Electronic Supplementary Information for Dalton Transactions

Electronic Supplementary Information (ESI)

Rare Earth Metal-Organic Complexes Constructed from Hydroxyl and Carboxyl Modified Arenesulfonate: Syntheses, Structure Evolutions, Ultraviolet, Visible and Near-Infrared Luminescence

Ying-Hui Xiao,[a,b] Zhao-Peng Deng,[*,a] Zhi-Biao Zhu,[a] Li-Hua Huo[a] and Shan Gao[*,a]

[a] *Key Laboratory of Functional Inorganic Material Chemistry, Ministry of Education, School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China*

[b] *School of Chemistry and Chemical Engineering, Qiqihar University, Qiqihar 161006, People's Republic of China*

[*] Correspondence author E-mail: dengzhaopeng@hlju.edu.cn; shangao67@yahoo.com

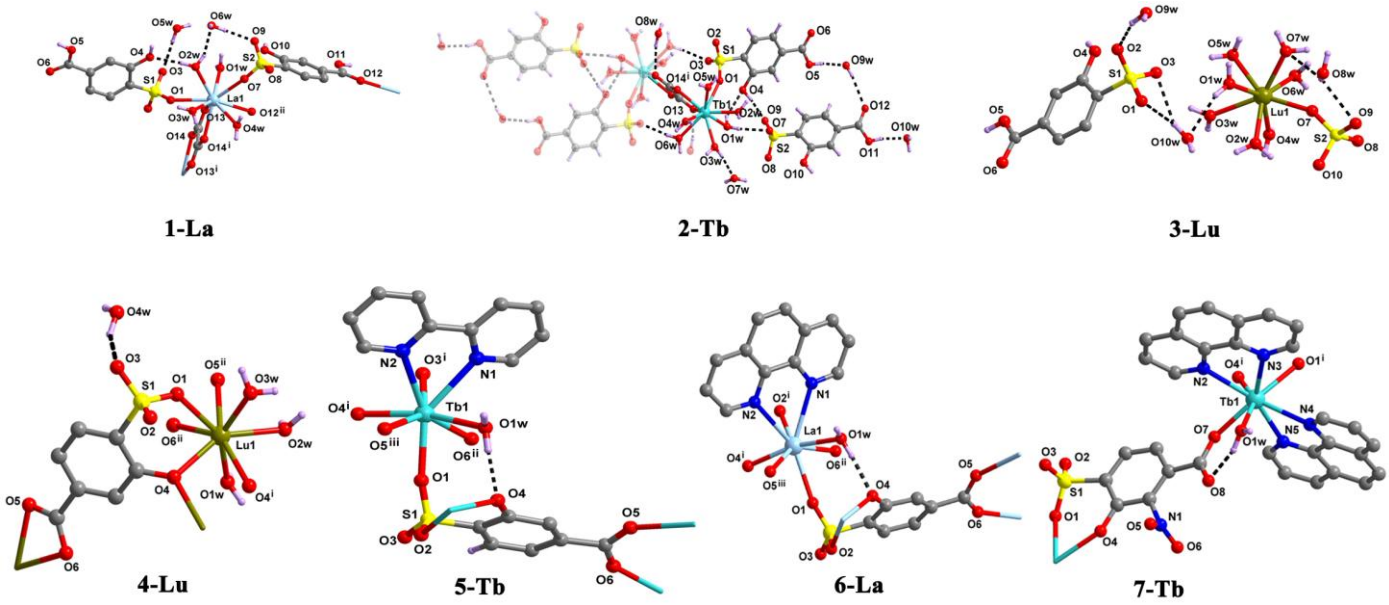


Fig. S1 Molecular structures of the 7 selected complexes with the hydrogen-bonding interactions denoted as black dashed lines.

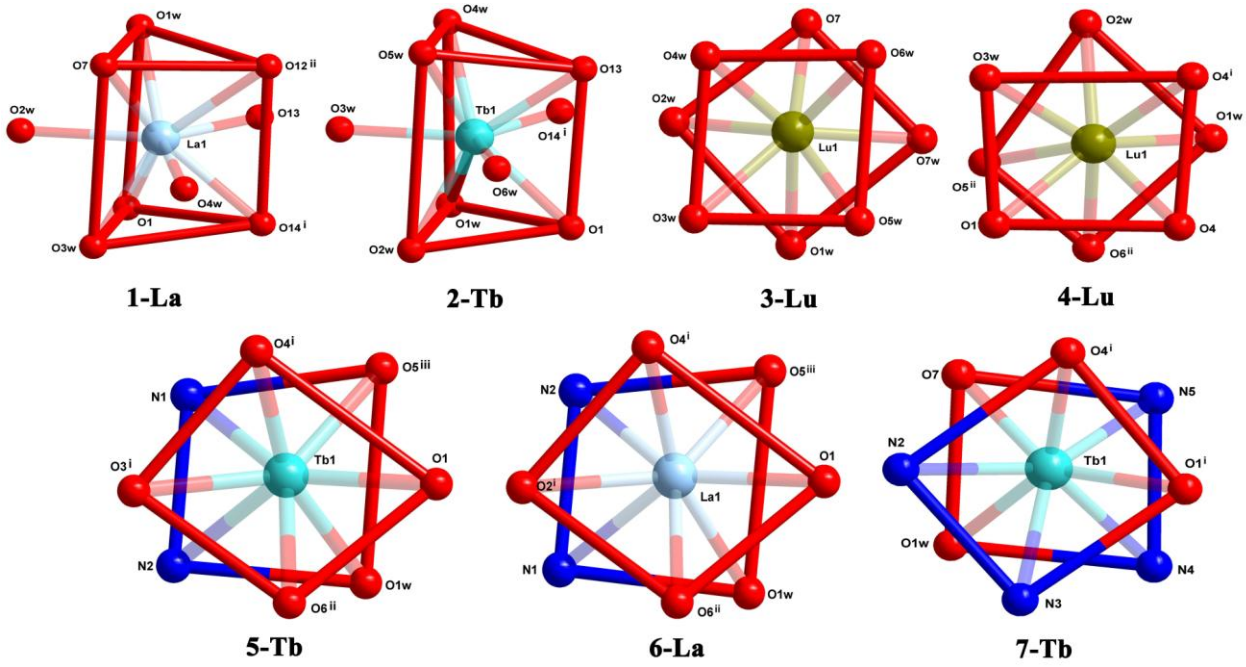


Fig. S2 Diverse polyhedra of RE cations in the 7 selected complexes.

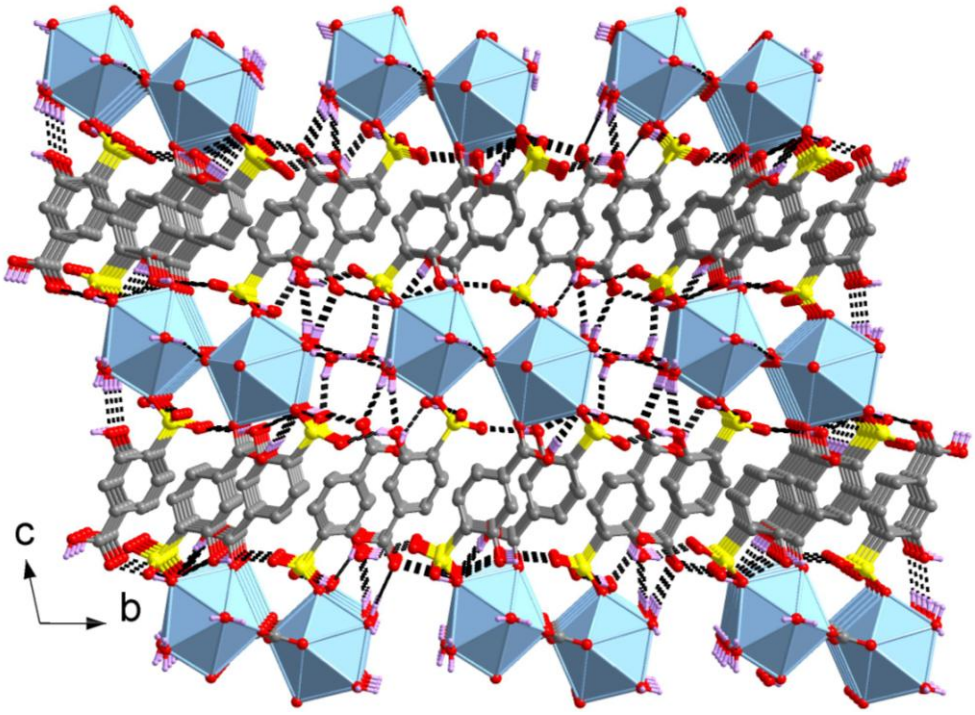


Fig. S3 3-D hybrid supramolecular network of complex **1-La**.

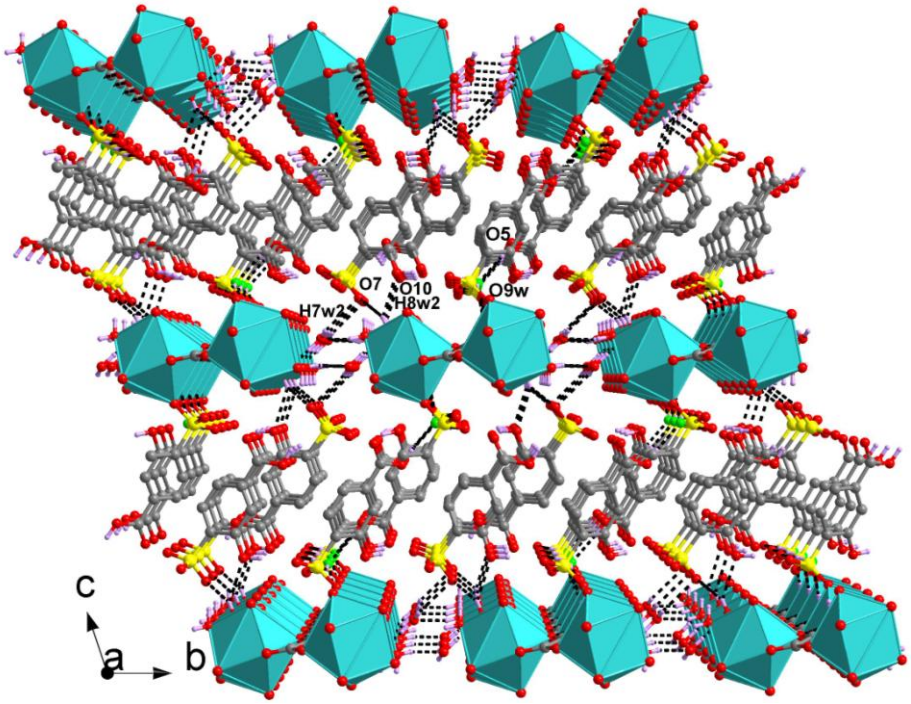


Fig. S4 3-D hybrid supramolecular network of complex **2-Tb**.

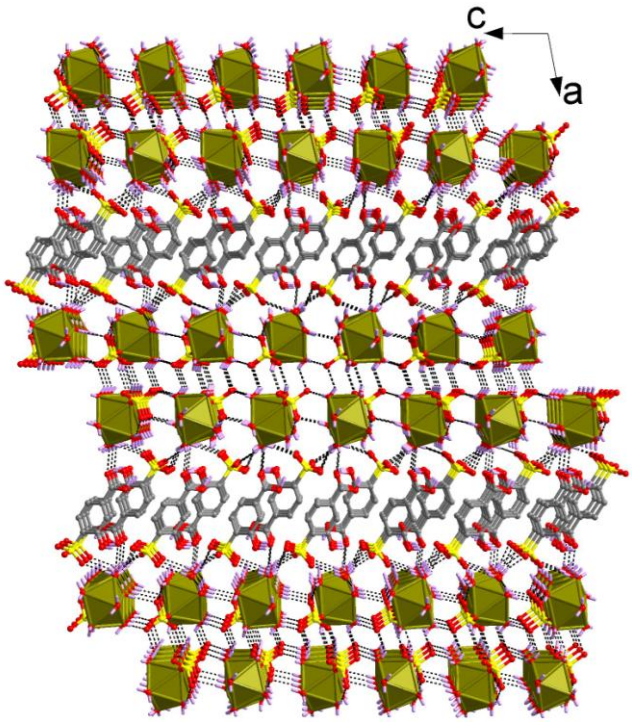


Fig. S5 3-D hybrid supramolecular network of complex **3-Lu**.

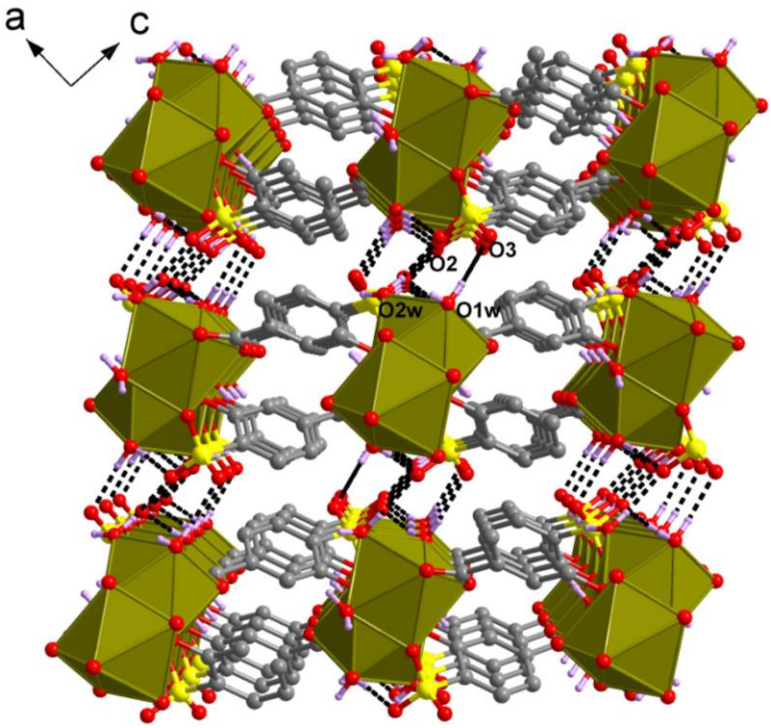


Fig. S6 3-D hybrid supramolecular network of complex **4-Lu**.

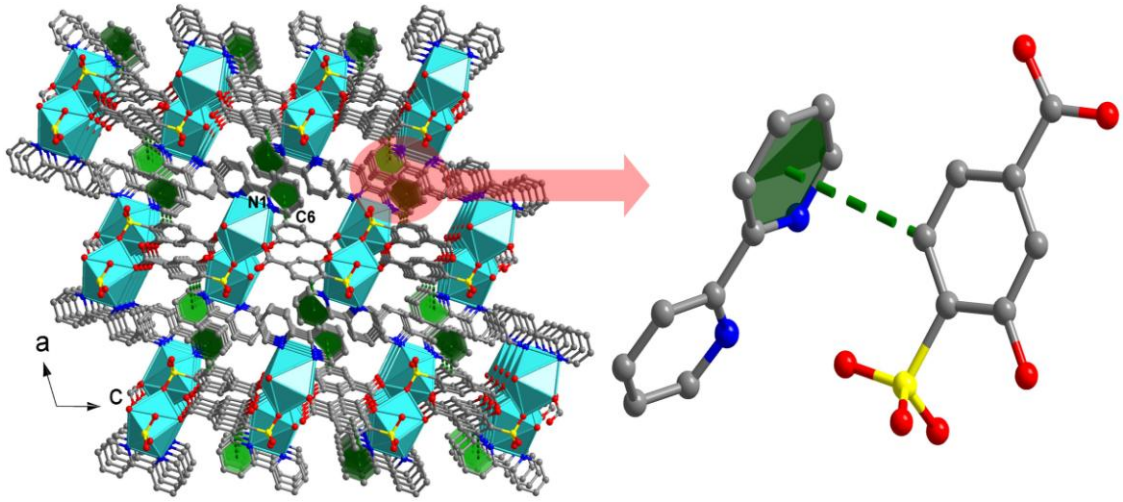


Fig. S7 3-D supramolecular network of complex **5-Tb**. The C-H···π interactions were denoted as green dashed lines.

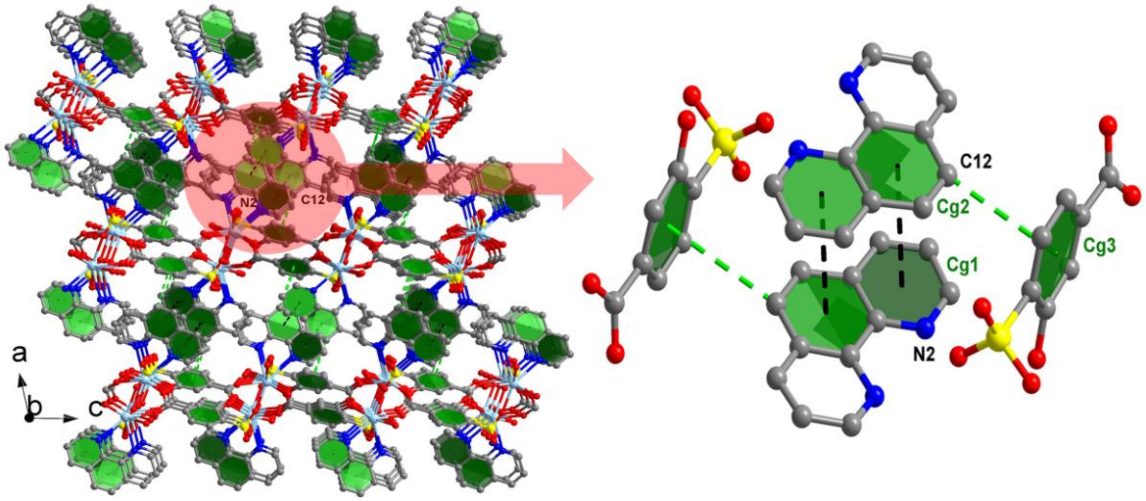


Fig. S8 3-D supramolecular network of complex **6-La**. The π···π and C-H···π interactions were denoted as black and green dashed lines.

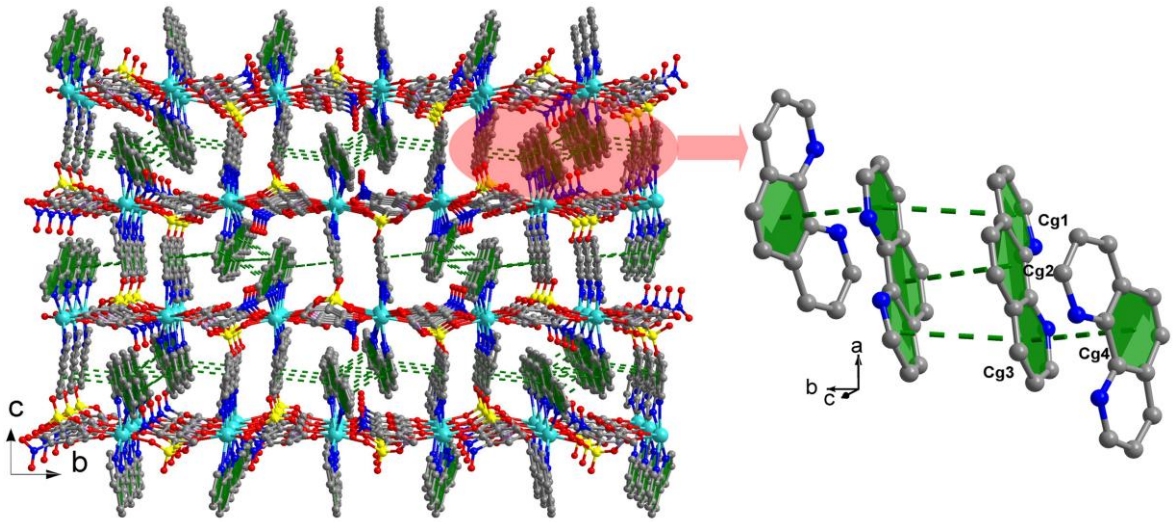


Fig. S9 3-D supramolecular network of complex **7-Tb**. The π···π interactions were denoted as black and green dashed lines.

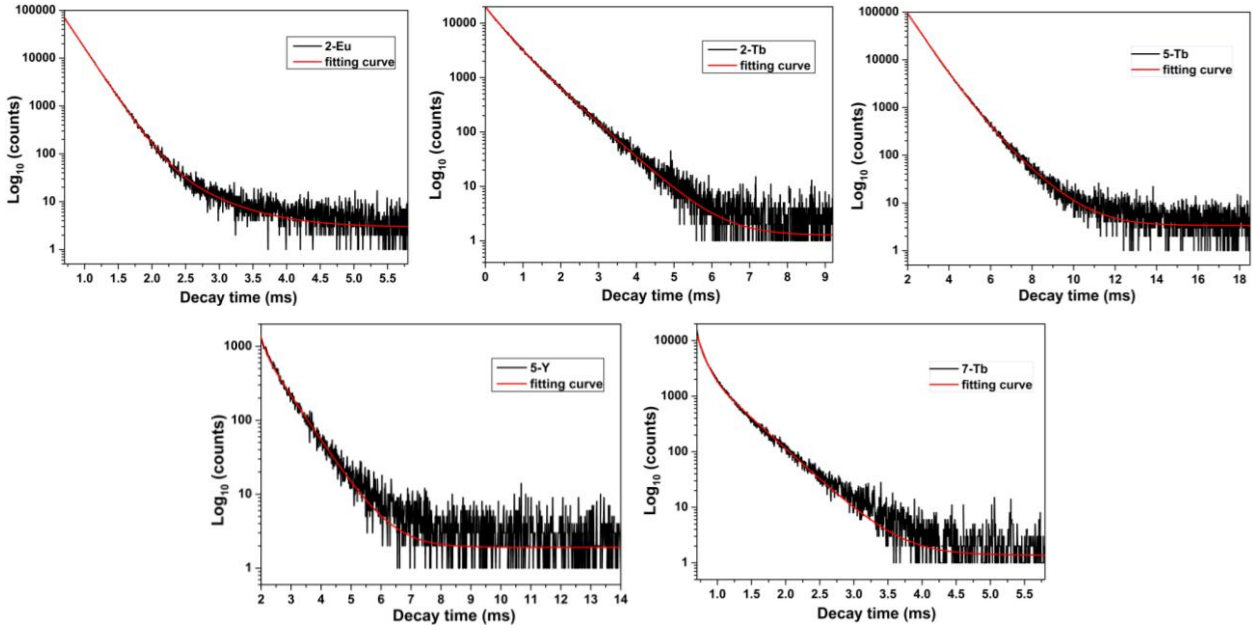
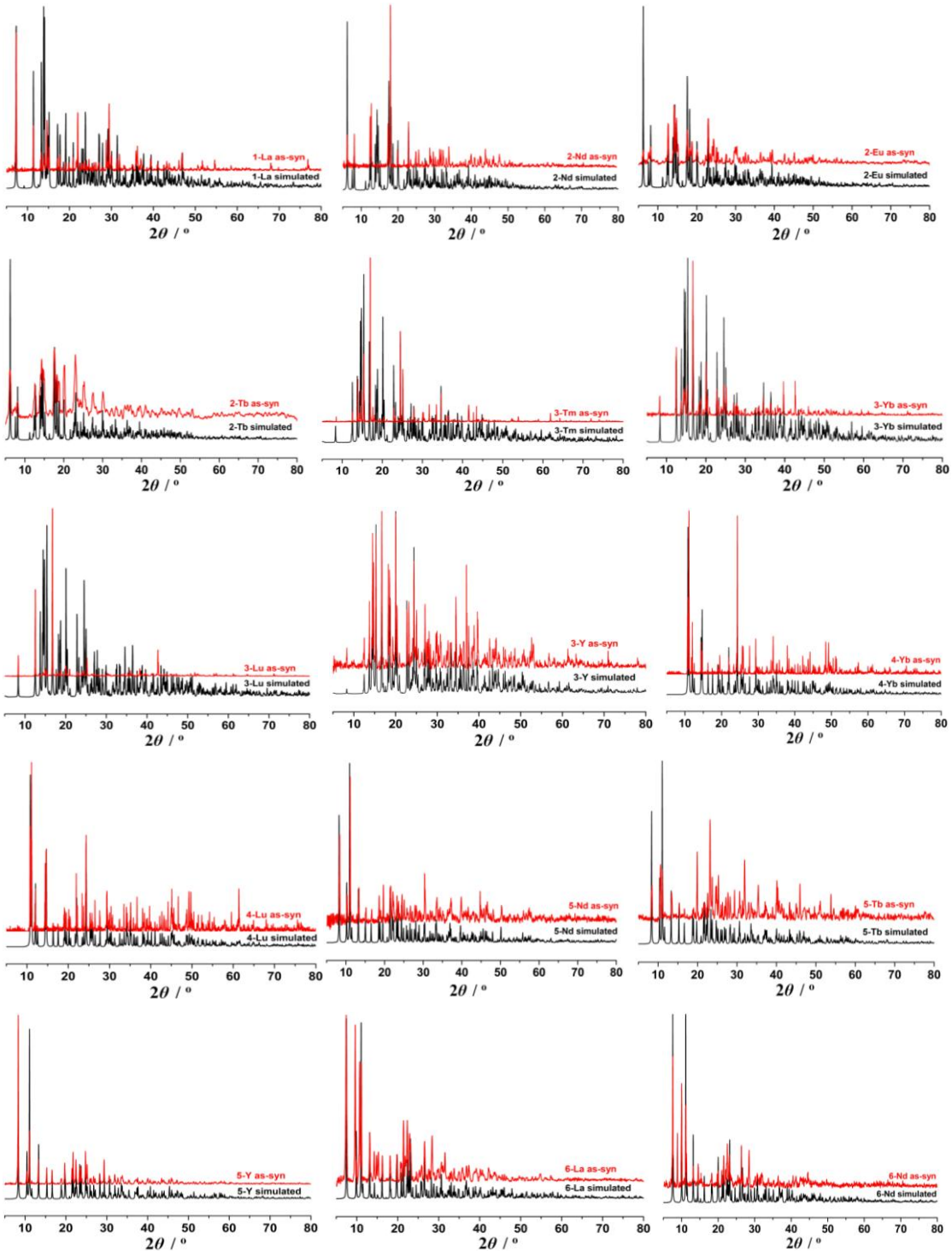


Fig. S10 Luminescence decay curves of complexes **2-Eu**, **2-Tb**, **5-Tb**, **5-Y** and **7-Tb**.


1-La as-syn
1-La simulated
2-Nd as-syn
2-Nd simulated
2-Eu as-syn
2-Eu simulated
2-Tb as-syn
2-Tb simulated
3-Tm as-syn
3-Tm simulated
3-Yb as-syn
3-Yb simulated
3-Lu as-syn
3-Lu simulated
3-Y as-syn
3-Y simulated
4-Yb as-syn
4-Yb simulated
4-Lu as-syn
4-Lu simulated
5-Nd as-syn
5-Nd simulated
5-Tb as-syn
5-Tb simulated
5-Y as-syn
5-Y simulated
6-La as-syn
6-La simulated
6-Nd as-syn
6-Nd simulated
10 20 30 40 50 60 70 80
2θ / º

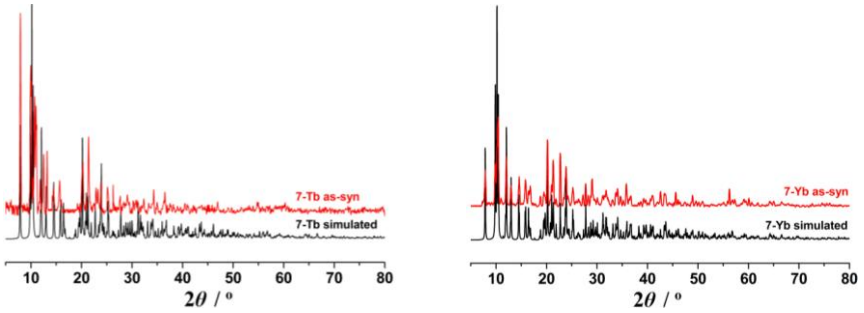


Fig. S11 PXRD patterns of the 17 luminescent complexes at room temperature.

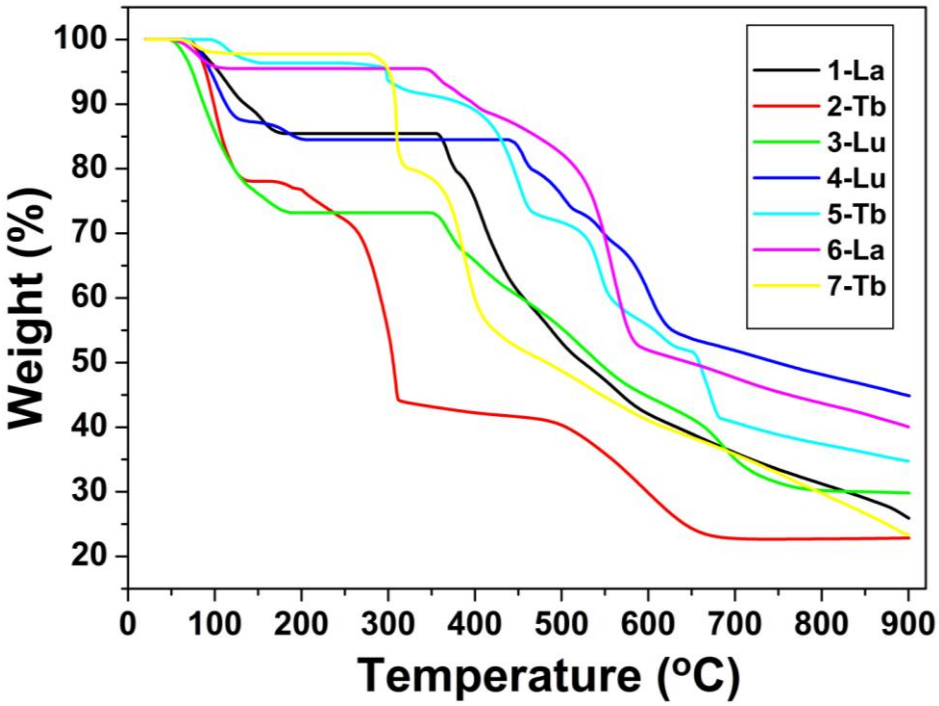


Fig. S12 TG curves of the 7 selected complexes.

Thermogravimetric analysis. To examine the thermal stability, powder X-ray diffraction (PXRD) patterns for solid samples of the 17 luminescent complexes are firstly measured at room temperature as illustrated in Figure S11 (*Supporting Information*). The patterns are highly similar to their simulated ones (based on the single-crystal X-ray diffraction data), indicating that the single-crystal structures are really representative of the bulk of the corresponding samples. Furthermore, owing to the seven types of

structures they presented, only the stabilities of the 7 selected complexes were analyzed on crystalline samples by thermogravimetric analyses (TGA) from room temperature to 900 °C at a rate of 10 °C min^{-1}, under N_2 atmosphere. As shown in Figure S12 (*Supporting Information*), all the seven complexes exhibit an obvious weight loss followed by gradually decompose of organic parts. Generally, the similar first weight loss corresponds to the release of solvent water molecules which occurred in the range of 68-172, 68-142, 52-186, 78-190, 60-106, 60-110 and 94-148 °C, respectively. The observed weight loss of 14.33% in **1-La**, 21.94% in **2-Tb**, 26.82% in **3-Lu**, 15.52% in **4-Lu**, 3.67% in **5-Tb**, 4.50% in **6-La** and 2.23% in **7-Tb** is reasonably close to their calculated value (14.90% in **1-La**, 22.04% in **2-Tb**, 26.95% in **3-Lu**, 15.59% in **4-Lu**, 3.29% in **5-Tb**, 4.10% in **6-La** and 2.26% in **7-Tb**). Then, the following weight losses starting from 357 °C for **1-La**, 180 °C for **2-Tb**, 355 °C for **3-Lu**, 450 °C for **4-Lu**, 288 °C for **5-Tb**, 348 °C for **6-La**, 280 °C for **7-Tb** indicated the decomposition of the organic components, leaving the residue corresponding to La_2O_3 for **1-La** and **6-La** (obsrd. 22.75%, calcd 22.46% in **1-La**, obsrd. 37.52%, calcd 37.06% in **6-La**), Tb_4O_7 for **2-Tb**, **5-Tb** and **7-Tb** (obsrd. 22.72%, calcd 22.87% in **2-Tb**, obsrd. 34.20%, calcd 34.09% in **5-Tb**, obsrd. 23.33%, calcd 23.44% in **7-Tb**), as well as Lu_2O_3 for **3-Lu** and **4-Lu** (obsrd. 30.04%, calcd 29.77% in **3-Lu**, obsrd. 43.65%, calcd 43.05% in **4-Lu**).

Table S1. Crystal data and structure refinement parameters of the other 21 complexes

Complexes	**2-Sm**	**2-Gd**	**2-Dy**	**3-Ho**
Empirical formula	$C_{30}H_{60}O_{48}S_4Sm_2$	$C_{30}H_{60}O_{48}S_4Gd_2$	$C_{30}H_{60}O_{48}S_4Dy_2$	$C_7H_{25}O_{20}S_2Ho$
Formula weight	1617.72	1631.52	1642.02	658.32
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\,2_1/c$
a/Å	7.9111(5)	7.9036(7)	7.8588(3)	21.6475(8)
b/Å	12.3804(6)	12.3541(8)	12.3336(6)	7.6506(3)
c/Å	15.0892(9)	15.0517(10)	15.0079(10)	12.2817(5)
α/°	107.252(5)	107.339(6)	107.378(5)	90.00
β/°	96.881(5)	96.737(6)	97.003(4)	101.053(4)
γ/°	96.565(5)	96.821(6)	96.478(3)	90.00
V/Å^3	1383.61(14)	1374.76(18)	1360.71(12)	1996.31(13)
Z	1	1	1	4
D_c/g cm^{-3}	1.942	1.971	2.004	2.190
μ (Mo Kα)/mm^{-1}	2.376	2.667	3.004	4.270
F(000)	812	816	820	1304
Reflections collected	8258	9118	9131	7344
Unique reflections	6315	6281	6216	4553
Parameters	439	439	451	325
R (int)	0.0269	0.0244	0.0277	0.0284
GOF on F^2	1.037	1.026	1.012	1.057
Final R indices	R_1 = 0.0433	R_1 = 0.0295	R_1 = 0.0341	R_1 = 0.0366
[$I \geq 2\sigma(I)$]	wR_2 = 0.0984	wR_2= 0.0632	wR_2 = 0.0574	wR_2 = 0.0809

Complexes	**3-Er**	**4-Er**	**4-Tm**	**5-La**
Empirical formula	$C_7H_{25}O_{20}S_2Er$	$C_7H_{11}O_{10}SEr$	$C_7H_{11}O_{10}STm$	$C_{17}H_{13}N_2O_7SLa$
Formula weight	660.65	454.48	456.15	528.26
Space group	$P\ 2_1/c$	$P2_1/n$	$P2_1/n$	$P\ 2_1/c$
a/Å	21.6150(9)	10.8891(3)	10.8795(3)	11.3057(3)
b/Å	7.6224(3)	9.3172(3)	9.3023(2)	8.60327(20)
c/Å	12.2659(7)	12.0758(3)	12.0554(3)	18.4261(4)
α/°	90.00	90.00	90.00	90.00
β/°	101.123(5)	91.687(3)	91.715(2)	107.497(3)
γ/°	90.00	90.00	90.00	90.00
V/Å^3	1982.95(16)	1224.63(6)	1219.52(5)	1709.31(7)
Z	4	4	4	4
D_c/g cm^{-3}	2.213	2.465	2.484	2.053
μ (Mo Kα)/mm^{-1}	4.541	7.070	7.493	2.668
F(000)	1308	868	872	1032
Reflections collected	6978	4329	4452	6145
Unique reflections	4530	2793	2784	3898
Parameters	325	196	196	259
R (int)	0.0302	0.0348	0.0313	0.0285
GOF on F^2	1.042	1.016	1.004	1.037
Final R indices	R_1 = 0.0389	R_1 = 0.0405	R_1 = 0.0332	R_1 = 0.0321
[$I \geq 2\sigma(I)$]	wR_2 = 0.0799	wR_2= 0.0782	wR_2 = 0.0507	wR_2 = 0.0585

Complexes	**5-Pr**	**5-Sm**	**5-Eu**	**5-Gd**
Empirical formula	$C_{17}H_{13}N_2O_7SPr$	$C_{17}H_{13}N_2O_7SSm$	$C_{17}H_{13}N_2O_7SEu$	$C_{17}H_{13}N_2O_7SGd$
Formula weight	530.26	539.70	541.31	546.60
Space group	$P\ 2_1/c$	$P\ 2_1/c$	$P\ 2_1/c$	$P\ 2_1/c$
a/Å	11.2702(3)	11.2394(3)	11.2266(4)	11.2180(5)
b/Å	8.58496(16)	8.5661(2)	8.5445(3)	8.5475(3)
c/Å	18.2760(4)	18.1081(4)	18.0467(6)	17.9929(9)
α/°	90.00	90.00	90.00	90.00
β/°	107.839(2)	107.825(3)	107.810(4)	107.729(5)
γ/°	90.00	90.00	90.00	90.00
V/Å^3	1683.26(6)	1659.72(7)	1648.18(10)	1643.33(13)
Z	4	4	4	4
D_c/g cm^{-3}	2.092	2.160	2.181	2.209
μ (Mo Kα)/mm^{-1}	3.066	3.712	3.981	4.212
F(000)	1040	1052	1056	1060
Reflections collected	6183	6873	5763	5652
Unique reflections	3876	3835	3780	3770
Parameters	259	259	259	259
R (int)	0.0279	0.0368	0.0261	0.0310
GOF on F^2	1.035	1.034	1.011	1.062
Final R indices	R_1 = 0.0303	R_1 = 0.0335	R_1 = 0.0313	R_1 = 0.0384
[$I \geq 2\sigma(I)$]	wR_2 = 0.0568	wR_2= 0.0584	wR_2 = 0.0564	wR_2 = 0.0669

Complexes	**5-Dy**	**5-Ho**	**6-Pr**	**6-Sm**
Empirical formula	$C_{17}H_{13}N_2O_7SDy$	$C_{17}H_{13}N_2O_7SHo$	$C_{19}H_{13}N_2O_7SPr$	$C_{19}H_{13}N_2O_7SSm$
Formula weight	551.85	554.28	554.28	563.72
Space group	$P\ 2_1/c$	$P\ 2_1/c$	$P\ 2_1/c$	$P\ 2_1/c$
a/Å	11.1794(2)	11.1687(4)	11.9937(4)	11.9619(3)
b/Å	8.50490(16)	8.4946(3)	8.5177(2)	8.48361(18)
c/Å	17.8416(4)	17.7855(6)	18.1162(5)	17.9950(4)
α/°	90.00	90.00	90.00	90.00
β/°	107.657(2)	107.588(4)	102.778(3)	103.186(2)
γ/°	90.00	90.00	90.00	90.00
V/Å^3	1616.45(6)	1608.50(9)	1804.89(9)	1777.99(7)
Z	4	4	4	4
D_c/g cm^{-3}	2.268	2.289	2.040	2.106
μ (Mo Kα)/mm^{-1}	4.801	5.099	2.865	3.470
F(000)	1068	1072	1088	1100
Reflections collected	5613	5614	6322	6593
Unique reflections	3691	3676	4122	4054
Parameters	259	259	277	277
R (int)	0.0250	0.0356	0.0268	0.0301
GOF on F^2	1.012	1.001	1.051	1.019
Final R indices	R_1 = 0.0296	R_1 = 0.0381	R_1 = 0.0303	R_1 = 0.0302
[$I \geq 2\sigma(I)$]	wR_2 = 0.0495	wR_2= 0.0579	wR_2 = 0.0648	wR_2 = 0.0534

Complexes	**6-Eu**	**7-Gd**	**7-Ho**	**7-Er**	**7-Lu**
Empirical formula	$C_{19}H_{13}N_2O_7SEu$	$C_{31}H_{20}N_5O_9SYb$	$C_{31}H_{20}N_5O_9SHo$	$C_{31}H_{20}N_5O_9SEr$	$C_{31}H_{20}N_5O_9SLu$
Formula weight	565.33	795.83	803.51	805.84	813.55
Space group	$P\ 2_1/c$	$P\ 2_1/c$	$P\ 2_1/c$	$P\ 2_1/c$	$P\ 2_1/c$
a/Å	11.9548(2)	11.6131(3)	11.6315(2)	11.6194(3)	11.6033(3)
b/Å	8.47498(17)	14.8734(4)	14.8756(3)	14.8842(3)	14.8669(4)
c/Å	17.9413(4)	17.5855(5)	17.5103(4)	17.4773(4)	17.4306(5)
α/°	90.00	90.00	90.00	90.00	90.00
β/°	103.253(2)	104.818(3)	104.705(2)	104.617(2)	104.603(3)
γ/°	90.00	90.00	90.00	90.00	90.00
V/Å^3	1769.34(6)	2936.46(14)	2930.49(11)	2924.80(11)	2909.72(14)
Z	4	4	4	4	4
D_c/g cm^{-3}	2.122	1.800	1.821	1.830	1.857
μ (Mo Kα)/mm^{-1}	3.713	2.396	2.838	3.008	3.532
F(000)	1104	1572	1584	1588	1600
Reflections collected	6279	10807	10615	10651	8913
Unique reflections	4025	6699	6712	6682	5095
Parameters	277	430	430	430	430
R (int)	0.0315	0.0346	0.0291	0.0340	0.0321
GOF on F^2	1.015	1.095	1.007	1.002	1.043
Final R indices	R_1 = 0.0348	R_1 = 0.0531	R_1 = 0.0366	R_1 = 0.0390	R_1 = 0.0809
[$I \geq 2\sigma(I)$]	wR_2 = 0.0629	wR_2= 0.1059	wR_2 = 0.0585	wR_2 = 0.0610	wR_2 = 0.2351

Table S2 Selected bond lengths of the 7 selected complexes (Å)[a]

1-La			
La(1)-O(7)	2.477(6)	La(1)-O(1)	2.542(6)
La(1)-O(14)^{i}	2.480(6)	La(1)-O(2W)	2.553(7)
La(1)-O(1W)	2.500(6)	La(1)-O(12)^{ii}	2.631(6)
La(1)-O(13)	2.526(5)	La(1)-O(4W)	2.777(6)
La(1)-O(3W)	2.538(6)		
2-Tb			
Tb(1)-O(5W)	2.360(3)	Tb(1)-O(2W)	2.459(3)
Tb(1)-O(14)^{i}	2.380(3)	Tb(1)-O(13)	2.474(3)
Tb(1)-O(3W)	2.400(3)	Tb(1)-O(6W)	2.478(3)
Tb(1)-O(1)	2.409(3)	Tb(1)-O(1W)	2.502(3)
Tb(1)-O(4W)	2.431(3)		
3-Lu			
Lu(1)-O(7)	2.247(4)	Lu(1)-O(5W)	2.318(5)
Lu(1)-O(6W)	2.297(4)	Lu(1)-O(1W)	2.321(4)
Lu(1)-O(7W)	2.306(5)	Lu(1)-O(2W)	2.326(4)
Lu(1)-O(4W)	2.308(4)	Lu(1)-O(3W)	2.391(5)
4-Lu			
Lu(1)-O(4)	2.287(4)	Lu(1)-O(1)	2.330(4)
Lu(1)-O(4)^{i}	2.287(3)	Lu(1)-O(5)^{ii}	2.349(4)
Lu(1)-O(3W)	2.287(4)	Lu(1)-O(2W)	2.364(4)
Lu(1)-O(1W)	2.303(4)	Lu(1)-O(6)^{ii}	2.379(4)
5-Tb			
Tb(1)-O(4)^{i}	2.274(4)	Tb(1)-O(1W)	2.443(4)
Tb(1)-O(6)^{ii}	2.292(4)	Tb(1)-O(2)^{i}	2.475(4)
Tb(1)-O(5)^{iii}	2.374(4)	Tb(1)-N(2)	2.569(4)
Tb(1)-O(1)	2.398(3)	Tb(1)-N(1)	2.586(4)
6-La			
La(1)-O(4)^{i}	2.369(2)	La(1)-O(1W)	2.592(3)
La(1)-O(6)^{ii}	2.394(2)	La(1)-O(2)^{i}	2.598(2)
La(1)-O(5)^{iii}	2.463(2)	La(1)-N(1)	2.715(3)
La(1)-O(1)	2.512(2)	La(1)-N(2)	2.720(3)
7-Tb			
Tb(1)-O(4)^{i}	2.232(6)	Tb(1)-N(5)	2.503(7)

Tb(1)-O(7)	2.316(6)	Tb(1)-N(2)	2.546(7)
Tb(1)-O(1W)	2.359(6)	Tb(1)-N(3)	2.587(7)
Tb(1)-O(1)^{i}	2.366(6)	Tb(1)-N(4)	2.594(7)

^{a} Symmetry operations: **For 1-La**, i -x+2,-y,-z+1; ii -x+1,-y,-z. **For 2-Tb**, i -x+1,-y+1,-z. **For 4-Lu**, i -x,-y+1,-z+2; ii -x+1/2,y-1/2,-z+3/2. **For 5-Tb**, i -x+1/2,y-1/2,-z+1/2; ii -x+1,-y+2,-z+1; iii x-1/2,-y+5/2,z-1/2. **For 6-La**, i -x+2,y+1/2,-z+1/2; ii -x+2,-y+1,-z+1; iii x,-y+1/2,z-1/2. **For 7-Tb**, i -x+2,y+1/2,-z+3/2.

Table S3 Hydrogen bond parameters of the 7 selected complexes (Å)^{a}

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
1-La				
O(1W)-H(1W1)...O(14)^{iii}	0.85(8)	2.69(8)	3.281(9)	127(8)
O(1W)-H(1W2)...O(13)^{iii}	0.85(8)	2.21(6)	2.911(9)	140(8)
O(2W)-H(2W1)...O(4)	0.85(8)	1.94(2)	2.783(9)	172(12)
O(2W)-H(2W2)...O(6W)	0.85(8)	1.99(7)	2.735(10)	145(11)
O(3W)-H(3W1)...O(6W)^{iv}	0.85	1.92	2.743(10)	163.3
O(3W)-H(3W2)...O(6)^{v}	0.85	1.99	2.814(8)	163.1
O(4W)-H(4W1)...O(6)^{vi}	0.85	2.04	2.836(9)	155.5
O(4W)-H(4W2)...O(9)^{iv}	0.85	2.07	2.867(8)	155.3
O(4)-H(4O)...O(8)^{vii}	0.85(8)	1.90(4)	2.709(8)	159(11)
O(5)-H(5O)...O(5W)^{viii}	0.82	1.78	2.574(9)	163.0
O(5W)-H(5W1)...O(3)	0.85	2.08	2.929(10)	179.4
O(5W)-H(5W2)...O(14)^{iii}	0.85	2.16	3.010(9)	179.2
O(6W)-H(6W1)...O(9)	0.85	1.90	2.724(12)	162.6
O(6W)-H(6W2)...O(2W)^{vii}	0.85	2.12	2.942(11)	162.2
O(10)-H(10O)...O(2)^{iii}	0.85(8)	1.88(4)	2.701(8)	161(11)
O(11)-H(11O)...O(4W)^{ii}	0.82	1.81	2.631(8)	179.1
2-Tb				
O(1W)-H(1W1)...O(8)^{ii}	0.85(5)	2.33(4)	3.029(5)	140(5)
O(1W)-H(1W2)...O(4)	0.85(5)	2.26(3)	2.992(5)	145(4)
O(1W)-H(1W2)...O(1)	0.85(5)	2.59(5)	3.024(5)	113(4)
O(2W)-H(2W1)...O(6)^{iii}	0.85(5)	1.92(2)	2.730(4)	157(6)
O(2W)-H(2W2)...O(7W)	0.85(5)	1.961(16)	2.805(6)	169(6)
O(3W)-H(3W1)...O(10W)^{iv}	0.85(5)	2.12(2)	2.902(5)	154(4)
O(3W)-H(3W2)...O(7W)^{v}	0.85(5)	1.860(19)	2.687(6)	165(6)

O(4)-H(4O)...O(9)^{ii}	0.85(5)	1.868(15)	2.700(4)	168(5)
O(4W)-H(4W1)...O(8W)^{vi}	0.85(5)	1.889(12)	2.731(5)	174(6)
O(4W)-H(4W2)...O(12)^{iv}	0.85(5)	2.032(14)	2.868(5)	170(5)
O(5)-H(5O)...O(9W)^{iii}	0.85(5)	1.867(18)	2.691(4)	165(6)
O(5W)-H(5W1)...O(14)^{vii}	0.85(5)	1.92(2)	2.736(4)	160(5)
O(5W)-H(5W2)...O(9W)	0.85(5)	1.958(18)	2.781(5)	163(4)
O(6W)-H(6W1)...O(3)^{i}	0.85(5)	2.059(12)	2.899(4)	169(4)
O(6W)-H(6W2)...O(7)^{i}	0.85(5)	1.918(17)	2.740(5)	162(5)
O(7W)-H(7W1)...O(8W)^{vi}	0.85(5)	1.92(4)	2.705(6)	151(7)
O(7W)-H(7W2)...O(7)^{viii}	0.85(5)	2.53(6)	3.026(5)	118(5)
O(8W)-H(8W1)...O(13)^{i}	0.85(5)	2.020(12)	2.868(5)	172(5)
O(8W)-H(8W2)...O(7)	0.85(5)	2.30(3)	3.081(5)	152(5)
O(8W)-H(8W2)...O(10)	0.85(5)	2.35(5)	2.935(5)	126(5)
O(9W)-H(9W1)...O(12)^{ix}	0.85(5)	2.32(3)	3.042(5)	144(4)
O(9W)-H(9W1)...O(2)	0.85(5)	2.52(4)	3.117(4)	128(4)
O(9W)-H(9W2)...O(3)^{vii}	0.85(5)	2.22(2)	3.013(4)	158(4)
O(9W)-H(9W2)...O(4)^{vii}	0.85(5)	2.62(4)	3.053(4)	113(4)
O(10)-H(10O)...O(2)	0.85(5)	1.871(13)	2.712(4)	173(6)
O(10W)-HAW...O(6)	0.85(5)	2.45(3)	3.164(5)	142(4)
O(10W)-HBW...O(8)^{ix}	0.85(5)	1.944(15)	2.781(5)	170(5)
O(11)-H(11O)...O(10W)	0.85(5)	1.85(2)	2.671(5)	165(6)
3-Lu				
O(1W)-H(1W1)...O(10)^{i}	0.85(6)	2.05(4)	2.850(6)	156(8)
O(1W)-H(1W2)...O(10W)	0.85(6)	2.18(3)	2.962(7)	151(6)
O(1W)-H(1W2)...O(3)	0.85(6)	2.62(7)	3.107(7)	117(6)
O(2W)-H(2W1)...O(10)	0.85(6)	2.01(3)	2.765(6)	148(6)
O(2W)-H(2W1)...O(3)^{ii}	0.85(6)	2.56(5)	3.149(6)	128(5)
O(2W)-H(2W2)...O(4)^{ii}	0.85(6)	2.42(5)	3.100(6)	138(6)
O(2W)-H(2W2)...O(10W)	0.85(6)	2.46(5)	3.112(6)	135(6)
O(2W)-H(2W2)...O(2)^{ii}	0.85(6)	2.63(6)	3.136(6)	120(5)
O(3W)-H(3W1)...O(6)^{iii}	0.85(6)	2.12(5)	2.831(7)	141(6)
O(3W)-H(3W1)...O(9W)^{iv}	0.85(6)	2.50(5)	3.168(7)	136(7)
O(3W)-H(3W2)...O(1)^{v}	0.85(6)	2.21(5)	2.970(6)	148(8)
O(4W)-H(4W1)...O(10)^{vi}	0.85(6)	1.916(13)	2.764(6)	176(6)
O(4W)-H(4W2)...O(9W)^{v}	0.85(6)	1.97(4)	2.750(6)	153(7)

O(4)-H(4O)...O(1)^{iv}	0.85(6)	1.883(12)	2.733(5)	178(7)
O(5)-H(5O)...O(10W)^{iii}	0.85(6)	1.89(2)	2.715(6)	163(7)
O(5W)-H(5W1)...O(8)^{i}	0.85	2.27	3.108(9)	169.1
O(5W)-H(5W1)...O(7W)	0.85	2.43	2.884(8)	114.2
O(5W)-H(5W2)...O(9W)^{iv}	0.85	1.98	2.817(7)	168.3
O(6W)-H(6W1)...O(9)^{vi}	0.85(6)	1.90(2)	2.739(6)	167(7)
O(6W)-H(6W2)...O(9)^{vii}	0.85(6)	2.25(6)	2.828(7)	125(6)
O(6W)-H(6W2)...O(7W)	0.85(6)	2.42(6)	2.846(6)	112(5)
O(7W)-H(7W1)...O(8)^{vii}	0.85(6)	2.13(5)	2.884(7)	147(7)
O(7W)-H(7W2)...O(8)^{i}	0.85(6)	1.97(3)	2.786(7)	159(6)
O(8W)-H(8W2)...O(7)	0.85	2.28	3.090(16)	159.0
O(8W)-H(8W2)...O(7W)	0.85	2.48	3.03(2)	123.2
O(8W)-H(8W1)...O(9)^{viii}	0.85	1.96	2.766(15)	157.7
O(9W)-H(9W1)...O(2)	0.85(6)	2.03(3)	2.824(6)	155(6)
O(9W)-H(9W1)...O(6)^{ix}	0.85(6)	2.55(6)	3.009(6)	115(5)
O(9W)-H(9W2)...O(3)^{x}	0.85(6)	2.045(15)	2.889(6)	173(7)
O(10W)-HAW...O(6)^{xi}	0.85	2.35	3.110(6)	149.0
O(10W)-HAW...O(2)^{ii}	0.85	2.35	2.907(6)	123.2
O(10W)-HBW...O(3)	0.85	2.31	3.053(6)	146.4
O(10W)-HBW...O(1)	0.85	2.37	3.127(6)	149.1
4-Lu				
O(1W)-H(1W1)...O(2)^{i}	0.85(6)	1.861(13)	2.703(6)	174(5)
O(1W)-H(1W2)...O(3)^{iv}	0.85(6)	1.934(15)	2.770(5)	171(5)
O(2W)-H(2W1)...O(4W)^{v}	0.85(6)	2.04(3)	2.845(6)	157(6)
O(2W)-H(2W2)...O(2)^{iv}	0.85(6)	1.943(15)	2.785(5)	172(7)
O(3W)-H(3W1)...O(4W)^{v}	0.85	1.87	2.721(7)	174.4
O(3W)-H(3W2)...O(5)^{vi}	0.85	2.06	2.903(5)	174.7
O(4W)-H(4W1)...O(6)^{vii}	0.85(6)	2.026(18)	2.851(5)	165(6)
O(4W)-H(4W2)...O(3)	0.85(6)	2.15(4)	2.831(6)	138(5)
5-Tb				
O(1W)-H(1W1)...O(3)^{iv}	0.85(5)	2.12(3)	2.918(5)	157(6)
O(1W)-H(1W1)...O(1)^{iv}	0.85(5)	2.61(4)	3.128(6)	120(4)
O(1W)-H(1W2)...O(4)	0.85(5)	1.925(15)	2.763(5)	170(6)
6-La				
O(1W)-H(1W1)...O(3)^{iv}	0.85(4)	2.094(16)	2.907(4)	162(4)

O(1W)-H(1W1)...O(1)[iv]	0.85(4)	2.65(3)	3.149(3)	119(3)
O(1W)-H(1W2)...O(4)	0.85(4)	1.915(10)	2.760(3)	176(4)
7-Tb				
O(1W)-H(1W1)...O(8)	0.85(4)	1.88(4)	2.680(9)	156(9)
O(1W)-H(1W2)...O(2)[iii]	0.85(4)	1.80(3)	2.622(9)	164(10)

[a] Symmetry operations: **For 1-La**, ii -x+1,-y,-z; iii -x+1,-y,-z+1; iv x+1,y,z; v -x+2,-y+1,-z+2; vi x,y,z-1; vii -x+1,-y+1,-z+1; viii -x+1,-y+1,-z+2. **For 2-Tb**, i -x+1,-y+1,-z; ii x,y+1,z; iii -x+2,-y+2,-z+1; iv x,y,z-1; v -x+2,-y+2,-z; vi -x+2,-y+1,-z; vii x+1,y,z; viii x+1,y+1,z; ix -x+2,-y+1,-z+1. **For 3-Lu**, i x,y+1,z; ii x,y-1,z; iii -x+2,-y+1,-z+2; iv x,-y+3/2,z-1/2; v x,-y+1/2,z-1/2; vi x,-y-1/2,z-1/2; vii -x+3,y+1/2,-z+5/2; viii -x+3,-y,-z+3; ix -x+2,y+1/2,-z+5/2; x x,-y+3/2,z+1/; xi -x+2,y-1/2,-z+5/2. **For 4-Lu**, i -x,-y+1,-z+2; iv x-1/2,-y+1/2,z-1/2; v -x,-y,-z+2; vi x-1/2,-y+1/2,z+1/2; vii x,y-1,z. **For 5-Tb**, iii x-1/2,-y+5/2,z-1/2; iv -x+1/2,y+1/2,-z+1/2. **For 6-La**, iv -x+2,y-1/2,-z+1/2; **For 7-Tb**, iii x-1,y,z.