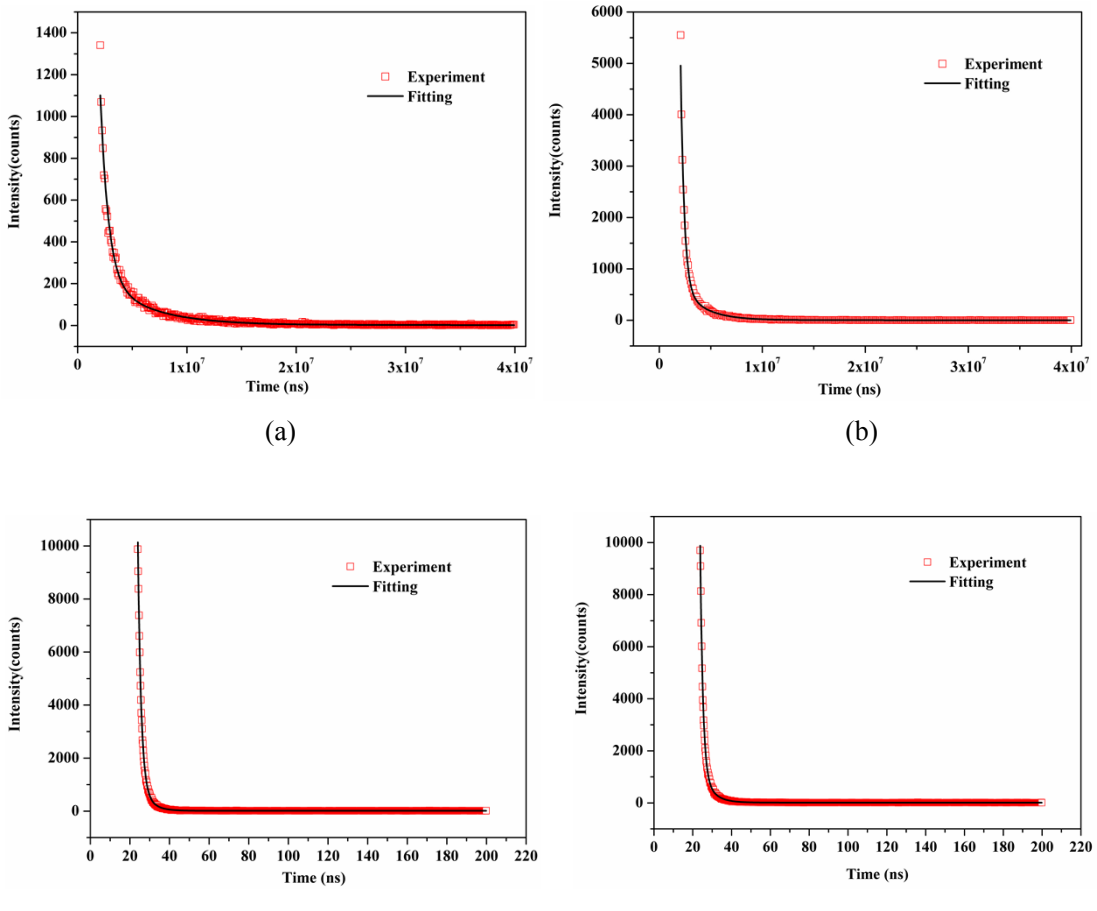


Fig. S6 Luminescence decay profiles for compounds **1**-(a), **2**-(b), **3**-(c) and H_3TZI ligand-(d) recorded at room temperature.

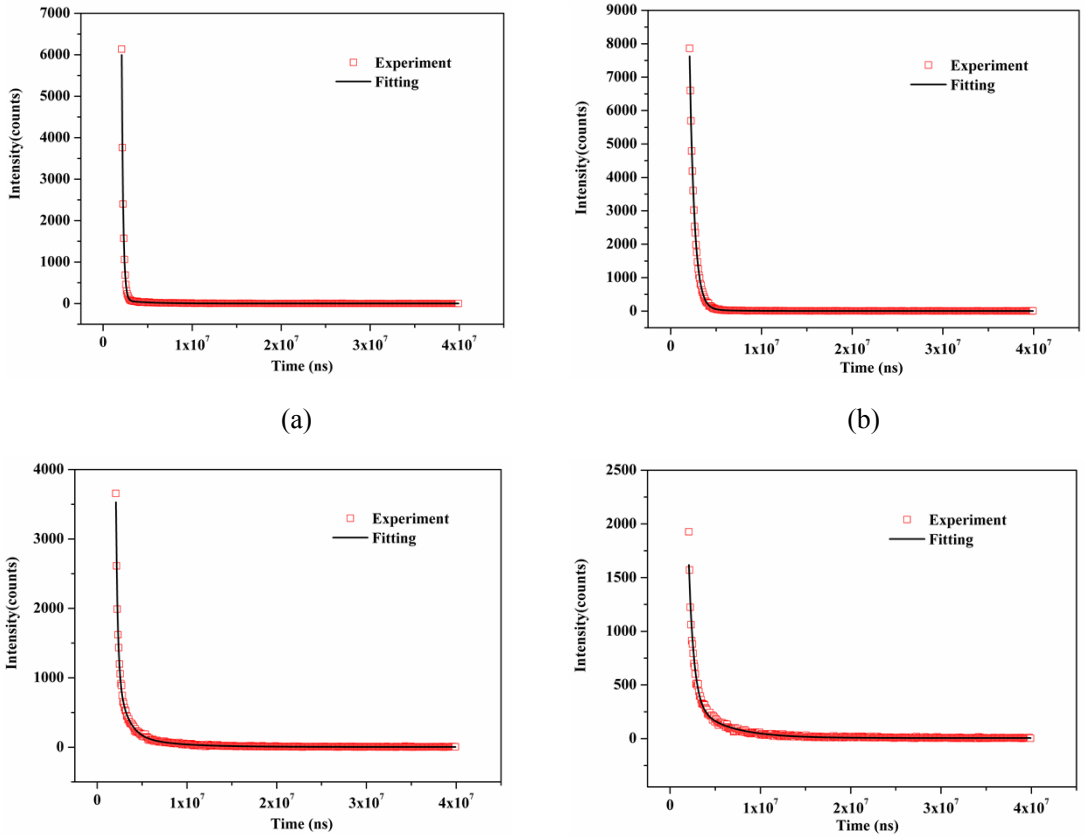


Fig.S7 Luminescence decay profiles for Eu^{3+}@1-(a), Tb^{3+}@1-(b), Dy^{3+}@1-(c) and Sm^{3+}@1-(d) recorded at room temperature. The $^5D_0$ decay curve of Eu^{3+}@1with emission was monitored at 616 nm (λ_{ex} = 350 nm). The red line is the best fitting to the data using a double exponential function, giving the value of τ_1 = 0.18ms and τ_2 = 2.66ms. The $^5D_4$ decay curve of Tb^{3+}@1 with emission was monitored at 544 nm (λ_{ex} = 350 nm), τ_1 = 0.53ms and τ_2 = 2.71ms. The decay curve of Dy^{3+}@1 with emission was monitored at 574 nm (λ_{ex} = 350 nm), τ_1 = 0.56ms and τ_2 = 4.01ms. The decay curve of Sm^{3+}@1with emission was monitored at 642 nm (λ_{ex} = 350 nm), τ_1 = 0.65ms and τ_2 = 4.28ms.

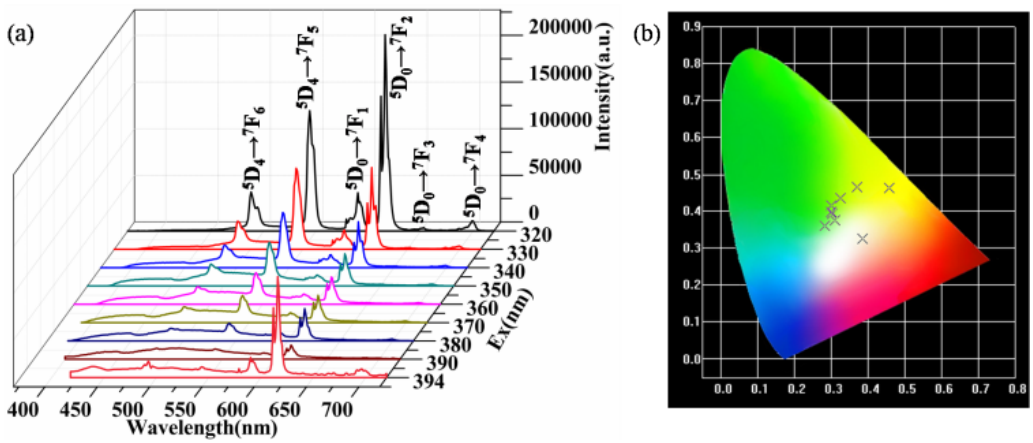
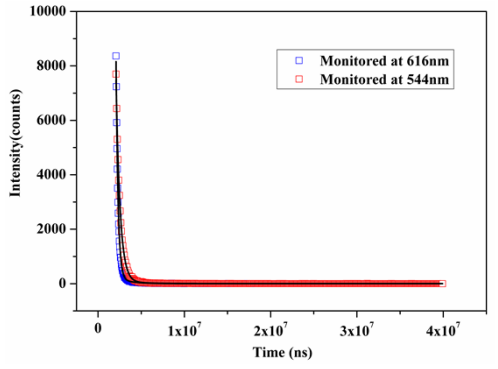
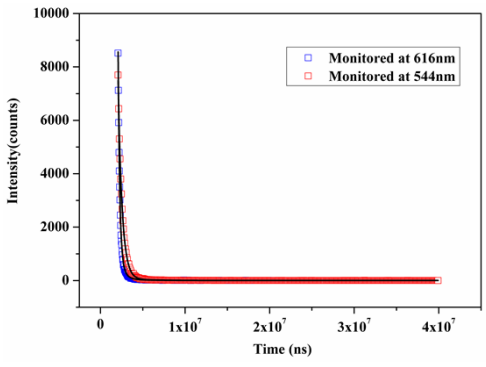


Fig. S8(a) Solid-state emission spectra of $Eu_{0.5}Tb_{0.5}$@l with excitation wavelengths varying from 320 to 394 nm. (b) The CIE chromaticity diagram for $Eu_{0.5}Tb_{0.5}$@l under excitation wavelengths from 320 to 394 nm.

$Eu_{0.5}Tb_{0.5}$@l mainly emits intense yellow luminescence upon excitation at 320 and 330 nm. Adjusting the excitation light from 340 to 390 nm, it mainly displays green light. When excited at 394nm, near white light emission is also obtained and its CIE coordination is (0.384, 0.325). The quantum yield is 3.07%.



(a)



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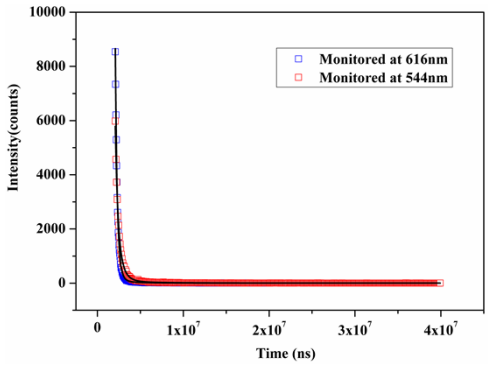

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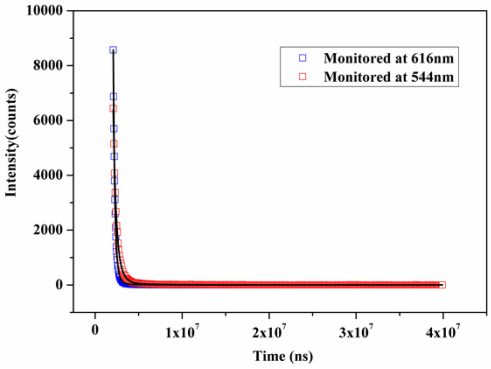

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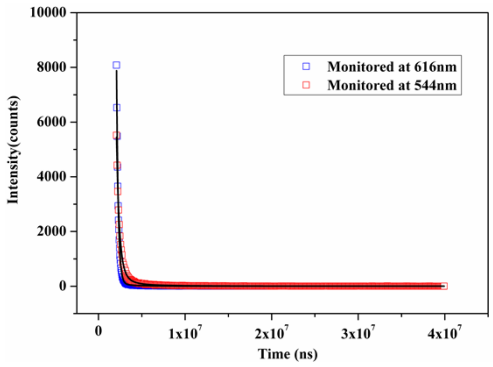

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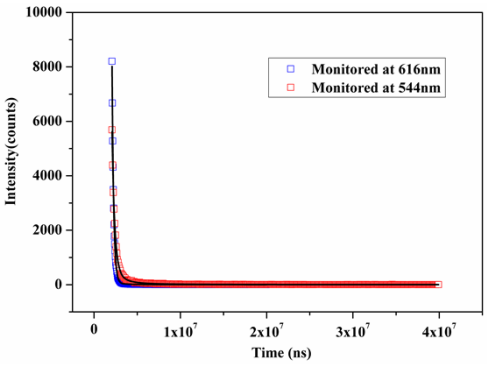

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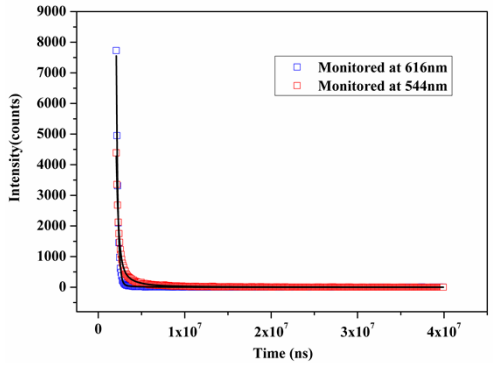


(g)

Fig. S9 Luminescence decay profiles for Eu^{3+}/Tb^{3+}-loaded samples recorded at room temperature. $Eu_{0.2}Tb_{0.8}$@l -(a), $Eu_{0.3}Tb_{0.7}$@l -(b), $Eu_{0.4}Tb_{0.6}$@l -(c), $Eu_{0.5}Tb_{0.5}$@l -(d), $Eu_{0.6}Tb_{0.4}$@l -(e), $Eu_{0.7}Tb_{0.3}$@l -(f) and $Eu_{0.8}Tb_{0.2}$@l -(g). The decay curves were recorded with emission monitored by the $^5D_4 \rightarrow {}^7F_5$ transition at 544 nm and the $^5D_0 \rightarrow {}^7F_2$ transition at 616 nm (λ_{ex} = 312 nm).

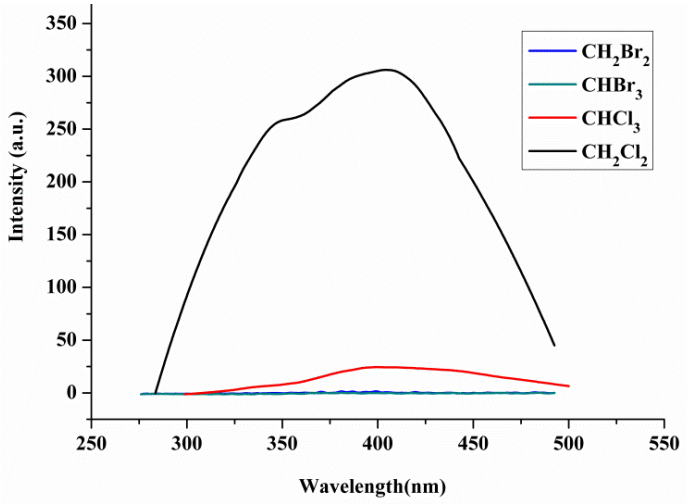


Fig. S10 The emission spectra of **1**-solvent emulsions at room temperature (excited at 256 nm).

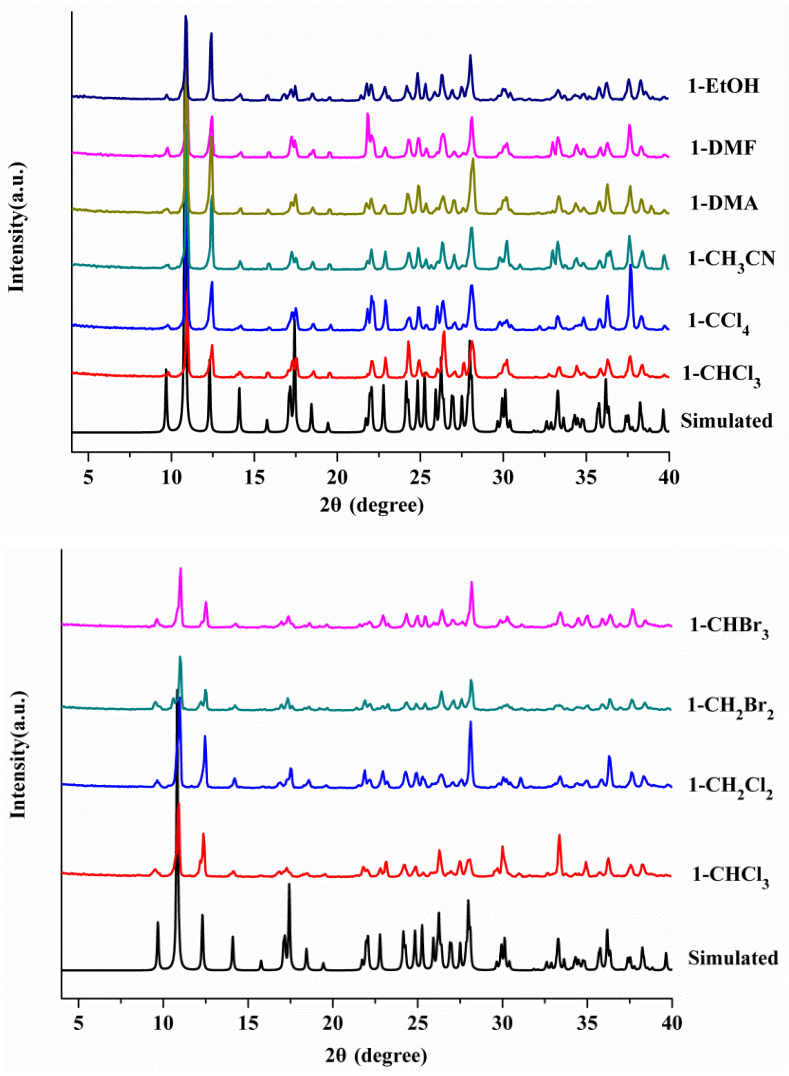


Fig. S11 PXRD patterns for **1** after soaking in different solvents.

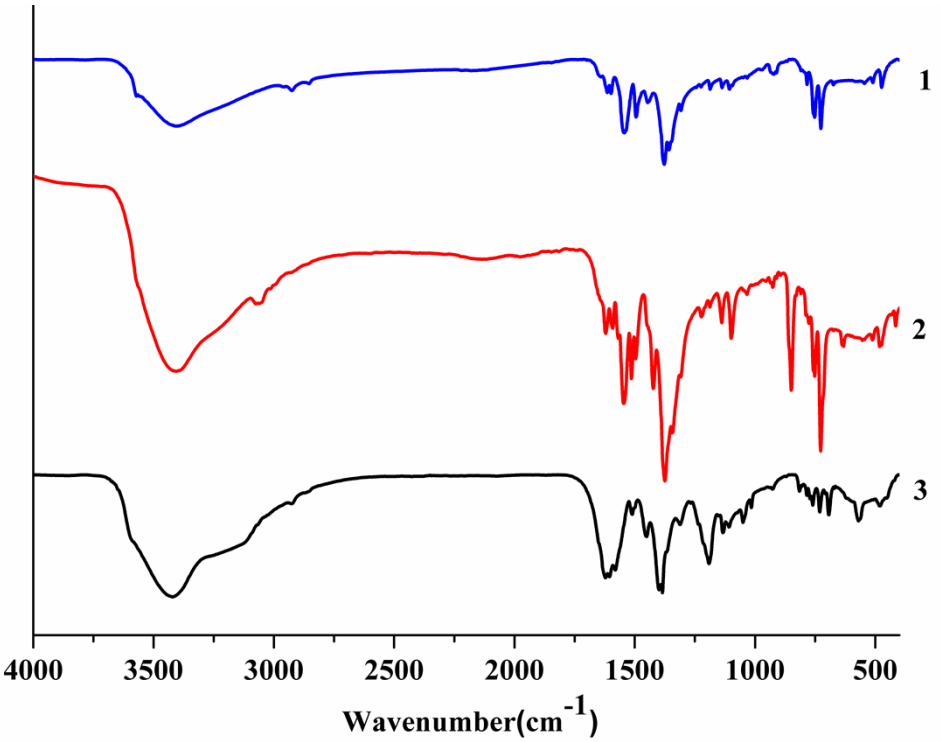
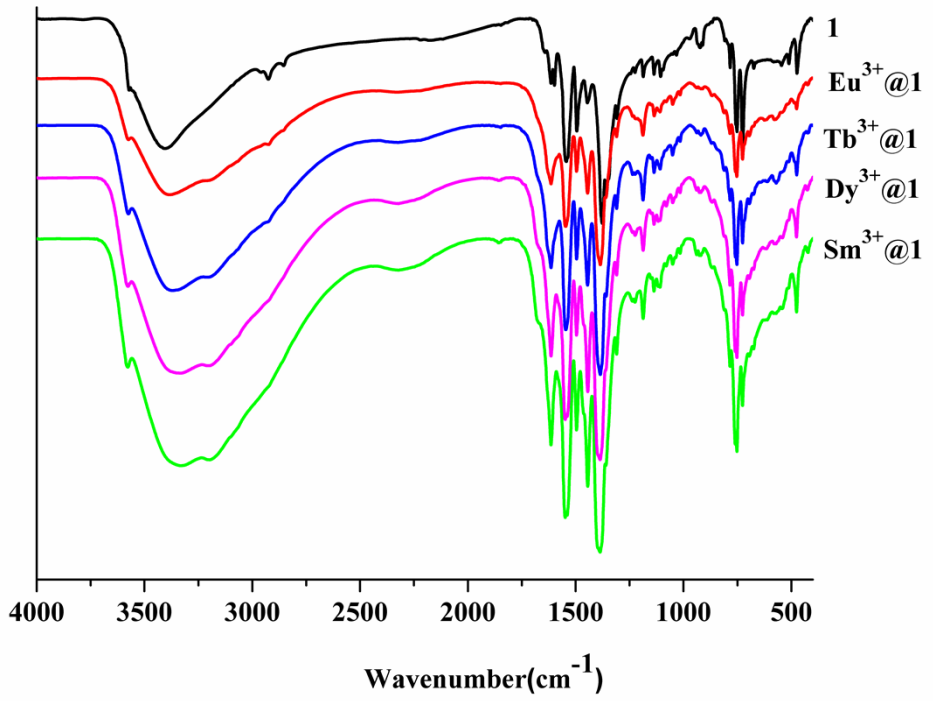


Fig. S12 IR spectra of compounds **1**-**3**.



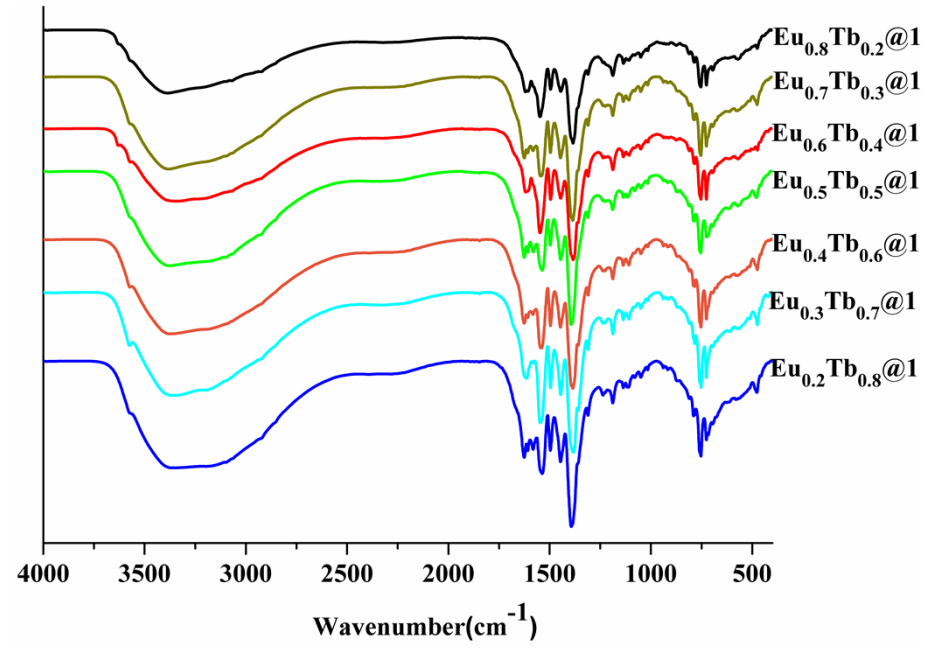


Fig. S13 IR spectra of **1**, Eu^{3+}@1, Tb^{3+}@1, Dy^{3+}@1 and Sm^{3+}@1 (top), $Eu_{0.8}Tb_{0.2}$@1, $Eu_{0.7}Tb_{0.3}$@1, $Eu_{0.6}Tb_{0.4}$@1, $Eu_{0.5}Tb_{0.5}$@1,$Eu_{0.4}Tb_{0.6}$@1, $Eu_{0.3}Tb_{0.7}$@1 and $Eu_{0.2}Tb_{0.8}$@1 (bottom).

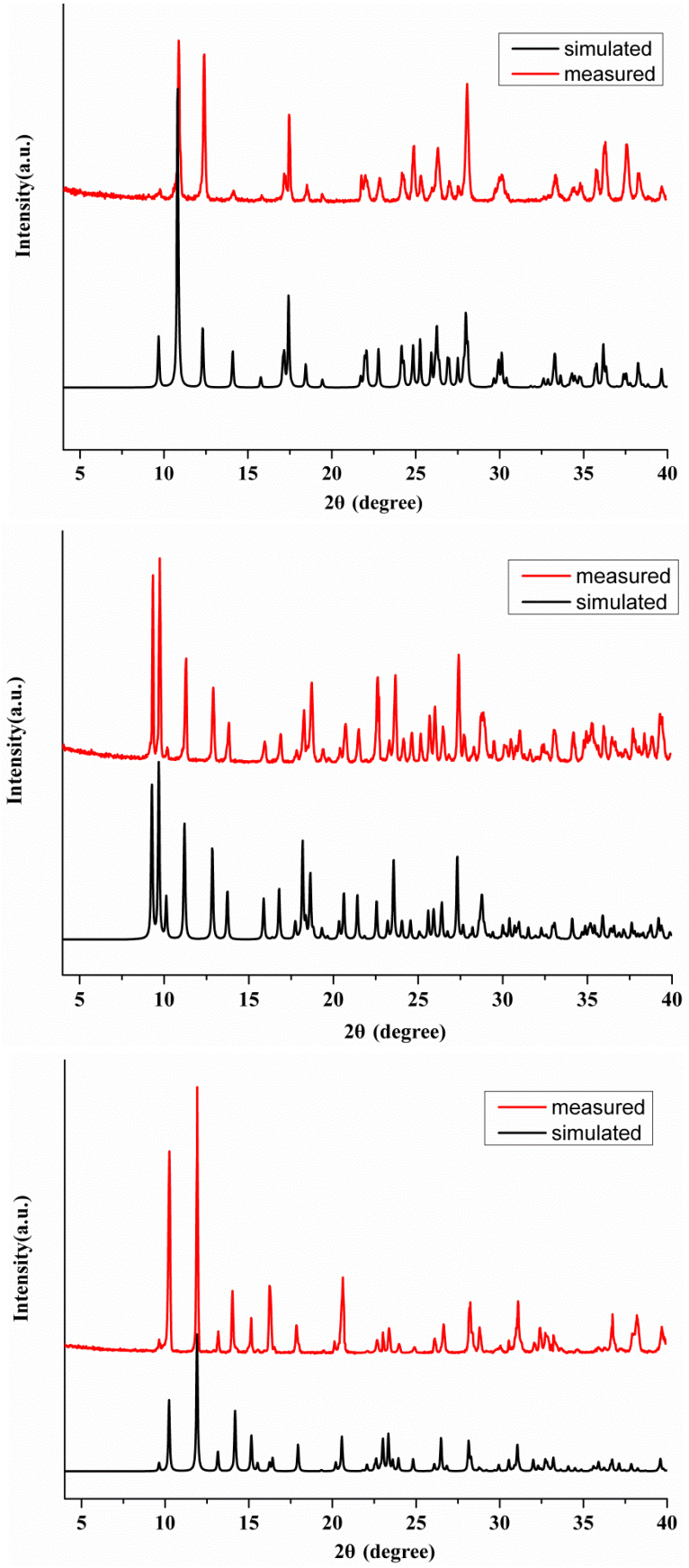


Fig. S14 Simulated and experimental X-ray diffraction patterns of compounds **1** (top), **2** (middle) and **3** (bottom).

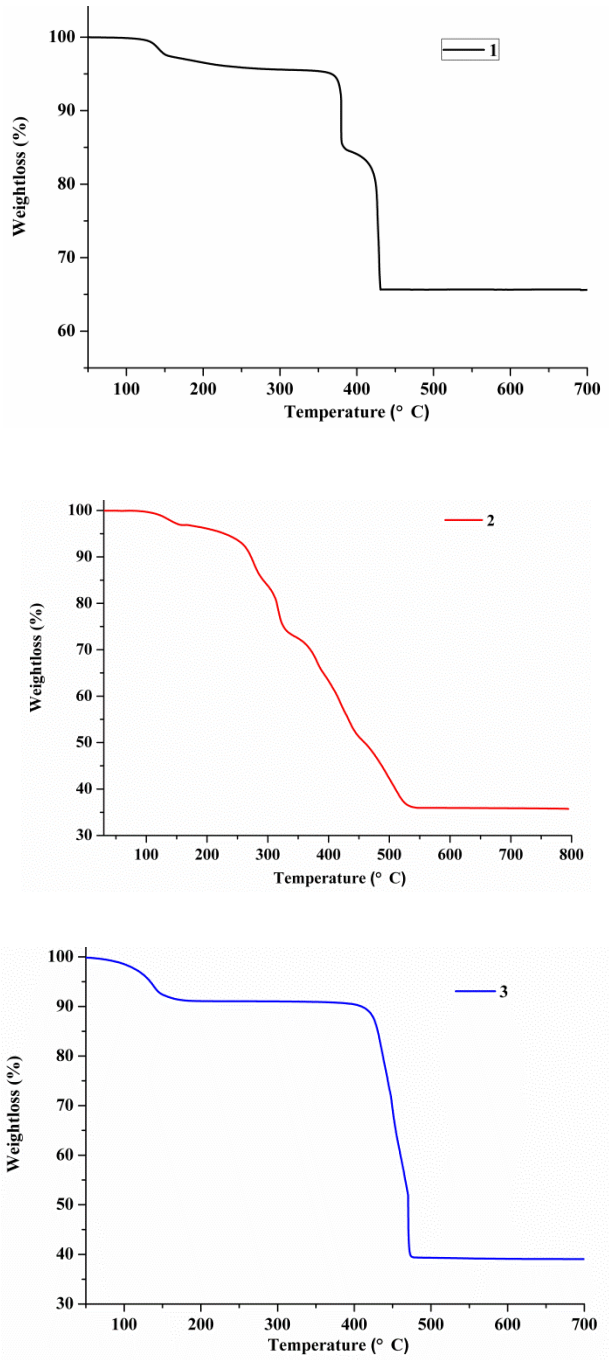


Fig. S15 TGA curves of the compounds **1** (top), **2** (middle) and **3** (bottom) measured in air atmosphere.

For **1**, the first step from 50°C to 220 °C corresponds to the removal of the coordinated and the free water molecules (weight loss ca. 4.46%, calculated 5.16%), and the structure then decomposed starting at 350 °C. The weight loss from 350 to 430 °C is attributed to the collapse of the framework of **1**. The remaining weight of 65.60% is attributed to the final product of PbO (cal. 64.00%). For **2**, the water molecule was lost at the temperature of 50°C to 167 °C (weight loss ca. 3.12%, calculated 2.82%) and the final product of PbO is 35.94% (cal. 35.01%). For **3**, the weight loss of 9.95% observed from 50 to 180 °C corresponds to the departure of the water molecules (cal. 10.61%), and the framework of **3** begins to collapse at 370°C. The final residue is ZnO with the weight of 39.26% (cal. 38.39%).

Table S1. Crystal data and structure refinement for compounds **1- 3**

Compounds	**1**	**2**	**3**
Formula	$C_9H_8N_4O_7Pb_2$	$C_{21}H_{14}N_6O_5Pb$	$C_9H_9N_4O_{7.5}Zn_2$
Fw (g mol^{-1})	698.59	637.57	423.97
Crystal system	triclinic	monoclinic	triclinic
space group	*P*-1	*P21/c*	*P*-1
a(Å)	7.8513(2)	11.2006(16)	7.794(2)
b(Å)	9.1456(2)	11.1967(16)	9.057(3)
c(Å)	10.6941(3)	18.5221(18)	9.169(3)
α(°)	112.083(2)	90	90.38(3)
β(°)	108.443(2)	121.700(6)	91.24(2)
γ(°)	96.4630(10)	90	107.59(2)
V(Å^3)	651.18(3)	1976.3(4)	616.8(3)
Z	2	4	2
D_{calc}(g· cm^{-3})	3.537	2.136	2.229
μ(mm^{-1})	25.864	8.588	3.935
F(000)	610	1208	410
*θ*range (°)	2.23 – 24.99	2.14 – 26.38	3.03 – 27.45
Limiting indices	$-8 \le h \le 8$	$-13 \le h \le 13$	$-9 \le h \le 10$
	$-10 \le k \le 10$	$-13 \le k \le 13$	$-11 \le k \le 11$
	$-12 \le l \le 12$	$-23 \le l \le 23$	$-11 \le l \le 10$
Refl.Collected / unique	5783/ 2254	14822/4028	5771 / 2709
R_{int}	0.1056	0.0331	0.0431
Data / restraints / parameters	2254 / 37 / 199	4028 / 0 / 302	2709 / 4 / 215
GOF	1.041	1.070	1.040
R_1 [$I>2\sigma(I)$]	0.0456	0.0210	0.0472
wR_2[$I>2\sigma(I)$]	0.1273	0.0523	0.1129
R_1 (all data)	0.0481	0.0242	0.0613
wR_2(all data)	0.1298	0.0535	0.1192
Largest diff.peakand hole(e·Å^{-3})	2.475 and -3.353	1.304 and -1.211	1.252 and -0.928
CCDC No.	1418713	1418704	1418639

Table S2. Selected bond lengths [Å] and angles [°] for compounds **1- 3**

1			
Pb(1)-O(6)#1	2.518(8)	Pb(2) -O(7)	2.829(9)
Pb(1)-O(3)#2	2.548(9)	Pb(2)-O(2)	2.429(8)
Pb(1)-O(5)	3.027(11)	Pb(2)-O(1)#5	2.869(7)
Pb(1)-Pb(1)#1	3.9256(8)	Pb(2)-N(4)#3	2.618(10)
Pb(1)-O(2)	2.690(7)	Pb(2)-O(1)	2.725(9)
Pb(1)-O(4)#2	2.620(8)	Pb(2)-O(4)#4	2.742(9)
Pb(1)-N(3)#3	2.668(9)	Pb(2)-Pb(1)#1	4.0103(6)
Pb(1)-Pb(2)#1	4.0103(6)	Pb(2)- O(6)	2.403(7)
Pb(1)- O(6)	2.331(8)	O(3)#2-Pb(1)-N(3)#3	75.7(3)
O(6)-Pb(1)-O(6)#1	72.0(3)	O(4)#2-Pb(1)-N(3)#3	120.0(3)
O(6)-Pb(1)-O(3)#2	72.3(3)	O(6)-Pb(1)-O(2)	65.7(3)
O(6)#1-Pb(1)-O(3)#2	100.5(3)	O(6)#1-Pb(1)-O(2)	85.9(2)
O(6)-Pb(1)-O(4)#2	104.9(3)	O(3)#2-Pb(1)-O(2)	133.1(3)
O(6)#1-Pb(1)-O(4)#2	76.2(3)	O(4)#2-Pb(1)-O(2)	161.8(3)
O(3)#2-Pb(1)-O(4)#2	49.7(3)	N(3)#3-Pb(1)-O(2)	73.9(3)
O(6)-Pb(1)-N(3)#3	74.6(3)	O(6)-Pb(1)-C(8)#2	89.2(3)
O(6)#1-Pb(1)-N(3)#3	145.7(3)	O(3)#2-Pb(1)-N(3)#3	75.8(3)
O(6)#1-Pb(1)-C(8)#2	89.1(3)	O(2)-Pb(1)-O(5)	108.4(3)
O(3)#2-Pb(1)-C(8)#2	24.8(3)	C(8)#2-Pb(1)-O(5)	91.4(3)
O(4)#2-Pb(1)-C(8)#2	24.9(3)	O(6)-Pb(1)-Pb(1)#1	37.58(18)
N(3)#3-Pb(1)-C(8)#2	97.5(3)	O(6)#1-Pb(1)-Pb(1)#1	34.38(17)
O(2)-Pb(1)-C(8)#2	154.8(3)	O(3)#2-Pb(1)-Pb(1)#1	86.3(2)
O(6)-Pb(1)-O(5)	136.0(3)	O(4)#2-Pb(1)-Pb(1)#1	90.0(2)
O(6)#1-Pb(1)-O(5)	64.0(3)	N(3)#3-Pb(1)-Pb(1)#1	111.8(2)
O(3)#2-Pb(1)-O(5)	116.2(3)	O(2)-Pb(1)-Pb(1)#1	73.12(19)
O(4)#2-Pb(1)-O(5)	66.6(3)	C(8)#2-Pb(1)-Pb(1)#1	89.0(2)
N(3)#3-Pb(1)-O(5)	148.5(3)	O(5)-Pb(1)-Pb(1)#1	98.42(19)
O(6)-Pb(1)-Pb(2)	34.17(17)	O(5)-Pb(1)-Pb(2)	141.61(18)
O(6)#1-Pb(1)-Pb(2)	90.96(16)	Pb(1)#1-Pb(1)-Pb(2)	61.274(12)
O(3)#2-Pb(1)-Pb(2)	95.9(2)	O(6)-Pb(1)-Pb(2)#1	92.17(17)
O(4)#2-Pb(1)-Pb(2)	138.3(2)	O(6)#1-Pb(1)-Pb(2)#1	34.48(16)
N(3)#3-Pb(1)-Pb(2)	56.3(2)	O(3)#2-Pb(1)-Pb(2)#1	80.6(2)
O(2)-Pb(1)-Pb(2)	37.27(17)	O(4)#2-Pb(1)-Pb(2)#1	42.8(2)
C(8)#2-Pb(1)-Pb(2)	118.3(2)	N(3)#3-Pb(1)-Pb(2)#1	155.4(2)
O(2)-Pb(1)-Pb(2)#1	119.90(18)	O(2)-Pb(2)-N(4)#3	76.5(3)
C(8)#2-Pb(1)-Pb(2)#1	61.0(2)	O(6)-Pb(2)-O(1)	118.4(2)
O(5)-Pb(1)-Pb(2)#1	51.15(19)	O(2)-Pb(2)-O(1)	49.8(2)
Pb(1)#1-Pb(1)-Pb(2)#1	59.587(11)	N(4)#3-Pb(2)-O(1)	89.7(3)
Pb(2)-Pb(1)-Pb(2)#1	120.860(11)	O(6)-Pb(2)-O(4)#4	75.8(2)
O(6)-Pb(2)-O(2)	69.1(3)	O(2)-Pb(2)-O(4)#4	75.1(3)
O(6)-Pb(2)-N(4)#3	83.2(3)	N(4)#3-Pb(2)-O(4)#4	149.2(3)
O(1)-Pb(2)-O(4)#4	80.9(3)	N(4)#3-Pb(2)-C(9)	84.9(3)

O(6)-Pb(2)-O(7)	78.4(3)	O(1)-Pb(2)-C(9)	25.4(2)
O(2)-Pb(2)-O(7)	137.2(3)	O(4)#4-Pb(2)-C(9)	74.0(3)
N(4)#3-Pb(2)-O(7)	72.7(3)	O(7)-Pb(2)-C(9)	156.7(3)
O(1)-Pb(2)-O(7)	154.7(3)	O(1)#5-Pb(2)-C(9)	98.5(3)
O(4)#4-Pb(2)-O(7)	123.4(3)	O(6)-Pb(2)-Pb(1)	33.02(19)
O(6)-Pb(2)-O(1)#5	168.5(3)	O(2)-Pb(2)-Pb(1)	42.05(17)
O(2)-Pb(2)-O(1)#5	122.3(3)	N(4)#3-Pb(2)-Pb(1)	62.84(19)
N(4)#3-Pb(2)-O(1)#5	97.6(3)	O(1)-Pb(2)-Pb(1)	91.01(17)
O(1)-Pb(2)-O(1)#5	73.2(3)	O(4)#4-Pb(2)-Pb(1)	87.89(18)
O(4)#4-Pb(2)-O(1)#5	107.5(2)	O(7)-Pb(2)-Pb(1)	96.6(2)
O(7)-Pb(2)-O(1)#5	90.9(2)	O(1)#5-Pb(2)-Pb(1)	155.4(2)
O(6)-Pb(2)-C(9)	93.0(3)	C(9)-Pb(2)-Pb(1)	66.6(2)
O(2)-Pb(2)-C(9)	24.8(3)	O(6)-Pb(2)-Pb(1)#1	36.38(19)
O(2)-Pb(2)-Pb(1)#1	73.7(2)	O(7)-Pb(2)-Pb(1)#1	96.2(2)
N(4)#3-Pb(2)-Pb(1)#1	118.87(19)	O(1)#5-Pb(2)-Pb(1)#1	143.33(19)
O(1)-Pb(2)-Pb(1)#1	108.43(17)	C(9)-Pb(2)-Pb(1)#1	88.98(19)
O(4)#4-Pb(2)-Pb(1)#1	40.44(16)	Pb(1)-Pb(2)-Pb(1)#1	59.140(11)
		2	
Pb(1)-O(2)	2.519(2)	Pb(1)-O(4)#2	2.834(2)
Pb(1)-O(4)#1	2.536(2)	Pb(1)-C(1)	2.977(3)
Pb(1)-N(2)	2.561(3)	Pb(1)-C(6)#1	2.999(3)
Pb(1)-N(1)	2.663(3)	Pb(1)-O(5)	3.075(4)
Pb(1)-O(1)	2.709(3)	Pb(1)-Pb(1)#3	4.376(5)
Pb(1)-O(3)#1	2.769(3)	O(2)-Pb(1)-O(4)#1	82.68(8)
O(2)-Pb(1)-N(2)	80.15(9)	O(4)#1-Pb(1)-O(3)#1	49.05(8)
O(4)#1-Pb(1)-N(2)	79.27(9)	N(2)-Pb(1)-O(3)#1	123.15(8)
O(2)-Pb(1)-N(1)	93.03(9)	N(1)-Pb(1)-O(3)#1	161.51(9)
O(4)#1-Pb(1)-N(1)	142.29(9)	O(1)-Pb(1)-O(3)#1	90.19(9)
N(2)-Pb(1)-N(1)	63.13(9)	O(2)-Pb(1)-O(4)#2	144.07(7)
O(2)-Pb(1)-O(1)	49.67(7)	O(4)#1-Pb(1)-O(4)#2	70.98(7)
O(4)#1-Pb(1)-O(1)	127.13(7)	N(2)-Pb(1)-O(4)#2	71.44(8)
N(2)-Pb(1)-O(1)	108.38(9)	N(1)-Pb(1)-O(4)#2	93.30(8)
N(1)-Pb(1)-O(1)	71.49(9)	O(1)-Pb(1)-O(4)#2	161.86(7)
O(2)-Pb(1)-O(3)#1	72.43(9)	O(3)#1-Pb(1)-O(4)#2	105.18(8)
O(2)-Pb(1)-C(1)	25.03(8)	N(1)-Pb(1)-C(6)#1	161.73(9)
O(4)#1-Pb(1)-C(1)	104.64(8)	O(1)-Pb(1)-C(6)#1	108.07(9)
N(2)-Pb(1)-C(1)	95.97(9)	O(3)#1-Pb(1)-C(6)#1	24.25(9)
N(1)-Pb(1)-C(1)	83.01(9)	O(4)#2-Pb(1)-C(6)#1	89.50(8)
O(1)-Pb(1)-C(1)	24.74(8)	C(1)-Pb(1)-C(6)#1	90.29(9)
O(3)#1-Pb(1)-C(1)	79.08(9)	O(2)-Pb(1)-O(5)	130.79(9)
O(4)#2-Pb(1)-C(1)	167.11(9)	O(4)#1-Pb(1)-O(5)	126.86(10)
O(2)-Pb(1)-C(6)#1	74.52(9)	N(2)-Pb(1)-O(5)	137.03(9)
O(4)#1-Pb(1)-C(6)#1	24.92(9)	N(1)-Pb(1)-O(5)	83.60(9)
N(2)-Pb(1)-C(6)#1	100.95(9)	O(1)-Pb(1)-O(5)	83.47(9)

O(3)#1-Pb(1)-O(5)	97.14(9)	N(2)-Pb(1)-Pb(1)#3	71.70(7)
O(4)#2-Pb(1)-O(5)	85.08(8)	N(1)-Pb(1)-Pb(1)#3	119.73(6)
C(1)-Pb(1)-O(5)	106.67(10)	O(1)-Pb(1)-Pb(1)#3	164.86(5)
C(6)#1-Pb(1)-O(5)	114.64(10)	O(3)#1-Pb(1)-Pb(1)#3	77.85(6)
O(2)-Pb(1)-Pb(1)#3	116.78(5)	O(4)#2-Pb(1)-Pb(1)#3	33.23(4)
O(4)#1-Pb(1)-Pb(1)#3	37.75(5)	C(1)-Pb(1)-Pb(1)#3	141.06(6)
C(6)#1-Pb(1)-Pb(1)#3	57.89(7)	O(5)-Pb(1)-Pb(1)#3	106.99(8)
		3	
Zn(1)- O(4)	2.226(5)	Zn(1)-O(3)	2.053(3)
Zn(1)-O(1)#1	2.076(3)	Zn(1)-O(7)	2.130(4)
Zn(1)-N(2)	2.133(4)	Zn(1)-O(1)	2.164(3)
Zn(1)-Zn(1)#1	3.1579(15)	Zn(1)-Zn(2)#1	3.3537(14)
Zn(1)-Zn(2)	3.3795(13)	Zn(2)-O(1)	1.966(3)
Zn(2)-O(2)#1	1.991(3)	Zn(2)-N(1)	2.051(4)
Zn(2)-O(6)#2	2.062(4)	Zn(2)-O(5)#2	2.336(5)
O(3)-Zn(1)-O(1)#1	95.07(14)	O(3)-Zn(1)-O(4)	81.37(19)
O(3)-Zn(1)-O(7)	88.55(15)	O(1)#1-Zn(1)-O(4)	171.24(19)
O(1)#1-Zn(1)-O(7)	95.77(17)	O(7)-Zn(1)-O(4)	92.2(2)
O(3)-Zn(1)-N(2)	165.78(16)	N(2)-Zn(1)-O(4)	85.6(2)
O(1)#1-Zn(1)-N(2)	98.59(14)	O(1)-Zn(1)-O(4)	88.53(17)
O(7)-Zn(1)-N(2)	86.19(16)	O(3)-Zn(1)-Zn(1)#1	96.25(11)
O(3)-Zn(1)-O(1)	94.24(13)	O(1)#1-Zn(1)-Zn(1)#1	42.94(9)
O(1)#1-Zn(1)-O(1)	83.74(13)	O(7)-Zn(1)-Zn(1)#1	138.64(14)
O(7)-Zn(1)-O(1)	177.19(14)	N(2)-Zn(1)-Zn(1)#1	96.43(11)
N(2)-Zn(1)-O(1)	91.15(13)	O(1)-Zn(1)-Zn(1)#1	40.80(8)
O(4)-Zn(1)-Zn(1)#1	129.20(15)	Zn(2)#1-Zn(1)-Zn(2)	124.06(3)
O(3)-Zn(1)-Zn(2)#1	64.38(11)	O(1)-Zn(2)-O(2)#1	111.06(14)
O(1)#1-Zn(1)-Zn(2)#1	32.89(8)	O(1)-Zn(2)-N(1)	97.48(14)
O(7)-Zn(1)-Zn(2)#1	83.48(13)	O(2)#1-Zn(2)-N(1)	97.21(15)
N(2)-Zn(1)-Zn(2)#1	127.89(11)	O(1)-Zn(2)-O(6)#2	134.43(14)
O(1)-Zn(1)-Zn(2)#1	97.49(9)	O(2)#1-Zn(2)-O(6)#2	93.07(15)
O(4)-Zn(1)-Zn(2)#1	145.51(15)	N(1)-Zn(2)-O(6)#2	117.84(15)
Zn(1)#1-Zn(1)-Zn(2)#1	62.44(3)	O(1)-Zn(2)-O(5)#2	90.60(15)
O(3)-Zn(1)-Zn(2)	122.05(10)	O(2)#1-Zn(2)-O(5)#2	151.15(15)
O(1)#1-Zn(1)-Zn(2)	98.58(9)	N(1)-Zn(2)-O(5)#2	98.62(18)
O(7)-Zn(1)-Zn(2)	144.49(11)	O(6)#2-Zn(2)-O(5)#2	58.17(15)
N(2)-Zn(1)-Zn(2)	59.68(11)	O(1)-Zn(2)-C(8)#2	113.20(15)
O(1)-Zn(1)-Zn(2)	33.21(8)	O(2)#1-Zn(2)-C(8)#2	122.26(15)
O(4)-Zn(1)-Zn(2)	76.86(13)	N(1)-Zn(2)-C(8)#2	111.55(16)
Zn(1)#1-Zn(1)-Zn(2)	61.62(3)	O(6)#2-Zn(2)-C(8)#2	29.29(16)
O(5)#2-Zn(2)-C(8)#2	28.91(16)	O(1)-Zn(2)-Zn(1)#1	34.98(9)
O(2)#1-Zn(2)-Zn(1)#1	76.39(10)	O(6)#2-Zn(2)-Zn(1)	146.00(11)
N(1)-Zn(2)-Zn(1)#1	97.62(11)	O(5)#2-Zn(2)-Zn(1)	87.87(11)
O(6)#2-Zn(2)-Zn(1)#1	144.15(11)	C(8)#2-Zn(2)-Zn(1)	116.79(12)

O(5)#2-Zn(2)-Zn(1)#1	124.79(13)	Zn(1)#1-Zn(2)-Zn(1)	55.94(3)
C(8)#2-Zn(2)-Zn(1)#1	141.20(11)	Zn(2)-O(1)-Zn(1)#1	112.12(14)
O(1)-Zn(2)-Zn(1)	37.08(9)	Zn(2)-O(1)-Zn(1)	109.72(14)
O(2)#1-Zn(2)-Zn(1)	120.93(10)	Zn(1)#1-O(1)-Zn(1)	96.26(13)
N(1)-Zn(2)-Zn(1)	61.42(10)	O(6)#2-Zn(2)-Zn(1)	146.00(11)

Symmetry transformations used to generate equivalent atoms for **1**: #1 -x+1, -y+1, -z+1; #2 x, y-1, z-1; #3 x, y-1, z; #4 -x+1, -y+2, -z+2; #5 -x+1, -y+1, -z+2, for **2**:#1 -x+1, y-1/2, -z+1/2; #2 x-1, -y+1/2, z-1/2; #3 –x, -y, -z, for **3**: #1 -x+2, -y, -z+1; #2 -x+2, -y+1, -z.

Table S3. ICP analysis for Ln(III)-encapsulated **1**.

Sample	Elemental contents (%)		The ratio of Ln^{3+} : Pb^{2+}
	Ln^{3+}	Pb^{2+}	
Eu^{3+}@1	3.02	33.90	1:11.22
Tb^{3+}@1	2.94	35.02	1:11.91
Dy^{3+}@1	2.86	34.27	1:11.98
Sm^{3+}@1	2.85	34.58	1:12.13

Table S4. Ratios of Eu^{3+}/Tb^{3+} added to **1** and determined by ICP in Ln(III)-encapsulated **1**.

Ratio of Eu^{3+}/Tb^{3+} added to **1**	Ratio of Eu^{3+}/Tb^{3+} determined by ICP in Ln(III)-encapsulated **1**
0.8:0.2	0.8:0.21
0.7:0.3	0.7:0.33
0.6:0.4	0.6:0.44
0.5:0.5	0.5:0.56
0.4:0.6	0.4:0.66
0.3:0.7	0.3:0.75
0.2:0.8	0.2:0.84

Table S5. EDX analysis for Ln(III)-encapsulated **1**.

Sample	Elemental contents (Wt %)		
	Ln^{3+}		Pb^{2+}
Eu^{3+}@1	24.83		28.01
Tb^{3+}@1	21.10		46.58
Dy^{3+}@1	21.14		33.66
Sm^{3+}@1	21.51		29.57
	Eu^{3+}	Tb^{3+}	Pb^{2+}
$Eu_{0.8}/Tb_{0.2}$@1	20.88	5.51	22.42
$Eu_{0.7}/Tb_{0.3}$@1	21.85	8.60	21.03
$Eu_{0.6}/Tb_{0.4}$@1	19.04	13.52	23.08
$Eu_{0.5}/Tb_{0.5}$@1	14.55	14.65	48.95
$Eu_{0.4}/Tb_{0.6}$@1	11.38	16.09	37.64
$Eu_{0.3}/Tb_{0.7}$@1	7.93	15.94	40.72
$Eu_{0.2}/Tb_{0.8}$@1	4.74	17.92	33.04

Table S6. CIE chromaticity coordinates (x, y) for Eu^{3+}@l.

λ_{ex} / nm	Eu^{3+}@l
310	(0.614, 0.354)
320	(0.589, 0.358)
330	(0.546, 0.355)
340	(0.436, 0.356)
350	(0.320, 0.346)
360	(0.301, 0.373)
370	(0.289, 0.372)
380	(0.300, 0.362)
390	(0.280, 0.351)
394	(0.345, 0.324)

Table S7. CIE chromaticity coordinates (x, y) for Eu^{3+}@1, Tb^{3+}@1 and Eu^{3+}/Tb^{3+}-loaded samples under excitation wavelengths at 312 nm.

Compounds	Coordinations
Eu^{3+}@1	(0.640, 0.345)
Tb^{3+}@1	(0.274, 0.611)
$Eu_{0.8}Tb_{0.2}$@l	(0.594, 0.372)
$Eu_{0.7}Tb_{0.3}$@l	(0.569, 0.394)
$Eu_{0.6}Tb_{0.4}$@l	(0.560, 0.400)
$Eu_{0.5}Tb_{0.5}$@l	(0.540, 0.424)
$Eu_{0.4}Tb_{0.6}$@l	(0.503, 0.447)
$Eu_{0.3}Tb_{0.7}$@l	(0.484, 0.470)
$Eu_{0.2}Tb_{0.8}$@l	(0.441, 0.510)

Table S8. CIE chromaticity coordinates (x, y) for $Eu_{0.5}Tb_{0.5}$@l.

λ_{ex} / nm	$Eu_{0.5}Tb_{0.5}$@l
320	(0.457, 0.463)
330	(0.371, 0.466)
340	(0.325, 0.435)
350	(0.301, 0.414)
360	(0.301, 0.398)
370	(0.302, 0.393)
380	(0.310, 0.374)
390	(0.283, 0.360)
394	(0.384, 0.325)

Table S9. Luminescence lifetimes of the Eu^{3+}/Tb^{3+}-loaded samples.

Compounds	luminescence lifetimes (τ_{Tb3+})	luminescence lifetimes (τ_{Eu3+})
$Eu_{0.8}Tb_{0.2}$@l	τ_1 = 0.39 ms	τ_1 = 0.19 ms
	τ_2 = 3.46 ms	τ_2 = 1.76 ms
$Eu_{0.7}Tb_{0.3}$@l	τ_1 = 0.36 ms	τ_1 = 0.19 ms
	τ_2 = 3.17 ms	τ_2 = 1.62 ms
$Eu_{0.6}Tb_{0.4}$@l	τ_1 = 0.39 ms	τ_1 = 0.21 ms
	τ_2 = 3.20 ms	τ_2 = 1.81 ms
$Eu_{0.5}Tb_{0.5}$@l	τ_1 = 0.41 ms	τ_1 = 0.21 ms
	τ_2 = 3.10 ms	τ_2 = 1.35 ms
$Eu_{0.4}Tb_{0.6}$@l	τ_1 = 0.42 ms	τ_1 = 0.25 ms
	τ_2 = 3.13ms	τ_2 = 2.14 ms
$Eu_{0.3}Tb_{0.7}$@l	τ_1 = 0.47 ms	τ_1 = 0.23 ms
	τ_2 = 3.25 ms	τ_2 = 1.69 ms
$Eu_{0.2}Tb_{0.8}$@l	τ_1 = 0.47 ms	τ_1 = 0.21 ms
	τ_2 = 2.79 ms	τ_2 = 1.35 ms