Supplementary Information

A Series of Color-Tunable Light-Emitting Open-Framework Lanthanide Sulfates Containing Extra-Large 36-Ring Channels

Yun-Shan Xue,[a,b] Dayou Shi,[a] Haitao Zhang,[a] Weiwei Ju,[a] Hua Mei[a] and Yan Xu*[a,c]

[a]*College of Chemical Engineering, State Key Laboratory of Materials-oriented Chemical Engineering, Nanjing Tech University, Nanjing, 210009 (China). E-mail: yanxu@njut.edu.cn; Tel: (+86)25-83587857.*

[b]*school of chemistry and environmental engineering，yancheng teachers university，yancheng，224002，China*

[c]*State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing 210093, P. R. China.*

Table of Contents

3. Tables

1. Experimental section

Synthesis of mix-Eu/TbSO$_4$-NTU1: [(CH$_3$)$_2$NH$_2$]$_{14}$[(Eu$_x$Tb$_{1-x}$)$_{10}$(μ_2-OH)$_4$(μ_3-OH)$_8$(SO$_4$)$_{16}$]·6H$_2$O (x = 0.1980, 0.0997, 0.0509, 0.0196, 0.0095, 0.0070, 0.0049, 0.0025, 0.0011). The Eu/Tb mixed lanthanide sulfates were synthesized similarly to LnSO$_4$-NTU1 except for the use of a mixture of EuCl$_3$·6H$_2$O and TbCl$_3$·6H$_2$O. Optimized synthesis condition for the synthesis of mix-Eu/TbSO$_4$-NTU1:

taking mix-Eu/TbSO$_4$-NTU1 (x = 0.1980) as an example, a mixture of EuCl$_3$·6H$_2$O (0.0729 g, 0.199 mmol), TbCl$_3$·6H$_2$O (0.3009 g, 0.8059 mmol), D-tartaric acid (0.0503 g, 0.335 mmol), H$_2$O (0.8007 g, 44.45 mmol) was added into N,N-dimethyl formamide (10 mL); aqueous HF (40 wt %, 0.1001 g, 2.001 mmol) and concentrated H$_2$SO$_4$ (98 wt %, 0.1435 g, 1.434 mmol) were added dropwise to the mixture. The resulting mixture was then vigorously stirred for two hours and was introduced into a 25 mL Teflon-lined stainless steel autoclave. The autoclave was sealed and heated at 393 K for 3 days. After cooling to room temperature, the product was washed with ethanol, and colorless block crystals were obtained (0.0806 g, 22.09% based on Eu). Anal. Calcd for C$_{28}$H$_{138}$N$_{14}$O$_{82}$S$_{16}$Eu$_{1.98}$Tb$_{8.02}$ (4071.95): C 8.26%, H 3.42%, N 4.82%. Found: C 8.15%, H 3.27%, N 4.78%.

2. Figures

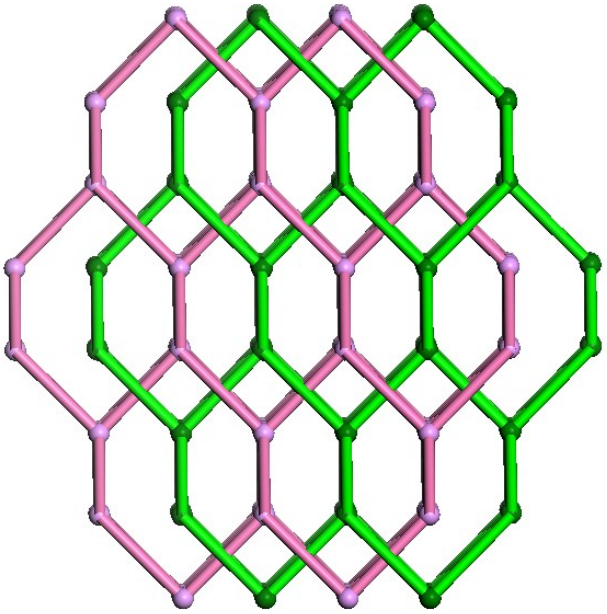


Figure S1. Topological views of $LnSO_4$-NTU1, showing 2-fold interpenetrated ***dia*** framework.

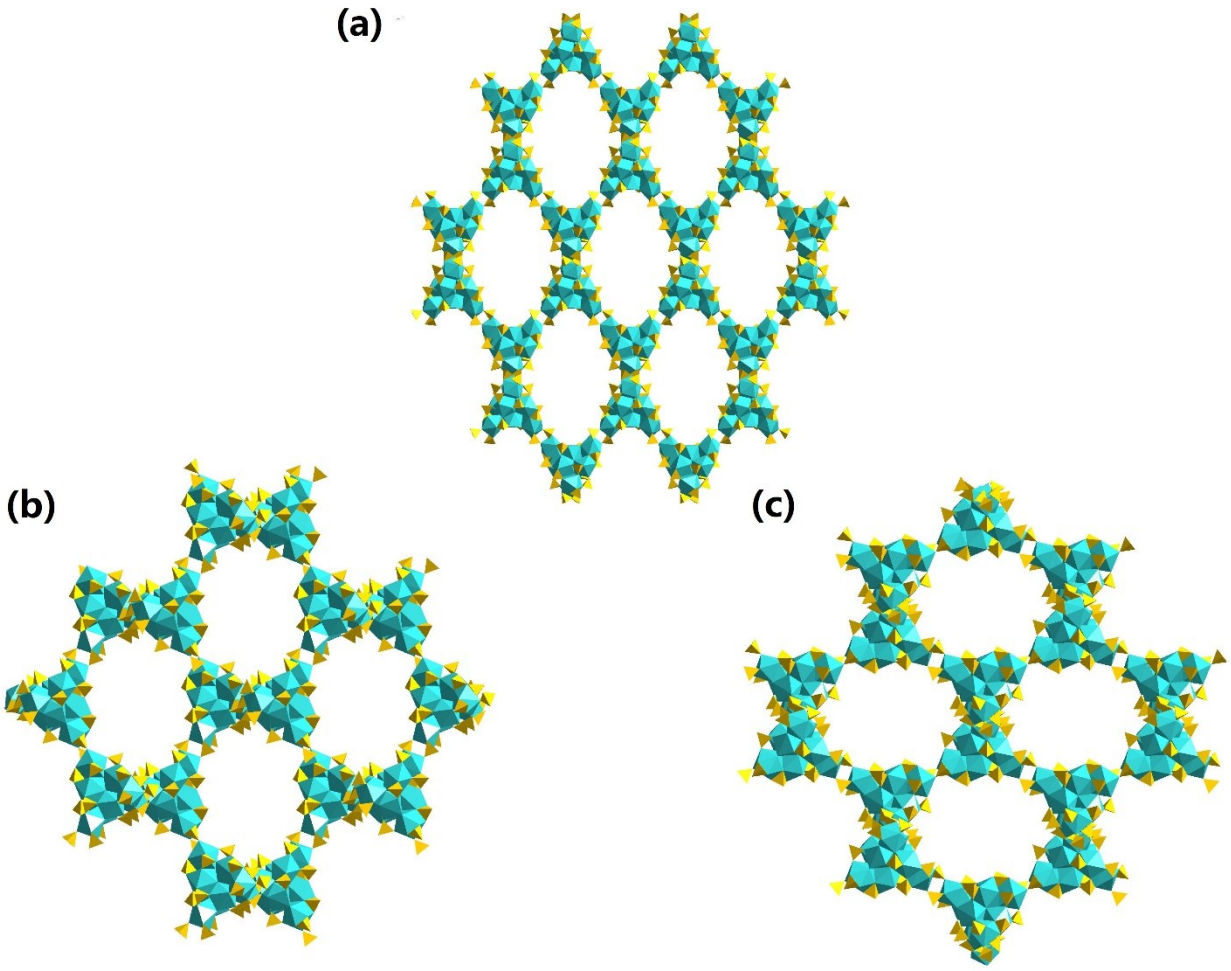


Figure S2. Channel system of the single ***dia*** net in $LnSO_4$-NTU1. (a) Views along the [110] direction; (b) views along the [011] direction; (c) views along the [101] direction.

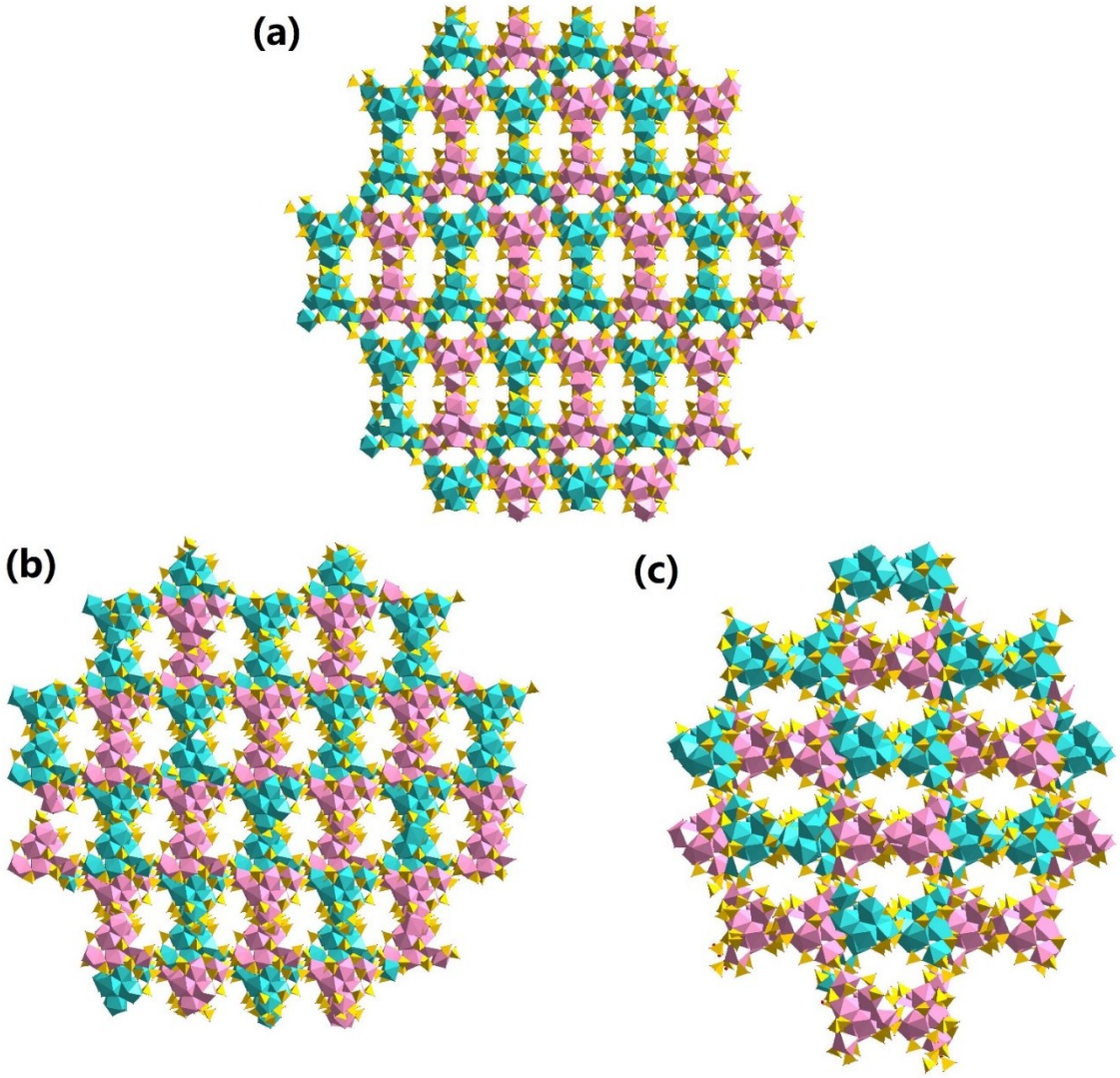


Figure S3. The structure of $LnSO_4$-NTU1 is represented by two interpenetrated ***dia*** nets. (a) Views along the [110] direction; (b) views along the [011] direction; (c) views along the [101] direction.

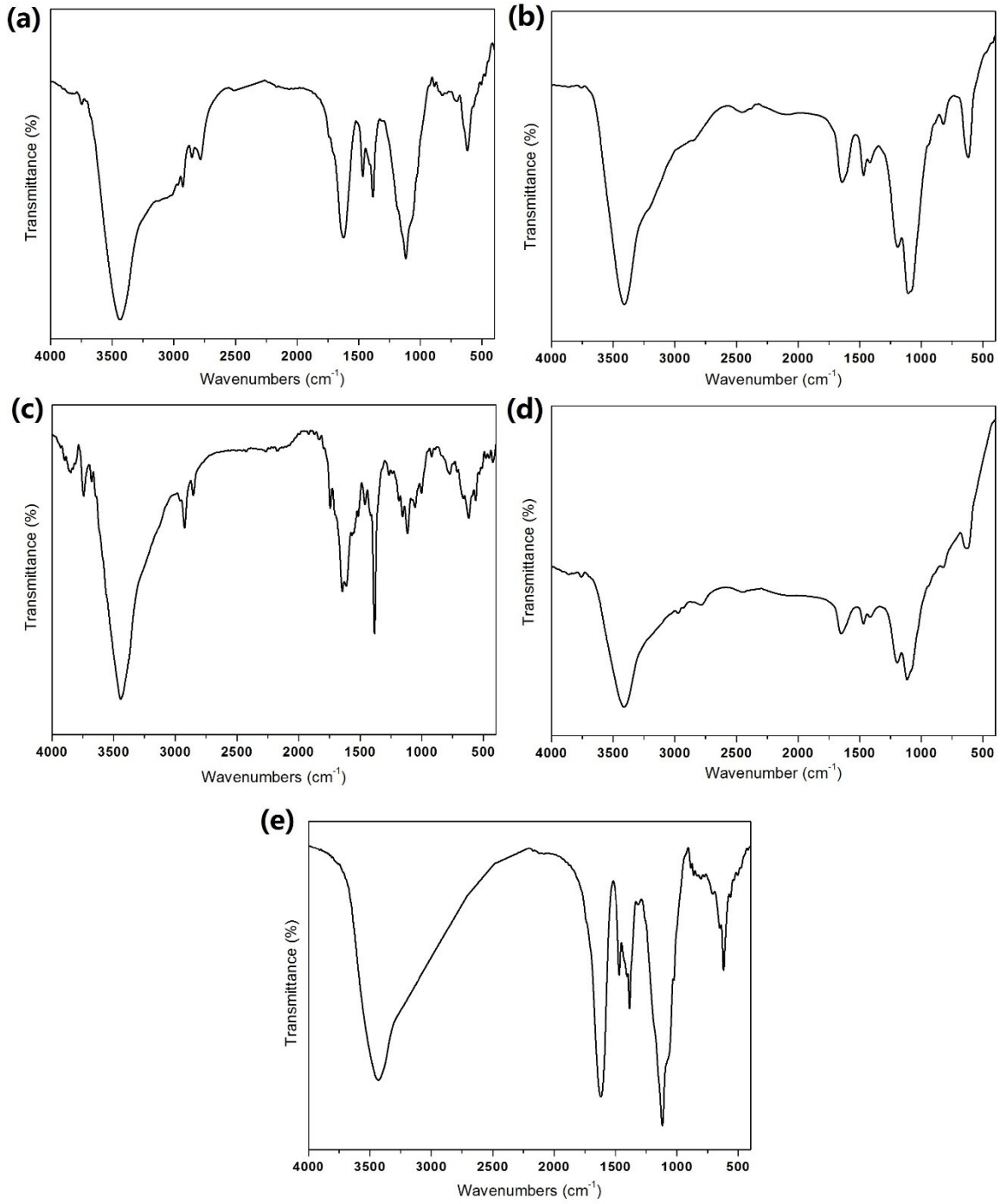


Figure S4. FTIR spectra of $LnSO_4$-NTU1: (a) Eu, (b) Tb, (c) Sm, (d) Dy and (e) Er.

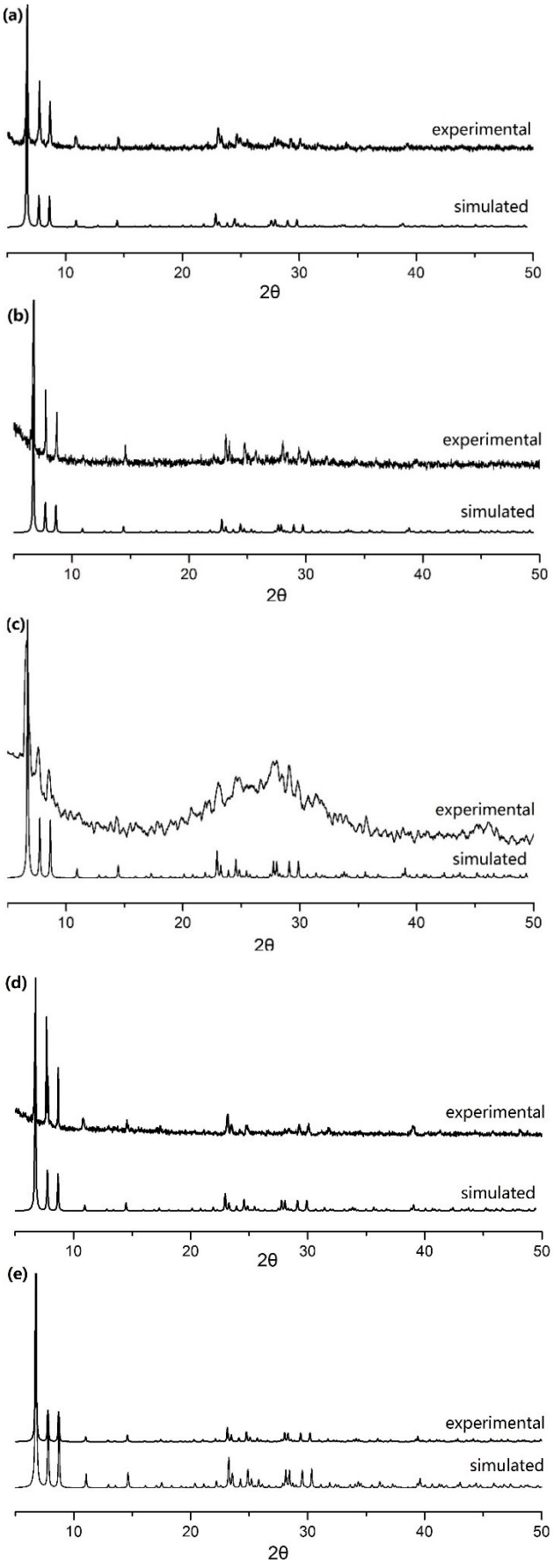


Figure S5. Powder XRD patterns of $LnSO_4$-NTU1: (a) Eu, (b) Tb, (c) Sm, (d) Dy and (e) Er.

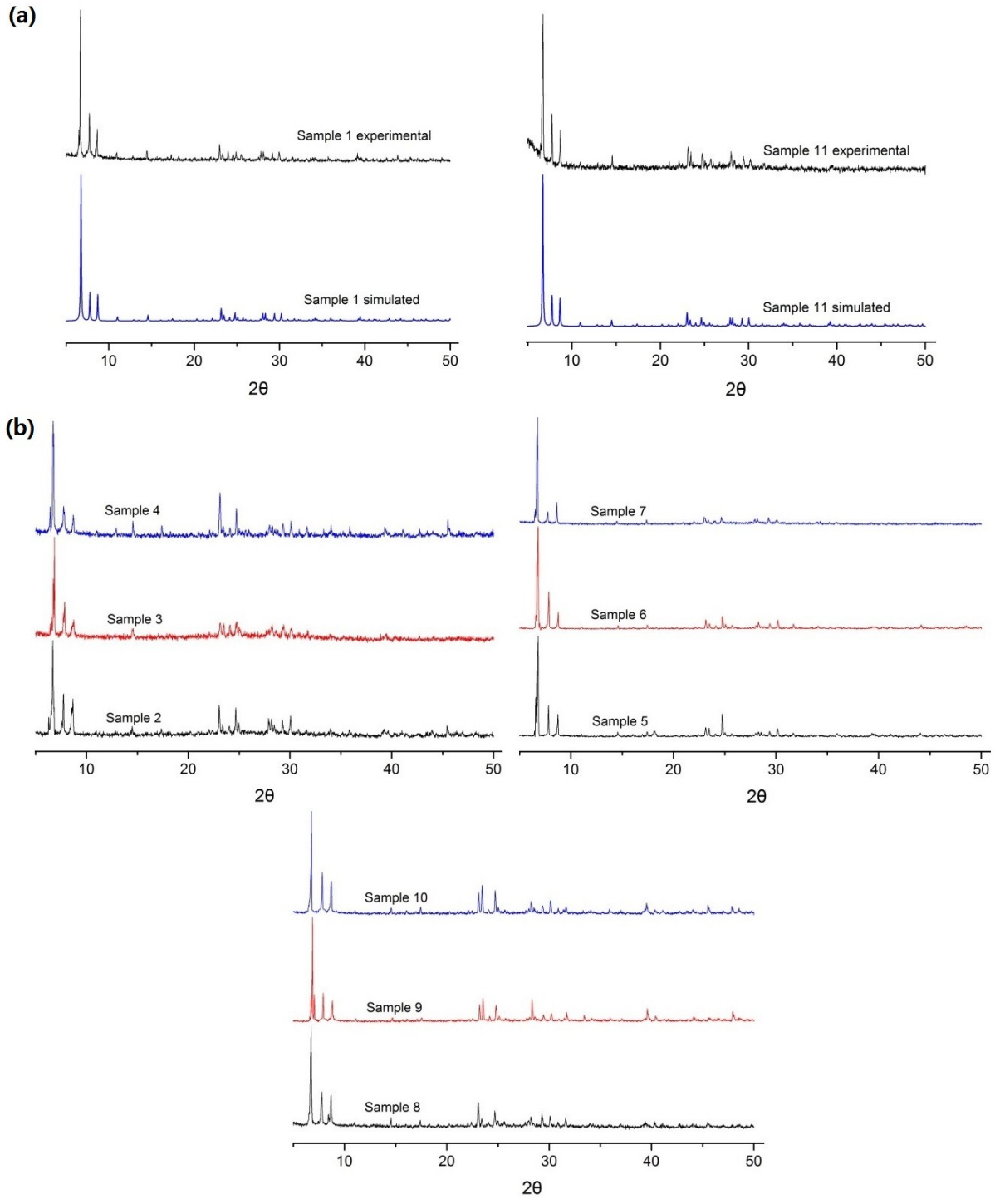


Figure S6. Powder XRD patterns of (a) $EuSO_4$-NTU1 (sample 1) and $TbSO_4$-NTU1 (sample 11), (b) mix-Eu/$TbSO_4$-NTU1 $\{[(CH_3)_2NH_2]_{14}[(Eu_xTb_{1-x})_{10}(\mu_2\text{-}OH)_4(\mu_3\text{-}OH)_8(SO_4)_{16}]\cdot 6H_2O\}$: sample 2 (x= 0.1980), sample 3 (x= 0.0997), sample 4 (x= 0.0509), sample 5 (x= 0.0196), sample 6 (x= 0.0095), sample 7 (x= 0.0070), sample 8 (x= 0.0049), sample 9 (x= 0.0025), sample 10 (x= 0.0011).

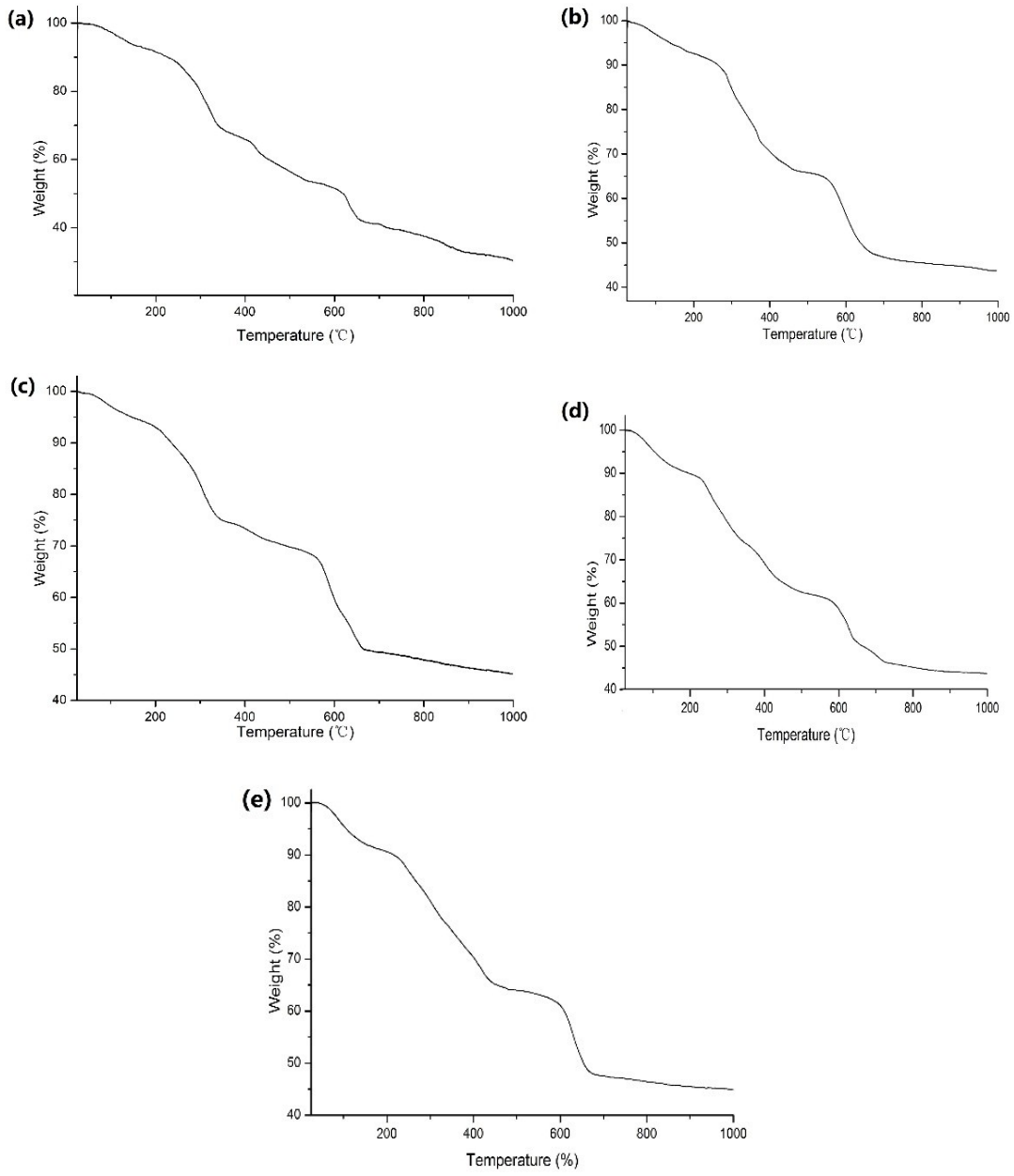


Figure S7. TGA profiles of $LuSO_4$-NTU1: (a) Eu, (b) Tb, (c) Sm, (d) Dy and (e) Er.

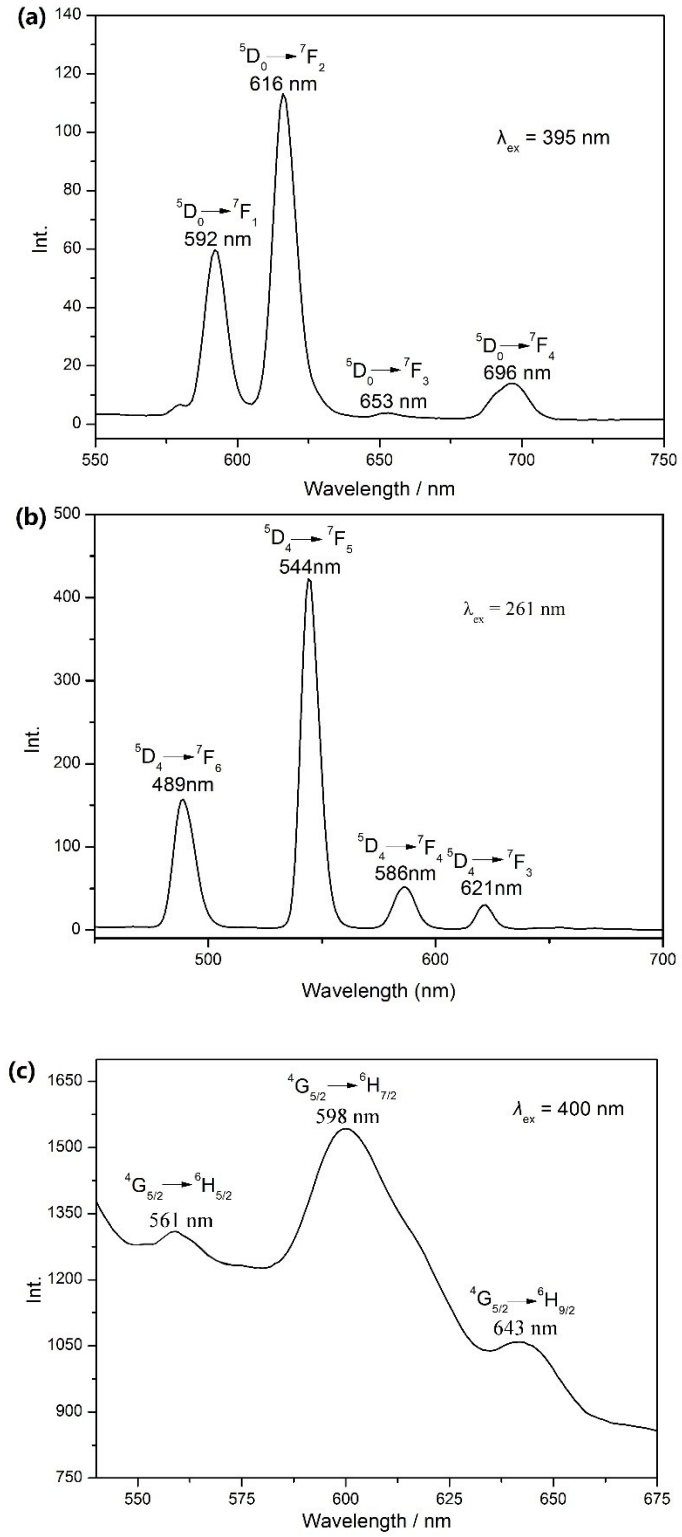
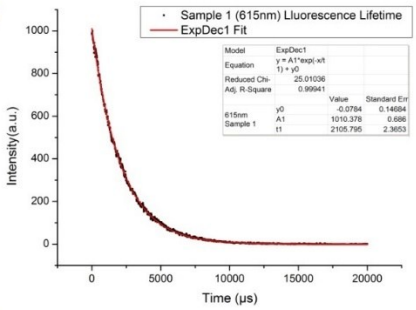
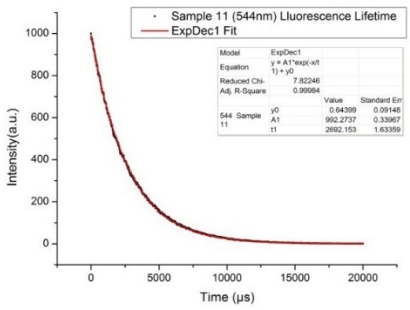


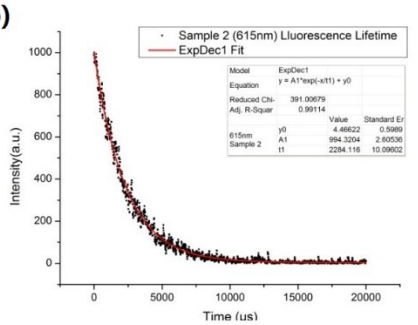
Figure S8. The emission spectra of $LnSO_4$-NTU1: (a) Eu, (b) Tb, (c) Sm.

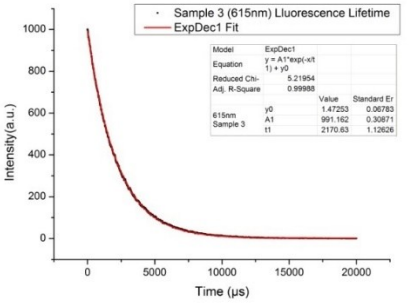
(a)

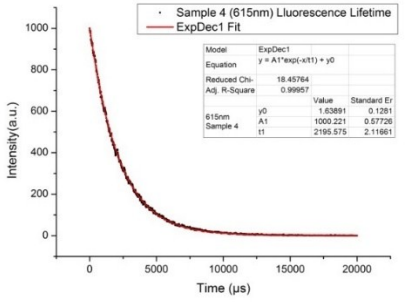

Sample 1 (615nm) Lluorescence Lifetime
ExpDec1 Fit
Model ExpDec1
Equation y = A1*exp(-x/t1) + y0
Reduced Chi-Sq 25.01036
Adj. R-Square 0.99941
Value Standard Err
615nm Sample 1 y0 -0.0784 0.14684
A1 1010.378 0.686
t1 2105.795 2.3653
Intensity(a.u.)
Time (μs)

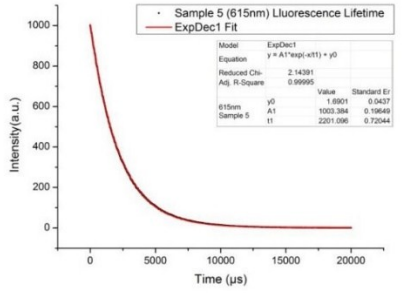

Sample 11 (544nm) Lluorescence Lifetime
ExpDec1 Fit
Model ExpDec1
Equation y = A1*exp(-x/t1) + y0
Reduced Chi-Sq 7.82246
Adj. R-Square 0.99984
Value Standard Err
544 Sample 11 y0 0.64399 0.09148
A1 992.2737 0.33967
t1 2692.153 1.63359
Intensity(a.u.)
Time (μs)

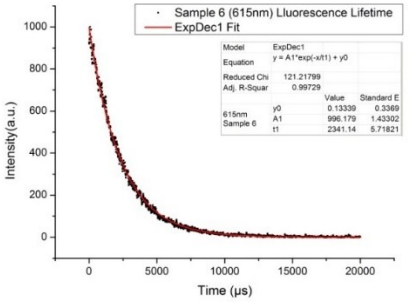
(b)

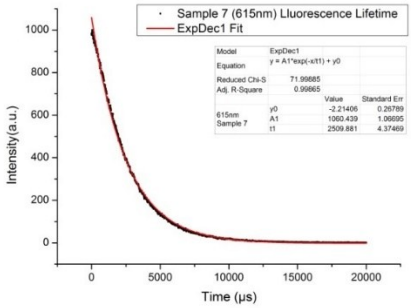

Sample 2 (615nm) Lluorescence Lifetime
ExpDec1 Fit
Model ExpDec1
Equation y = A1*exp(-x/t1) + y0
Reduced Chi-Sq 391.00679
Adj. R-Square 0.99114
Value Standard Er
615nm Sample 2 y0 4.46622 0.5986
A1 994.3204 2.60536
t1 2284.116 10.09602
Intensity(a.u.)
Time (μs)

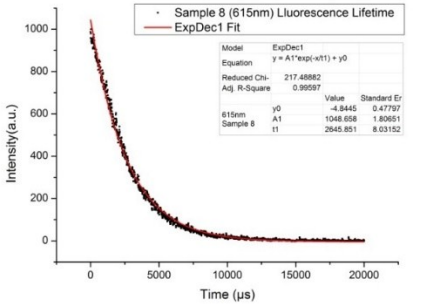

Sample 3 (615nm) Lluorescence Lifetime
ExpDec1 Fit
Model ExpDec1
Equation y = A1*exp(-x/t1) + y0
Reduced Chi-Sq 5.21954
Adj. R-Square 0.99988
Value Standard Er
615nm Sample 3 y0 1.47253 0.06783
A1 991.162 0.30871
t1 2170.63 1.12626
Intensity(a.u.)
Time (μs)

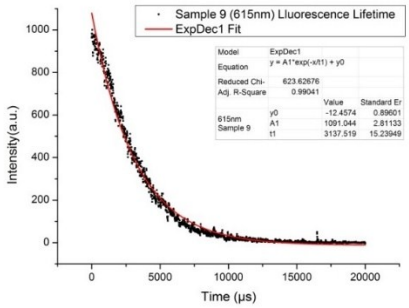

Sample 4 (615nm) Lluorescence Lifetime
ExpDec1 Fit
Model ExpDec1
Equation y = A1*exp(-x/t1) + y0
Reduced Chi-Sq 18.45764
Adj. R-Square 0.99957
Value Standard Er
615nm Sample 4 y0 1.63891 0.1281
A1 1009.221 0.57726
t1 2195.575 2.11661
Intensity(a.u.)
Time (μs)

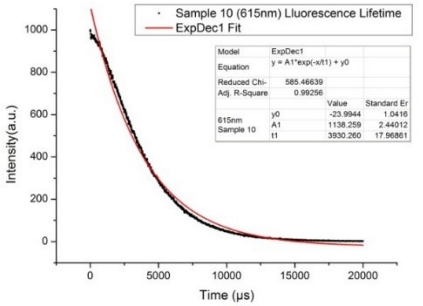

Sample 5 (615nm) Lluorescence Lifetime
ExpDec1 Fit
Model ExpDec1
Equation y = A1*exp(-x/t1) + y0
Reduced Chi-Sq 2.14391
Adj. R-Square 0.99995
Value Standard Er
615nm Sample 5 y0 1.6901 0.0437
A1 1003.384 0.19649
t1 2201.096 0.72044
Intensity(a.u.)
Time (μs)


Sample 6 (615nm) Lluorescence Lifetime
ExpDec1 Fit
Model ExpDec1
Equation y = A1*exp(-x/t1) + y0
Reduced Chi-Sq 121.21799
Adj. R-Square 0.99729
Value Standard E
615nm Sample 6 y0 0.13339 0.3369
A1 996.179 1.43302
t1 2341.14 5.71821
Intensity(a.u.)
Time (μs)


Sample 7 (615nm) Lluorescence Lifetime
ExpDec1 Fit
Model ExpDec1
Equation y = A1*exp(-x/t1) + y0
Reduced Chi-Sq 71.99685
Adj. R-Square 0.99865
Value Standard Err
615nm Sample 7 y0 -2.21406 0.26789
A1 1060.439 1.06695
t1 2509.881 4.37469
Intensity(a.u.)
Time (μs)


Sample 8 (615nm) Lluorescence Lifetime
ExpDec1 Fit
Model ExpDec1
Equation y = A1*exp(-x/t1) + y0
Reduced Chi-Sq 217.48882
Adj. R-Square 0.99597
Value Standard Er
615nm Sample 8 y0 -4.8445 0.47797
A1 1048.658 1.80651
t1 2645.851 8.03152
Intensity(a.u.)
Time (μs)


Sample 9 (615nm) Lluorescence Lifetime
ExpDec1 Fit
Model ExpDec1
Equation y = A1*exp(-x/t1) + y0
Reduced Chi-Sq 623.62676
Adj. R-Square 0.99041
Value Standard Er
615nm Sample 9 y0 -12.4574 0.89601
A1 1091.044 2.81133
t1 3137.519 15.23949
Intensity(a.u.)
Time (μs)


Sample 10 (615nm) Lluorescence Lifetime
ExpDec1 Fit
Model ExpDec1
Equation y = A1*exp(-x/t1) + y0
Reduced Chi-Sq 585.46639
Adj. R-Square 0.99256
Value Standard Er
615nm Sample 10 y0 -23.9944 1.0416
A1 1138.259 2.44012
t1 3930.260 17.56861
Intensity(a.u.)
Time (μs)

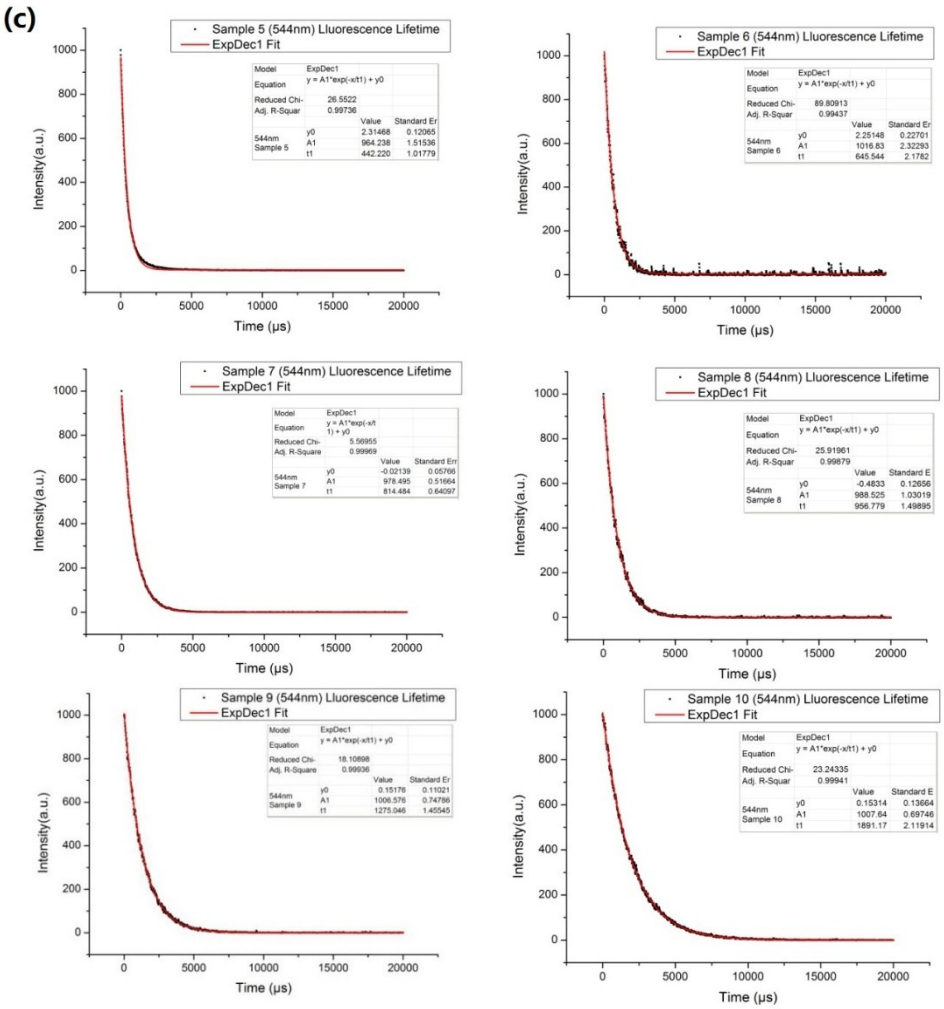


Figure S9. Luminescence decay profiles of (a) $EuSO_4$-NTU1 (sample 1), $TbSO_4$-NTU1 (sample 11), (b) mix-Eu/$TbSO_4$-NTU1 (samples 2-10) monitored at 615 nm, (c) mix-Eu/$TbSO_4$-NTU1 (samples 5-10) monitored at 544 nm.

3. Tables

Table S1. Crystallographic Data collection and Refinement result for $LnSO_4$-NTU1.

Compound reference	$EuSO_4$-NTU1(**1**)	$TbSO_4$-NTU1(**2**)	$SmSO_4$-NTU1(**3**)	$DySO_4$-NTU1(**4**)	$ErSO_4$-NTU1(**5**)
chemical formula	$C_{28}H_{136}Eu_{10}N_{14}O_{82}S_{16}$	$C_{28}H_{136}Tb_{10}N_{14}O_{82}S_{16}$	$C_{28}H_{136}Sm_{10}N_{14}O_{82}S_{16}$	$C_{28}H_{136}Dy_{10}N_{14}O_{82}S_{16}$	$C_{28}H_{138}Er_{10}N_{14}O_{82}S_{16}$
Crystal system	tetragonal	tetragonal	tetragonal	tetragonal	tetragonal
Space group	P42/*n*	P42/*n*	P42/*n*	P42/*n*	P42/*n*
a/Å	16.0974(13)	16.144(6)	16.0748(4)	16.0542(5)	15.9800(7)
b/Å	16.0974(13)	16.144(6)	16.0748(4)	16.0542(5)	15.9800(7)
c/Å	22.8640(18)	22.809(9)	22.7327(13)	22.7238(14)	22.646(2)
Unit cell volume/Å^3	5924.7(11)	5945(5)	5874.1(4)	5856.8(5)	5783.0(7)
Temperature/K	296(2)	296(2)	296(2)	296(2)	296(2)
Z	2	2	2	2	2
μ(mm^{-1})	5.599	6.253	5.307	6.688	7.569
No. of reflections measured	43204	19281	25854	42736	41342
No. of independent reflections	5498	5437	4622	5482	5365
R_{int}	0.1772	0.1206	0.0759	0.1081	0.1322
Final R_1 values ($I > 2\sigma(I)$)	0.0888	0.0530	0.0373	0.0502	0.0981
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.1888	0.1270	0.1055	0.1222	0.1810
Final R_1[a] values (all data)	0.1101	0.0989	0.0615	0.0734	0.1297
Final $wR(F^2)$[b] values (all data)	0.1959	0.1392	0.1221	0.1304	0.1900
Goodness of fit on F^2	1.180	1.112	1.092	1.051	1.169

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = \Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]^{1/2}$.

Table S2. Selected bond lengths (Å) and angles (deg) for $LnSO_4$-NTU1.

$EuSO_4$-NTU1 (**1**)					
Eu1-O2	2.823(9)	Eu1-O17	2.604(15)	Eu3-O1^{iv}	2.379(10)
Eu1-O3	2.302(11)	Eu1-O18^{i}	2.319(12)	Eu3-O2	2.492(9)
Eu1-O5	2.366(12)	Eu2-O1	2.345(8)	Eu3^{iv}-O6	2.452(11)
Eu1-O6	2.465(11)	Eu2-O2	2.432(10)	Eu3-O7	2.338(11)
Eu1-O11	2.521(12)	Eu2-O3^{ii}	2.220(9)	Eu3-O8^{iii}	2.356(14)
Eu1-O12	2.335(13)	Eu2-O4^{ii}	2.396(12)	Eu3-O2^{iii}	2.655(9)
Eu1-O13	2.482(12)	Eu3-O1	2.358(10)	Eu3-O19^{iii}	2.721(15)
O3-Eu1-O2	63.4(3)	O3^{ii}-Eu2-O1	93.7(3)	O10-Eu3-O1^{iv}	80.5(4)
O3-Eu1-O5	81.8(4)	O3-Eu2-O1	137.4(4)	O10-Eu3-O2^{iii}	132.6(4)
O3-Eu1-O6	71.2(4)	O3^{ii}-Eu2-O3	113.3(5)	O10-Eu3-O2	75.1(4)
O3-Eu1-O11	76.1(4)	O3^{ii}-Eu2-O4^{ii}	78.6(4)	O10-Eu3-O6^{iii}	77.5(4)
O3-Eu1-O12	130.9(4)	O3-Eu2-O4^{ii}	75.3(4)	O10-Eu3-O7	84.7(5)
O3-Eu1-O13	77.9(4)	O3^{ii}-Eu2-O2^{ii}	71.7(3)	O10-Eu3-O8^{iii}	133.9(5)
O3-Eu1-O17	121.1(4)	O4^{ii}-Eu2-O2^{ii}	77.9(4)	O10-Eu3-O19^{iii}	68.4(5)
O3-Eu1-O18^{i}	147.7(4)	O4-Eu2-O2^{ii}	128.8(4)	O11-Eu1-O2	130.5(4)
O5-Eu1-O2	73.4(3)	O4^{ii}-Eu2-O4	131.6(5)	O11-Eu1-O17	118.4(4)
O5-Eu1-O6	137.0(4)	O5-Eu1-O17	155.1(5)	O12-Eu1-O2	67.8(4)
O5-Eu1-O11	73.8(4)	O6-Eu1-O2	64.8(3)	O12-Eu1-O5	80.4(5)
O5-Eu1-O13	128.9(4)	O6-Eu1-O11	127.8(4)	O12-Eu1-O6	92.5(5)
O1-Eu2-O1^{ii}	86.5(4)	O6-Eu1-O13	77.8(4)	O12-Eu1-O11	139.2(4)
O1-Eu3-O1^{iv}	82.4(4)	O6-Eu1-O17	54.8(4)	O12-Eu1-O13	145.1(5)
O1-Eu2-O2^{ii}	67.2(3)	O6^{iii}-Eu3-O2	139.2(4)	O12-Eu1-O17	77.0(5)
O1-Eu3-O2^{iii}	63.6(3)	O6^{iii}-Eu3-O2^{iii}	67.7(4)	O13-Eu1-O2	132.5(4)
O1-Eu3-O2	68.1(3)	O6^{iii}-Eu3-O19^{iii}	54.0(5)	O13-Eu1-O11	56.0(4)
O1^{iv}-Eu3-O2	65.9(3)	O7-Eu3-O1^{iv}	140.5(4)	O13-Eu1-O17	70.0(5)
O1^{ii}-Eu2-O2^{ii}	69.3(3)	O7-Eu3-O1	88.1(4)	O17-Eu1-O2	106.7(3)
O1-Eu2-O4	77.2(4)	O7-Eu3-O2^{iii}	142.6(4)	O18^{i}-Eu1-O2	139.8(4)

O1^{ii}-Eu2-O4	144.9(4)	O7-Eu3-O2	74.9(3)	O18^{i}-Eu1-O5	85.7(5)
O1-Eu3-O6^{iii}	131.0(4)	O7-Eu3-O6^{iii}	131.7(4)	O18^{i}-Eu1-O6	133.7(5)
O1^{iv}-Eu3-O6^{iii}	80.2(4)	O7-Eu3-O8^{iii}	77.5(4)	O18^{i}-Eu1-O11	71.8(5)
O1-Eu3-O8^{iii}	78.9(4)	O7-Eu3-O19^{iii}	77.7(4)	O18^{i}-Eu1-O12	75.3(4)
O1^{iv}-Eu3-O19^{iii}	128.3(4)	O8^{iii}-Eu3-O1^{iv}	136.8(4)	O18^{i}-Eu1-O13	87.3(4)
O2^{ii}-Eu2-O2	118.9(4)	O8^{iii}-Eu3-O2^{iii}	73.6(4)	O18^{i}-Eu1-O17	78.9(5)
O2-Eu3-O2^{iii}	112.1(4)	O8^{iii}-Eu3-O2	137.1(4)	O8^{iii}-Eu3-O19^{iii}	66.4(5)
O2-Eu3-O19^{iii}	135.8(4)	O8^{iii}-Eu3-O6^{iii}	83.3(4)	O10-Eu3-O1	143.1(4)
O2^{iii}-Eu3-O19^{iii}	110.8(4)	O3-Eu2-O2^{ii}	150.9(3)		
$TbSO_4$-NTU1 (**2**)					
Tb1-O1	2.345(7)	Tb1-O17	2.741(10)	Tb2-O16^{iii}	2.569(10)
Tb1-O1^{ii}	2.357(7)	Tb2-O2^{i}	2.866(7)	Tb2-O19^{iv}	2.336(9)
Tb1-O2	2.463(7)	Tb2-O3	2.279(7)	Tb3-O1^{i}	2.332(6)
Tb1-O2^{iii}	2.625(7)	Tb2-O4	2.340(9)	Tb3-O2	2.409(7)
Tb1-O6^{i}	2.320(8)	Tb2-O9^{iii}	2.450(9)	Tb3-O3^{i}	2.228(7)
Tb1-O8^{ii}	2.312(9)	Tb2-O11	2.454(8)	Tb3-O5^{i}	2.384(9)
Tb1-O9	2.411(8)	Tb2-O12	2.514(9)	Tb2-O13	2.309(9)
Tb1-O10^{i}	2.283(9)				
O1-Tb1-O1^{ii}	84.4(3)	O6^{i}-Tb1-O1	86.8(3)	O8^{ii}-Tb1-O2^{iii}	73.6(3)
O1^{ii}-Tb1-O2	66.4(2)	O6^{i}-Tb1-O1^{ii}	140.2(3)	O9-Tb1-O2^{iii}	67.2(3)
O1-Tb1-O2	68.1(2)	O6^{i}-Tb1-O2	74.3(3)	O9-Tb1-O17	54.7(3)
O1-Tb1-O2^{iii}	63.9(2)	O6^{i}-Tb1-O9	132.8(3)	O9-Tb1-O2	139.6(3)
O1^{ii}-Tb1-O2^{iii}	63.5(2)	O6^{i}-Tb1-O2^{iii}	142.4(3)	O10^{i}-Tb1-O1^{ii}	81.2(3)
O1-Tb1-O9	130.7(3)	O6^{i}-Tb1-O17	78.1(3)	O10^{i}-Tb1-O1	143.9(3)
O1^{ii}-Tb1-O9	79.3(3)	O8^{ii}-Tb1-O1^{ii}	137.1(3)	O10^{i}-Tb1-O6^{i}	83.6(3)
O1-Tb1-O17	144.3(3)	O8^{ii}-Tb1-O2	136.9(3)	O10^{i}-Tb1-O8^{ii}	132.7(3)
O1^{ii}-Tb1-O17	127.1(3)	O8^{ii}-Tb1-O1	78.2(3)	O10^{i}-Tb1-O9	78.5(3)
O2^{iii}-Tb1-O17	111.6(2)	O8^{ii}-Tb1-O6^{i}	77.9(3)	O10^{i}-Tb1-O2	75.9(3)
O2-Tb1-O2^{iii}	111.7(3)	O8^{ii}-Tb1-O9	83.0(3)	O10^{i}-Tb1-O2^{iii}	134.0(3)

O2-Tb1-O17	135.3(3)	O8^{ii}-Tb1-O17	67.1(3)	O13-Tb2-O9^{iii}	91.2(3)
O3-Tb2-O4	82.4(3)	O4-Tb2-O16^{iii}	154.6(3)	O10^{i}-Tb1-O17	66.6(3)
O3-Tb2-O2^{i}	62.9(2)	O9^{iii}-Tb2-O2^{i}	62.8(2)	O13-Tb2-O11	145.7(3)
O3-Tb2-O9^{iii}	70.1(3)	O9^{iii}-Tb2-O11	80.1(3)	O13-Tb2-O12	139.5(3)
O3-Tb2-O11	78.6(3)	O9^{iii}-Tb2-O12	129.1(3)	O13-Tb2-O16^{iii}	77.4(3)
O3-Tb2-O12	76.2(3)	O9^{iii}-Tb2-O16^{iii}	55.7(3)	O13-Tb2-O19^{iv}	74.4(3)
O3-Tb2-O16^{iii}	120.5(3)	O11-Tb2-O2^{i}	133.1(2)	O16^{iii}-Tb2-O2^{i}	106.1(2)
O3-Tb2-O13	129.5(3)	O11-Tb2-O16^{iii}	70.2(3)	O19^{iv}-Tb2-O4	85.9(3)
O3-Tb2-O19^{iv}	150.1(3)	O11-Tb2-O12	56.3(3)	O19^{iv}-Tb2-O9^{iii}	134.0(3)
O4-Tb2-O2^{i}	72.9(2)	O12-Tb2-O2^{i}	129.8(3)	O19^{iv}-Tb2-O12	74.1(3)
O4-Tb2-O9^{iii}	134.8(3)	O12-Tb2-O16^{iii}	119.6(3)	O19^{iv}-Tb2-O11	88.0(3)
O4-Tb2-O11	129.6(3)	O13-Tb2-O2^{i}	66.8(2)	O19^{iv}-Tb2-O16^{iii}	78.4(3)
O4-Tb2-O12	74.0(3)	O13-Tb2-O4	79.1(3)	O19^{iv}-Tb2-O2^{i}	138.4(3)
O1^{i}-Tb3-O1	88.2(3)	O3-Tb3-O3^{i}	113.2(3)	O3-Tb3-O5	78.1(3)
O1^{i}-Tb3-O2	67.4(2)	O3-Tb3-O1^{i}	137.3(2)	O3^{i}-Tb3-O5	75.1(3)
O1-Tb3-O2	69.2(2)	O3^{i}-Tb3-O1^{i}	93.2(2)	O5^{i}-Tb3-O2	78.4(3)
O1^{i}-Tb3-O5^{i}	145.7(3)	O3-Tb3-O2	151.0(2)	O5-Tb3-O2	129.3(3)
O1-Tb3-O5^{i}	77.1(3)	O3^{i}-Tb3-O2	72.1(2)	O5^{i}-Tb3-O5	130.3(4)
O2-Tb3-O2^{i}	118.0(3)				
$SmSO_4$-NTU1 (**3**)					
Sm1-O1	2.317(6)	Sm1-O19^{i}	2.763(9)	Sm2-O11	2.479(9)
Sm1-O1^{ii}	2.346(6)	Sm2-O2	2.910(6)	Sm2-O17	2.567(8)
Sm1-O2	2.437(6)	Sm2-O3	2.262(6)	Sm2-O18^{iii}	2.312(7)
Sm1-O2^{i}	2.568(6)	Sm2-O5	2.323(7)	Sm3-O1	2.321(6)
Sm1-O6^{i}	2.407(7)	Sm2-O6	2.432(7)	Sm3-O2^{iv}	2.384(6)
Sm1-O7	2.305(7)	Sm2-O12	2.300(7)	Sm3-O3	2.215(5)
Sm1-O8^{i}	2.311(7)	Sm2-O13	2.428(7)	Sm3-O4	2.372(7)
Sm1-O10	2.272(8)				
O1^{ii}-Sm1-O2	65.61(19)	O6^{i}-Sm1-O2	139.7(2)	O8^{i}-Sm1-O6^{i}	82.7(3)

O1-Sm1-O2	67.68(19)	O6^{i}-Sm1-O2^{i}	68.3(2)	O8^{i}-Sm1-O2	137.1(2)
O1-Sm1-O2^{i}	63.86(19)	O6^{i}-Sm1-O19^{i}	54.2(2)	O8^{i}-Sm1-O2^{i}	74.6(2)
O1^{ii}-Sm1-O2^{i}	63.47(19)	O7-Sm1-O1^{ii}	139.8(2)	O8^{i}-Sm1-O19^{i}	66.6(3)
O1-Sm1-O1^{ii}	85.6(3)	O7-Sm1-O1	86.1(2)	O10-Sm1-O1	143.8(2)
O1-Sm1-O6^{i}	131.5(2)	O7-Sm1-O8^{i}	77.7(3)	O10-Sm1-O1^{ii}	80.7(2)
O1^{ii}-Sm1-O6^{i}	79.8(2)	O7-Sm1-O6^{i}	132.2(3)	O10-Sm1-O7	83.3(3)
O1-Sm1-O19^{i}	143.7(2)	O7-Sm1-O2	74.9(2)	O10-Sm1-O8^{i}	132.2(3)
O1^{ii}-Sm1-O19^{i}	126.9(2)	O7-Sm1-O2^{i}	142.5(2)	O10-Sm1-O6^{i}	78.5(2)
O2-Sm1-O2^{i}	110.1(3)	O7-Sm1-O19^{i}	78.1(2)	O10-Sm1-O2	76.2(2)
O2-Sm1-O19^{i}	136.0(2)	O8^{i}-Sm1-O1	78.2(2)	O10-Sm1-O2^{i}	134.2(2)
O2^{i}-Sm1-O19^{i}	112.5(2)	O8^{i}-Sm1-O1^{ii}	138.0(2)	O10-Sm1-O19^{i}	66.7(3)
O3-Sm2-O2	62.15(18)	O5-Sm2-O17	154.6(3)	O12-Sm2-O17	77.0(3)
O3-Sm2-O6	70.4(2)	O6-Sm2-O17	56.3(2)	O13-Sm2-O2	132.7(2)
O3-Sm2-O5	81.5(2)	O6-Sm2-O11	129.6(3)	O13-Sm2-O6	80.1(2)
O3-Sm2-O12	128.5(2)	O6-Sm2-O2	62.3(2)	O13-Sm2-O11	57.0(3)
O3-Sm2-O18^{iii}	149.9(2)	O11-Sm2-O2	129.5(2)	O13-Sm2-O17	70.1(3)
O3-Sm2-O13	79.4(2)	O11-Sm2-O17	119.9(3)	O17-Sm2-O2	106.4(2)
O3-Sm2-O11	76.4(2)	O12-Sm2-O5	79.8(3)	O18^{iii}-Sm2-O2	138.9(2)
O3-Sm2-O17	121.5(2)	O12-Sm2-O18^{iii}	75.2(3)	O18^{iii}-Sm2-O6	134.3(3)
O5-Sm2-O2	73.1(2)	O12-Sm2-O13	145.4(3)	O18^{iii}-Sm2-O5	86.1(3)
O5-Sm2-O6	134.5(2)	O12-Sm2-O6	90.4(3)	O18^{iii}-Sm2-O13	87.8(3)
O5-Sm2-O13	129.6(3)	O12-Sm2-O2	66.6(2)	O18^{iii}-Sm2-O11	73.7(3)
O5-Sm2-O11	73.3(3)	O12-Sm2-O11	139.9(3)	O18^{iii}-Sm2-O17	78.1(3)
O1^{iv}-Sm3-O1	89.0(3)	O3^{iv}-Sm3-O3	113.8(3)	O3^{iv}-Sm3-O2^{iv}	72.6(2)
O1^{iv}-Sm3-O4	146.6(2)	O3^{iv}-Sm3-O1^{iv}	136.6(2)	O3-Sm3-O2^{iv}	151.7(2)
O1-Sm3-O4	76.7(2)	O3-Sm3-O1^{iv}	93.0(2)	O4-Sm3-O4^{iv}	129.9(4)
O1^{iv}-Sm3-O2^{iv}	68.5(2)	O3^{iv}-Sm3-O4	75.0(2)	O4-Sm3-O2^{iv}	128.9(2)
O1-Sm3-O2^{iv}	66.81(19)	O3-Sm3-O4	78.3(2)	O4^{iv}-Sm3-O2^{iv}	79.8(2)
O2^{iv}-Sm3-O2	115.6(3)				

$DySO_4$-NTU1 (**4**)					
Dy1-O1	2.323(4)	Dy1-O10	2.270(6)	Dy2-O13	2.421(5)
Dy1-O1^{ii}	2.343(4)	Dy1-O19^{i}	2.767(6)	Dy2-O17	2.563(6)
Dy1-O2	2.425(4)	Dy2-O3	2.265(4)	Dy2-O18^{iii}	2.309(6)
Dy1-O2^{i}	2.589(4)	Dy2-O5	2.331(5)	Dy3-O1	2.310(4)
Dy1-O6^{i}	2.402(5)	Dy2-O6	2.430(5)	Dy3-O2^{iv}	2.373(4)
Dy1-O7	2.299(5)	Dy2-O11	2.491(5)	Dy3-O3	2.197(4)
Dy1-O8^{i}	2.316(5)	Dy2-O12	2.294(5)	Dy3-O4^{iv}	2.357(5)
O1-Dy1-O1^{ii}	84.7(2)	O6^{i}-Dy1-O2^{i}	68.47(16)	O8^{i}-Dy1-O2	136.76(16)
O1-Dy1-O2^{i}	63.54(13)	O6^{i}-Dy1-O19^{i}	54.10(18)	O8^{i}-Dy1-O2^{i}	74.94(16)
O1^{ii}-Dy1-O2	65.94(13)	O7-Dy1-O19^{i}	77.80(18)	O8^{i}-Dy1-O19^{i}	66.5(2)
O1-Dy1-O2	67.31(14)	O7-Dy1-O2^{i}	143.02(16)	O10-Dy1-O1	143.59(17)
O1^{ii}-Dy1-O2^{i}	62.90(13)	O7-Dy1-O2	74.60(16)	O10-Dy1-O1^{ii}	80.91(17)
O1-Dy1-O6^{i}	131.45(16)	O7-Dy1-O1	86.90(16)	O10-Dy1-O2	76.28(17)
O1^{ii}-Dy1-O6^{i}	79.99(16)	O7-Dy1-O1^{ii}	139.86(16)	O10-Dy1-O2^{i}	133.97(16)
O1-Dy1-O19^{i}	143.94(17)	O7-Dy1-O8^{i}	77.92(19)	O10-Dy1-O6^{i}	78.51(18)
O1^{ii}-Dy1-O19^{i}	127.27(16)	O7-Dy1-O6^{i}	131.90(19)	O10-Dy1-O7	83.01(19)
O2-Dy1-O2^{i}	109.93(18)	O8^{i}-Dy1-O1^{ii}	137.76(17)	O10-Dy1-O8^{i}	132.4(2)
O2-Dy1-O19^{i}	136.14(16)	O8^{i}-Dy1-O1	78.57(17)	O10-Dy1-O19^{i}	67.0(2)
O2^{i}-Dy1-O19^{i}	112.67(15)	O8^{i}-Dy1-O6^{i}	82.64(18)	O12-Dy2-O13	145.41(19)
O3-Dy2-O5	81.20(17)	O5-Dy2-O17	154.41(19)	O12-Dy2-O6	90.21(18)
O3-Dy2-O6	70.75(17)	O5-Dy2-O13	129.62(17)	O13-Dy2-O6	80.17(17)
O3-Dy2-O12	128.33(16)	O6-Dy2-O11	130.00(18)	O13-Dy2-O11	56.74(18)
O3-Dy2-O18^{iii}	149.66(17)	O6-Dy2-O17	55.85(18)	O13-Dy2-O17	70.43(18)
O3-Dy2-O13	79.69(17)	O11-Dy2-O17	119.68(18)	O18^{iii}-Dy2-O5	86.3(2)
O3-Dy2-O11	77.17(16)	O12-Dy2-O17	76.66(19)	O18^{iii}-Dy2-O13	87.43(19)
O3-Dy2-O17	121.68(17)	O12-Dy2-O11	139.61(18)	O18^{iii}-Dy2-O6	134.0(2)
O5-Dy2-O6	134.58(18)	O12-Dy2-O5	79.81(19)	O18^{iii}-Dy2-O11	72.80(19)
O5-Dy2-O11	73.73(18)	O12-Dy2-O18^{iii}	75.59(19)	O18^{iii}-Dy2-O17	78.3(2)

O1-Dy3-O1^{iv}	88.40(19)	O3-Dy3-O2^{iv}	151.39(15)	O3-Dy3-O4	77.83(17)
O1-Dy3-O4	77.20(15)	O3^{iv}-Dy3-O2^{iv}	72.52(14)	O3^{iv}-Dy3-O4	75.52(17)
O1^{iv}-Dy3-O4	145.97(16)	O3^{iv}-Dy3-O2	151.39(15)	O4-Dy3-O4^{iv}	129.9(2)
O1-Dy3-O2^{iv}	66.89(14)	O3-Dy3-O3^{iv}	114.1(2)	O4-Dy3-O2^{iv}	129.65(16)
O1^{iv}-Dy3-O2^{iv}	68.39(14)	O3^{iv}-Dy3-O1	93.02(14)	O4^{iv}-Dy3-O2^{iv}	79.13(16)
O2^{iv}-Dy3-O2	115.90(19)	O3^{iv}-Dy3-O1^{iv}	136.68(15)		
$ErSO_4$-NTU1 (**5**)					
Er1-O1^{ii}	2.305(12)	Er1-O10	2.258(16)	Er2-O13	2.393(15)
Er1-O1	2.311(12)	Er1-O19^{i}	2.818(19)	Er2-O17	2.54(2)
Er1-O2	2.379(11)	Er2-O3	2.250(13)	Er2-O18^{iii}	2.279(16)
Er1-O2^{i}	2.540(12)	Er2-O5	2.306(15)	Er3-O1	2.292(11)
Er1-O6^{i}	2.370(14)	Er2-O6	2.396(15)	Er3-O2^{iv}	2.359(13)
Er1-O7	2.285(14)	Er2-O11	2.472(16)	Er3-O4^{iv}	2.309(13)
Er1-O8^{i}	2.286(16)	Er2-O12	2.266(16)	Er3-O3^{iv}	2.176(11)
O1^{ii}-Er1-O1	86.1(5)	O6^{i}-Er1-O2	141.3(5)	O8^{i}-Er1-O1	78.4(5)
O1^{ii}-Er1-O6^{i}	80.8(5)	O6^{i}-Er1-O2^{i}	69.3(5)	O8^{i}-Er1-O6^{i}	81.4(6)
O1-Er1-O6^{i}	131.7(5)	O6^{i}-Er1-O19^{i}	53.1(6)	O8^{i}-Er1-O2	137.0(5)
O1^{ii}-Er1-O2	66.1(4)	O7-Er1-O2^{i}	142.9(5)	O8^{i}-Er1-O19^{i}	65.6(6)
O1-Er1-O2	67.7(4)	O7-Er1-O1^{ii}	140.8(5)	O10-Er1-O1	143.7(5)
O1^{ii}-Er1-O2^{i}	63.0(4)	O7-Er1-O1	86.9(5)	O10-Er1-O1^{ii}	80.3(5)
O1-Er1-O2^{i}	63.4(4)	O7-Er1-O8^{i}	76.9(6)	O10-Er1-O7	82.9(6)
O1^{ii}-Er1-O19^{i}	126.8(5)	O7-Er1-O6^{i}	130.0(6)	O10-Er1-O8^{i}	131.9(6)
O1-Er1-O19^{i}	143.0(5)	O7-Er1-O2	75.6(4)	O10-Er1-O6^{i}	79.2(5)
O2-Er1-O2^{i}	109.3(5)	O7-Er1-O19^{i}	76.9(5)	O10-Er1-O2	76.0(5)
O2-Er1-O19^{i}	136.4(5)	O8^{i}-Er1-O2^{i}	75.8(5)	O10-Er1-O19^{i}	67.5(6)
O2^{i}-Er1-O19^{i}	113.1(4)	O8^{i}-Er1-O1^{ii}	138.6(5)	O10-Er1-O2^{i}	134.2(5)
O3-Er2-O6	71.7(6)	O5-Er2-O6	133.4(5)	O12-Er2-O13	146.5(7)
O3-Er2-O5	80.6(5)	O5-Er2-O13	130.5(6)	O12-Er2-O18^{iii}	76.6(5)
O3-Er2-O13	81.0(5)	O6-Er2-O11	131.9(6)	O13-Er2-O6	81.6(5)

O3-Er2-O12	126.0(5)	O6-Er2-O17	55.9(6)	O13-Er2-O11	57.3(6)
O3-Er2-O18^{iii}	150.3(5)	O11-Er2-O17	120.2(6)	O13-Er2-O17	70.4(6)
O3-Er2-O17	122.4(5)	O12-Er2-O11	139.6(6)	O18^{iii}-Er2-O6	133.5(7)
O3-Er2-O11	77.7(5)	O12-Er2-O17	77.5(6)	O18^{iii}-Er2-O5	86.7(6)
O5-Er2-O11	74.0(5)	O12-Er2-O6	88.5(6)	O18^{iii}-Er2-O13	87.2(5)
O5-Er2-O17	153.8(6)	O12-Er2-O5	78.3(6)	O18^{iii}-Er2-O11	73.0(6)
O1^{iv}-Er3-O1	89.3(5)	O3^{iv}-Er3-O3	114.9(7)	O18^{iii}-Er2-O17	77.9(6)
O1^{iv}-Er3-O4	146.3(5)	O3^{iv}-Er3-O1^{iv}	136.8(5)	O3-Er3-O2^{iv}	151.5(4)
O1-Er3-O4	77.8(4)	O3-Er3-O1^{iv}	92.1(4)	O4-Er3-O4^{iv}	128.4(7)
O1^{iv}-Er3-O2^{iv}	68.3(4)	O3^{iv}-Er3-O4	75.4(5)	O4-Er3-O2^{iv}	130.2(5)
O1-Er3-O2^{iv}	66.2(4)	O3-Er3-O4	77.5(5)	O4^{iv}-Er3-O2^{iv}	80.1(5)
O2^{iv}-Er3-O2	114.1(5)	O3^{iv}-Er3-O2^{iv}	72.9(4)		

Symmetry codes for **1**: (i) 1-x, 1-y, -z; (ii) 0.5-x, 0.5-y, z; (iii) y, 0.5-x, 0.5-z; (iv) 0.5-y, x, 0.5-z; (v) 0.5-x, 1.5-y, z. For **2**: (i) 1.5-x, 1.5-y, z; (ii) y, 1.5-x, 0.5-z; (iii) 1.5-y, x, 0.5-z; (iv) 2-x, 1-y, -z; (v) 0.5-x, 0.5-y, z; (vi) 2.5-x, 1.5-y, z. For **3**: (i) y, 0.5-x, 0.5-z; (ii) 0.5-y, x, 0.5-z; (iii) 1-x, 1-y, -z; (iv) 0.5-x, 0.5-y, z; (v) 0.5-x, 1.5-y, z. For **4**: (i) y, 0.5-x, 0.5-z; (ii) 0.5-y, x, 0.5-z; (iii) 1-x, 1-y, -z; (iv) 0.5-x, 0.5-y, z; (v) 0.5-x, 1.5-y, z. For **5**: (i) y, 0.5-x, 0.5-z; (ii) 0.5-y, x, 0.5-z; (iii) 1-x, 1-y, -z; (iv) 0.5-x, 0.5-y, z; (v) 0.5-x, 1.5-y, z.