Supporting information

Preparation, Crystal structure and Luminescence Properties of Lanthanide Complexes with 2,4,6-tri(pyridin-2-yl)-1,3,5-triazine and Organic Carboxylic Acid

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1. Calculation of luminescent quantum efficiency

As for europium compound, with the emission spectrum and the lifetime of the Eu^{3+} first excited level (τ, $^5D_0$), the emission quantum efficiency (η) of the $^5D_0$ Eu^{3+} excited state can be determined. Assuming that only nonradiative and radiative processes are essentially involved in the depopulation of the $^5D_0$ statea, η can be defined as follows:

$$\eta=\frac{A_r}{A_r+A_{nr}} \qquad (1)$$

Where A_r and A_{nr} are radiative and nonradiative transition rates, respectively. A_r can also be obtained by summing over the radiative rates A_{0J} for each $^5D_0\rightarrow{}^7F_J$ (J=0–4) transitions of Eu^{3+}.

$$Ar=\sum A_{0J}=A_{00}+A_{01}+A_{02}+A_{03}+A_{04} \qquad (2)$$

The branching ratio for the $^5D_0\rightarrow{}^7F_{5,6}$ transitions can be neglected as they are not detected experimentally. In the above eqn (2), A_{0J} can be calculated from the following equation:

$$A_{0J}=A_{01}\left(\frac{I_{0J}}{I_{01}}\right)\left(\frac{\upsilon_{01}}{\upsilon_{0J}}\right) \qquad (3)$$

Here, A_{0J} is the experimental coefficient of spontaneous emission. A_{01} is Einstein's coefficient of spontaneous emission between the $^5D_0$ and $^7F_1$ energy levels. A_{01} can be determined to be about 50 s^{-1}, which can be considered as a reference for the whole spectra. I_{0J} corresponds to the intensities of the $^5D_0\rightarrow{}^7F_J$ transitions (J =0–4). I_{01} corresponds to the intensity of the transition $^5D_0\rightarrow{}^7F_1$ with ν_{0J} ($\nu_{0J}=1/\lambda_J$) energy centers, respectively.

The lifetime (τ), radiative (A_r), and nonradiative (A_{nr}) transition rates are related via

the following equation:

$A_{tot}=1/\tau=A_r+A_{nr}$ (4)

By the described in the above computing method, luminescence quantum yield was obtained.

2. Crystallographic informations

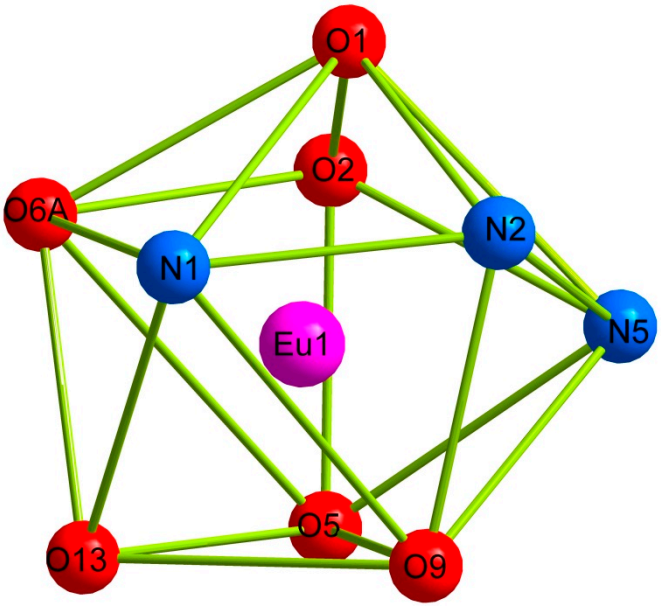

Figure S1. Coordination polyhedron of Eu^{3+} ions in crystal **1**

Table S1. Selected Bond lengths [Å] and angles [°]for crystal 1

Bond			
Eu(1)-O(5)	2.333(4)	Eu(1)-O(2)	2.532(4)
Eu(1)-O(9)	2.368(4)	Eu(1)-N(2)	2.598(4)
Eu(1)-O(6)#1	2.410(4)	Eu(1)-N(1)	2.629(5)
Eu(1)-O(1)	2.478(3)	Eu(1)-N(5)	2.635(5)
Eu(1)-O(13)	2.503(3)		
Angle			
O(5)-Eu(1)-O(9)	82.52(13)	O(1)-Eu(1)-N(2)	67.05(12)
O(5)-Eu(1)-O(6)#1	100.81(13)	O(13)-Eu(1)-N(2)	123.48(12)
O(9)-Eu(1)-O(6)#1	143.32(14)	O(2)-Eu(1)-N(2)	110.06(12)
O(5)-Eu(1)-O(1)	124.54(13)	O(5)-Eu(1)-N(1)	149.68(13)
O(9)-Eu(1)-O(1)	135.39(12)	O(9)-Eu(1)-N(1)	84.37(14)
O(6)#1-Eu(1)-O(1)	72.12(12)	O(6)#1-Eu(1)-N(1)	74.56(14)
O(5)-Eu(1)-O(13)	75.27(13)	O(1)-Eu(1)-N(1)	83.26(13)

O(9)-Eu(1)-O(13)	72.29(12)	O(13)-Eu(1)-N(1)	74.73(13)
O(6)#1-Eu(1)-O(13)	73.35(12)	O(2)-Eu(1)-N(1)	129.72(13)
O(1)-Eu(1)-O(13)	142.85(13)	N(2)-Eu(1)-N(1)	61.80(14)
O(5)-Eu(1)-O(2)	73.13(12)	O(5)-Eu(1)-N(5)	77.87(13)
O(9)-Eu(1)-O(2)	142.63(14)	O(9)-Eu(1)-N(5)	74.85(13)
O(6)#1-Eu(1)-O(2)	70.58(14)	O(6)#1-Eu(1)-N(5)	141.78(13)
O(1)-Eu(1)-O(2)	52.27(11)	O(1)-Eu(1)-N(5)	77.48(13)
O(13)-Eu(1)-O(2)	125.58(11)	O(13)-Eu(1)-N(5)	139.65(12)
O(5)-Eu(1)-N(2)	135.90(14)	O(2)-Eu(1)-N(5)	72.64(13)
O(9)-Eu(1)-N(2)	69.32(12)	N(2)-Eu(1)-N(5)	62.69(14)
O(6)#1-Eu(1)-N(2)	122.17(13)	N(1)-Eu(1)-N(5)	124.46(13)

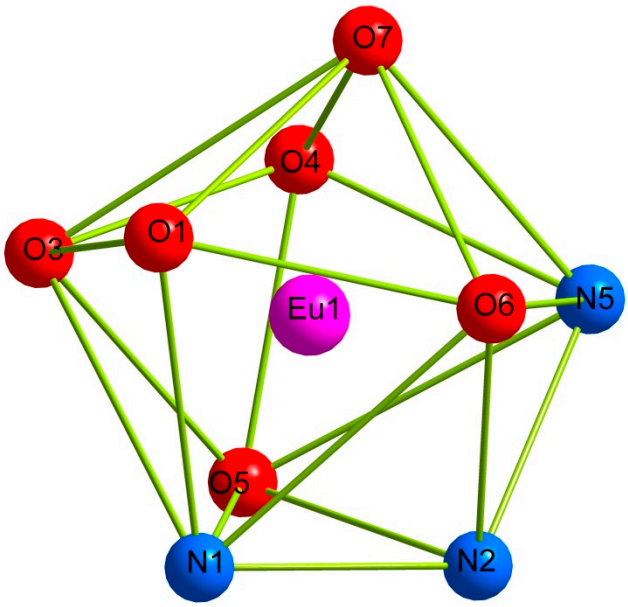

Figure S2. Coordination polyhedron of Eu^{3+} ions in crystal **2**

Table S2. Selected Bond lengths [Å] and angles [°] for crystal 2

Bond			
Eu(1)-O(5)	2.406(9)	Eu(1)-O(4)	2.497(9)
Eu(1)-O(1)	2.420(12)	Eu(1)-N(2)	2.585(11)
Eu(1)-O(6)	2.435(12)	Eu(1)-N(1)	2.592(10)
Eu(1)-O(7)	2.437(9)	Eu(1)-N(5)	2.628(11)
Eu(1)-O(3)	2.446(14)		

Angle			
O(5)-Eu(1)-O(1)	130.5(4)	O(5)-Eu(1)-N(5)	86.6(3)
O(5)-Eu(1)-O(6)	139.1(4)	O(1)-Eu(1)-N(5)	142.6(4)
O(1)-Eu(1)-O(6)	73.8(5)	O(6)-Eu(1)-N(5)	73.8(4)
O(5)-Eu(1)-O(7)	138.6(3)	O(7)-Eu(1)-N(5)	80.2(4)
O(1)-Eu(1)-O(7)	73.3(4)	O(3)-Eu(1)-N(5)	139.6(4)
O(6)-Eu(1)-O(7)	73.8(4)	O(4)-Eu(1)-N(5)	70.5(3)
O(5)-Eu(1)-O(3)	73.9(4)	N(2)-Eu(1)-N(5)	62.1(3)
O(1)-Eu(1)-O(3)	67.9(5)	N(1)-Eu(1)-N(5)	122.8(3)
O(6)-Eu(1)-O(3)	141.5(5)	O(5)-Eu(1)-H(5A)	16.6
O(7)-Eu(1)-O(3)	91.3(4)	O(1)-Eu(1)-H(5A)	113.9
O(5)-Eu(1)-O(4)	70.1(3)	O(6)-Eu(1)-H(5A)	144.7
O(1)-Eu(1)-O(4)	120.8(4)	O(7)-Eu(1)-H(5A)	141.3
O(6)-Eu(1)-O(4)	131.3(3)	O(3)-Eu(1)-H(5A)	60.7
O(7)-Eu(1)-O(4)	68.4(4)	O(4)-Eu(1)-H(5A)	76.4
O(3)-Eu(1)-O(4)	69.6(4)	N(2)-Eu(1)-H(5A)	77.4
O(5)-Eu(1)-N(2)	68.8(3)	N(1)-Eu(1)-H(5A)	65.5
O(1)-Eu(1)-N(2)	121.6(4)	N(5)-Eu(1)-H(5A)	103.2
O(6)-Eu(1)-N(2)	70.2(4)	O(5)-Eu(1)-H(5B)	16.6
O(7)-Eu(1)-N(2)	133.4(4)	O(1)-Eu(1)-H(5B)	135.7
O(3)-Eu(1)-N(2)	135.1(4)	O(6)-Eu(1)-H(5B)	122.4
O(4)-Eu(1)-N(2)	117.5(3)	O(7)-Eu(1)-H(5B)	147.5
O(5)-Eu(1)-N(1)	74.6(3)	O(3)-Eu(1)-H(5B)	89.1
O(1)-Eu(1)-N(1)	72.7(4)	O(4)-Eu(1)-H(5B)	81.3
O(6)-Eu(1)-N(1)	86.1(3)	N(2)-Eu(1)-H(5B)	52.2
O(7)-Eu(1)-N(1)	144.2(3)	N(1)-Eu(1)-H(5B)	68.3
O(3)-Eu(1)-N(1)	86.2(3)	N(5)-Eu(1)-H(5B)	78.5
O(4)-Eu(1)-N(1)	141.5(3)	H(5A)-Eu(1)-H(5B)	28.7
N(2)-Eu(1)-N(1)	60.7(3)		

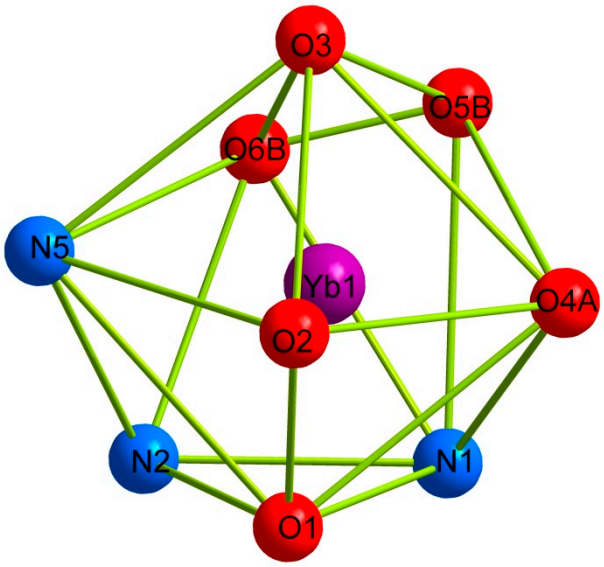

Figure S3. Coordination polyhedron of Yb^{3+} ions in crystal **3**

Table S3. Selected Bond lengths [Å] and angles [°] for crystal 3

Bond			
Yb(1)-O(4)#1	2.172(11)	Yb(1)-O(5)#2	2.48(3)
Yb(1)-O(3)	2.234(13)	Yb(1)-N(2)	2.482(16)
Yb(1)-O(6)#2	2.326(15)	Yb(1)-N(5)	2.498(19)
Yb(1)-O(1)	2.336(13)	Yb(1)-N(1)	2.506(19)
Yb(1)-O(2)	2.460(13)		
Angle			
O(4)#1-Yb(1)-O(3)	90.0(4)	O(4)#1-Yb(1)-N(1)	77.5(5)
O(4)#1-Yb(1)-O(6)#2	123.2(6)	O(3)-Yb(1)-N(1)	146.5(5)
O(3)-Yb(1)-O(6)#2	80.1(5)	O(6)#2-Yb(1)-N(1)	81.2(6)
O(4)#1-Yb(1)-O(1)	85.1(5)	O(1)-Yb(1)-N(1)	79.5(5)
O(3)-Yb(1)-O(1)	130.8(5)	O(2)-Yb(1)-N(1)	126.9(5)
O(6)#2-Yb(1)-O(1)	140.8(5)	O(5)#2-Yb(1)-N(1)	76.0(9)
O(4)#1-Yb(1)-O(2)	76.4(5)	N(2)-Yb(1)-N(1)	63.5(6)
O(3)-Yb(1)-O(2)	78.2(5)	N(5)-Yb(1)-N(1)	127.9(6)
O(6)#2-Yb(1)-O(2)	150.7(7)	O(4)#1-Yb(1)-C(19)	80.6(6)
O(1)-Yb(1)-O(2)	53.0(5)	O(3)-Yb(1)-C(19)	104.8(6)

O(4)#1-Yb(1)-O(5)#2	79.9(7)	O(6)#2-Yb(1)-C(19)	156.0(7)
O(3)-Yb(1)-O(5)#2	71.2(9)	O(1)-Yb(1)-C(19)	26.1(6)
O(6)#2-Yb(1)-O(5)#2	43.9(8)	O(2)-Yb(1)-C(19)	26.9(6)
O(1)-Yb(1)-O(5)#2	153.5(10)	O(5)#2-Yb(1)-C(19)	160.1(8)
O(2)-Yb(1)-O(5)#2	141.0(8)	N(2)-Yb(1)-C(19)	87.3(6)
O(4)#1-Yb(1)-N(2)	134.9(5)	N(5)-Yb(1)-C(19)	76.1(6)
O(3)-Yb(1)-N(2)	135.1(5)	N(1)-Yb(1)-C(19)	103.5(6)
O(6)#2-Yb(1)-N(2)	73.7(6)	O(4)#1-Yb(1)-C(26)#2	101.8(9)
O(1)-Yb(1)-N(2)	67.2(5)	O(3)-Yb(1)-C(26)#2	76.4(10)
O(2)-Yb(1)-N(2)	109.2(5)	O(6)#2-Yb(1)-C(26)#2	21.5(9)
O(5)#2-Yb(1)-N(2)	109.5(7)	O(1)-Yb(1)-C(26)#2	152.3(10)
O(4)#1-Yb(1)-N(5)	148.9(5)	O(2)-Yb(1)-C(26)#2	154.6(10)
O(3)-Yb(1)-N(5)	76.5(5)	O(5)#2-Yb(1)-C(26)#2	22.5(7)
O(6)#2-Yb(1)-N(5)	82.4(6)	N(2)-Yb(1)-C(26)#2	90.2(8)
O(1)-Yb(1)-N(5)	83.0(5)	N(5)-Yb(1)-C(26)#2	102.0(10)
O(2)-Yb(1)-N(5)	73.5(5)	N(1)-Yb(1)-C(26)#2	76.0(11)
O(5)#2-Yb(1)-N(5)	120.3(8)	C(19)-Yb(1)-C(26)#2	177.4(8)
N(2)-Yb(1)-N(5)	64.5(5)		

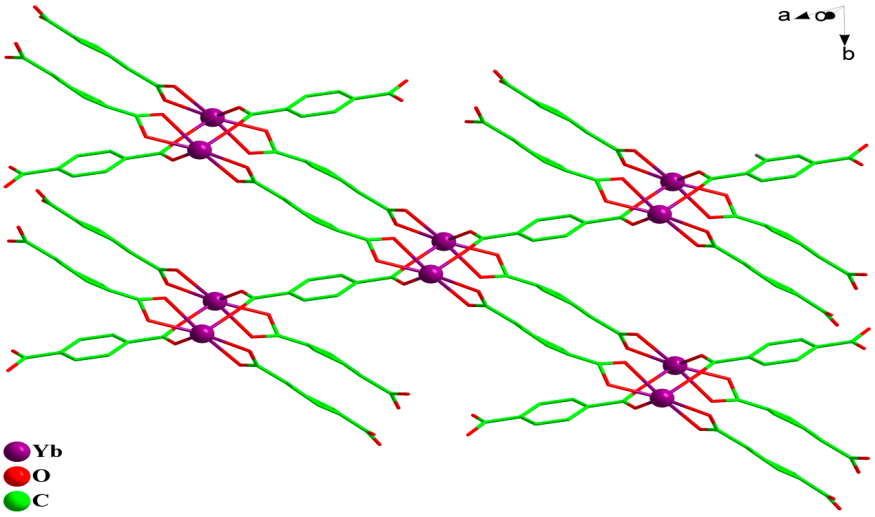

Figure S4. The coordination environment of $BDC^{2-}$and Yb^{3+} in crystal **3**

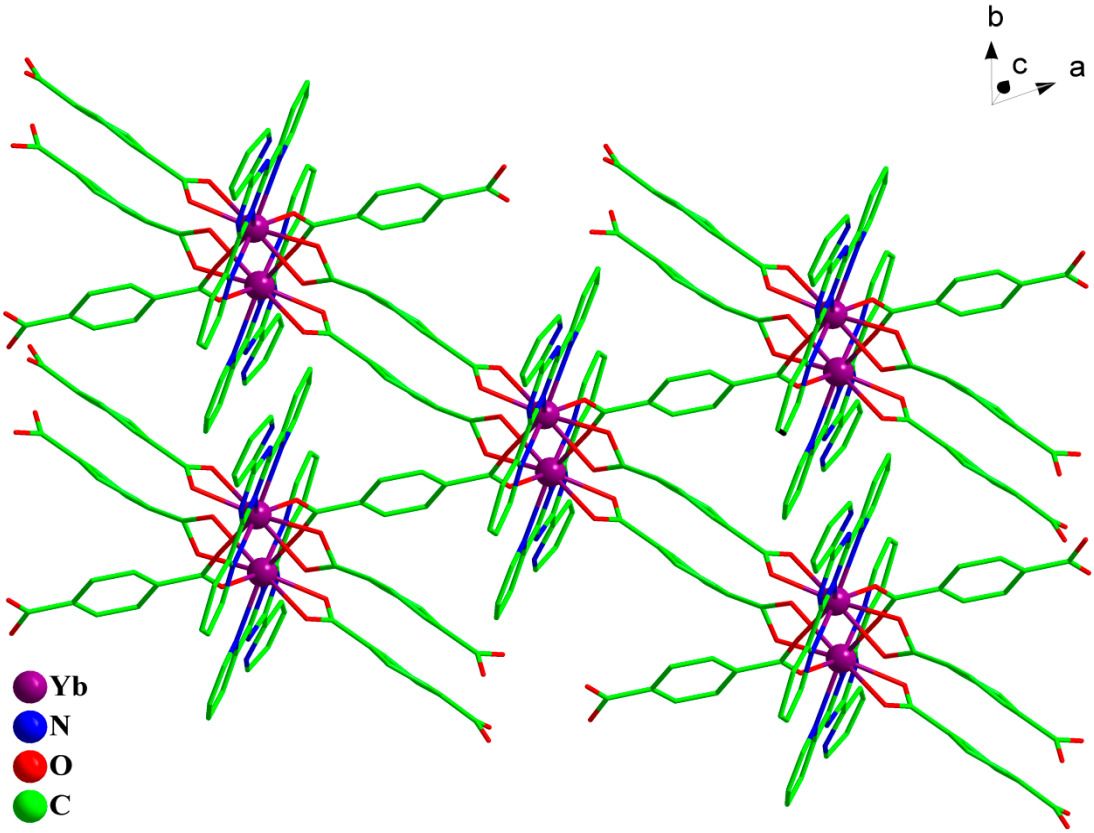

Figure S5. The 2D layered structure of crystal **3**

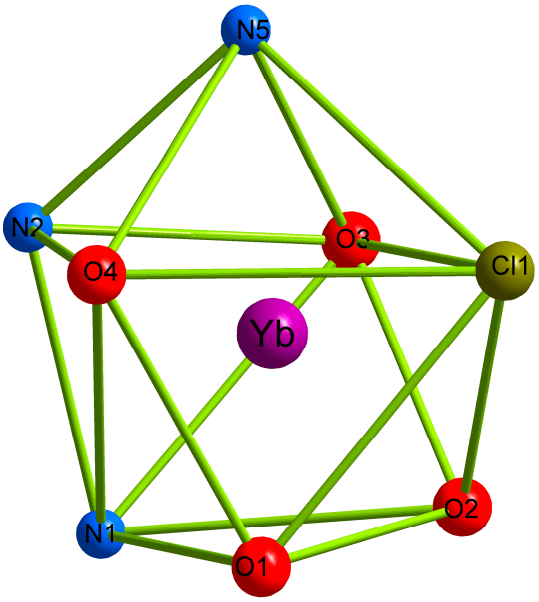

Figure S6. Coordination polyhedron of Yb^{3+} ions in crystal **4**

Table S4. Selected Bond lengths [Å] and angles [º] for crystal 4

Bond			
Yb(1)-O(3)	2.289(6)	Yb(1)-N(2)	2.457(7)
Yb(1)-O(4)	2.325(6)	Yb(1)-N(1)	2.524(7)
Yb(1)-O(2)	2.336(6)	Yb(1)-N(5)	2.548(6)
Yb(1)-O(1)	2.385(5)	Yb(1)-Cl(1)	2.614(2)
Angle			
O(3)-Yb(1)-O(4)	141.1(2)	N(2)-Yb(1)-N(1)	64.1(2)
O(3)-Yb(1)-O(2)	70.7(2)	O(3)-Yb(1)-N(5)	72.6(2)
O(4)-Yb(1)-O(2)	148.11(19)	O(4)-Yb(1)-N(5)	74.0(2)
O(3)-Yb(1)-O(1)	143.2(2)	O(2)-Yb(1)-N(5)	133.3(2)
O(4)-Yb(1)-O(1)	73.9(2)	O(1)-Yb(1)-N(5)	143.6(2)
O(2)-Yb(1)-O(1)	74.7(2)	N(2)-Yb(1)-N(5)	64.8(2)
O(3)-Yb(1)-N(2)	74.9(2)	N(1)-Yb(1)-N(5)	128.3(2)
O(4)-Yb(1)-N(2)	73.2(2)	O(3)-Yb(1)-Cl(1)	106.80(17)
O(2)-Yb(1)-N(2)	129.0(2)	O(4)-Yb(1)-Cl(1)	87.34(15)
O(1)-Yb(1)-N(2)	120.2(2)	O(2)-Yb(1)-Cl(1)	82.17(15)
O(3)-Yb(1)-N(1)	87.3(2)	O(1)-Yb(1)-Cl(1)	80.20(15)
O(4)-Yb(1)-N(1)	98.2(2)	N(2)-Yb(1)-Cl(1)	144.60(15)
O(2)-Yb(1)-N(1)	77.6(2)	N(1)-Yb(1)-Cl(1)	149.85(15)
O(1)-Yb(1)-N(1)	73.1(2)	N(5)-Yb(1)-Cl(1)	81.75(16)

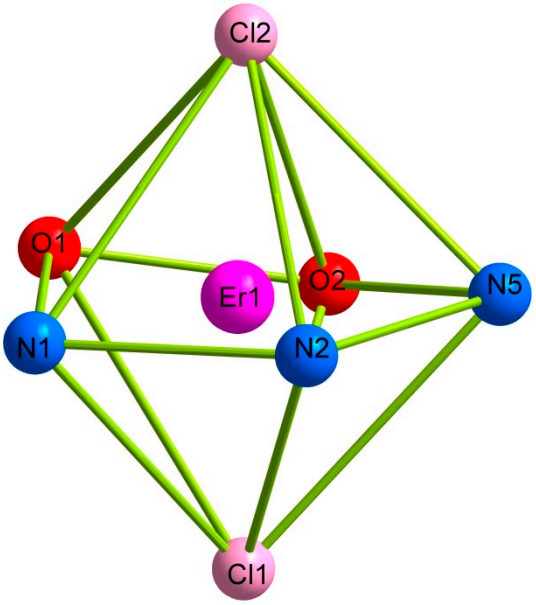

Figure S7. Coordination polyhedron of Yb^{3+} ions in crystal **5**

Table S5. Selected Bond lengths [Å] and angles [°] for crystal 5

Bond			
Er(1)-O(2)	2.242(7)	Er(1)-N(5)	2.528(7)
Er(1)-O(1)	2.280(7)	Er(1)-Cl(2)	2.566(3)
Er(1)-N(2)	2.434(8)	Er(1)-Cl(1)	2.577(3)
Er(1)-N(1)	2.522(7)		
Angle			
O(2)-Er(1)-O(1)	75.3(2)	O(1)-Er(1)-Cl(2)	88.65(19)
O(2)-Er(1)-N(2)	140.5(2)	N(2)-Er(1)-Cl(2)	88.64(19)
O(1)-Er(1)-N(2)	143.9(2)	N(1)-Er(1)-Cl(2)	91.9(2)
O(2)-Er(1)-N(1)	151.4(2)	N(5)-Er(1)-Cl(2)	85.04(19)
O(1)-Er(1)-N(1)	79.0(2)	O(2)-Er(1)-Cl(1)	90.86(19)
N(2)-Er(1)-N(1)	65.2(2)	O(1)-Er(1)-Cl(1)	101.55(19)
O(2)-Er(1)-N(5)	77.9(2)	N(2)-Er(1)-Cl(1)	78.36(19)
O(1)-Er(1)-N(5)	150.9(2)	N(1)-Er(1)-Cl(1)	82.3(2)
N(2)-Er(1)-N(5)	64.3(2)	N(5)-Er(1)-Cl(1)	89.69(19)
N(1)-Er(1)-N(5)	129.5(3)	Cl(2)-Er(1)-Cl(1)	166.99(10)
O(2)-Er(1)-Cl(2)	99.62(19)		

3. Excitation spectra of complexes 1 and 2

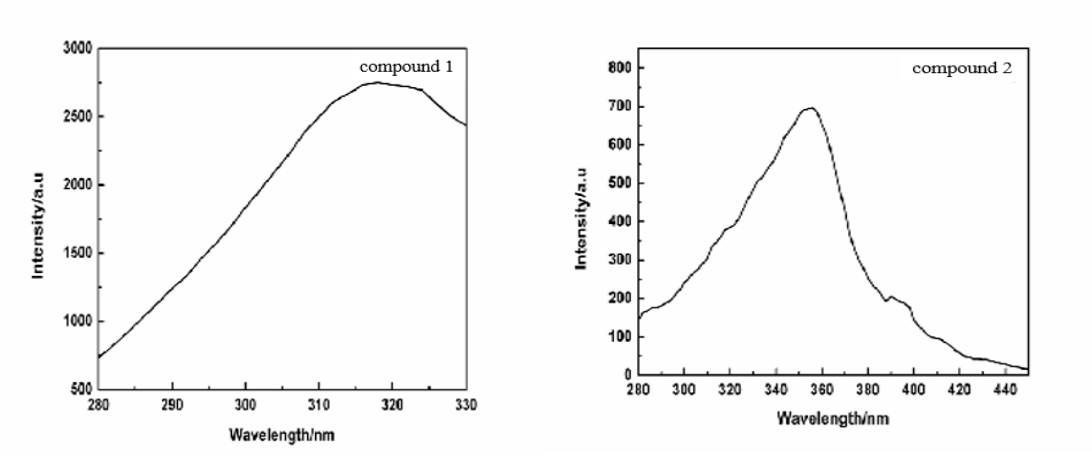

Figure S8. Excitation spectra of complexes 1 and 2

4. Fluorescence fit curves of complexes 1 and 2

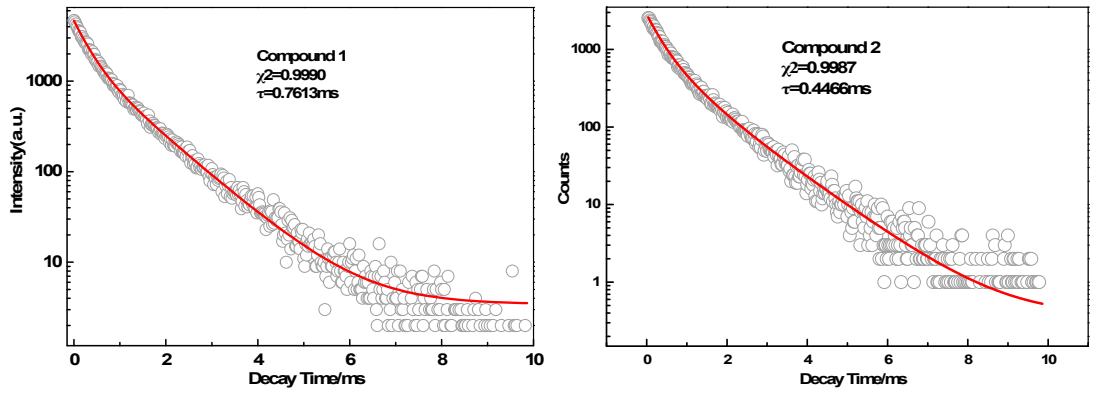

Figure S9. Fluorescence fit curves of complexes 1 and 2