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Supporting Information

Syntheses and crystal structures of new dinuclear lanthanide complexes based on 3-(4-hydroxyphenyl)propanoic acid: Hirshfeld surface analyses and photoluminescence sensing

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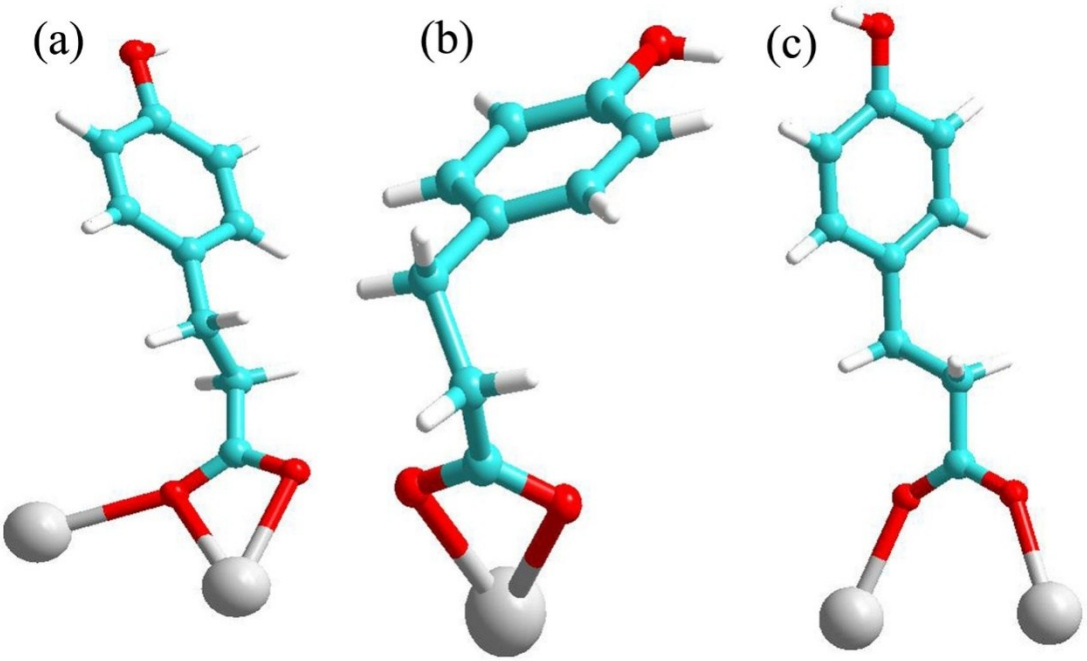

Scheme S1 view of the three types of coordination modes of HPA in this work.

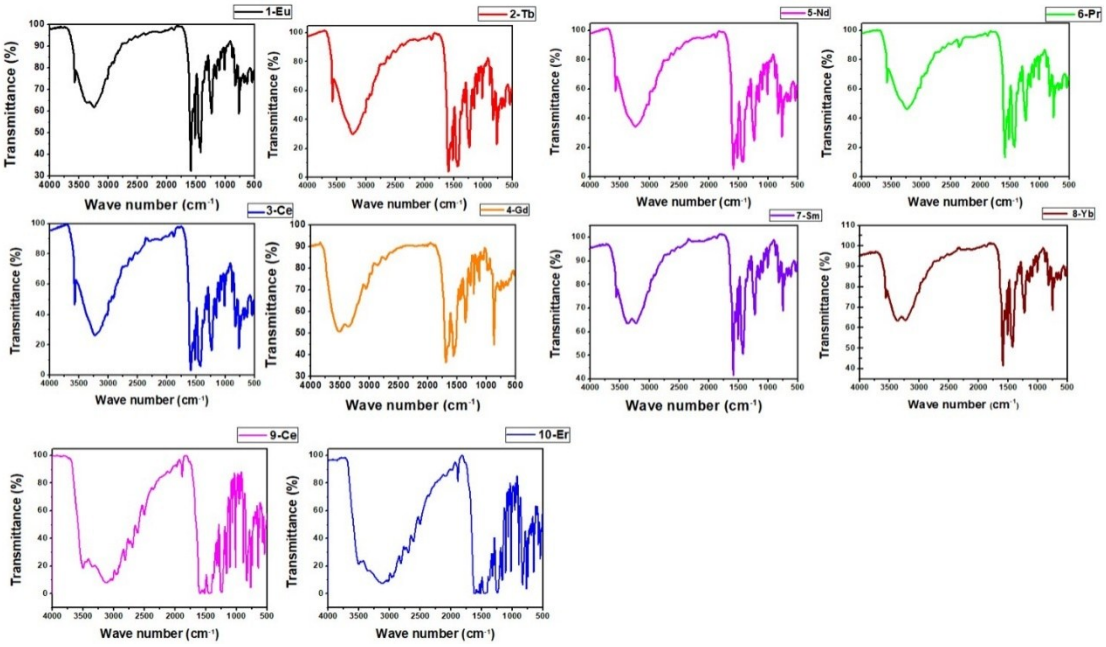

Fig. S1. FTIR spectra for the lanthanide complexes.

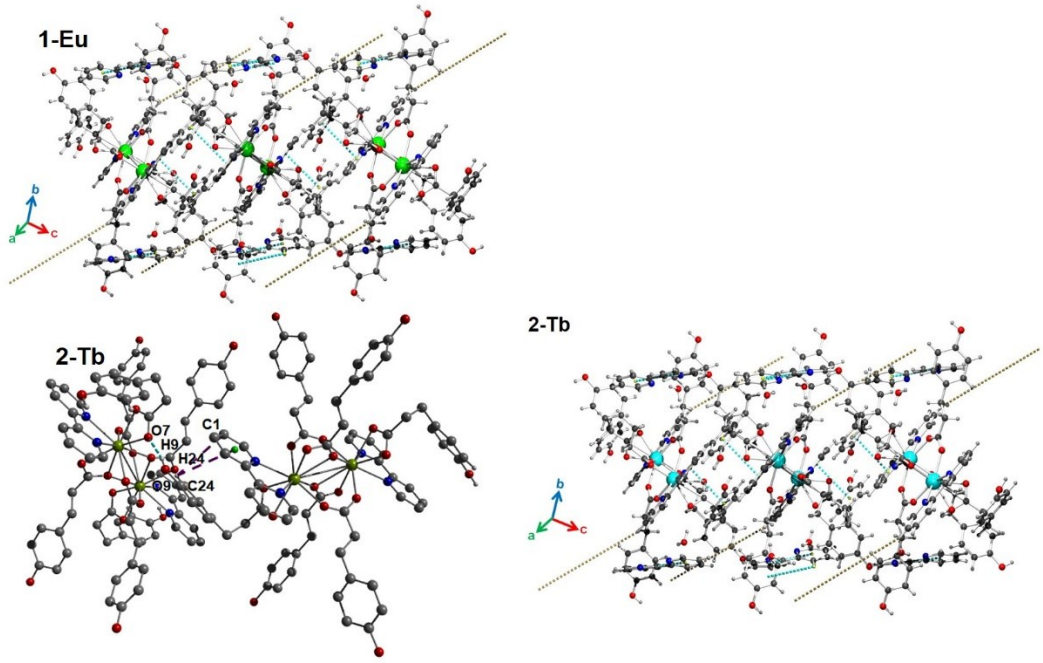

Fig. S2. Intermolecular packing representing O-H···O interaction and C-H···π, π···π interactions for **1** and **2**.

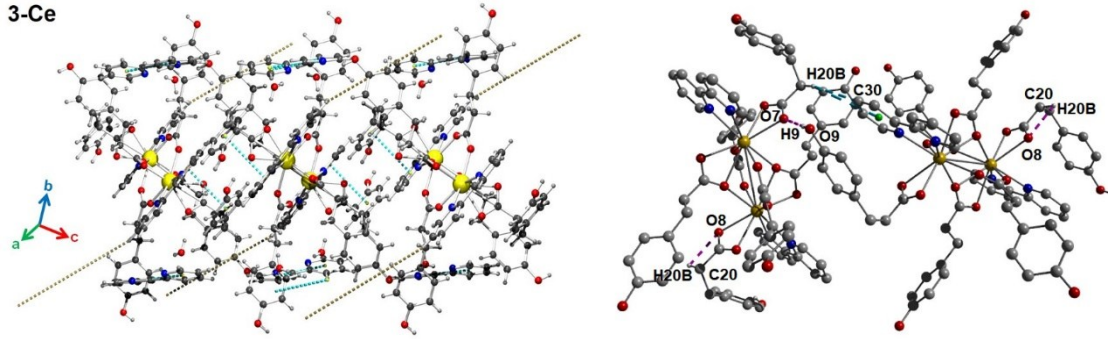

Fig. S3.Intermolecular packing representing O-H···O interaction and C-H···π, π···π interactions for**3**.

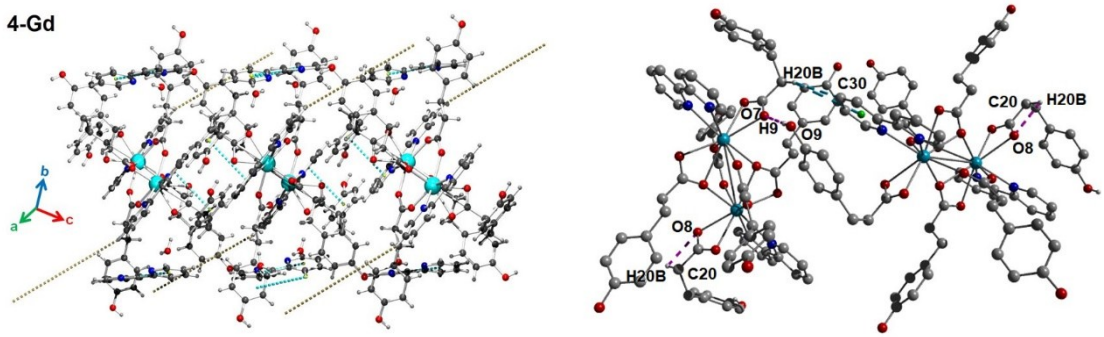

Fig. S4.Intermolecular packing representing O-H···O interaction and C-H···π, π···π interactions for**4**.

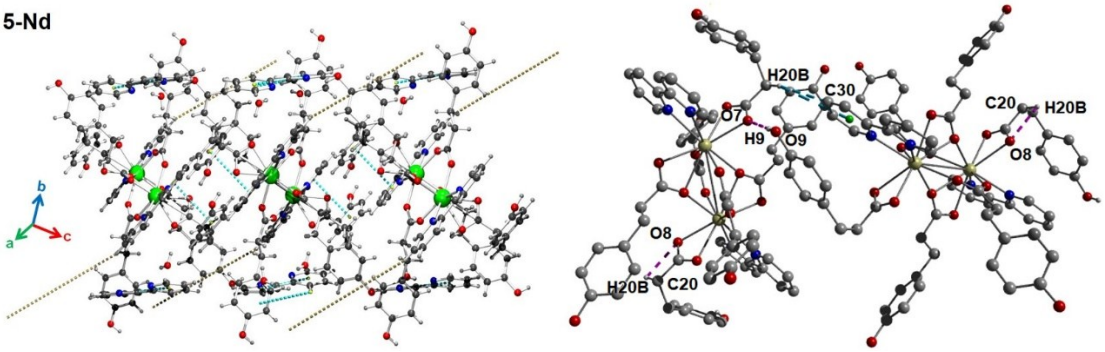

Fig. S5.Intermolecular packing representing O-H···O interaction and C-H···π, π···π interactions for**5**.

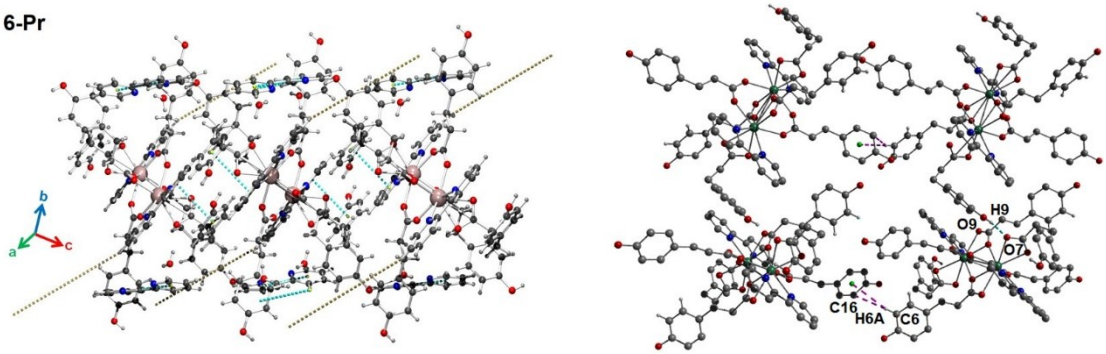

Fig. S6.Intermolecular packing representing O-H···O interaction and C-H···π, π···π interactions for**6**.

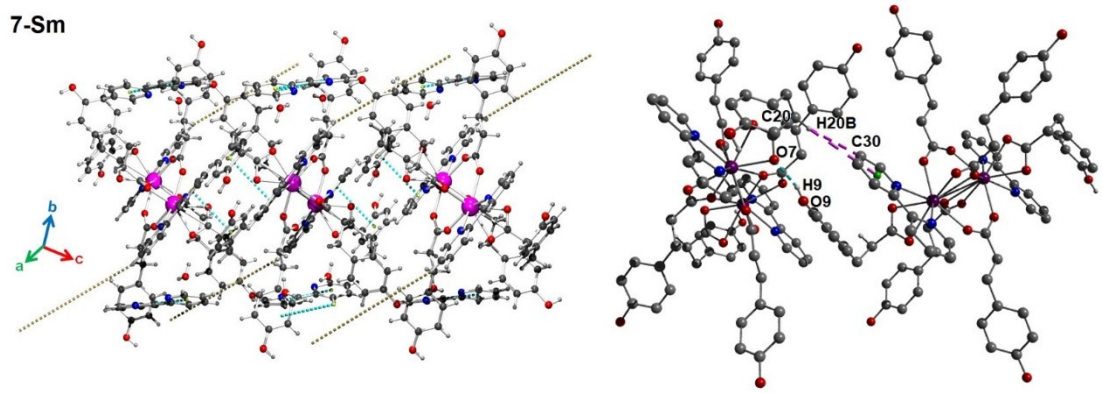

Fig. S7.Intermolecular packing representing O-H···O interaction and C-H···π, π···π interactions for**7**.

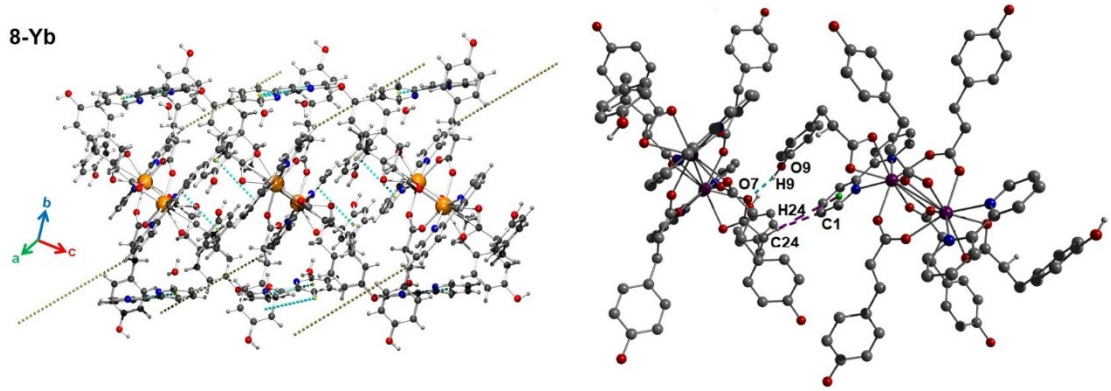

Fig. S8.Intermolecular packing representing O-H···O interaction and C-H···π, π···π interactions for**8**.

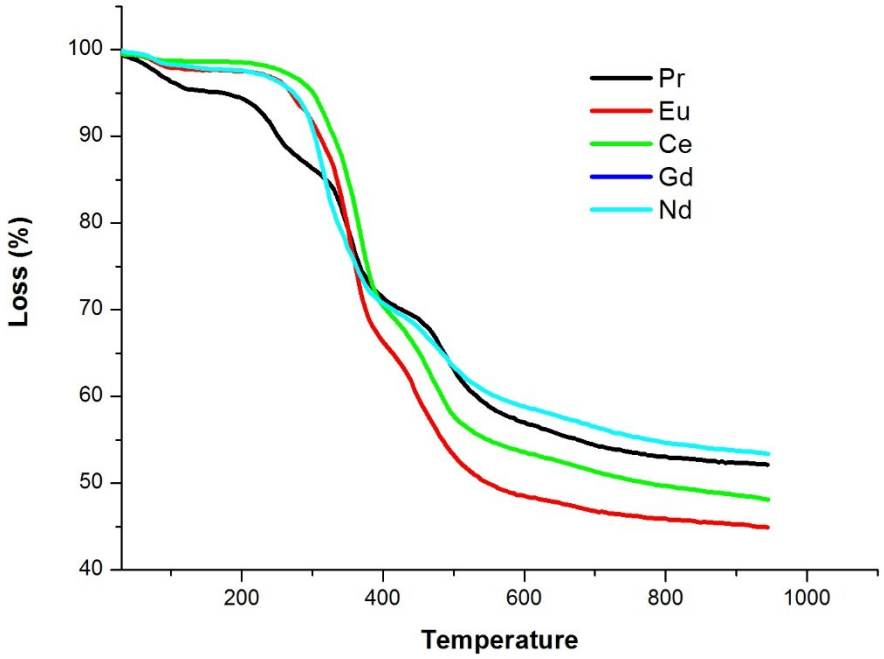

Fig.S9Thermogravimetric plots for the complexes.

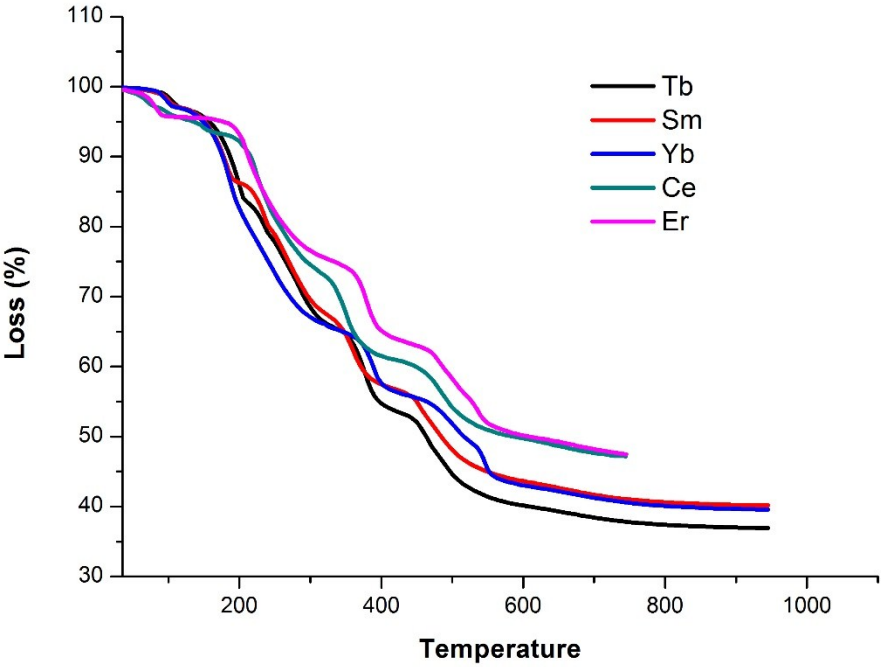

Fig.S10Thermogravimetric plots for the complexes.

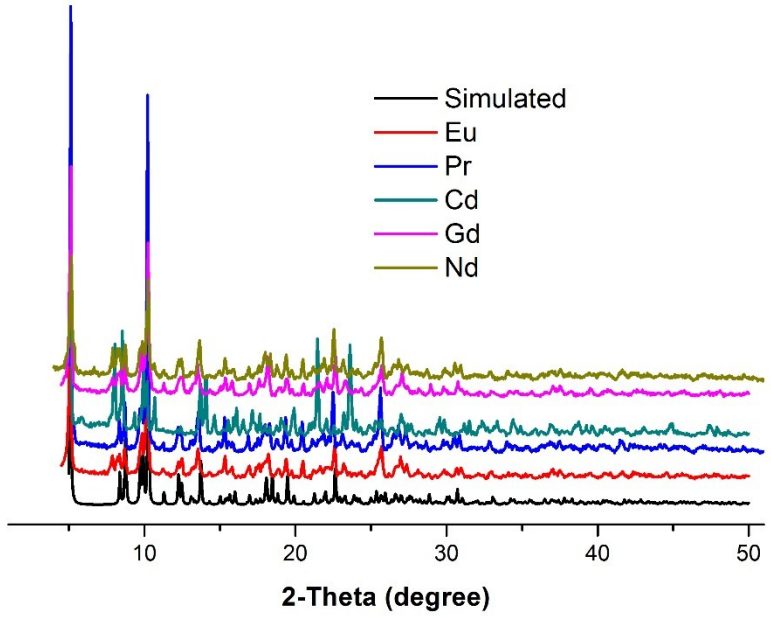

Fig.S11 view of the PXRD pattern for simulated and as-synthesized ones for **1-5**.

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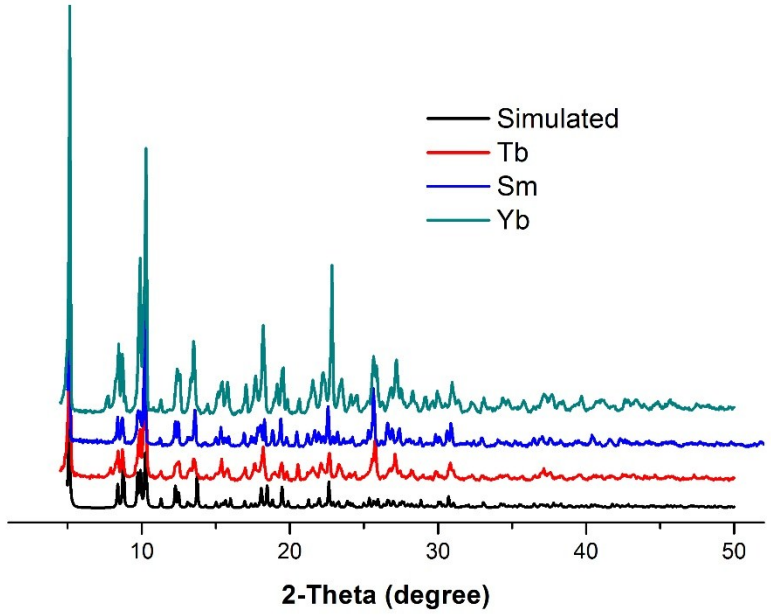

Fig. S12 view of the PXRD patterns of **6-8**.

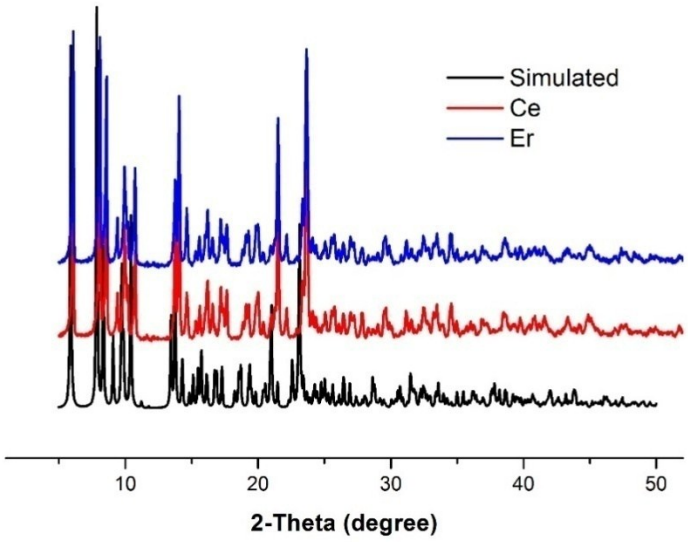

Fig. S13 view of the PXRD patterns of **9**-**10**.

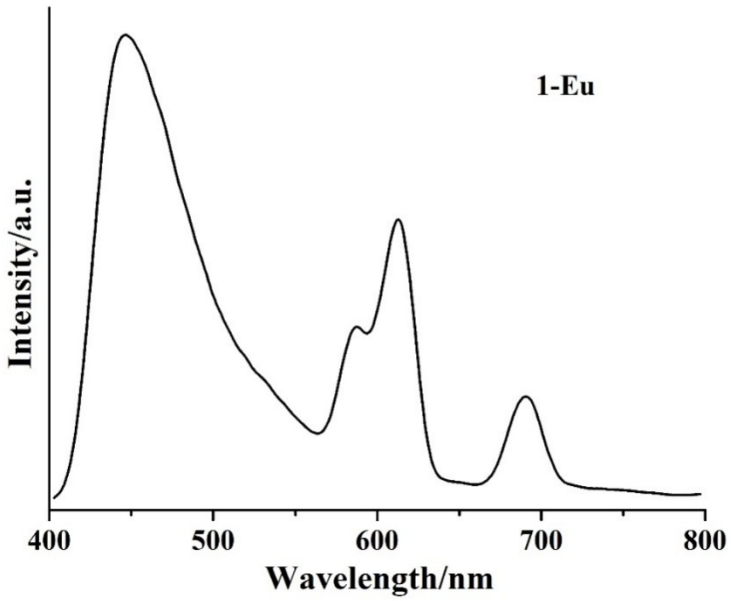

Fig.S14 emission spectrumfor complex **1**.

Table S1. Crystal data and structure refinement information for **1-5**

Compound	**1**	**2**	**3**
Empirical formula	$C_{94}H_{92}N_8O_{22}Eu_2$	$C_{94}H_{94}N_8O_{22}Tb_2$	$C_{94}H_{94}N_8O_{22}Ce_2$
Formula wt	1989.67	2005.61	1968.01
Crystal system	Monoclinic	Monoclinic	Monoclinic
space group	$P2_1/c$	$P2_1/c$	$P2_1/c$
a (Å)	17.2607(8)	17.1988(12)	17.1988(12)
b (Å)	12.3502(6)	12.2560(9)	12.2560(9)
c (Å)	20.2823(9)	20.2497(14)	20.2497(14)
α (deg)	90.00	90.00	90.00
β (deg)	92.0553(7)	92.024(1)	92.024(1)
γ (deg)	90.00	90.00	90.00
V (Å^3)	4320.9(3)	4265.7(5)	4265.7(5)
Z	2	2	2
ρ_{calc}(g·cm^{-3})	1.529	1.561	1.532
μ (mm^{-1})	1.519	1.726	1.135
F(000)	2028	2040	2012
θ Range, deg	2.0-28.6	1.9-28.1	1.9-29.8
Reflns collected	27287	26468	27955
Reflns unique	10746	10262	11466
Independent reflections (R_{int})	0.030	0.054	0.059
R_1, wR_2(I> 2σ(I))*	0.0292, 0.0672	0.0384, 0.0749	0.0489, 0.1242
R_1, wR_2 (all data)**	0.0415, 0.0734	0.0680, 0.0855	0.0932, 0.1570

Compound	**4**	**5**
Empirical formula	$C_{94}H_{94}N_8O_{22}Gd_2$	$C_{94}H_{94}N_8O_{22}Nd_2$
Formula wt	2002.27	1976.25
Crystal system	Monoclinic	Monoclinic
space group	$P2_1/c$	$P2_1/c$
a (Å)	17.1988(12)	17.2971(9)

b (Å)	12.2560(9)	12.3645(6)
c (Å)	20.2497(14)	20.2045(10)
α (deg)	90	90
β (deg)	92.0240(10)	92.2910(8)
γ (deg)	90	90
V (Å^3)	4265.7(5)	4317.7(4)
Z	2	2
ρ_{calc}(g·cm^{-3})	1.559	1.520
μ (mm^{-1})	1.623	1.270
F(000)	2036	2020
θ Range, deg	1.9-28.5	1.9-28.5
Reflns collected	27188	26825
Reflns unique	10582	10715
Independent reflections (R_{int})	0.035	0.037
R_1, wR_2(I> 2σ(I))*	0.0295, 0.0625	0.0314, 0.0668
R_1, wR_2 (all data)**	0.0457, 0.0692	0.0474, 0.0732

Table S1a. Crystal data and structure refinement information for **6-10**

Compound	**6**	**7**	**8**
Empirical formula	$C_{94}H_{94}N_8O_{22}Pr_2$	$C_{94}H_{94}N_8O_{22}Sm_2$	$C_{94}H_{94}N_8O_{22}Yb_2$
Formula wt	1969.59	1988.47	2033.85
Crystal system	Monoclinic	Monoclinic	Monoclinic
space group	$P2_1/c$	$P2_1/c$	$P2_1/c$
a (Å)	17.2971(9)	17.3228(8)	17.3073(9)
b (Å)	12.3645(6)	12.3831(5)	12.3374(6)
c (Å)	20.2045(10)	20.3030(9)	20.4274(10)
α (deg)	90	90	90.00
β (deg)	92.2910(8)	92.0594(7)	91.7501(8)
γ (deg)	90	90	90.00
V (Å^3)	4317.7(4)	4352.4(3)	4359.8(4)
Z	2	2	2
ρ_{calc}(g·cm^{-3})	1.515	1.517	1.549

μ (mm^{-1})	1.196	1.416	2.212
F(000)	2016	2028	2060
θ Range, deg	1.9-28.6	2.0-28.4	1.9-28.1
Reflns collected	27593	27451	26273
Reflns unique	10807	10755	10302
Independent reflections (R_{int})	0.038	0.028	0.033
R_1, wR_2(I> 2σ(I))*	0.0325, 0.0678	0.0262, 0.0607	0.0287, 0.0593
R_1, wR_2 (all data)**	0.0508, 0.0749	0.0367, 0.0654	0.0447, 0.0648

Compound	**9**	**10**
Empirical formula	$C_{74}H_{78}N_4O_{22}Ce_2$	$C_{74}H_{78}N_4O_{22}Er_2$
Formula wt	1655.64	1709.92
Crystal system	Triclinic	Triclinic
space group	P-1	P-1
a (Å)	11.4683(17)	11.3201(10)
b (Å)	12.1254(18)	12.0641(10)
c (Å)	15.092(2)	15.0263(12)
α (deg)	88.418(3)	88.384(1)
β (deg)	95.900(3)	83.721(2)
γ (deg)	111.890(3)	68.535(1)
V (Å3)	1936.9 (5)	1898.2(3)
Z	2	2
ρcalc ($g \cdot cm^{-3}$)	1.419	1.496
μ (mm^{-1})	1.234	2.270
F(000)	842	862
θ Range, deg	1.8-28.7	1.9-28.0
Reflns collected	12150	10968
Reflns unique	8982	8142
Independent reflections (Rint)	0.062	0.040
R1, wR2 (I > 2σ(I))*	0.0853, 0.1912	0.0550, 0.1282

R1, wR2 (all data)**	0.1696, 0.2361	0.0928, 0.1553	

Table S2. Selected bond distances (Å) and angles (deg) for **1-5**

		1	
Eu(1)-O(1)	2.464(2)	Eu(1)-O(2)	2.5643(18)
Eu(1)-O(4)	2.3287(17)	Eu(1)-O(7)	2.488(2)
Eu(1)-O(8)	2.4663(19)	Eu(1)-N(1)	2.577(2)
Eu(1)-N(2)	2.594(2)		
O(1)-Eu(1)-O(2)	51.07(6)	O(1)-Eu(1)-O(4)	80.23(7)
O(1)-Eu(1)-O(7)	143.45(7)	O(1)-Eu(1)-O(8)	141.78(6)
O(1)-Eu(1)-N(1)	74.96(7)	O(1)-Eu(1)-N(2)	69.50(7)
O(2)-Eu(1)-O(7)	141.13(6)	O(2)-Eu(1)-O(8)	150.71(6)
O(2)-Eu(1)-N(1)	120.91(6)	O(2)-Eu(1)-N(2)	109.97(7)
O(2)-Eu(1)-O(4)	70.69(6)	O(4)-Eu(1)-O(7)	77.58(6)
O(4)-Eu(1)-O(8)	129.33(7)	O(4)-Eu(1)-N(1)	79.13(7)
O(4)-Eu(1)-N(2)	135.31(6)	O(7)-Eu(1)-O(8)	51.79(7)
O(7)-Eu(1)-N(1)	72.59(7)	O(7)-Eu(1)-N(2)	108.30(7)
O(8)-Eu(1)-N(1)	86.61(7)	O(8)-Eu(1)-N(2)	72.29(7)
		2	
Tb(1)- O(1)	2.428(3)	Tb(1)-O(2)	2.544(2)
Tb(1)- O(4)	2.294(2)	Tb(1)- O(7)	2.466(2)
Tb(1)- O(8)	2.438(2)	Tb(1)- N(1)	2.539(4)
Tb(1)- N(2)	2.562(3)		
O(1)-Tb(1)-O(2)	51.21(8)	O(1)-Tb(1)-O(4)	80.28(9)
O(1)-Tb(1)-O(7)	143.37(9)	O(1)-Tb(1)-O(8)	141.79(9)
O(1)-Tb(1)-N(1)	75.18(9)	O(1)-Tb(1)-N(2)	69.37(9)
O(2)-Tb(1)- O(4)	70.79(8)	O(2)-Tb(1)- O(7)	140.87(8)
O(2)-Tb(1)- O(8)	150.26(8)	O(2)-Tb(1)- N(1)	121.09(9)
O(2)-Tb(1)- N(2)	109.79(9)	O(4)-Tb(1)- O(7)	77.31(8)
O(4)-Tb(1)- O(8)	129.49(8)	O(4)-Tb(1)- N(1)	78.72(9)
O(4)-Tb(1)-N(2)	135.46(9)	O(7)-Tb(1)-O(8)	52.23(8)
O(7)-Tb(1)-N(1)	72.29(9)	O(7)-Tb(1)-N(2)	108.76(9)
N(1)-Tb(1)-N(2)	62.78(9)		
		3	
Ce(1)-O(1)	2.526(4)	Ce(1)-O(2)	2.608(3)

Ce(1)-O(4)	2.381(3)	Ce(1)-O(7)	2.564(4)
Ce(1)-O(8)	2.520(4)	Ce(1)-N(1)	2.619(4)
Ce(1)-N(2)	2.636(4)		
O(1)-Ce(1)-O(2)	49.08(10)	O(1)-Ce(1)-O(4)	80.88(12)
O(1)-Ce(1)-O(7)	144.70(12)	O(1)-Ce(1)-O(8)	142.32(12)
O(1)-Ce(1)-N(1)	75.93(12)	O(1)-Ce(1)-N(2)	69.44(11)
O(2)-Ce(1)-O(4)	71.05(11)	O(2)-Ce(1)-O(7)	142.67(10)
O(2)-Ce(1)-O(8)	152.19(10)	O(2)-Ce(1)-N(1)	120.19(10)
O(2)-Ce(1)-N(2)	108.88(11)	O(4)-Ce(1)-O(7)	78.05(11)
O(4)-Ce(1)-O(8)	128.21(12)	O(4)-Ce(1)-N(1)	79.93(12)
O(4)-Ce(1)-N(2)	135.10(12)	O(7)-Ce(1)-O(8)	50.20(11)
N(1)-Ce(1)-N(2)	61.01(12)		
	4		
Gd(1)-O(1)	2.442(2)	Gd(1)-O(2)	2.5513(18)
Gd(1)-O(4)	2.3115(18)	Gd(1)-O(7)	2.4765(19)
Gd(1)-O(8)	2.4495(18)	Gd(1)-N(1)	2.551(2)
Gd(1)-N(2)	2.575(2)		
O(1)-Gd(1)-O(2)	51.00(6)	O(1)-Gd(1)-O(4)	80.14(7)
O(1)-Gd(1)-O(7)	143.40(7)	O(1)-Gd(1)-O(8)	141.89(7)
O(1)-Gd(1)-N(1)	75.18(7)	O(1)-Gd(1)-N(2)	69.62(7)
O(2)-Gd(1)-O(4)	70.63(6)	O(2)-Gd(1)-O(7)	141.01(6)
O(2)-Gd(1)-O(8)	150.52(6)	O(2)-Gd(1)-N(1)	120.97(6)
O(2)-Gd(1)-N(2)	109.90(6)	O(4)-Gd(1)-O(7)	77.51(6)
O(4)-Gd(1)-O(8)	129.48(6)	O(4)-Gd(1)-N(1)	78.94(7)
O(4)-Gd(1)-N(2)	135.52(7)	O(7)-Gd(1)-O(8)	52.02(6)
O(7)-Gd(1)-N(1)	72.36(7)	O(7)-Gd(1)-N(2)	108.51(7)
O(8)-Gd(1)-N(1)	86.78(7)	O(8)-Gd(1)-N(2)	72.28(7)
N(1)-Gd(1)-N(2)	62.55(7)		
	5		
Nd(1)-O(2)	2.500(2)	Nd(1)-O(2)	2.5825(17)
Nd(1)-O(4)	2.3673(16)	Nd(1)-O(7)	2.5179(19)
Nd(1)-O(8)	2.5053(18)	Nd(1)-N(1)	2.607(2)
Nd(1)-N(2)	2.627(2)		
O(1)-Nd(1)-O(2)	50.22(6)	O(1)-Nd(1)-O(4)	80.31(6)
O(1)-Nd(1)-O(7)	143.96(6)	O(1)-Nd(1)-O(8)	141.97(7)

O(1)-Nd(1)-N(1)	75.09(7)	O(1)-Nd(1)-N(2)	69.61(7)
O(2)-Nd(1)-O(4)	70.38(6)	O(2)-Nd(1)-O(7)	141.64(6)
O(2)-Nd(1)-O(8)	151.61(6)	O(2)-Nd(1)-N(1)	120.32(6)
O(2)-Nd(1)-N(2)	109.83(6)	O(4)-Nd(1)-O(7)	78.02(6)
O(4)-Nd(1)-O(8)	129.05(6)	O(4)-Nd(1)-N(1)	79.75(7)
O(4)-Nd(1)-N(2)	135.19(7)	O(7)-Nd(1)-O(8)	51.07(6)
N(1)-Nd(1)-N(2)	61.20(7)		

Table S2a. Selected bond distances (Å) and angles (deg) for **6-10**

6			
Pr(1)-O(1)	2.518(2)	Pr(1)-O(2)	2.5958(17)
Pr(1)-O(4)	2.3780(16)	Pr(1)-O(7)	2.5316(19)
Pr(1)-O(8)	2.5157(18)	Pr(1)-N(1)	2.619(2)
Pr(1)-N(2)	2.642(2)		
O(1)-Pr(1)-O(2)	49.90(6)	O(1)-Pr(1)-O(4)	80.23(6)
O(1)-Pr(1)-O(7)	144.17(6)	O(1)-Pr(1)-O(8)	142.09(6)
O(1)-Pr(1)-N(1)	75.07(7)	O(1)-Pr(1)-N(2)	69.73(7)
O(2)-Pr(1)-O(4)	70.37(6)	O(2)-Pr(1)-O(7)	141.90(6)
O(2)-Pr(1)-O(8)	151.76(6)	O(2)-Pr(1)-N(1)	120.08(6)
O(2)-Pr(1)-N(2)	109.78(6)	O(4)-Pr(1)-O(7)	78.25(6)
O(4)-Pr(1)-O(8)	129.05(6)	O(4)-Pr(1)-N(1)	79.84(7)
O(4)-Pr(1)-N(2)	135.03(7)	O(7)-Pr(1)-O(8)	50.83(6)
O(7)-Pr(1)-N(1)	73.18(6)	O(7)-Pr(1)-N(2)	107.61(6)
O(8)-Pr(1)-N(1)	86.21(7)	O(8)-Pr(1)-N(2)	72.36(6)
N(1)-Pr(1)-N(2)	60.89(7)		
7			
Sm(1)-O(1)	2.4810(18)	Sm(1)-O(2)	2.5737(16)
Sm(1)-O(4)	2.3474(15)	Sm(1)-O(7)	2.5046(17)
Sm(1)-O(8)	2.4858(16)	Sm(1)-N(1)	2.5949(19)
Sm(1)-N(2)	2.6114(19)		
O(1)-Sm(1)-O(2)	50.77(5)	O(1)-Sm(1)-O(4)	80.39(6)
O(1)-Sm(1)-O(7)	143.63(6)	O(1)-Sm(1)-O(8)	141.70(6)
O(1)-Sm(1)-N(2)	69.58(6)	O(2)-Sm(1)-O(4)	70.63(5)
O(2)-Sm(1)-O(7)	141.29(5)	O(2)-Sm(1)-N(1)	120.66(6)
O(2)-Sm(1)-N(2)	109.94(6)	O(4)-Sm(1)-O(7)	77.63(5)
O(4)-Sm(1)-N(1)	79.30(6)	O(4)-Sm(1)-N(2)	135.44(5)

O(7)-Sm(1)-N(2)	108.15(6)	O(8)-Sm(1)-N(2)	72.13(6)
N(1)-Sm(1)-N(2)	61.91(6)		
		8	
Yb(1)-O(1)	2.385(2)	Yb(1)-O(2)	2.564(2)
Yb(1)-O(5)	2.2627(18)	Yb(1)-O(7)	2.448(2)
Yb(1)-O(8)	2.408(2)	Yb(1)-N(1)	2.517(2)
Yb(1)-N(2)	2.543(2)		
O(1)-Yb(1)-O(2)	51.86(6)	O(1)-Yb(1)-O(4)	80.10(7)
O(1)-Yb(1)-O(7)	143.21(7)	O(1)-Yb(1)-O(8)	141.48(7)
O(1)-Yb(1)-N(1)	75.38(8)	O(1)-Yb(1)-N(2)	69.46(7)
O(2)-Yb(1)-O(4)	70.34(7)	O(2)-Yb(1)-O(7)	139.84(6)
O(2)-Yb(1)-O(8)	149.55(6)	O(2)-Yb(1)-N(1)	121.41(7)
O(2)-Yb(1)-N(2)	110.27(7)	O(4)-Yb(1)-O(7)	77.06(7)
O(4)-Yb(1)-O(8)	130.31(7)	O(7)-Yb(1)-N(1)	71.93(7)
O(7)-Yb(1)-N(2)	109.38(7)	O(7)-Yb(1)-O(8)	53.29(7)
N(1)-Yb(1)-N(2)	64.02(8)		
		9	
Ce(1)-O(1)	2.494(7)	Ce(1)-O(4)	2.611(7)
Ce(1)-O(5)	2.705(7)	Ce(1)-O(7)	2.585(7)
Ce(1)-O(8)	2.655(6)	Ce(1)-N(1)	2.702(8)
Ce(1)-N(1)	2.759(10)		
O(1)-Ce(1)-O(4)	84.3(2)	O(1)-Ce(1)-O(5)	122.1(2)
O(1)-Ce(1)-O(7)	93.7(2)	O(1)-Ce(1)-N(1)	139.6(3)
O(1)-Ce(1)-N(2)	79.2(3)	O(4)-Ce(1)-O(5)	49.6(2)
O(4)-Ce(1)-O(7)	143.9(3)	O(4)-Ce(1)-N(1)	82.8(2)
O(5)-Ce(1)-O(7)	144.1(2)	O(5)-Ce(1)-O(8)	138.6(2)
O(5)-Ce(1)-N(1)	75.2(2)	O(5)-Ce(1)-N(2)	107.6(3)
O(7)-Ce(1)-N(2)	74.4(2)	O(8)-Ce(1)-N(1)	121.0(2)
O(8)-Ce(1)-N(2)	113.4(3)	N(1)-Ce(1)-N(2)	60.4(3)
		10	
Er(1)-O(1)	2.341(6)	Er(1)-O(4)	2.596(5)
Er(1)-O(5)	2.432(6)	Er(1)-O(7)	2.607(5)
Er(1)-O(8)	2.471(5)	Er(1)-N(1)	2.583(7)
Er(1)-N(2)	2.584(6)		
O(1)-Er(1)-O(4)	70.30(17)	O(1)-Er(1)-O(5)	79.99(19)

O(1)-Er(1)-O(7)	74.82(18)	O(1)-Er(1)-O(8)	126.45(19)
O(1)-Er(1)-N(1)	137.7(2)	O(1)-Er(1)-N(2)	78.2(2)
O(4)-Er(1)-O(5)	52.05(18)	O(4)-Er(1)-O(7)	136.5(2)
O(4)-Er(1)-O(8)	151.40(17)	O(4)-Er(1)-N(1)	114.52(19)
O(4)-Er(1)-N(2)	122.51(19)	O(5)-Er(1)-O(7)	143.43(17)
O(5)-Er(1)-O(8)	144.2(2)	O(5)-Er(1)-N(1)	73.8(2)
O(5)-Er(1)-N(2)	76.36(18)	O(7)-Er(1)-O(8)	51.6(2)
O(8)-Er(1)-N(1)	70.5(2)	N(1)-Er(1)-N(2)	63.8(2)

Table S3. Selected the hydrogen bond distances (Å) for **1-10**

Contact D–H···A	Distance, Å			Angle D–H···A, deg
	D–H	H···A	D···A	
1				
O(1W)-H(1W1)···N(3)	0.8400	1.9200	2.760(5)	174.00
O(3)-H(3)···O(1W)	0.8400	1.9400	2.771(5)	172.00
O(2W)-H(2W2)··· O(8)	0.8500	1.9800	2.823(3)	171.00
O(6)-H(6)···O(2W)	0.8400	1.8700	2.706(3)	176.00
O(9)-H(9)··· O(7)	0.8400	1.9300	2.758(3)	167.00
2				
O(1W)-H(1W1)···N(3)	0.8400	1.9100	2.750(6)	174.00
O(3)-H(3)···O(1W)	0.8400	1.9300	2.769(5)	177.00
O(2W)-H(2W2)··· O(8)	0.8500	1.9700	2.815(4)	176.00
O(6)-H(6)···O(2W)	0.8400	1.8700	2.706(4)	177.00
O(9)-H(9)··· O(7)	0.8400	1.9300	2.758(4)	170.00
3				
O(1W)-H(1W1)···N(3)	0.8400	1.9100	2.745(8)	172.00
O(3)-H(3)···O(1W)	0.8400	1.9600	2.797(8)	174.00
O(2W)-H(2W2)··· O(8)	0.8500	2.0000	2.806(5)	158.00
O(6)-H(6)···O(2W)	0.8400	1.8600	2.692(6)	173.00
O(9)-H(9)··· O(7)	0.8400	1.9300	2.765(5)	170.00
4				
O(1W)-H(1W1)···N(3)	0.8400	1.9100	2.743(5)	174.00
O(3)-H(3)···O(1W)	0.8400	1.9500	2.767(4)	164.00
O(2W)-H(2W2)··· O(8)	0.8500	1.9700	2.812(3)	171.00

O(6)-H(6)···O(2W)	0.8400	1.8700	2.705(3)	176.00
O(9)-H(9)··· O(7)	0.8400	1.9400	2.750(3)	163.00
5				
O(1W)-H(1W1)···N(3)	0.8400	1.9200	2.761(4)	173.00
O(3)-H(3)···O(1W)	0.8400	1.9200	2.757(5)	176.00
O(2W)-H(2W2)··· O(8)	0.8500	1.9600	2.807(3)	178.00
O(6)-H(6)···O(2W)	0.8400	1.8600	2.695(3)	176.00
O(9)-H(9)··· O(7)	0.8400	1.9500	2.763(3)	164.00
6				
O(1W)-H(1W1)···N(3)	0.8400	1.9100	2.753(4)	173.00
O(3)-H(3)···O(1W)	0.8400	1.9300	2.768(4)	172.00
O(2W)-H(2W2)··· O(8)	0.8500	1.9600	2.802(3)	173.00
O(6)-H(6)···O(2W)	0.8400	1.8500	2.692(3)	174.00
O(9)-H(9)··· O(7)	0.8400	1.9400	2.768(3)	168.00
7				
O(1W)-H(1W1)···N(3)	0.8500	1.9300	2.771(4)	173.00
O(3)-H(3)···O(1W)	0.8400	1.9400	2.774(4)	175.00
O(2W)-H(2W2)··· O(8)	0.8500	1.9800	2.815(2)	169.00
O(6)-H(6)···O(2W)	0.8400	1.8700	2.706(3)	176.00
O(9)-H(9)··· O(7)	0.8400	1.9500	2.773(3)	165.00
8				
O(1W)-H(1W1)···N(3)	0.8500	1.9300	2.771(5)	174.00
O(3)-H(3)···O(1W)	0.8400	1.9700	2.792(5)	165.00
O(2W)-H(2W2)··· O(8)	0.8500	2.0100	2.857(3)	173.00
O(6)-H(6)···O(2W)	0.8400	1.8900	2.729(4)	175.00
O(9)-H(9)··· O(7)	0.8400	1.9400	2.769(3)	170.00
9				
O(1W)-H(1W1)···O(6)	0.8500	2.5600	2.936(14)	108.00
O(3)-H(3)···O(1W)	0.8400	1.8500	2.683(15)	174.00
O(2W)-H(2W2)··· O(8)	0.8400	2.2600	3.020(13)	151.00
O(6)-H(6)···O(5)	0.8200	1.9400	2.737(12)	165.00
O(9)-H(9)··· O(4)	0.8400	1.9800	2.753(13)	153.00
10				
O(1W)-H(1W1)···O(9)	0.8400	2.2500	2.923(12)	137.00
O(3)-H(3)···O(1W)	0.8400	1.9200	2.758(13)	174.00

O(2W)-H(2W2)··· O(6)	0.8400	2.1100	2.954(11)	179.00
O(9)-H(9)··· O(7)	0.8400	1.9500	2.747(10)	157.00