Seven Ln (III) Coordination Polymers with Two Kinds of Geometric Coordination but the Same 3D Topological Property: Luminescence Sensing and Magnetic Properties

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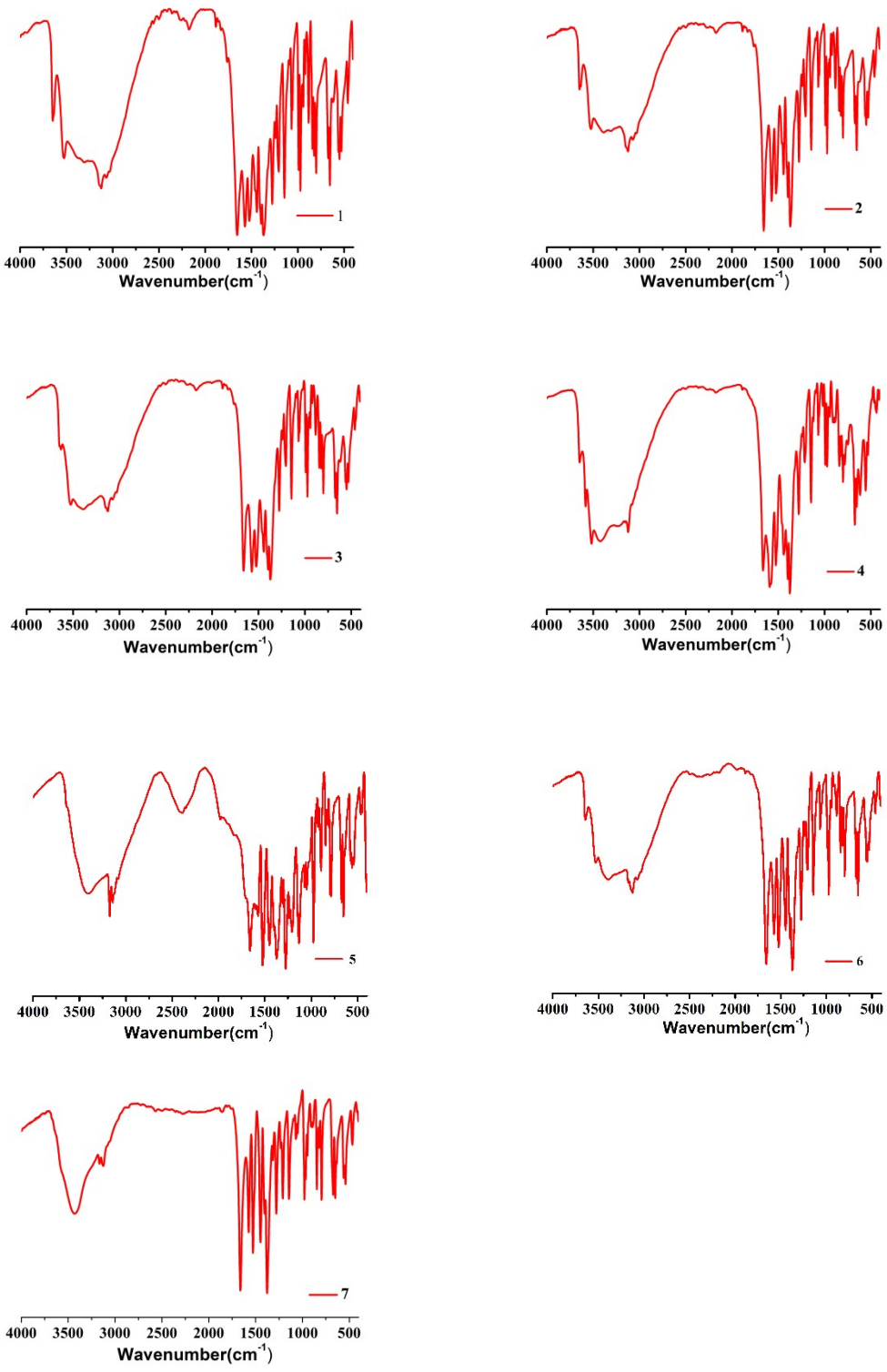

Fig. S1 IR spectra of complexes **1-7**.

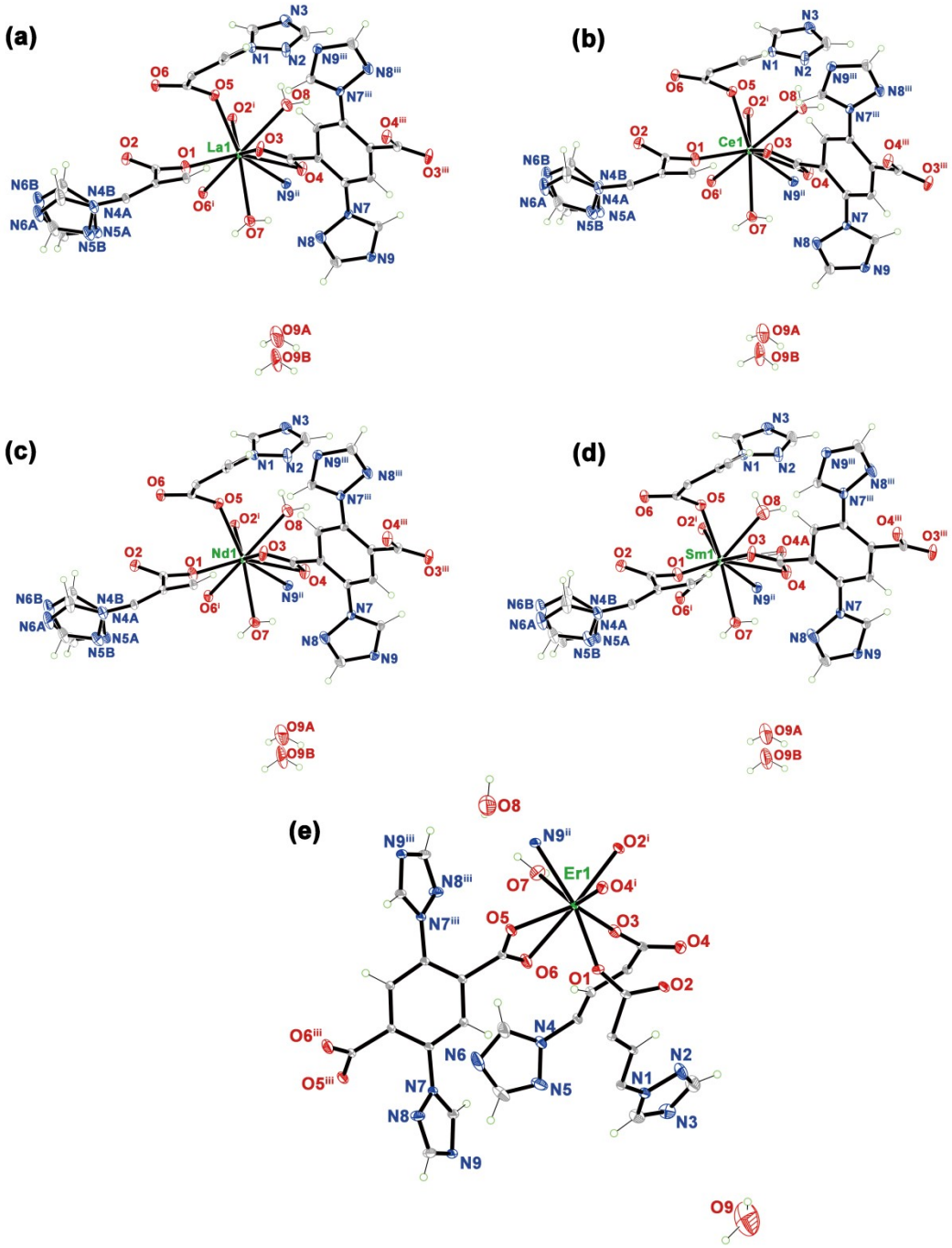

Fig. S2 Coordination environment of the La^{3+} ion in **1** (a), the Ce^{3+} ion in **2** (b), the Nd^{3+} ion in **3** (c), the Sm^{3+} ion in **4** (d) and the Er^{3+} ion in **7** (e).

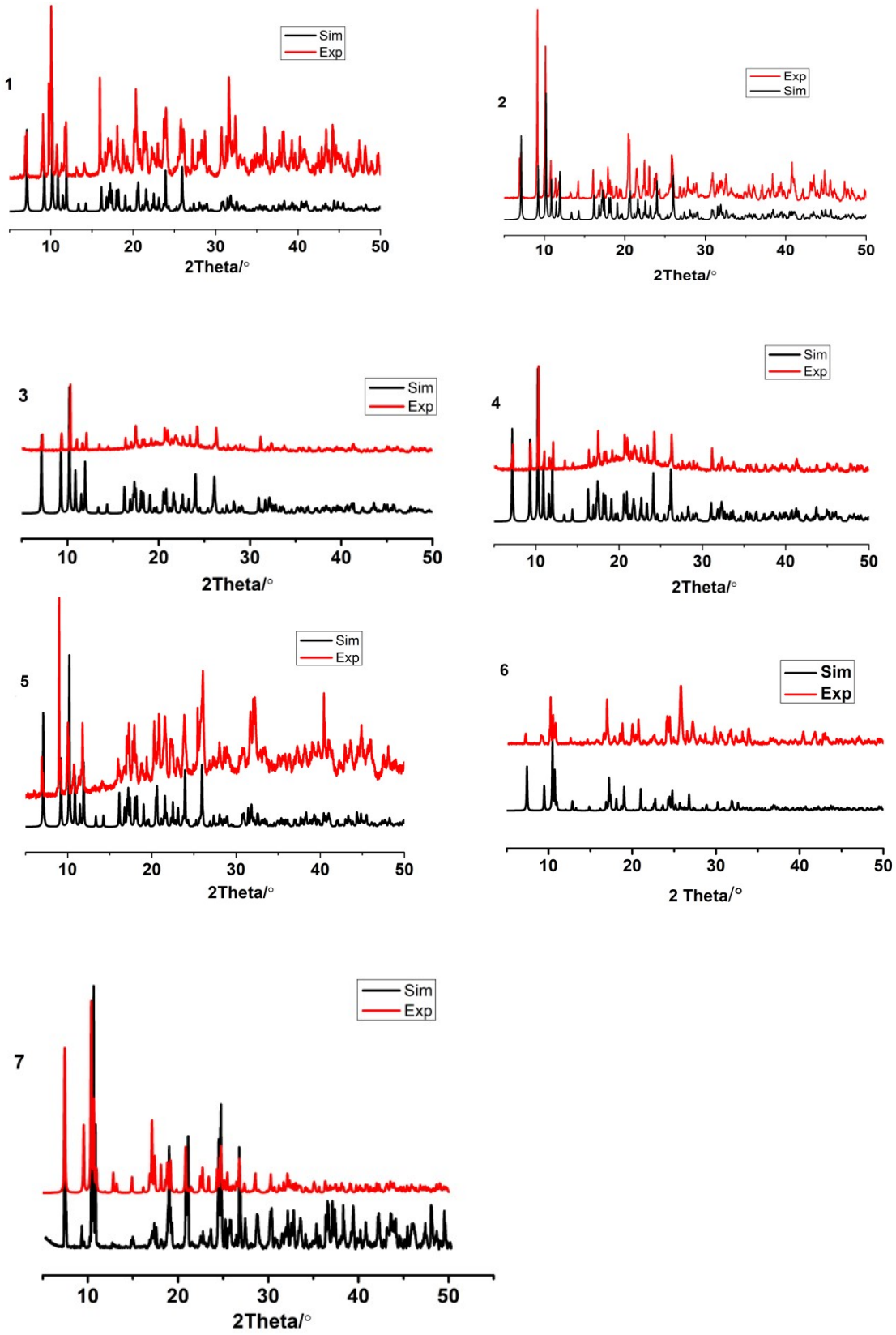

Fig. S3 PXRD patterns of complexes **1-7**.

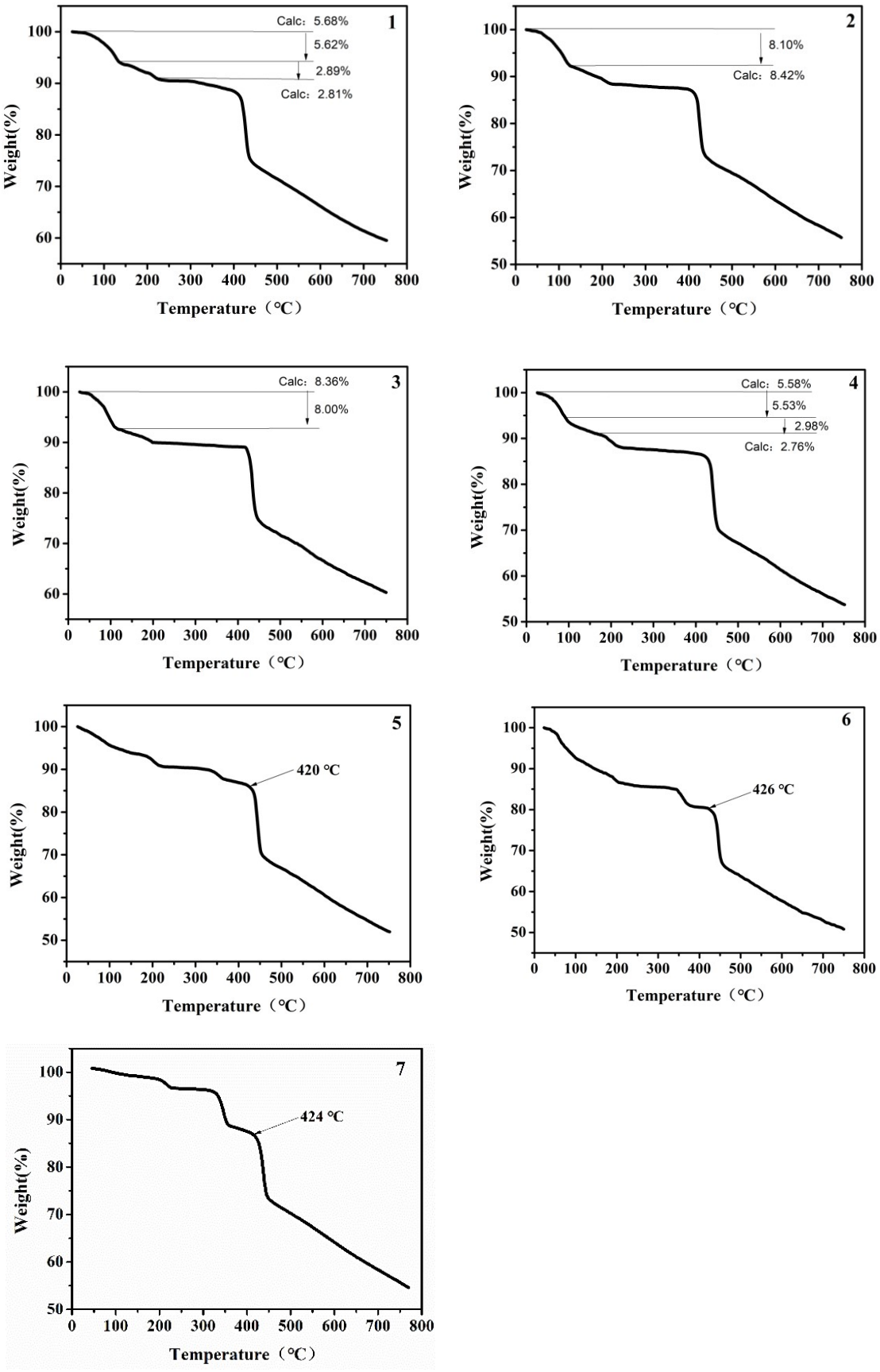

Fig. S4 TGA spectra of complexes **1-7**.

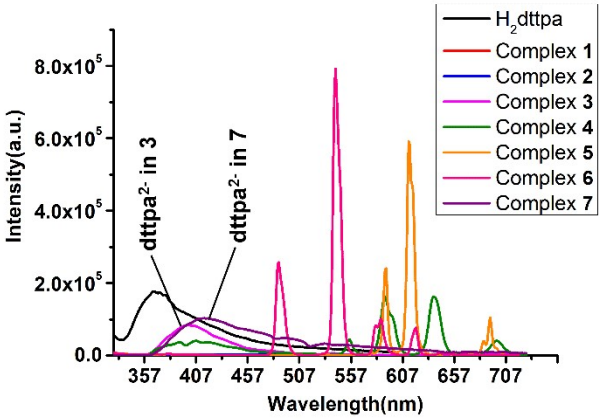

Fig. S5 Solid-state emission spectra of H_2dttpa and complexes **1**−**7** with λ_{ex} = 311 nm.

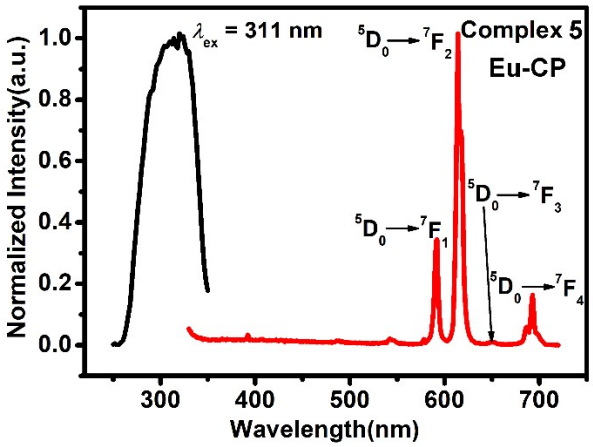

Fig. S6 Solid-state excitation (black line) and emission (red line) spectra of complex **5** (λ_{ex} = 311 nm) at room temperature.

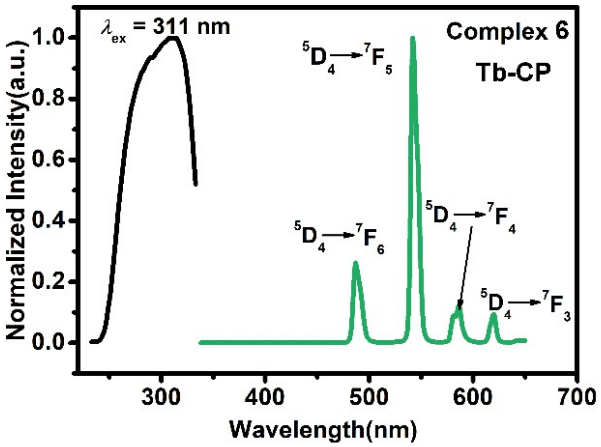

Fig. S7 Solid-state excitation (black line) and emission (green line) spectra of complex **6** (λ_{ex} = 311 nm) at room temperature.

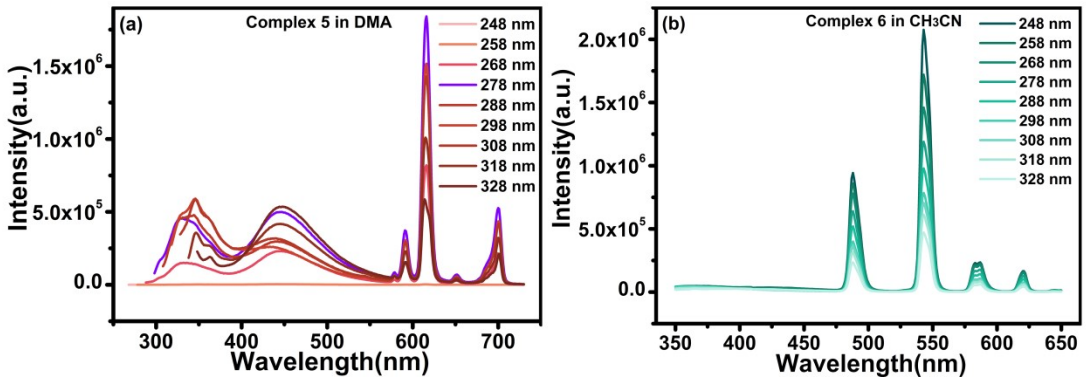

Fig. S8 The emission spectra of complex **5** in DMA (a) and **6** in CH_3CN (b) with different excitation wavelengths.

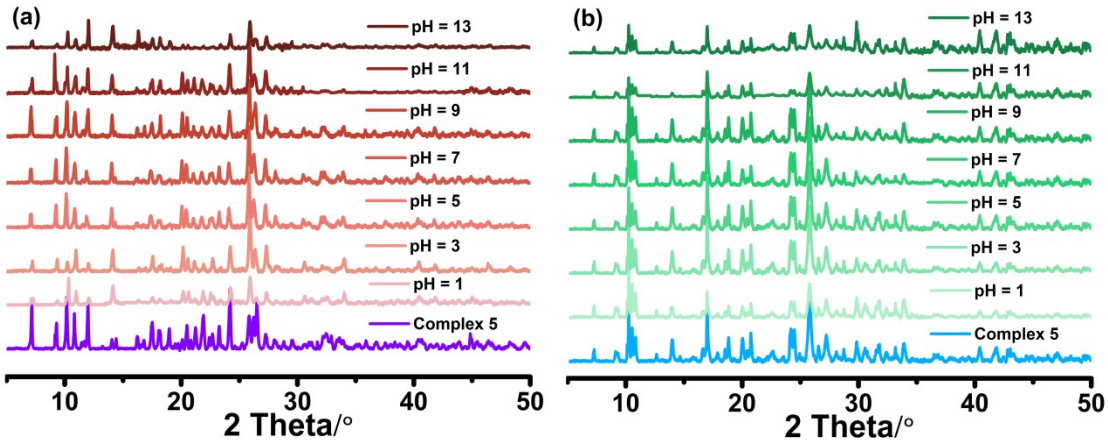

Fig. S9 PXRD of recycled powders for complexes **5** (a) and **6** (b) from different pH detection systems.

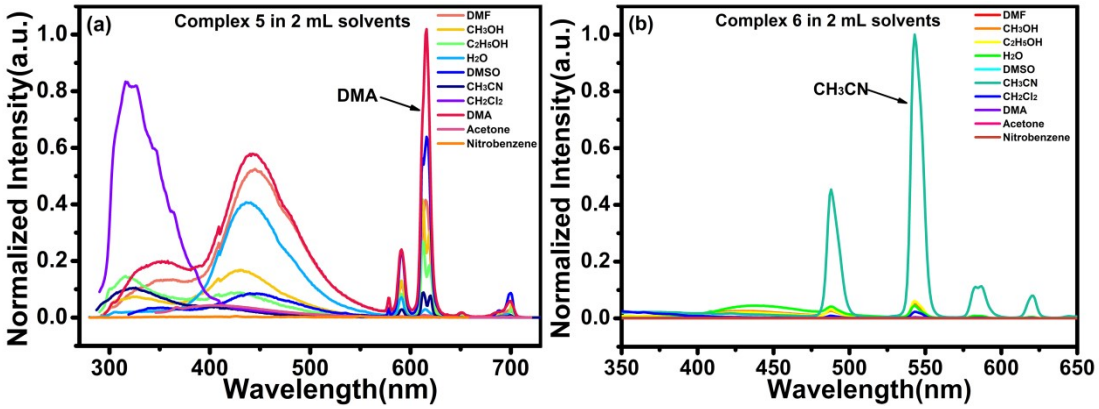

Fig. S10 (a) Fluorescence intensities of complex **5** (λ_{ex} = 278 nm) and (b) complex **6** (λ_{ex} = 248 nm) in different solvents.

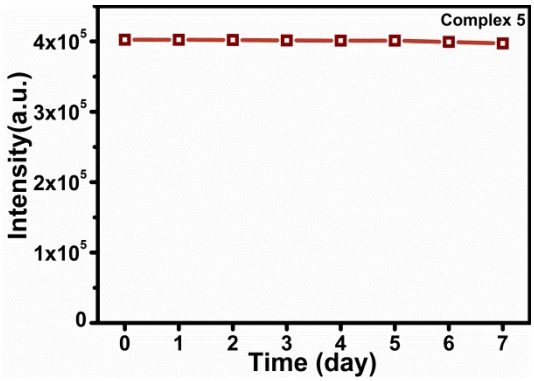

Fig. S11 The stability for complex **5** in DMA within 7 days.

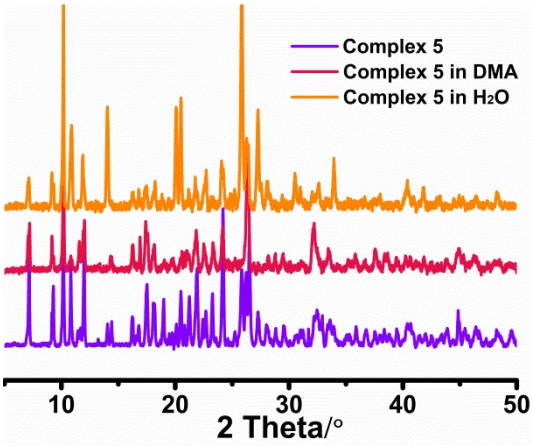

Fig. S12 PXRD of complex **5** and complex **5** in DMA and H_2O for 7 days.

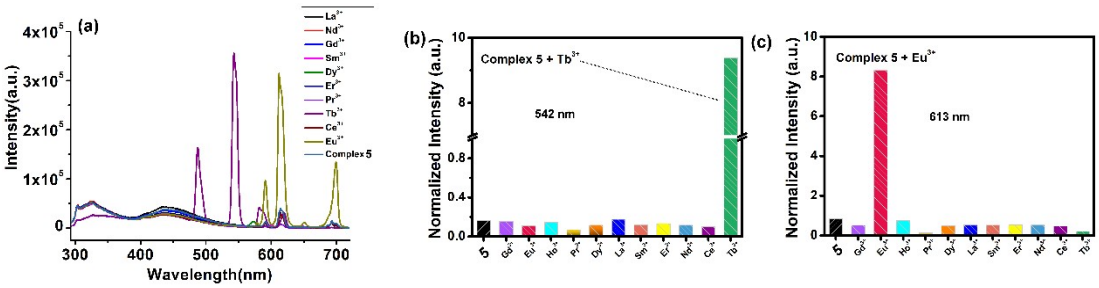

Fig. S13 (a) Luminescence responses of **5** (5.0 mg dispersed in 50.0 mL of DMA) toward different lanthanide cations solution (λ_{ex} = 278 nm); (b) Luminescence intensity of **5** with the additional different lanthanide cations solution at 542 nm; (c) Luminescence intensity of **5** with different lanthanide cations solution at 613 nm.

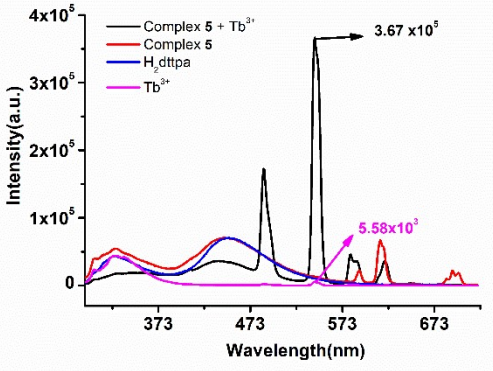

Fig. S14 Luminescence spectra of **5** in DMA (5.0 mg dispersed in 50.0 mL of DMA), complex **5** with additional Tb^{3+}, ligand H_2dttpa and Tb^{3+} in DMA.

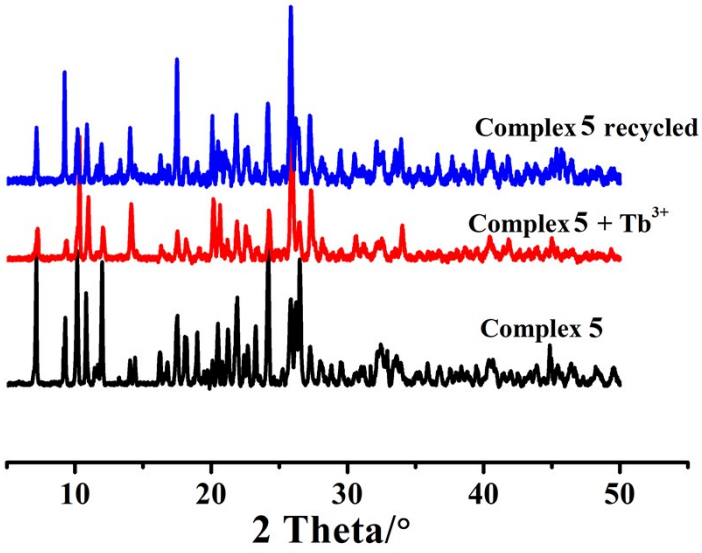

Fig. S15 PXRD of complex **5**, the solid samples after sensing Tb^{3+} ions and after the 5 cycle experiments.

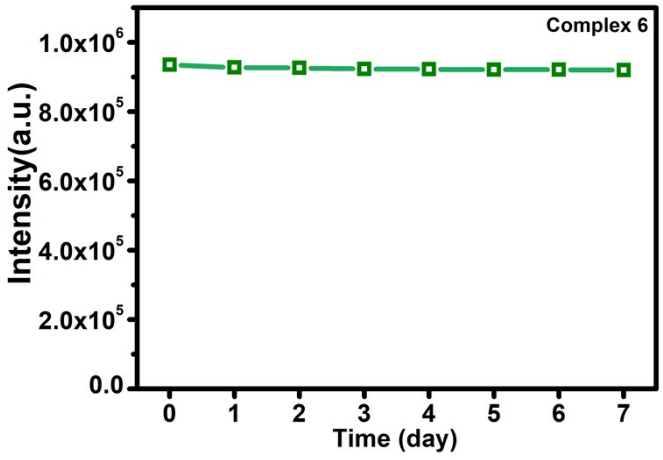

Fig. S16 The stability for complex **6** in CH_3CN for 7 days.

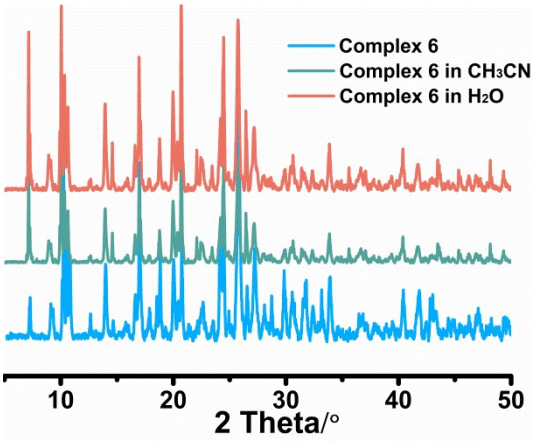

Fig. S17 PXRD of complex **6** and complex **6** in CH_3CN and H_2O for 7 days.

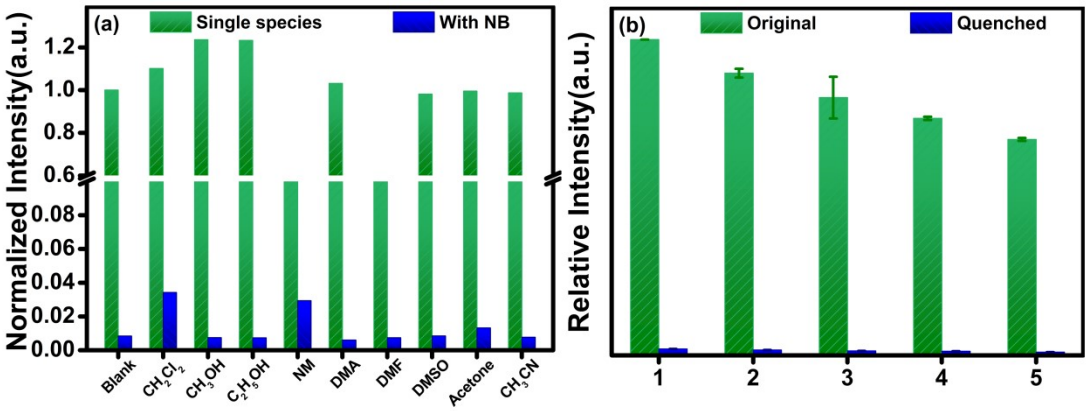

Fig. S18 (a) Interference study of complex 6 (Tb-CP) for sensing NB in the presence of other solvents; (b) Reproducibility of the quenching ability of 6 in CH3CN and in NB (60 μM of NB).

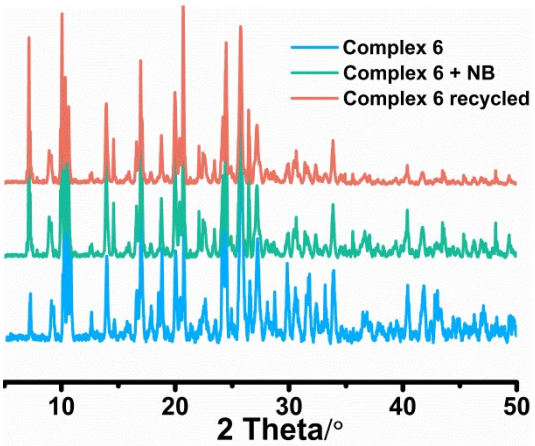

Fig. S19 PXRD of complex **6**, the solid samples after sensing NB and after the 5 cycle experiments.

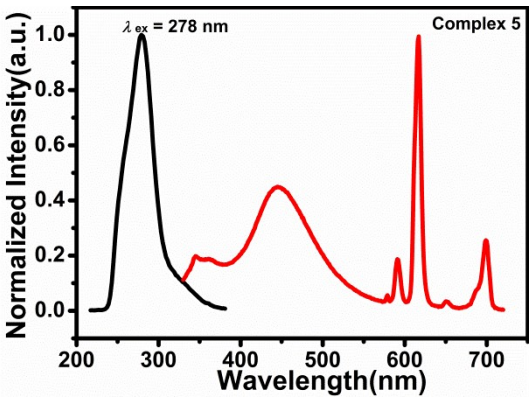

Fig. S20 The excitation and emission spectra of complex **5** in DMA (λ_{ex} = 278 nm)

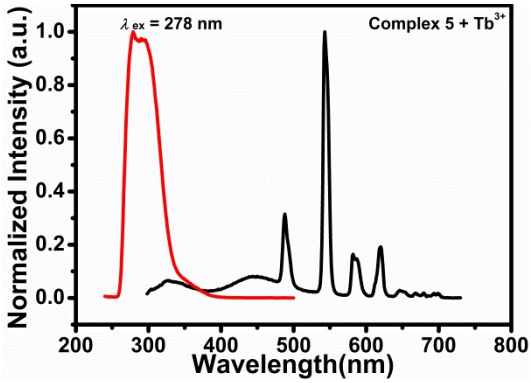

Fig. S21 The excitation and emission spectra of complex **5** in DMA plus Tb^{3+} (λ_{ex} = 278 nm with the maximum emission of Tb^{3+})

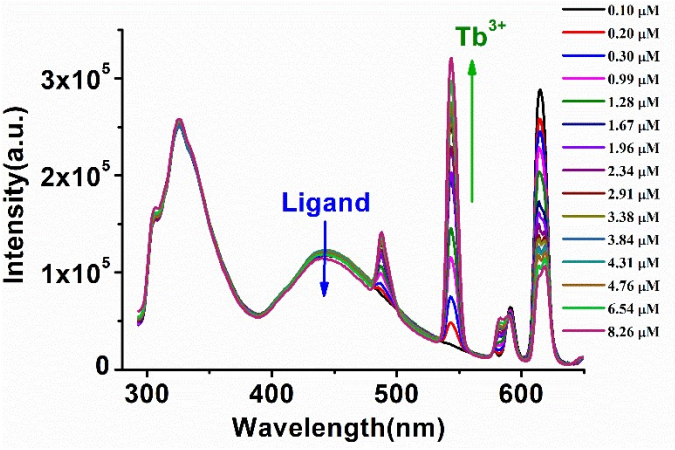

Fig. S22 Two-dimensional luminescence responses of compound **5** toward different concentrations of $TbCl_3$ solution.

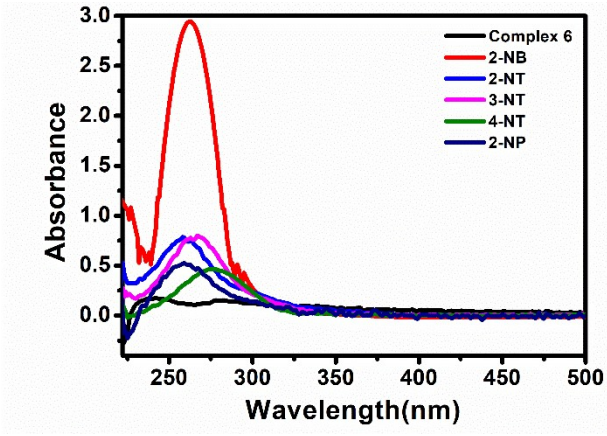

Fig. S23 UV-vis spectra of complex **6** and **6** after adding NB, 2-NT, 2-NP, 3-NT and 4-NT in CH_3CN.

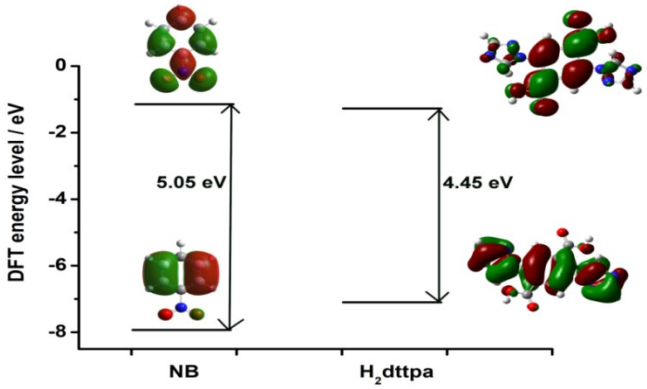

Fig. S24 Energy gap of the HOMO and LUMO for H_2dttpa and NB.

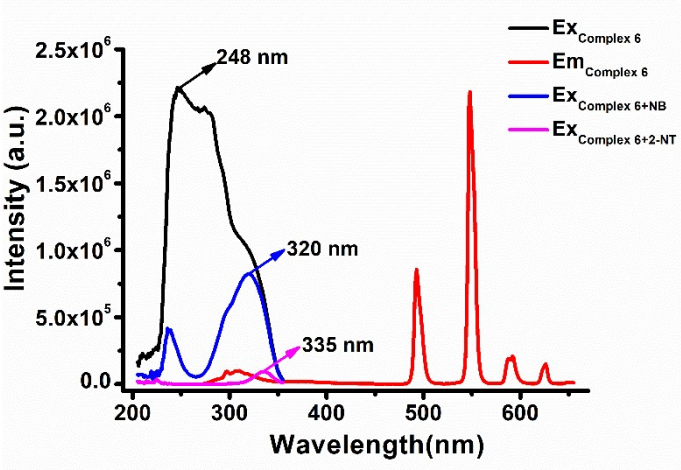

Fig. S25 The excitation spectra of complex **6** in CH_3CN and **6** in CH_3CN after adding NB and 2-NT, respectively.

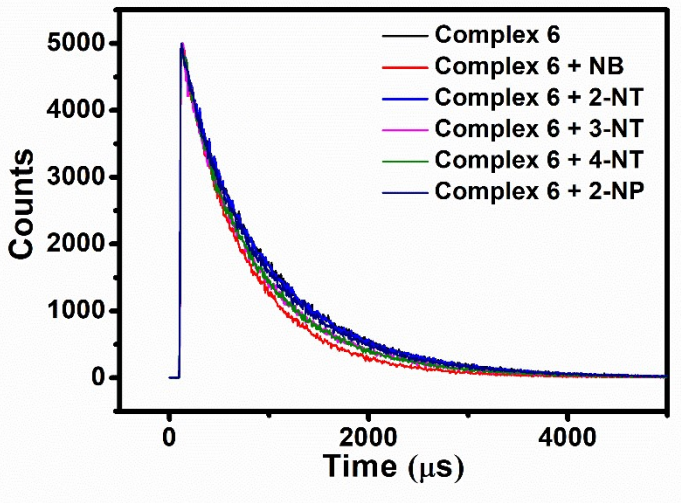

Fig. S26 Lifetime for $^5D_4$ emission of **6** in CH_3CN and after adding NB, 2-NT, 2-NP, 3-NT and 4-NT.

Table S1 Crystal data and structure refinement for complexes **1-7**

Comp.	**1**	**2**	**3**	**4**	**5**	**6**	**7**
CCDC	2096052	2096053	2096054	2096055	2096056	2096057	2096058
Formula	$C_{18}H_{15}LaN_9O_9$	$C_{18}H_{15}CeN_9O_9$	$C_{18}H_{15}NdN_9O_9$	$C_{18}H_{15}SmN_9O_9$	$C_{18}H_{15}EuN_9O_9$	$C_{36}H_{30}N_{18}O_{15.5}Tb_2$	$C_{36}H_{25}Er_2N_{18}O_{15.5}$
M_r	640.30	641.51	645.63	651.74	653.35	1275.60	1292.26
Crystal	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic
Space	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
Temp. (K)	296 (2)	296 (2)	296 (2)	296 (2)	296 (2)	296 (2)	298 (2)
Size	0.26 × 0.25 × 0.24	0.26 × 0.25 × 0.24	0.26 × 0.25 × 0.23	0.23 × 0.22 × 0.20	0.26 × 0.25 × 0.23	0.26 × 0.24 × 0.22	0.26 × 0.24 × 0.23
a (Å)	9.5199 (5)	9.4853 (4)	9.4901 (4)	9.4774 (4)	9.4618 (4)	9.3859 (5)	9.3751 (5)
b (Å)	10.4152 (6)	10.3887 (5)	10.3535 (5)	10.3232 (4)	10.3098 (5)	10.4122 (5)	10.3758 (5)
c (Å)	12.6533 (7)	12.6157 (6)	12.5438 (5)	12.4655 (5)	12.4302 (6)	12.1355 (6)	12.0667 (5)

α (°)	84.4347 (15)	84.4594 (15)	84.3246 (13)	84.0976 (13)	83.9872 (17)	97.9575 (15)	98.0007 (14)
β (°)	79.2703 (15)	79.4366 (14)	79.5509 (13)	80.0670 (13)	80.5410 (18)	92.8219 (15)	93.1898 (14)
γ (°)	67.2952 (14)	67.3666 (14)	67.1626 (13)	66.9366 (12)	66.8943 (16)	114.2386 (15)	114.3485 (13)
V (Å^3)	1136.70 (11)	1127.50 (9)	1116.50 (9)	1104.45 (8)	1099.04 (9)	1063.60 (9)	1050.62 (9)
Z	2	2	2	2	2	1	1
μ (mm^{-1})	1.950	2.09	2.40	2.73	2.93	3.39	4.07
R_{int}	0.030	0.024	0.027	0.026	0.025	0.024	0.024
GOF	1.08	1.09	1.12	1.10	1.10	1.03	1.05
F_{000}	630	632	636	640	642	614	621
R_1 [$I >$ 2σ(I)][a]	0.023	0.014	0.015	0.017	0.021	0.014	0.014
ωR_2 [$I >$ 2$\sigma(I)$][b]	0.048	0.036	0.038	0.045	0.053	0.037	0.036
$\Delta\rho_{max}$ (e Å^{-3})	0.67	0.41	0.72	0.68	0.73	0.40	0.74
$\Delta\rho_{min}$ (e Å^{-3})	-0.35	-0.34	-0.51	-0.83	-1.11	-0.57	-0.68

[a] R_1=∑IIF_oI-IF_cII/∑IF_oI

[b] ωR_2=[Σω (F_o^2- F_c^2)^2/Σω(F_o^2)^2]$^{1/2}$

The B alerts in the structures of 1-5 maybe due to the structure, then resulting in the absence of suitable hydrogen bond acceptors.

The B alerts in the structures of 6 and 7 maybe due to the water molecules removed from the SQUEEZE form hydrogen bonds with the H7A around O7.

Table S2 The selected bond lengths and angles of all the complexes

Complex **1**			
Bond	Distance(Å)	Bond	Distance(Å)

La1—O5	2.4702 (16)	La1—O7	2.5749 (17)
La1—O1	2.4730 (16)	La1—O3	2.6268 (17)
La1—O6^{i}	2.5283 (16)	La1—O4	2.6520 (17)
La1—O2^{i}	2.5424 (16)	La1—N9^{ii}	2.7230 (19)
La1—O8	2.5613 (18)		
Angle	Degree(°)	Angle	Degree(°)
O5—La1—O1	73.93 (6)	O2^{i}—La1—O8	67.22 (6)
O5—La1—O6^{i}	118.06 (5)	O5—La1—O7	147.06 (6)
O1—La1—O6^{i}	78.03 (5)	O1—La1—O7	78.23 (6)
O5—La1—O2^{i}	75.27 (6)	O6^{i}—La1—O7	71.82 (6)
O1—La1—O2^{i}	118.84 (6)	O2^{i}—La1—O7	135.01 (6)
O6^{i}—La1—O2^{i}	72.08 (6)	O8—La1—O7	127.58 (6)
O5—La1—O8	70.15 (6)	O5—La1—O3	77.33 (6)
O1—La1—O8	140.30 (6)	O1—La1—O3	74.25 (5)
O6^{i}—La1—O8	134.46 (6)	O6^{i}—La1—O3	142.72 (6)
Symmetry codes: (i) -*x*, -*y*+2, -*z*+1; (ii) -*x*, -*y*+2, -*z*+2;			
Complex **2**			
Bond	Distance(Å)	Bond	Distance(Å)
Ce1—O5	2.4456 (10)	Ce1—O7	2.5491 (12)
Ce1—O1	2.4533 (10)	Ce1—O3	2.6044 (11)
Ce1—O6^{i}	2.5055 (10)	Ce1—O4	2.6429 (11)
Ce1—O2^{i}	2.5202 (10)	Ce1—N9^{ii}	2.6996 (12)
Ce1—O8	2.5391 (13)		
Angle	Degree(°)	Angle	Degree(°)
O5—Ce1—O1	74.34 (4)	O5—Ce1—O7	147.21 (4)
O5—Ce1—O6^{i}	117.82 (4)	O1—Ce1—O7	77.86 (4)
O1—Ce1—O6^{i}	77.97 (4)	O6^{i}—Ce1—O7	71.93 (4)
O5—Ce1—O2^{i}	75.03 (4)	O2^{i}—Ce1—O7	135.01 (4)
O1—Ce1—O2^{i}	118.89 (4)	O8—Ce1—O7	127.75 (4)
O6^{i}—Ce1—O2^{i}	71.83 (4)	O5—Ce1—O3	77.27 (4)
O5—Ce1—O8	70.08 (4)	O1—Ce1—O3	74.07 (4)

O1—Ce1—O8	140.60 (4)	O6^{i}—Ce1—O3	142.90 (4)
O6^{i}—Ce1—O8	134.20 (4)	O2^{i}—Ce1—O3	143.99 (4)
O2^{i}—Ce1—O8	67.19 (4)	O8—Ce1—O3	82.03 (5)
Symmetry codes: (i) -*x*, -*y*+2, -*z*+1; (ii) -*x*, -*y*+2, -*z*+2;			
Complex **3**			
Bond	Distance(Å)	Bond	Distance(Å)
Nd1—O5	2.4129 (12)	Nd1—O8	2.5104 (15)
Nd1—O1	2.4202 (12)	Nd1—O3	2.5698 (13)
Nd1—O6^{i}	2.4717 (12)	Nd1—O4	2.6185 (13)
Nd1—O2^{i}	2.4864 (12)	Nd1—N9^{ii}	2.6559 (14)
Nd1—O7	2.5087 (13)		
Angle	Degree(°)	Angle	Degree(°)
O5—Nd1—O1	74.71 (5)	O5—Nd1—O8	69.96 (5)
O5—Nd1—O6^{i}	117.72 (4)	O1—Nd1—O8	140.92 (5)
O1—Nd1—O6^{i}	77.61 (4)	O6^{i}—Nd1—O8	134.18 (5)
O5—Nd1—O2^{i}	74.81 (4)	O2^{i}—Nd1—O8	67.08 (5)
O1—Nd1—O2^{i}	118.81 (4)	O7—Nd1—O8	127.96 (5)
O6^{i}—Nd1—O2^{i}	71.88 (4)	O5—Nd1—O3	76.69 (4)
O5—Nd1—O7	147.06 (4)	O1—Nd1—O3	74.07 (4)
O1—Nd1—O7	77.41 (5)	O6^{i}—Nd1—O3	143.15 (5)
O6^{i}—Nd1—O7	72.07 (4)	O2^{i}—Nd1—O3	143.45 (5)
O2^{i}—Nd1—O7	135.33 (4)	O7—Nd1—O3	79.08 (5)
Symmetry codes: (i) -*x*, -*y*+2, -*z*+1; (ii) -*x*, -*y*+2, -*z*+2;			
Complex **4**			
Bond	Distance(Å)	Bond	Distance(Å)
Sm1—O5	2.3805 (14)	Sm1—O4A	2.377 (8)
Sm1—O1	2.3902 (14)	Sm1—O8	2.504 (2)
Sm1—O6^{i}	2.4360 (14)	Sm1—O3	2.5466 (15)
Sm1—O2^{i}	2.4458 (14)	Sm1—O4	2.607 (3)
Sm1—O7	2.4680 (15)	Sm1—N9^{ii}	2.6231 (17)
Angle	Degree(°)	Angle	Degree(°)

O4A—Sm1—O5	97.0 (4)	O4A—Sm1—O7	82.6 (5)
O5—Sm1—O1	75.18 (6)	O5—Sm1—O7	147.07 (5)
O4A—Sm1—O6^{i}	143.4 (4)	O1—Sm1—O7	77.80 (6)
O5—Sm1—O6^{i}	118.41 (5)	O6^{i}—Sm1—O7	72.62 (5)
O1—Sm1—O6^{i}	77.31 (5)	O2^{i}—Sm1—O7	135.63 (5)
O5—Sm1—O2^{i}	75.22 (5)	O4A—Sm1—O8	48.4 (5)
O1—Sm1—O2^{i}	119.38 (5)	O5—Sm1—O8	69.23 (7)
O6^{i}—Sm1—O2^{i}	72.43 (5)	O1—Sm1—O8	140.81 (7)
Symmetry codes: (i) -*x*, -*y*+2, -*z*+1; (ii) -*x*, -*y*+2, -*z*+2.			
Complex **5**			
Bond	Distance(Å)	Bond	Distance(Å)
Eu1—O5	2.3651 (18)	Eu1—O4A	2.357 (7)
Eu1—O1	2.3779 (18)	Eu1—O8	2.511 (3)
Eu1—O6^{i}	2.4194 (18)	Eu1—O3	2.5415 (19)
Eu1—O2^{i}	2.4274 (17)	Eu1—O4	2.604 (4)
Eu1—O7	2.4472 (19)	Eu1—N9^{ii}	2.614 (2)
Angle	Degree(°)	Angle	Degree(°)
O4A—Eu1—O5	96.0 (4)	O6^{i}—Eu1—O7	73.07 (7)
O5—Eu1—O1	75.33 (7)	O2^{i}—Eu1—O7	135.81 (7)
O4A—Eu1—O6^{i}	143.9 (3)	O4A—Eu1—O8	47.6 (4)
O5—Eu1—O6^{i}	118.87 (6)	O5—Eu1—O8	68.84 (9)
O1—Eu1—O6^{i}	77.30 (6)	O1—Eu1—O8	140.67 (9)
O5—Eu1—O2^{i}	75.52 (6)	O6^{i}—Eu1—O8	134.66 (9)
O1—Eu1—O2^{i}	119.78 (7)	O2^{i}—Eu1—O8	66.29 (9)
O6^{i}—Eu1—O2^{i}	72.76 (7)	O7—Eu1—O8	126.87 (8)
O4A—Eu1—O7	82.8 (4)	O5—Eu1—O3	75.95 (7)
O5—Eu1—O7	147.05 (6)	O1—Eu1—O3	74.03 (6)
O1—Eu1—O7	78.22 (7)	O6^{i}—Eu1—O3	142.73 (7)
Symmetry codes: (i) -*x*, -*y*+2, -*z*+1; (ii) -*x*, -*y*+2, -*z*+2;			
Complex **6**			

Bond	Distance(Å)	Bond	Distance(Å)
Tb1—O3	2.2951 (13)	Tb1—O2^{i}	2.3672 (12)
Tb1—O1	2.3470 (13)	Tb1—O7	2.3770 (15)
Tb1—O4^{i}	2.3642 (13)	Tb1—N9^{ii}	2.5585 (15)
Tb1—O5	2.3669 (13)	Tb1—O6	2.5679 (14)
Angle	Degree(°)	Angle	Degree(°)
O3—Tb1—O1	77.03 (5)	O3—Tb1—O7	83.24 (6)
O3—Tb1—O4^{i}	122.93 (5)	O1—Tb1—O7	144.65 (5)
O1—Tb1—O4^{i}	76.45 (5)	O4^{i}—Tb1—O7	138.56 (5)
O3—Tb1—O5	130.46 (5)	O5—Tb1—O7	90.00 (6)
O1—Tb1—O5	81.22 (5)	O2^{i}—Tb1—O7	78.83 (5)
O4^{i}—Tb1—O5	93.52 (5)	O3—Tb1—N9^{ii}	146.80 (5)
O3—Tb1—O2^{i}	78.04 (5)	O1—Tb1—N9^{ii}	135.38 (5)
O1—Tb1—O2^{i}	124.11 (5)	O4^{i}—Tb1—N9^{ii}	70.35 (5)
O4^{i}—Tb1—O2^{i}	76.75 (5)	O5—Tb1—N9^{ii}	72.14 (5)
O5—Tb1—O2^{i}	148.27 (5)	O2^{i}—Tb1—N9^{ii}	76.15 (5)
Symmetry codes: (i) -*x*+1, -*y*, -*z*+1; (ii) *x*, *y*-1, *z*;			
Complex **7**			
Bond	Distance(Å)	Bond	Distance(Å)
Er1—O3	2.2625 (13)	Er1—O2^{i}	2.3329 (13)
Er1—O1	2.3103 (13)	Er1—O7	2.3363 (15)
Er1—O4^{i}	2.3264 (13)	Er1—N9^{ii}	2.5204 (15)
Er1—O5	2.3293 (14)	Er1—O6	2.5603 (15)
Angle	Degree(°)	Angle	Degree(°)
O3—Er1—O1	77.33 (5)	O5—Er1—O2^{i}	148.59 (5)
O3—Er1—O4^{i}	122.97 (5)	O3—Er1—O7	82.33 (6)
O1—Er1—O4^{i}	76.25 (5)	O1—Er1—O7	144.17 (5)
O3—Er1—O5	130.21 (5)	O4^{i}—Er1—O7	139.31 (5)
O1—Er1—O5	80.85 (5)	O5—Er1—O7	90.47 (6)
O4^{i}—Er1—O5	93.64 (5)	O2^{i}—Er1—O7	79.13 (5)
O3—Er1—O2^{i}	78.09 (5)	O3—Er1—N9^{ii}	146.54 (5)

O1—Er1—O2^{i}	123.97 (5)	O1—Er1—N9^{ii}	135.43 (5)
O4^{i}—Er1—O2^{i}	76.51 (5)	O4^{i}—Er1—N9^{ii}	70.79 (5)
Symmetry codes: (i) -*x*+1, -*y*, -*z*+1; (ii) *x*, *y*-1.			

Table S3 Hydrogen-bond geometry (Å, º) for complexes **1-7**

Complex **1**				
D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7*A*···O4	0.82	2.30	2.794 (2)	119
O7—H7*B*···N3^{vii}	0.82	1.93	2.731 (3)	167
O8—H8*A*···O9*A*^{viii}	0.82	1.91	2.731 (8)	174
O9*A*—H9*A*···N6*A*^{ix}	0.83	2.30	2.964 (11)	138
O9*A*—H9*A*···N6*B*^{ix}	0.83	2.05	2.710 (15)	136
O9*A*—H9*B*···O8^{vii}	0.83	2.05	2.731 (8)	139
Symmetry codes: (vii) *x*+1, *y*, *z*; (viii) *x*-1, *y*, *z*; (ix) *x*, *y*, *z*+1.				
Complex **2**				
D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O9*A*—H9*B*···O8^{viii}	0.82	2.06	2.732 (6)	139
O9*A*—H9*A*···N6*B*^{vii}	0.83	2.06	2.727 (11)	137
O9*A*—H9*A*···N6*A*^{vii}	0.83	2.29	2.953 (9)	137
O8—H8*A*···O9*A*^{vi}	0.82	1.92	2.732 (6)	174
O7—H7*B*···N3^{viii}	0.82	1.93	2.7310 (18)	168
O7—H7*A*···O4	0.82	2.29	2.7818 (17)	120
Symmetry codes: (vi) *x*-1, *y*, *z*; (vii) *x*, *y*, *z*+1; (viii) *x*+1, *y*, *z*;				
Complex **3**				
D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7*A*···O4	0.81	2.26	2.7596 (19)	120
O7—H7*B*···N3^{vii}	0.82	1.92	2.728 (2)	168
O8—H8*A*···O9*A*^{viii}	0.81	1.90	2.709 (6)	174
O9*A*—H9*A*···N6*A*^{ix}	0.82	2.28	2.935 (9)	138
O9*A*—H9*A*···N6*B*^{ix}	0.82	2.05	2.702 (13)	136

O9*A*—H9*B*···O8^{vii}	0.82	2.03	2.709 (6)	139
Symmetry codes: (vii) *x*+1, *y*, *z*; (viii) *x*-1, *y*, *z*; (ix) *x*, *y*, *z*+1.				
Complex **4**				
D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O9*B*—H9*B*···O8^{viii}	0.94	2.01	2.624 (14)	121
O9*B*—H9*C*···O4*A*^{viii}	0.82	1.57	2.39 (2)	172
O9*A*—H9*B*···O8^{viii}	0.82	2.01	2.673 (5)	138
O9*A*—H9*A*···N6*B*^{vii}	0.82	2.05	2.693 (14)	135
O8—H8*A*···O9*B*^{vi}	0.81	1.89	2.624 (14)	150
O8—H8*A*···O9*A*^{vi}	0.81	1.87	2.673 (5)	172
O7—H7*B*···N3^{viii}	0.82	1.91	2.721 (3)	169
O7—H7*A*···O4	0.81	2.23	2.729 (4)	120
Symmetry codes: (vi) *x*-1, *y*, *z*; (vii) *x*, *y*, *z*+1; (viii) *x*+1, *y*, *z*;				
Complex **5**				
D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O9*B*—H9*B*···O8^{viii}	0.96	2.01	2.65 (3)	122
O9*B*—H9*C*···O4*A*^{viii}	0.82	1.63	2.45 (3)	172
O9*A*—H9*B*···O8^{viii}	0.82	2.01	2.667 (5)	137
O9*A*—H9*A*···N6*B*^{vii}	0.81	2.03	2.666 (16)	135
O9*A*—H9*A*···N6*A*^{vii}	0.81	2.27	2.915 (9)	137
O8—H8*A*···O9*B*^{vi}	0.81	1.91	2.65 (3)	151
O8—H8*A*···O9*A*^{vi}	0.81	1.86	2.667 (5)	170
O7—H7*B*···N3^{viii}	0.82	1.91	2.717 (3)	170
Symmetry codes: (vi) *x*-1, *y*, *z*; (vii) *x*, *y*, *z*+1; (viii) *x*+1, *y*, *z*;				
Complex **6**				

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O8—H8*A*···O8^{i}	0.85	2.02	2.570 (10)	122
O8—H8*A*···N6^{ii}	0.85	2.49	2.953 (5)	115
O7—H7*B*···N3^{viii}	0.81	1.93	2.734 (2)	173
O7—H7*A*···O8	0.82	1.98	2.739 (5)	153
Symmetry codes: (i) -*x*+2, -*y*, -*z*+2; (ii) *x*, *y*-1, *z*; (viii) -*x*+2, -*y*+1, -*z*+1.				
Complex **7**				
D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O8—H8*A*···O8^{viii}	0.85	2.04	2.578 (10)	121
O8—H8*A*···N6^{ii}	0.85	2.46	2.923 (5)	115
O7—H7*B*···N3^{v}	0.81	1.93	2.739 (2)	174
O7—H7*A*···O8	0.82	1.98	2.735 (5)	153
Symmetry codes: (ii) *x*, *y*-1, *z*; (v) -*x*+2, -*y*+1, -*z*+1; (viii) -*x*+2, -*y*, -*z*+2;				

Table S4 Quantum yields of Eu-CP, Eu-CP after loaded Tb^{3+} and Tb-CP.

Sample	Quantum yield
Eu-CP	17 %
Tb^{3+}@ Eu-CP	4 %
Tb-CP	15 %

Table S5 The detection limitation of complex **5** in this paper and of previously reported compounds for the detection of Tb^{3+}

No.	Complex	Analyte	LOD(nM)	Media	Ref
1	$[(CH_3)_2NH_2]_2[Cd_3(BPTC)_2]\cdot(DMF)$	Tb^{3+}	1.0×10^4	DMF	S1
2	$(Cd_3(L)_{2.5}(4\text{-PTZ})(DMF)_3$	Tb^{3+}	10	DMF	S2
3	$[Zn_3(L)(DCTP)_3]_n$	Tb^{3+}	11.5	Ethanol–H_2O	S3
4	cy(WQETR)	Tb^{3+}	5×10^4	Tris buffer	S4
5	PPH	Tb^{3+}	56	--	S5
4	$\{[Eu(dttpa)_{1.5}(H_2O)_2]\cdot H_2O\}_n$	Tb^{3+}	9.88	DMA	Complex **5**

Table S6 The detection limitation of complex **6** in this paper and of previously reported compounds for the detection of nitrobenzene (NB)

No.	Complex	Analyte	K_{SV}/M^{-1}	LOD(nM)	Media	Ref
1	{[Eu(L)(DMF)(H_2O)]·0.5DMF}$_n$	NB	4.74×10^6	1.38×10^3	DMF	S6
2	[Eu(L)(DEF)(H_2O)]$_n$	NB	1.20×10^6	1.09×10^4	DMF	S6
3	EuL	NB	302	1.0×10^3	DMF	S7
4	TbL	NB	320	5.0×10^3	DMF	S7
5	2**a**	NB	2.14×10^4	--	DMF	S8
6	2**b**	NB	2.48×10^4	--	DMF	S8
7	Porous Silicon	NB	--	5.0×10^3	Air	S9
8	OMCN-x	NB	--	1.8×10^5	PBS	S10
9	{[Zn(L)]·DMA}$_n$ (1)	NB	--	7.5×10^3	DMF	S11
10	1-Eu	NB	--	--	DMF	S12
11	3	NB	2.7×10^3	2.54×10^6	DMA	S13
12	{[Cd(tdc)(hedn)(H_2O)]·3H$_2$O}$_n$	NB	2.5×10^5	6.7×10^6	DMSO+EtOH	S14
13	{[Cd(tdc)(hdin)(H_2O)]·H_2O} n	NB	6.4×10^5	--	--	S14
14	{[Cd_2(tdc) (hdn)(H_2O)$_4$]·H_2O}n	NB	8.4×10^5	--	--	S14
15	{[Cd2(tdc) (pdn)(H_2O)$_2$]·4H_2O}n	NB	4.1×10^5	--	--	S14
16	[Cd(tdc)(pdin)]$_n$	NB	7.4×10^5	--	--	S14
17	$Eu_2Ti_4(\mu_2\text{-}O)_2(\mu_3\text{-}O)_4(phen)_2(tbza)^{10}\cdot4CH_3CN$	NB	0.095 (ppm^{-1})	10.5	CH_2Cl_2	S15
18	Au-NPs	NB	--	16.0	--	S16
19	IFMC-36-Eu	NB	--	1.0×10^4	DMA	S17
20	IFMC-3	NB	--	--	DMA	S18
21	{[Cd(dms)(4-pmina)]·2.5H_2O}$_n$	NB	--	--	DMSO+EtOH	S19
22	UiO-66-NH_2	NB	--	0.9×10^3	Trizma base	S20
23	$[NH_2(CH_3)_2]_2[Cd_{17}(L)_{12}(\mu_3\text{-}H_2O)_4(DMF)_2(H_2O)_2]$·solvent	NB	--	135	DMF	S21

24	$[Zn_3(TDPAT)(H_2O)_3]$	NB	--	5.0×10^4	Methanol	S22
25	Tb-1	NB	5.61×10^3	1.0×10^5	EtOH	S23
26	Tb− MOF	NB	6.03×10^5	41.4	H_2O	S24
27	M-15/OA	NB	--	1.22×10^3	H_2O	S25
28	Tb− MOF	NB	--	40.6	DMF	S26
29	Complex 1	NB	6.55×10^3	1.13×10^4	EtOH	S27
30	Complex 1	NB	1.19×10^5	147	EtOH	S28
30	Complex 2	NB	5.13×10^5	1142	EtOH	S28
30	Complex 3	NB	6.18×10^5	33.0	EtOH	S28
30	Complex 4	NB	2.62×10^5	192	EtOH	S28
31	$\{[Tb(dttpa)_{1.5}(H_2O)]\cdot0.42H_2O\}_n$	NB	5.6×10^6	12.5	CH_3CN	Complex **6**

Table S7 Lifetime for $^5D_4$ emission of **6** and after adding NB, 2-NT, 2-NP, 3-NT and 4-NT.

Sample	τ_1 (μs)	Rel_1 %	τ_2 (μs)	Rel_2 %	τ (μs)
Complex 6	310	5.47	917	94.54	884
Complex 6+NB	529	45.52	808	54.48	681
Complex 6+2-NT	412	9.86	928	90.14	877
Complex 6+3-NT	462	21.91	887	78.09	794
Complex 6+4-NT	411	17.11	859	82.89	782
Complex 6+2-NP	436	14.17	918	85.83	850

References:

S1 S. -M. Chen and T.-T. Lian, *Inorg. Chem. Comm*., 2011, **14**, 447-449.

S2 F. -Y. Yi, M. L. Gu, S. -C. Wang, J. -Q. Zheng, L. Q. Pan and L Han. Inorg. Chem. 2018, 57, 2654-2662.

S3 M.-M. Fu, L. S. Fu and G.-H. Cui, Dalton Trans, 2021, 50, 10180- 10186.

S4 F. Ji, S. Shao, Z. Li, S. Wang, R. Chaudhuri, Z. Guo, N. Perkins, P. Sarkar and M. Xue, Analyst. 2021, 146, 3474-3481.

S5 H. Zamani, M. Ranjkesh, M. R. Abedi, Int. J. Electrochem. Sci. 2014, 9, 8435–8445.

S6 R. R. Ma, Z. W. Chen, S. N. Wang, Q. X. Yao, Y. W. Li, J. Lu, D. C. Li, J. M. Dou. J. Solid State Chem., 2017, 252, 142–151.

S7 W. Liu, X. Huang, C. Y. Chen, C. Xu, J. X. Ma, L. Z. Yang, W. J. Wang, W. Dou and W. S. Liu. Chem. Eur. J. 2019, 25, 1090-1097.

S8 M. Z. K. Baig, P. K. Sahu, M. Sarkar and M. Chakravarty. J. Org. Chem. 2017, 82, 13359−13367

S9 S. Content, W. C. Trogler, M. J. Sailor. Chem. Eur. J. 2000, 6, 2205-2213.

S10 Y. F. Zhang, X. X. Bo, A. Nsabimana, C. Luhana, G. Wang, H. Wang, M. Li, L.P. Guo. Biosens. Bioelectron., 2014, 53, 250–256.

S11 D. M. Chen, X. –Z. Ma, W. Shi, P. Cheng. Cryst. Growth Des. 2015, 15, 3999−4004

S12 R. -C. Gao, F.-S. Guo, N. -N. Bai, Y. –L. Wu, F. Yang, J. -Y. Liang, Z. –J. Li, Y. -Y. Wang. Inorg. Chem. 2016, 55, 11323−11330.

S13 Y. –T. Yan, J. Liu, G.-P. Yang, F. Zhang, Y.- K. Fan, W. -Y. Zhang, Y. -Y. Wang. CrystEngComm, 2018, 20, 477–486.

S14 J. J. Przybyla, R. L. LaDuca. Inorganica Chimica Acta, 2019, 486 , 314–323

S15 H. Zheng, Y. -K. Deng, M.-Yu Ye, Q. -F. Xu, X. –J. Kong, L. –S. Long, L. –S. Zheng. Inorg. Chem. 2020, 59, 12404−12409

S16 R. Emmanuel, C. Karuppiaha, S. M. Chen, S. Palanisamya, P. Prakash. J. Hazard. Mater., 2014, 279, 117-124.

S17 S. -R. Zhang, D. –Y. Du, J. –S. Qin, S. –L. Li, W. –W. He, Y. –Q. Lan, Z. –M. Su. Inorg. Chem. 2014, 53, 8105−8113.

S18 J. –S. Qin, S. –J. Bao, P. Li, W. Xie, D. -Y.Du, L. Zhao, Y. –Q. Lan, Z. –M. Su. Chem. Asian J. 2014, 9, 749 – 753.

S19 C.L. White, R. L. LaDuca. Inorg. Chim. Acta, 2016, 441, 169–180

S20 K. Vellingiri, D. W. Boukhvalov, S. K. Pandey, A. Deep, K. –H. Kim. Sensors. Actuat. B., 2017, 245, 305–313.

S21 D. Tian, Y. Li, R.-Y. Chen, Z. Chang, G.-Y. Wang, X.-H. Bu, J. Mater. Chem.A, 2014, 2, 1465–1470.

S22 D. Ma, B. Li, X. Zhou, Q. Zhou, K. Liu, G. Zeng, G. Li, Z. Shi, S. Feng. Chem. Comm. 2013, 49, 8964–8966.

S23 Y. H. Pham, V. A. Trush, M. Korabik, V. M. Amirkhanov, P. Gawryszewska. Dyes and Pigments, 2021, 186, 108986.

S24 X. -L. Chen, L. Shang, L. Liu, H. Yang, H. -L. Cui, J. -J. Wang. Dyes and Pigments, 2021, 196, 109809.

S25 X. P. Quan, B.Yan. J. Hazard. Mater., 2022, 427, 127869.

S26 C. -H. Zhan, D. -P. Huang, Y. Wang, W. -T. Mao, X. -J. Wang, Z. -G. Jiang. CrystEngComm, 2021, 23, 2788–2792.

S27 L. -L. Ren, Y. -Y. Cui, A. -L. Cheng, E. -Q. Gao. J. Solid. State. Chem., 2019, 270, 463–469.

S28 X. Yang, Y. X Ren, H. M. Chai, X. F. Hou, Z. X. Wang, J. J. Wang. RSC Adv., 2021, 11, 23975–23984.