Electronic Supplementary Information

Lanthanide Coordination Polymers Based on 5-(2′- Carboxylphenyl) Nicotinate: Syntheses, Structure Diversity, Dehydration/Hydration, Luminescence and Magnetic Properties

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Table S1 Crystal data and structure refinements for the compounds **2, 3, 5, 7, 8, 12**.

Complex	**2**	**3**	**5**	**7**	**8**	**12**
Empirical formula	$C_{38}H_{25}TbN_4O_9$	$C_{38}H_{25}HoN_4O_9$	$C_{39}H_{35}Y_2N_3O_{19}$	$C_{39}H_{35}Dy_2N_3O_{19}$	$C_{39}H_{35}Ho_2N_3O_{19}$	$C_{25}H_{15}LuN_4O_7$
Formula weight	840.54	846.55	1027.52	1174.70	1179.56	658.38
Crystal system	Trigonal	Trigonal	Triclinic	Triclinic	Triclinic	Monoclinic
Space group	*R*-3	*R*-3	*P*-1	*P*-1	*P*-1	$P2_1/n$
a (Å)	30.870(8)	30.7627(5)	12.725(19)	12.825(9)	12.7551(18)	12.385(4)
b(Å)	30.870(8)	30.7627(5)	13.57(2)	13.672(10)	13.617(2)	10.429(3)
c (Å)	17.963(4)	17.9693(3)	14.12(2)	14.227(10)	14.137(2)	17.436(5)
α(°)	90	90	66.224(14)	66.182(6)	66.2800(10)	90
β(°)	90	90	67.182(15)	66.800(6)	67.1400(10)	93.704(3)
γ(°)	120	120	77.113(14)	77.064(6)	77.1490(10)	90
Volume ($Å^3$)	14825(6)	14726.8	2051(5)	2091(3)	2065.1(5)	2247.2(11)
Z	18	18	2	2	2	4
Dcalcd (g cm^{-3})	1.695	1.718	1.664	1.866	1.897	1.946
M (Mo Kα) (mm^{-1})	2.213	5.080	2.900	3.629	3.888	4.450
F(000)	7524	7560	1040	1148	1152	1280
Data/restraints/parameters	6136/0/470	6395/0/470	7504/0/569	7513 / 0 / 568	7562/0/572	4186/6/ 334
Goodness-of-fit on F^2	1.047	1.069	1.036	1.064	1.039	1.038
Final R indices, [I > $2\sigma(I)$]	$R_1 = 0.0266$,	$R_1 = 0.0299$,	$R_1 = 0.0625$	$R_1 = 0.0357$	$R_1 = 0.0274$	$R_1 = 0.0310$
R indices (all data)	$R_1 = 0.0411$	$R_1 = 0.0323$	$R_1 = 0.1161$	$R_1 = 0.0465$	$R_1 = 0.0338$	$R_1 = 0.0409$

Table S2 Selected bond lengths [Å] and angles [°] for the compounds **1-12**[a].

1					
Sm(1)-O(1)	2.500(6)	Sm(1)-O(2)	2.496(6)	Sm(1)-O(5)	2.596(6)
Sm(1)-O(6)	2.612(6)	Sm(1)-O(6)#1	2.391(5)	Sm(1)-O(7)#3	2.439(5)
Sm(1)-O(8)#2	2.404(5)	Sm(1)-N(3)	2.616(7)	Sm(1)-N(4)	2.636(7)
Sm(1)#1-O(6)-Sm(1)	107.25(19)	O(6)#1-Sm(1)-O(8)#2	71.51(19)	O(6)#1-Sm(1)-O(7)#3	76.09(19)
O(8)#2-Sm(1)-O(7)#3	137.22(18)	O(6)#1-Sm(1)-O(2)	76.95(19)	O(8)#2-Sm(1)-O(2)	120.41(19)
O(7)#3-Sm(1)-O(2)	77.02(19)	O(6)#1-Sm(1)-O(1)	95.5(2)	O(8)#2-Sm(1)-O(1)	81.5(2)
O(7)#3-Sm(1)-O(1)	129.31(19)	O(2)-Sm(1)-O(1)	52.61(19)	O(6)#1-Sm(1)-O(5)	122.32(18)
O(8)#2-Sm(1)-O(5)	94.94(19)	O(7)#3-Sm(1)-O(5)	79.43(17)	O(2)-Sm(1)-O(5)	144.41(19)
O(1)-Sm(1)-O(5)	138.91(19)	O(6)#1-Sm(1)-O(6)	72.75(19)	O(8)#2-Sm(1)-O(6)	72.68(18)
O(7)#3-Sm(1)-O(6)	71.55(19)	O(2)-Sm(1)-O(6)	140.46(18)	O(1)-Sm(1)-O(6)	153.89(18)
O(5)-Sm(1)-O(6)	50.03(16)	O(6)#1-Sm(1)-N(3)	146.30(19)	O(8)#2-Sm(1)-N(3)	138.8(2)
O(7)#3-Sm(1)-N(3)	81.6(2)	O(2)-Sm(1)-N(3)	73.58(19)	O(1)-Sm(1)-N(3)	79.4(2)
O(5)-Sm(1)-N(3)	76.92(18)	O(6)-Sm(1)-N(3)	123.30(17)	O(6)#1-Sm(1)-N(4)	146.94(19)
O(8)#2-Sm(1)-N(4)	76.3(2)	O(7)#3-Sm(1)-N(4)	135.50(19)	O(2)-Sm(1)-N(4)	114.6(2)
O(1)-Sm(1)-N(4)	72.3(2)	O(5)-Sm(1)-N(4)	67.14(19)	O(6)-Sm(1)-N(4)	104.6(2)
2					
Tb(1)-O(1)	2.542(2)	Tb(1)-O(2)	2.550(2)	Tb(1)-O(2)#1	2.340(2)
Tb(1)-O(3)#3	2.370(2)	Tb(1)-O(4)#2	2.343(2)	Tb(1)-O(5)	2.439(2)
Tb(1)-O(6)	2.449(2)	Tb(1)-N(3)	2.564(3)	Tb(1)-N(4)	2.545(3)
O(2)#1-Tb(1)-O(4)#2	71.44(8)	O(2)#1-Tb(1)-O(3)#3	76.00(8)	O(4)#2-Tb(1)-O(3)#3	137.67(8)
O(2)#1-Tb(1)-O(5)	96.17(9)	O(4)#2-Tb(1)-O(5)	80.46(8)	O(3)#3-Tb(1)-O(5)	129.95(8)
O(2)#1-Tb(1)-O(6)	76.85(8)	O(4)#2-Tb(1)-O(6)	119.41(8)	O(3)#3-Tb(1)-O(6)	77.17(8)
O(5)-Tb(1)-O(6)	53.16(8)	O(2)#1-Tb(1)-O(1)	122.59(8)	O(4)#2-Tb(1)-O(1)	96.55(9)
O(3)#3-Tb(1)-O(1)	78.85(8)	O(5)-Tb(1)-O(1)	138.23(8)	O(6)-Tb(1)-O(1)	143.78(8)
O(2)#1-Tb(1)-N(4)	145.63(8)	O(4)#2-Tb(1)-N(4)	139.55(9)	O(3)#3-Tb(1)-N(4)	80.75(8)
O(5)-Tb(1)-N(4)	79.74(9)	O(6)-Tb(1)-N(4)	73.53(8)	O(1)-Tb(1)-N(4)	76.14(8)
O(2)#1-Tb(1)-O(2)	72.63(8)	O(4)#2-Tb(1)-O(2)	72.70(8)	O(3)#3-Tb(1)-O(2)	72.28(8)
O(5)-Tb(1)-O(2)	152.98(8)	O(6)-Tb(1)-O(2)	140.93(8)	O(1)-Tb(1)-O(2)	50.67(7)
N(4)-Tb(1)-O(2)	123.39(8)	O(2)#1-Tb(1)-N(3)	146.96(9)	O(4)#2-Tb(1)-N(3)	76.13(9)
O(3)#3-Tb(1)-N(3)	135.36(8)	O(5)-Tb(1)-N(3)	72.04(9)	O(6)-Tb(1)-N(3)	115.12(8)
O(1)-Tb(1)-N(3)	66.89(8)	N(4)-Tb(1)-N(3)	64.31(9)	Tb(1)#1-O(2)-Tb(1)	107.37(8)
3					
Ho(1)-O(1)	2.4144(19)	Ho(1)-O(2)	2.4221(18)	Ho(1)-O(5)	2.5178(18)
Ho(1)-O(6)	2.5269(17)	Ho(1)-O(6)#2	2.3218(17)	Ho(1)-O(7)#3	2.3503(16)
Ho(1)-O(8)#1	2.3202(17)	Ho(1)-N(3)	2.554(2)	Ho(1)-N(4)	2.523(2)
O(8)#1-Ho(1)-O(6)#2	71.83(6)	O(8)#1-Ho(1)-O(7)#3	138.09(6)	O(6)#2-Ho(1)-O(7)#3	75.98(6)
O(8)#1-Ho(1)-O(1)	79.87(7)	O(6)#2-Ho(1)-O(1)	96.23(7)	O(7)#3-Ho(1)-O(1)	130.31(6)
O(8)#1-Ho(1)-O(2)	119.51(7)	O(6)#2-Ho(1)-O(2)	76.67(6)	O(7)#3-Ho(1)-O(2)	76.92(6)
O(1)-Ho(1)-O(2)	53.78(7)	O(8)#1-Ho(1)-O(5)	97.14(7)	O(6)#2-Ho(1)-O(5)	122.69(6)
O(7)#3-Ho(1)-O(5)	78.35(6)	O(1)-Ho(1)-O(5)	138.21(7)	O(2)-Ho(1)-O(5)	143.11(7)
O(8)#1-Ho(1)-N(4)	139.59(6)	O(6)#2-Ho(1)-N(4)	145.21(6)	O(7)#3-Ho(1)-N(4)	80.32(6)
O(1)-Ho(1)-N(4)	80.09(7)	O(2)-Ho(1)-N(4)	73.39(7)	O(5)-Ho(1)-N(4)	75.81(6)
O(8)#1-Ho(1)-O(6)	72.64(6)	O(6)#2-Ho(1)-O(6)	72.42(6)	O(7)#3-Ho(1)-O(6)	72.54(6)
O(1)-Ho(1)-O(6)	152.32(6)	O(2)-Ho(1)-O(6)	140.69(6)	O(5)-Ho(1)-O(6)	51.16(5)
N(4)-Ho(1)-O(6)	123.66(6)	O(8)#1-Ho(1)-N(3)	75.62(7)	O(6)#2-Ho(1)-N(3)	146.90(6)
O(7)#3-Ho(1)-N(3)	135.35(7)	O(1)-Ho(1)-N(3)	72.00(7)	O(2)-Ho(1)-N(3)	115.62(7)
O(5)-Ho(1)-N(3)	66.99(6)	N(4)-Ho(1)-N(3)	64.92(7)	O(6)-Ho(1)-N(3)	103.50(6)
Ho(1)#2-O(6)-Ho(1)	107.59(6)				

4					
Sm(1)-O(1)	2.471(3)	Sm(1)-O(2)	2.495(3)	Sm(1)-O(5)	2.426(3)
Sm(1)-O(6)#2	2.392(3)	Sm(1)-O(7)#3	2.396(3)	Sm(1)-O(8)#1	2.375(3)
Sm(1)-O(8)#3	2.756(4)	Sm(1)-N(3)	2.601(4)	Sm(1)-N(4)	2.592(4)
O(8)#1-Sm(1)-O(6)#2	74.50(11)	O(8)#1-Sm(1)-O(7)#3	127.45(12)	O(6)#2-Sm(1)-O(7)#3	89.64(12)
O(8)#1-Sm(1)-O(5)	77.50(11)	O(6)#2-Sm(1)-O(5)	136.31(11)	O(7)#3-Sm(1)-O(5)	81.48(12)
O(8)#1-Sm(1)-O(1)	88.86(12)	O(6)#2-Sm(1)-O(1)	81.28(11)	O(7)#3-Sm(1)-O(1)	138.66(11)
O(5)-Sm(1)-O(1)	131.05(11)	O(8)#1-Sm(1)-O(2)	77.45(12)	O(6)#2-Sm(1)-O(2)	125.37(12)
O(7)#3-Sm(1)-O(2)	143.52(13)	O(5)-Sm(1)-O(2)	78.95(12)	O(1)-Sm(1)-O(2)	52.13(11)
O(8)#1-Sm(1)-N(4)	143.65(12)	O(6)#2-Sm(1)-N(4)	139.80(12)	O(7)#3-Sm(1)-N(4)	74.79(13)
O(5)-Sm(1)-N(4)	78.63(12)	O(1)-Sm(1)-N(4)	86.53(12)	O(2)-Sm(1)-N(4)	71.36(13)
O(8)#1-Sm(1)-N(3)	147.47(12)	O(6)#2-Sm(1)-N(3)	77.24(12)	O(7)#3-Sm(1)-N(3)	67.53(12)
O(5)-Sm(1)-N(3)	134.96(12)	O(1)-Sm(1)-N(3)	71.12(12)	O(2)-Sm(1)-N(3)	107.04(12)
N(4)-Sm(1)-N(3)	62.58(13)	O(8)#1-Sm(1)-O(8)#3	77.79(12)	O(6)#2-Sm(1)-O(8)#3	72.96(11)
O(7)#3-Sm(1)-O(8)#3	49.69(10)	O(5)-Sm(1)-O(8)#3	68.78(10)	O(1)-Sm(1)-O(8)#3	153.31(11)
O(2)-Sm(1)-O(8)#3	142.73(10)	N(4)-Sm(1)-O(8)#3	117.79(12)	N(3)-Sm(1)-O(8)#3	108.86(11)
Sm(1)#1-O(8)-Sm(1)#4	102.21(12)				
5					
Y(1)-O(1)	2.284(5)	Y(1)-O(3)#3	2.366(5)	Y(1)-O(3)#4	2.496(5)
Y(1)-O(4)#4	2.390(5)	Y(1)-O(5)	2.322(6)	Y(1)-O(6)#2	2.340(5)
Y(1)-O(11)#1	2.212(5)	Y(1)-O(13)	2.335(6)	Y(2)-O(2)	2.242(5)
Y(2)-O(7)	2.290(5)	Y(2)-O(8)#5	2.381(5)	Y(2)-O(9)	2.388(6)
Y(2)-O(10)	2.471(6)	Y(2)-O(12)#1	2.298(5)	Y(2)-O(14)	2.394(5)
Y(2)-O(15)	2.395(6)	O(11)#1-Y(1)-O(1)	82.16(19)	O(11)#1-Y(1)-O(5)	88.1(2)
O(1)-Y(1)-O(5)	77.17(19)	O(11)#1-Y(1)-O(13)	80.9(2)	O(1)-Y(1)-O(13)	74.26(19)
O(5)-Y(1)-O(13)	150.50(16)	O(11)#1-Y(1)-O(6)#2	106.00(19)	O(1)-Y(1)-O(6)#2	142.55(18)
O(5)-Y(1)-O(6)#2	138.27(17)	O(13)-Y(1)-O(6)#2	71.24(18)	O(11)#1-Y(1)-O(3)#3	80.89(17)
O(1)-Y(1)-O(3)#3	145.75(19)	O(5)-Y(1)-O(3)#3	72.74(17)	O(13)-Y(1)-O(3)#3	131.33(17)
O(6)#2-Y(1)-O(3)#3	71.17(19)	O(11)#1-Y(1)-O(4)#4	152.81(17)	O(1)-Y(1)-O(4)#4	73.3(2)
O(5)-Y(1)-O(4)#4	97.5(2)	O(13)-Y(1)-O(4)#4	81.3(2)	O(6)#2-Y(1)-O(4)#4	87.4(2)
O(3)#3-Y(1)-O(4)#4	126.20(17)	O(11)#1-Y(1)-O(3)#4	152.12(17)	O(1)-Y(1)-O(3)#4	111.69(17)
O(5)-Y(1)-O(3)#4	72.5(2)	O(13)-Y(1)-O(3)#4	125.4(2)	O(6)#2-Y(1)-O(3)#4	78.16(17)
O(3)#3-Y(1)-O(3)#4	74.38(17)	O(4)#4-Y(1)-O(3)#4	52.76(16)	O(2)-Y(2)-O(7)	89.2(2)
O(2)-Y(2)-O(12)#1	89.5(2)	O(7)-Y(2)-O(12)#1	156.65(17)	O(2)-Y(2)-O(8)#5	146.18(17)
O(7)-Y(2)-O(8)#5	85.99(19)	O(12)#1-Y(2)-O(8)#5	82.2(2)	O(2)-Y(2)-O(9)	85.9(2)
O(7)-Y(2)-O(9)	132.21(18)	O(12)#1-Y(2)-O(9)	70.90(18)	O(8)#5-Y(2)-O(9)	121.29(17)
O(2)-Y(2)-O(14)	74.63(18)	O(7)-Y(2)-O(14)	77.26(19)	O(12)#1-Y(2)-O(14)	79.93(18)
O(8)#5-Y(2)-O(14)	71.66(17)	O(9)-Y(2)-O(14)	144.97(19)	O(2)-Y(2)-O(15)	147.84(19)
O(7)-Y(2)-O(15)	86.7(2)	O(12)#1-Y(2)-O(15)	106.3(2)	O(8)#5-Y(2)-O(15)	65.27(18)
O(9)-Y(2)-O(15)	73.6(2)	O(14)-Y(2)-O(15)	134.85(18)	O(2)-Y(2)-O(10)	77.23(18)
O(7)-Y(2)-O(10)	79.70(19)	O(12)#1-Y(2)-O(10)	122.63(19)	O(8)#5-Y(2)-O(10)	134.23(18)
O(9)-Y(2)-O(10)	52.86(16)	O(14)-Y(2)-O(10)	143.56(16)	O(15)-Y(2)-O(10)	70.65(18)
Y(1)#6-O(3)-Y(1)#4	105.62(17)				
6					
Tb(1)-O(1)	2.248(3)	Tb(1)-O(5)	2.418(3)	Tb(1)-O(6)	2.528(3)
Tb(1)-O(6)#4	2.392(3)	Tb(1)-O(7)#1	2.311(3)	Tb(1)-O(11)#3	2.368(3)
Tb(1)-O(12)#2	2.365(3)	Tb(1)-O(13)	2.383(3)	Tb(2)-O(2)	2.338(3)
Tb(2)-O(3)#5	2.494(3)	Tb(2)-O(4)#5	2.431(3)	Tb(2)-O(8)#1	2.275(3)
Tb(2)-O(9)	2.400(3)	Tb(2)-O(10)#3	2.318(3)	Tb(2)-O(14)	2.407(3)
Tb(2)-O(15)	2.411(4)	O(1)-Tb(1)-O(7)#1	82.27(12)	O(1)-Tb(1)-O(12)#2	106.86(12)

O(7)#1-Tb(1)-O(12)#2	142.58(12)	O(1)-Tb(1)-O(11)#3	87.88(12)	O(7)#1-Tb(1)-O(11)#3	77.47(11)
O(12)#2-Tb(1)-O(11)#3	137.62(10)	O(1)-Tb(1)-O(13)	80.29(12)	O(7)#1-Tb(1)-O(13)	74.68(12)
O(12)#2-Tb(1)-O(13)	71.46(11)	O(11)#3-Tb(1)-O(13)	150.91(11)	O(1)-Tb(1)-O(6)#4	81.38(11)
O(7)#1-Tb(1)-O(6)#4	146.14(12)	O(12)#2-Tb(1)-O(6)#4	70.93(11)	O(11)#3-Tb(1)-O(6)#4	72.48(11)
O(13)-Tb(1)-O(6)#4	130.74(12)	O(1)-Tb(1)-O(5)	153.10(11)	O(7)#1-Tb(1)-O(5)	73.38(12)
O(12)#2-Tb(1)-O(5)	86.69(12)	O(11)#3-Tb(1)-O(5)	97.64(12)	O(13)-Tb(1)-O(5)	82.35(12)
O(6)#4-Tb(1)-O(5)	125.42(10)	O(1)-Tb(1)-O(6)	152.57(11)	O(7)#1-Tb(1)-O(6)	110.83(11)
O(12)#2-Tb(1)-O(6)	77.82(11)	O(11)#3-Tb(1)-O(6)	72.49(11)	O(13)-Tb(1)-O(6)	125.75(11)
O(6)#4-Tb(1)-O(6)	74.63(11)	O(5)-Tb(1)-O(6)	51.83(10)	O(8)#1-Tb(2)-O(10)#3	88.63(12)
O(8)#1-Tb(2)-O(2)	89.61(11)	O(10)#3-Tb(2)-O(2)	156.30(11)	O(8)#1-Tb(2)-O(9)	145.99(11)
O(10)#3-Tb(2)-O(9)	86.44(11)	O(2)-Tb(2)-O(9)	81.90(11)	O(8)#1-Tb(2)-O(14)	74.12(12)
O(10)#3-Tb(2)-O(14)	77.18(11)	O(2)-Tb(2)-O(14)	79.61(11)	O(9)-Tb(2)-O(14)	71.97(11)
O(8)#1-Tb(2)-O(15)	147.74(13)	O(10)#3-Tb(2)-O(15)	86.24(15)	O(2)-Tb(2)-O(15)	107.20(15)
O(9)-Tb(2)-O(15)	65.39(12)	O(14)-Tb(2)-O(15)	134.97(12)	O(8)#1-Tb(2)-O(4)#5	86.39(13)
O(10)#3-Tb(2)-O(4)#5	132.38(11)	O(2)-Tb(2)-O(4)#5	71.03(11)	O(9)-Tb(2)-O(4)#5	120.93(12)
O(14)-Tb(2)-O(4)#5	144.77(12)	O(15)-Tb(2)-O(4)#5	74.00(14)	O(8)#1-Tb(2)-O(3)#5	77.49(11)
O(10)#3-Tb(2)-O(3)#5	80.15(11)	O(2)-Tb(2)-O(3)#5	122.43(11)	O(9)-Tb(2)-O(3)#5	134.29(11)
O(14)-Tb(2)-O(3)#5	143.78(11)	O(15)-Tb(2)-O(3)#5	70.26(12)	O(4)#5-Tb(2)-O(3)#5	52.55(11)
Tb(1)#4-O(6)-Tb(1)	105.37(11)				
7					
Dy(1)-O(1)	2.234(4)	Dy(1)-O(5)	2.419(4)	Dy(1)-O(6)	2.523(4)
Dy(1)-O(6)#2	2.384(4)	Dy(1)-O(8)#1	2.309(4)	Dy(1)-O(11)	2.356(4)
Dy(1)-O(12)#2	2.366(4)	Dy(1)-O(13)	2.367(4)	Dy(2)-O(2)	2.342(4)
Dy(2)-O(3)#4	2.425(4)	Dy(2)-O(4)#4	2.495(4)	Dy(2)-O(7)#1	2.261(4)
Dy(2)-O(9)	2.315(4)	Dy(2)-O(10)#3	2.389(4)	Dy(2)-O(14)	2.411(4)
Dy(2)-O(15)	2.421(5)	O(1)-Dy(1)-O(8)#1	82.36(15)	O(1)-Dy(1)-O(11)	88.00(16)
O(8)#1-Dy(1)-O(11)	77.07(14)	O(1)-Dy(1)-O(12)#2	106.36(15)	O(8)#1-Dy(1)-O(12)#2	142.76(14)
O(11)-Dy(1)-O(12)#2	137.98(13)	O(1)-Dy(1)-O(13)	80.55(16)	O(8)#1-Dy(1)-O(13)	74.95(15)
O(11)-Dy(1)-O(13)	150.89(13)	O(12)#2-Dy(1)-O(13)	71.12(13)	O(1)-Dy(1)-O(6)#2	81.24(14)
O(8)#1-Dy(1)-O(6)#2	145.89(15)	O(11)-Dy(1)-O(6)#2	72.67(14)	O(12)#2-Dy(1)-O(6)#2	70.96(14)
O(13)-Dy(1)-O(6)#2	130.80(14)	O(1)-Dy(1)-O(5)	152.81(14)	O(8)#1-Dy(1)-O(5)	72.96(15)
O(11)-Dy(1)-O(5)	97.21(16)	O(12)#2-Dy(1)-O(5)	87.51(16)	O(13)-Dy(1)-O(5)	82.16(15)
O(6)#2-Dy(1)-O(5)	125.81(13)	O(1)-Dy(1)-O(6)	152.32(14)	O(8)#1-Dy(1)-O(6)	111.06(14)
O(11)-Dy(1)-O(6)	72.50(14)	O(12)#2-Dy(1)-O(6)	78.04(13)	O(13)-Dy(1)-O(6)	125.61(15)
O(6)#2-Dy(1)-O(6)	74.38(14)	O(5)-Dy(1)-O(6)	52.34(13)	O(7)#1-Dy(2)-O(9)	88.86(16)
O(7)#1-Dy(2)-O(2)	89.60(15)	O(9)-Dy(2)-O(2)	156.68(13)	O(7)#1-Dy(2)-O(10)#3	145.77(14)
O(9)-Dy(2)-O(10)#3	86.27(15)	O(2)-Dy(2)-O(10)#3	81.99(15)	O(7)#1-Dy(2)-O(14)	73.93(14)
O(9)-Dy(2)-O(14)	77.30(14)	O(2)-Dy(2)-O(14)	79.92(14)	O(10)#3-Dy(2)-O(14)	71.94(13)
O(7)#1-Dy(2)-O(15)	147.73(15)	O(9)-Dy(2)-O(15)	85.71(19)	O(2)-Dy(2)-O(15)	107.33(18)
O(10)#3-Dy(2)-O(15)	65.56(15)	O(14)-Dy(2)-O(15)	134.99(15)	O(7)#1-Dy(2)-O(3)#4	86.61(16)
O(9)-Dy(2)-O(3)#4	132.02(14)	O(2)-Dy(2)-O(3)#4	71.07(14)	O(10)#3-Dy(2)-O(3)#4	121.01(15)
O(14)-Dy(2)-O(3)#4	145.09(15)	O(15)-Dy(2)-O(3)#4	73.90(18)	O(7)#1-Dy(2)-O(4)#4	77.72(14)
O(9)-Dy(2)-O(4)#4	79.50(14)	O(2)-Dy(2)-O(4)#4	122.79(14)	O(10)#3-Dy(2)-O(4)#4	134.12(14)
O(14)-Dy(2)-O(4)#4	143.41(14)	O(15)-Dy(2)-O(4)#4	70.01(15)	O(3)#4-Dy(2)-O(4)#4	52.87(13)
Dy(1)#2-O(6)-Dy(1)	105.62(14)				
8					
Ho(1)-O(1)	2.219(3)	Ho(1)-O(5)	2.498(3)	Ho(1)-O(5)#4	2.368(3)
Ho(1)-O(6)	2.400(3)	Ho(1)-O(8)#1	2.286(3)	Ho(1)-O(11)#2	2.336(3)
Ho(1)-O(12)#3	2.340(3)	Ho(1)-O(13)	2.360(3)	Ho(2)-O(2)	2.311(3)
Ho(2)-O(3)#5	2.404(3)	Ho(2)-O(4)#5	2.482(3)	Ho(2)-O(7)#1	2.249(3)

Ho(2)-O(9)	2.375(3)	Ho(2)-O(10)#2	2.291(3)	Ho(2)-O(14)	2.382(3)
Ho(2)-O(15)	2.408(4)	O(1)-Ho(1)-O(8)#1	82.03(11)	O(1)-Ho(1)-O(11)#2	88.01(11)
O(8)#1-Ho(1)-O(11)#2	77.26(11)	O(1)-Ho(1)-O(12)#3	106.30(11)	O(8)#1-Ho(1)-O(12)#3	142.52(11)
O(11)#2-Ho(1)-O(12)#3	138.15(10)	O(1)-Ho(1)-O(13)	80.72(12)	O(8)#1-Ho(1)-O(13)	74.43(11)
O(11)#2-Ho(1)-O(13)	150.69(10)	O(12)#3-Ho(1)-O(13)	71.17(10)	O(1)-Ho(1)-O(5)#4	81.13(11)
O(8)#1-Ho(1)-O(5)#4	145.65(11)	O(11)#2-Ho(1)-O(5)#4	72.44(10)	O(12)#3-Ho(1)-O(5)#4	71.35(11)
O(13)-Ho(1)-O(5)#4	131.32(11)	O(1)-Ho(1)-O(6)	152.76(11)	O(8)#1-Ho(1)-O(6)	73.11(11)
O(11)#2-Ho(1)-O(6)	97.02(11)	O(12)#3-Ho(1)-O(6)	87.69(12)	O(13)-Ho(1)-O(6)	82.01(11)
O(5)#4-Ho(1)-O(6)	125.94(10)	O(1)-Ho(1)-O(5)	152.23(11)	O(8)#1-Ho(1)-O(5)	111.88(10)
O(11)#2-Ho(1)-O(5)	72.76(10)	O(12)#3-Ho(1)-O(5)	77.76(10)	O(13)-Ho(1)-O(5)	125.42(11)
O(5)#4-Ho(1)-O(5)	74.14(10)	O(6)-Ho(1)-O(5)	52.56(10)	O(7)#1-Ho(2)-O(10)#2	89.10(11)
O(7)#1-Ho(2)-O(2)	89.60(11)	O(10)#2-Ho(2)-O(2)	156.62(11)	O(7)#1-Ho(2)-O(9)	145.94(11)
O(10)#2-Ho(2)-O(9)	86.24(11)	O(2)-Ho(2)-O(9)	81.84(10)	O(7)#1-Ho(2)-O(14)	74.12(11)
O(10)#2-Ho(2)-O(14)	77.47(11)	O(2)-Ho(2)-O(14)	79.73(10)	O(9)-Ho(2)-O(14)	71.94(10)
O(7)#1-Ho(2)-O(3)#5	86.26(12)	O(10)#2-Ho(2)-O(3)#5	132.12(10)	O(2)-Ho(2)-O(3)#5	71.05(10)
O(9)-Ho(2)-O(3)#5	121.06(11)	O(14)-Ho(2)-O(3)#5	144.80(11)	O(7)#1-Ho(2)-O(15)	148.01(13)
O(10)#2-Ho(2)-O(15)	85.86(15)	O(2)-Ho(2)-O(15)	106.96(15)	O(9)-Ho(2)-O(15)	65.20(12)
O(14)-Ho(2)-O(15)	134.77(12)	O(3)#5-Ho(2)-O(15)	74.16(14)	O(7)#1-Ho(2)-O(4)#5	77.39(11)
O(10)#2-Ho(2)-O(4)#5	79.39(10)	O(2)-Ho(2)-O(4)#5	122.99(10)	O(9)-Ho(2)-O(4)#5	134.29(10)
O(14)-Ho(2)-O(4)#5	143.26(10)	O(3)#5-Ho(2)-O(4)#5	53.10(10)	O(15)-Ho(2)-O(4)#5	70.63(13)
Ho(1)#4-O(5)-Ho(1)	105.86(10)				

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Lu(1)-O(1)	2.309(3)	Lu(1)-O(2)#3	2.314(3)	Lu(1)-O(5)	2.348(3)
Lu(1)-O(6)	2.503(3)	Lu(1)-O(6)#3	2.333(3)	Lu(1)-O(7)#2	2.254(3)
Lu(1)-O(12)#1	2.186(3)	Lu(1)-O(13)	2.284(3)	Lu(2)-O(3)	2.127(4)
Lu(2)-O(8)#2	2.162(3)	Lu(2)-O(9)	2.198(3)	Lu(2)-O(10)#4	2.181(3)
Lu(2)-O(11)#1	2.209(3)	Lu(2)-O(14)	2.248(3)	O(12)#1-Lu(1)-O(7)#2	83.35(12)
O(12)#1-Lu(1)-O(13)	80.89(14)	O(7)#2-Lu(1)-O(13)	71.61(12)	O(12)#1-Lu(1)-O(1)	96.90(12)
O(7)#2-Lu(1)-O(1)	74.89(11)	O(13)-Lu(1)-O(1)	146.46(12)	O(12)#1-Lu(1)-O(2)#3	96.56(12)
O(7)#2-Lu(1)-O(2)#3	144.75(11)	O(13)-Lu(1)-O(2)#3	73.58(12)	O(1)-Lu(1)-O(2)#3	139.45(10)
O(12)#1-Lu(1)-O(6)#3	78.05(11)	O(7)#2-Lu(1)-O(6)#3	139.10(11)	O(13)-Lu(1)-O(6)#3	138.71(12)
O(1)-Lu(1)-O(6)#3	71.65(11)	O(2)#3-Lu(1)-O(6)#3	74.06(11)	O(12)#1-Lu(1)-O(5)	152.86(11)
O(7)#2-Lu(1)-O(5)	72.37(12)	O(13)-Lu(1)-O(5)	80.09(13)	O(1)-Lu(1)-O(5)	88.48(12)
O(2)#3-Lu(1)-O(5)	96.43(13)	O(6)#3-Lu(1)-O(5)	128.57(10)	O(12)#1-Lu(1)-O(6)	154.07(11)
O(7)#2-Lu(1)-O(6)	115.20(11)	O(13)-Lu(1)-O(6)	121.05(13)	O(1)-Lu(1)-O(6)	72.63(10)
O(2)#3-Lu(1)-O(6)	78.74(10)	O(6)#3-Lu(1)-O(6)	76.14(11)	O(5)-Lu(1)-O(6)	52.53(10)
O(3)-Lu(2)-O(8)#2	88.14(15)	O(3)-Lu(2)-O(10)#4	87.27(15)	O(8)#2-Lu(2)-O(10)#4	166.35(13)
O(3)-Lu(2)-O(9)	96.83(15)	O(8)#2-Lu(2)-O(9)	85.30(13)	O(10)#4-Lu(2)-O(9)	108.01(13)
O(3)-Lu(2)-O(11)#1	176.99(14)	O(8)#2-Lu(2)-O(11)#1	94.65(12)	O(10)#4-Lu(2)-O(11)#1	90.27(13)
O(9)-Lu(2)-O(11)#1	82.28(12)	O(3)-Lu(2)-O(14)	90.67(14)	O(8)#2-Lu(2)-O(14)	83.90(11)
O(10)#4-Lu(2)-O(14)	83.31(12)	O(9)-Lu(2)-O(14)	166.64(12)	O(11)#1-Lu(2)-O(14)	90.77(11)
Lu(1)#3-O(6)-Lu(1)	103.86(11)				

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Y(1)-O(2)	2.310(4)	Y(1)-O(5)#1	2.269(4)	Y(1)-O(6)	2.351(4)
Y(1)-O(7)#2	2.299(4)	Y(1)-O(8)#3	2.329(4)	Y(1)-O(13)	2.452(4)
Y(1)-N(1)	2.557(5)	Y(1)-N(2)	2.533(5)	Y(2)-O(4)	2.175(4)
Y(2)-O(9)	2.363(4)	Y(2)-O(10)	2.551(4)	Y(2)-O(10)#6	2.344(4)
Y(2)-O(11)#5	2.306(4)	Y(2)-O(12)#4	2.305(4)	Y(2)-N(5)	2.529(5)
Y(2)-N(6)	2.549(5)	O(5)#1-Y(1)-O(7)#2	76.35(15)	O(5)#1-Y(1)-O(2)	83.24(14)
O(7)#2-Y(1)-O(2)	82.28(14)	O(5)#1-Y(1)-O(8)#3	79.55(14)	O(7)#2-Y(1)-O(8)#3	123.63(14)

O(2)-Y(1)-O(8)#3	143.53(14)	O(5)#1-Y(1)-O(6)	123.72(13)	O(7)#2-Y(1)-O(6)	77.98(13)
O(2)-Y(1)-O(6)	140.55(14)	O(8)#3-Y(1)-O(6)	74.65(14)	O(5)#1-Y(1)-O(13)	142.80(14)
O(7)#2-Y(1)-O(13)	73.19(14)	O(2)-Y(1)-O(13)	72.05(14)	O(8)#3-Y(1)-O(13)	135.81(14)
O(6)-Y(1)-O(13)	69.67(14)	O(5)#1-Y(1)-N(2)	139.45(16)	O(7)#2-Y(1)-N(2)	144.09(16)
O(2)-Y(1)-N(2)	101.41(15)	O(8)#3-Y(1)-N(2)	73.17(15)	O(6)-Y(1)-N(2)	77.07(15)
O(13)-Y(1)-N(2)	74.14(15)	O(5)#1-Y(1)-N(1)	79.56(16)	O(7)#2-Y(1)-N(1)	146.39(15)
O(2)-Y(1)-N(1)	71.85(15)	O(8)#3-Y(1)-N(1)	73.54(15)	O(6)-Y(1)-N(1)	135.45(15)
O(13)-Y(1)-N(1)	116.60(15)	N(2)-Y(1)-N(1)	64.39(17)	O(4)-Y(2)-O(12)#4	99.12(14)
O(4)-Y(2)-O(11)#5	104.30(14)	O(12)#4-Y(2)-O(11)#5	138.48(13)	O(4)-Y(2)-O(10)#6	81.89(13)
O(12)#4-Y(2)-O(10)#6	73.45(14)	O(11)#5-Y(2)-O(10)#6	76.50(13)	O(4)-Y(2)-O(9)	149.63(14)
O(12)#4-Y(2)-O(9)	96.05(14)	O(11)#5-Y(2)-O(9)	80.45(14)	O(10)#6-Y(2)-O(9)	127.84(13)
O(4)-Y(2)-N(5)	83.45(14)	O(12)#4-Y(2)-N(5)	77.06(16)	O(11)#5-Y(2)-N(5)	138.85(16)
O(10)#6-Y(2)-N(5)	144.34(15)	O(9)-Y(2)-N(5)	74.51(14)	O(4)-Y(2)-N(6)	73.74(14)
O(12)#4-Y(2)-N(6)	141.85(15)	O(11)#5-Y(2)-N(6)	78.33(15)	O(10)#6-Y(2)-N(6)	139.08(14)
O(9)-Y(2)-N(6)	78.07(14)	N(5)-Y(2)-N(6)	64.99(17)	O(4)-Y(2)-O(10)	157.25(13)
O(12)#4-Y(2)-O(10)	74.75(13)	O(11)#5-Y(2)-O(10)	70.38(13)	O(10)#6-Y(2)-O(10)	75.36(13)
O(9)-Y(2)-O(10)	52.85(13)	N(5)-Y(2)-O(10)	115.51(13)	N(6)-Y(2)-O(10)	124.54(13)
Y(2)#6-O(10)-Y(2)	104.63(13)				
11					
Tm(1)-O(1)	2.310(6)	Tm(1)-O(2)	2.339(6)	Tm(1)-O(3)#1	2.208(6)
Tm(1)-O(4)#2	2.222(5)	Tm(1)-O(5)	2.412(7)	Tm(1)-O(6)	2.389(7)
Tm(1)-N(1)	2.475(7)	Tm(1)-N(2)	2.498(6)	O(3)#1-Tm(1)-O(4)#2	94.61(19)
O(3)#1-Tm(1)-O(1)	85.4(2)	O(4)#2-Tm(1)-O(1)	136.3(2)	O(3)#1-Tm(1)-O(2)	87.0(2)
O(4)#2-Tm(1)-O(2)	81.10(19)	O(1)-Tm(1)-O(2)	55.26(19)	O(3)#1-Tm(1)-O(6)	149.5(2)
O(4)#2-Tm(1)-O(6)	92.4(2)	O(1)-Tm(1)-O(6)	109.3(3)	O(2)-Tm(1)-O(6)	123.5(2)
O(3)#1-Tm(1)-O(5)	158.5(2)	O(4)#2-Tm(1)-O(5)	88.5(3)	O(1)-Tm(1)-O(5)	77.8(3)
O(2)-Tm(1)-O(5)	72.5(2)	O(6)-Tm(1)-O(5)	51.2(2)	O(3)#1-Tm(1)-N(1)	81.6(2)
O(4)#2-Tm(1)-N(1)	147.0(2)	O(1)-Tm(1)-N(1)	76.4(2)	O(2)-Tm(1)-N(1)	131.0(2)
O(6)-Tm(1)-N(1)	76.4(2)	O(5)-Tm(1)-N(1)	106.9(3)	O(3)#1-Tm(1)-N(2)	81.2(2)
O(4)#2-Tm(1)-N(2)	80.3(2)	O(1)-Tm(1)-N(2)	142.1(2)	O(2)-Tm(1)-N(2)	157.0(2)
O(6)-Tm(1)-N(2)	70.9(2)	O(5)-Tm(1)-N(2)	120.3(2)	N(1)-Tm(1)-N(2)	66.7(2)
12					
Lu(1)-O(1)	2.329(3)	Lu(1)-O(2)	2.296(4)	Lu(1)-O(3)#1	2.185(3)
Lu(1)-O(4)#2	2.214(3)	Lu(1)-O(5)	2.399(5)	Lu(1)-O(6)	2.380(4)
Lu(1)-N(1)	2.462(4)	Lu(1)-N(2)	2.470(4)	O(3)#1-Lu(1)-O(4)#2	94.55(12)
O(3)#1-Lu(1)-O(2)	86.33(15)	O(4)#2-Lu(1)-O(2)	136.29(12)	O(3)#1-Lu(1)-O(1)	86.82(14)
O(4)#2-Lu(1)-O(1)	80.87(12)	O(2)-Lu(1)-O(1)	55.50(12)	O(3)#1-Lu(1)-O(6)	149.69(14)
O(4)#2-Lu(1)-O(6)	91.88(16)	O(2)-Lu(1)-O(6)	108.88(17)	O(1)-Lu(1)-O(6)	123.46(15)
O(3)#1-Lu(1)-O(5)	158.93(14)	O(4)#2-Lu(1)-O(5)	87.71(17)	O(2)-Lu(1)-O(5)	77.75(17)
O(1)-Lu(1)-O(5)	72.83(15)	O(6)-Lu(1)-O(5)	50.79(15)	O(3)#1-Lu(1)-N(1)	81.95(13)
O(4)#2-Lu(1)-N(1)	147.00(13)	O(2)-Lu(1)-N(1)	76.48(13)	O(1)-Lu(1)-N(1)	131.27(12)
O(6)-Lu(1)-N(1)	76.68(16)	O(5)-Lu(1)-N(1)	107.18(17)	O(3)#1-Lu(1)-N(2)	80.83(13)
O(4)#2-Lu(1)-N(2)	80.16(12)	O(2)-Lu(1)-N(2)	142.43(13)	O(1)-Lu(1)-N(2)	156.40(13)
O(6)-Lu(1)-N(2)	71.14(14)	O(5)-Lu(1)-N(2)	120.14(14)	N(1)-Lu(1)-N(2)	66.87(13)

[a] Symmetry transformations used to generate equivalent atoms: #1 –*x*+4/3, –*y*+5/3, –*z*+2/3; #2 *x*–*y*+1, *x*, –*z*+1; #3 –*x*+*y*+1/3, –*x*+5/3, *z*–1/3 for **1**; #1 –*x*+2/3, –*y*+1/3, –*z*+4/3; #2 *x*–*y*, *x*, –*z*+1; #3 –*x*+*y*+2/3, –*x*+1/3, *z*+1/3 for **2**; #1 *x*–*y*+1/3, *x*–1/3, –*z*+2/3; #2 –*x*+1, –*y*+1, –*z*+1; #3 –*x*+*y*+2/3, –*x*+4/3, *z*+1/3 for **3**; #1 –*x*+2, –*y*+1, –*z*; #2 –*x*+1, –*y*+1, –*z*; #3 *x*–1, *y*, *z*; #4 *x*+1, *y*, *z* for **4**; #1 –*x*+2, –*y*, –*z*+1; #2 –*x*+2, –*y*+1, –*z*+1; #3 *x*+1, *y*, *z*; #4 –*x*+1, –*y*+1, –*z*+1; #5 –*x*+2,

–*y*+1, –*z*; #6 *x*–1, *y*, *z* for **5**; #1 –*x*, –*y*+2, –*z*+2; #2 *x*, *y*, *z*+1; #3 –*x*+1, –*y*+2, –*z*+1; #4 –*x*+1, –*y*+2, –*z*+2; #5 –*x*+1, –*y*+1, –*z*+2 for **6**; #1 –*x*+2, –*y*+1, –*z*+1; #2 –*x*+1, –*y*+1, –*z*+1; #3 –*x*+1, –*y*+1, –*z*+2; #4 –*x*+1, –*y*+2, –*z*+1 for **7**; #1 –*x*, –*y*+2, –*z*+2; #2 –*x*+1, –*y*+2, –*z*+1; #3 *x*, *y*, *z*+1; #4 –*x*+1, –*y*+2, –*z*+2; #5 –*x*+1, –*y*+1, –*z*+2 for **8**; #1 –*x*+1, –*y*+1, –*z*+2; #2 –*x*+1, –*y*, –*z*+1; #3 –*x*+1, –*y*+1, –*z*+1; #4 –*x*+2, –*y*+1, –*z*+2 for **9**; #1 –*x*, –*y*+2, –*z*+1; #2 –*x*–1, –*y*+2, –*z*+1; #3 *x*+1, *y*, *z*; #4 –*x*+1, –*y*+1, –*z*; #5 *x*–1, *y*, *z*; #6 –*x*, –*y*+1, –*z* for **10**; #1 –*x*+1, –*y*+2, –*z*; #2 *x*, *y*–1, *z* for **11**; #1 –*x*+1, –*y*+1, –*z*+2; #2 *x*, *y*–1, *z* for **12**.

Table S3 Hydrogen bonds in crystal packing [Å, °] of **1-10**.

Complexes	D-H…A	*d*(D-H)	*d*(H…A)	*d*(D…A)	∠DHA	Symmetry code
1	O(9)-H(1W)···O(1)	0.85	2. 12	2. 974	179. 5	
	O(3)-H(3)···N(2)	0.82	1. 98	2. 711	148. 0	–*y* + 4/3, *x* – *y* + 2/3, *z* – 1/3
2	O(9)-H(1W) ···O(5)	0.85	2.09	2.937	179.6	
	O(8)-H(8) ···N(1)	0.82	1.87	2.686	174.7	–*y* + 2/3, *x* – *y* + 1/3, *z* + 1/3
3	O(9)-H(1W)···O(1)	0.85	2.12	2.972	179.3	
	O(3)-H(3)···N(2)	0.82	1.88	2.678	165.4	–*y* + 2/3, *x* – *y* + 1/3, *z* + 1/3
4	O(3)-H(5)···N(2)	0.82	1.91	2.712	164.3	-*x*+1, -*y*, -*z*
	O(9)-H(1W)···N(1)	0.85	2.00	2.846	179.3	*x*-1, *y*, *z*
	O(9)-H(2W)···O(10)	0.72	2.31	2.895	139.4	
	O(10)-H(3W)···O(1)	0.85	2.05	2.903	179.0	
5	O(13)-H(1W)···O(6)	0.85	1.87	2.723	180.0	-*x*+2, -*y*+1, -*z*+1
	O(13)-H(2W)···N(3)	0.85	1.90	2.748	179.1	
	O(14)-H(3W)···O(5)	0.85	1.96	2.806	179.6	
	O(14)-H(4W)···O(7)	0.85	2.08	2.925	179.8	
	O(15)-H(5W)···O(16)	0.85	1.86	2.713	179.2	
	O(15)-H(6W)···O(8)	0.85	1.73	2.576	179.7	-*x*+2, -*y*+1, -*z*
	O(16)-H(7W)···N(2)	0.85	1.94	2.788	179.8	*x*, *y*-1, *z*
	O(17)-H(9W)···O(9)	0.85	2.01	2.861	179.9	-*x*+2, -*y*, -*z*+1
	O(17)-H(10W)···O(13)	0.85	2.05	2.902	180.0	
	O(18)-H(12W)···O(17)	0.85	2.22	3.07	180.0	*x*, *y*+1, *z*
	O(19)-H(13W)···O(10)	0.86	2.28	3.14	175.4	*x*, *y*, *z*+1
6	O(13)-H(1W) ···N(1)	0.85	1.93	2.763	165.2	-*x*+1, -*y*+1, -*z*+2
	O(13)-H(2W) ···O(12)	0.85	1.92	2.773	179.7	*x*, *y*, *z*+1
	O(14)-H(3W) ···O(11)	0.85	1.95	2.796	171.3	-*x*+1, -*y*+2, -*z*+1
	O(14)-H(4W) ···O(10)	0.83	2.09	2.844	150.3	
	O(15)-H(5W) ···O(16)	0.85	1.89	2.737	175.3	-*x*+1, -*y*+1, -*z*+1
	O(15)-H(6W) ···O(9)	0.85	1.75	2.599	180.0	

	O(16)-H(7W) ···N(3)	0.85	1.96	2.812	179.9	
	O(17)-H(9W) ···O(4)	0.85	2.00	2.853	179.6	*x*, *y*, *z*–1
	O(17)-H(10W) ···O(13)	0.85	2.03	2.874	179.6	*x*, *y*, *z*–1
	O(18)-H(11W) ···O(17)	0.85	2.23	3.085	180.0	-*x*+1, -*y*+1, -*z*+1
	O(18)-H(12W) ···O(2)	0.85	2.23	3.081	179.9	
	O(19)-H(13W) ···O(3)	0.85	2.20	3.047	178.1	*x*, *y*, *z*–1
7	O(13)-H(2W) ···N(1)	0.57	2.30	2.778	143.9	-*x*+1, -*y*+2, -*z*+1
	O(14)-H(3W) ···O(11)	0.85	1.96	2.808	179.8	
	O(14)-H(4W) ···O(9)	0.85	1.99	2.837	179.8	-*x*+1, -*y*+1, -*z*+2
	O(15)-H(5W) ···O(10)	0.85	1.76	2.605	179.9	-*x*+1, -*y*+1, -*z*+2
	O(15)-H(6W)···O(16)	0.73	2.06	2.729	153.0	
	O(16)-H(7W) ···N(3)	0.85	1.97	2.821	179.9	*x*, *y*+1, *z*
	O(17)-H(9W)···O(3)	0.85	2.02	2.872	179.8	
	O(17)-H(10W)···O(13)	0.83	2.25	2.876	132.0	
	O(18)-H(11W)···O(17)	0.85	2.21	3.061	179.5	-*x*+1, -*y*+2, -*z*+1
	O(19)-H(13W)···O(4)	0.85	2.21	3.060	179.8	*x*, *y*-1, *z*+1
8	O(13)-H(1W)···N(1)	0.84	1.93	2.760	165.1	-*x*+1, -*y*+1, -*z*+2
	O(13)-H(2W)···O(12)	0.85	1.88	2.735	179.7	*x*, *y*, *z*+1
	O(14)-H(3W)···O(10)	0.84	2.11	2.834	143.8	
	O(14)-H(4W)···O(11)	0.85	1.95	2.801	171.7	-*x*+1, -*y*+2, -*z*+1
	O(15)-H(5W)···O(4)	0.85	1.98	2.827	179.6	-*x*+1, -*y*+1, -*z*+2
	O(16)-H(7W)···N(3)	0.85	1.93	2.783	179.6	
	O(16)-H(8W)···O(15)	0.73	2.06	2.742	155.0	-*x*+1, -*y*+1, -*z*+1
	O(17)-H(9W)···O(3)	0.85	2.01	2.857	179.2	*x*, *y*, *z*–1
	O(17)-H(10W)···O(13)	0.85	2.03	2.883	179.6	*x*, *y*, *z*–1
	O(18)-H(11W)···O(17)	0.85	2.19	3.036	179.9	-*x*+1, -*y*+1, -*z*+1
	O(18)-H(12W)···O(2)	0.85	2.19	3.044	179.9	
	O(19)-H(13W) ···O(4)	0.85	2.17	3.023	177.1	*x*, *y*, *z*–1
9	O(13)-H(1W)···O(4)	0.85	1.81	2.658	179.3	*x*-1, *y*, *z*
	O(13)-H(2W)···N(3)	0.85	2.35	3.195	179.5	
	O(14)-H(3W)···O(1)	0.85	1.92	2.774	179.5	
	O(14)-H(4W)···N(1)	0.85	1.87	2.717	179.4	-*x*+2, -*y*+1, -*z*+1
10	O(13)-H(1W) ···O(2)	0.85	1.83	2.683	180.0	*x*+1, *y*, *z*
	O(13)-H(2W)···O(6)	0.85	1.90	2.745	180.0	
	O(14)-H(3W)···O(3)	0.85	2.09	2.938	179.7	*x*+1, *y*, *z*
	O(14)-H(4W) ···N(4)	0.88	2.51	3.089	123.9	-*x*, -*y*+1, -*z*+1

Table S4 Luminescent Data for Complexes **2** and **6.**

complexes	λ_{max}[a] (nm)	assignment	lifetime (ms)	excited/emission (nm)	quantum yield Φ (%)
2	489	$^5D_4 \rightarrow {}^7F_6$			
	544	$^5D_4 \rightarrow {}^7F_5$	1.3	331/544	58
	584	$^5D_4 \rightarrow {}^7F_4$			
	622	$^5D_4 \rightarrow {}^7F_3$			
6	488	$^5D_4 \rightarrow {}^7F_6$			
	542	$^5D_4 \rightarrow {}^7F_5$	1.0	312/542	20
	582	$^5D_4 \rightarrow {}^7F_4$			
	621	$^5D_4 \rightarrow {}^7F_3$			
6 dehydrated	488	$^5D_4 \rightarrow {}^7F_6$			
	542	$^5D_4 \rightarrow {}^7F_5$	1.2	312/542	37
	582	$^5D_4 \rightarrow {}^7F_4$			
	621	$^5D_4 \rightarrow {}^7F_3$			
6 re-hydrated	488	$^5D_4 \rightarrow {}^7F_6$			
	542	$^5D_4 \rightarrow {}^7F_5$	0.8	312/542	18
	582	$^5D_4 \rightarrow {}^7F_4$			
	621	$^5D_4 \rightarrow {}^7F_3$			

[a]EX slit = 0.2 nm, and EM slit = 0.2 nm

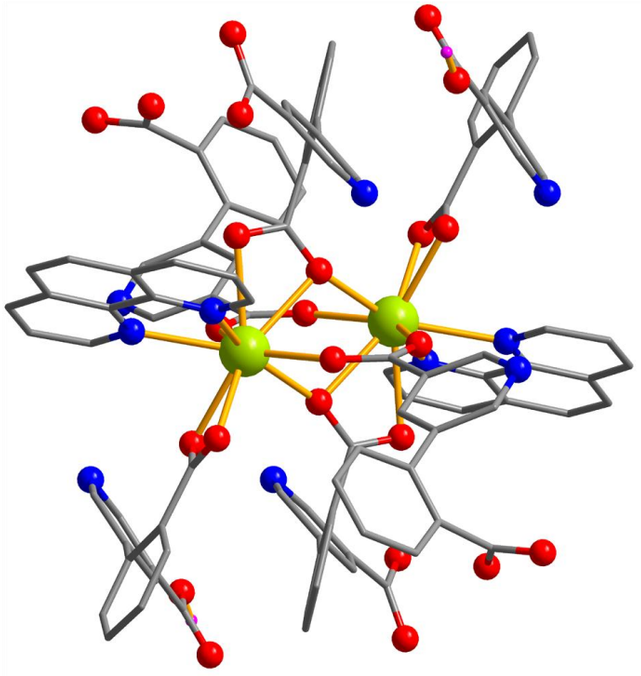

Fig. S1 Dinuclear unit in **1**. The hydrogen atoms are omitted for clarity.

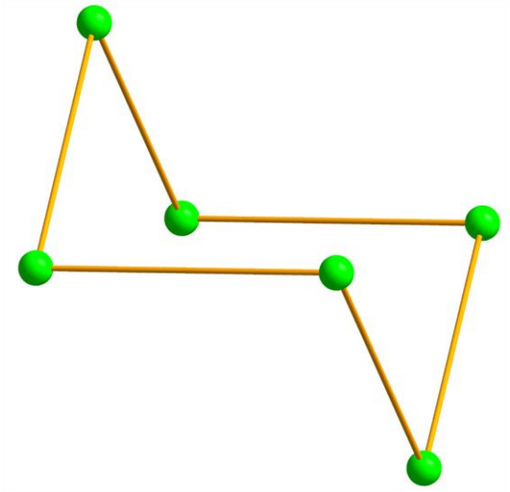

Fig. S2 The chair conformation resembling cyclohexane. The green balls represent the dinuclear units.

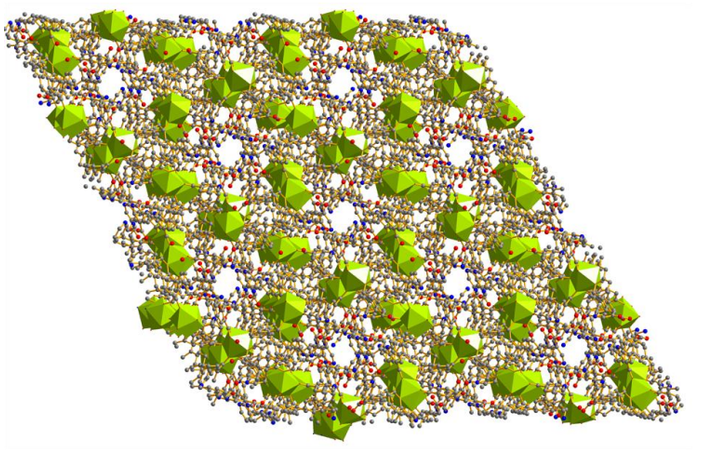

Fig. S3 A perspective of 3D framework along the *c*-axis in **1**.

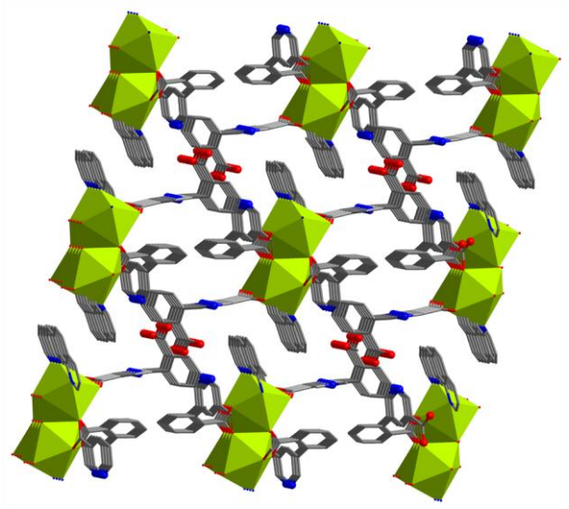

Fig. S4 A perspective of 3D framework along the *b*-axis in **4**.

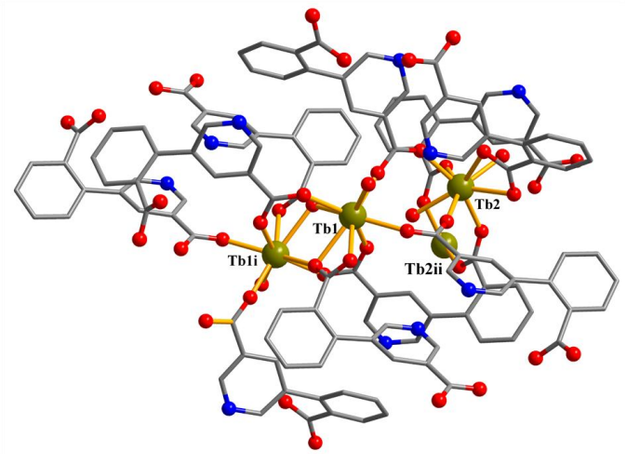

Fig. S5 Tetranuclear unit in **6**. The hydrogen atoms are omitted for clarity.

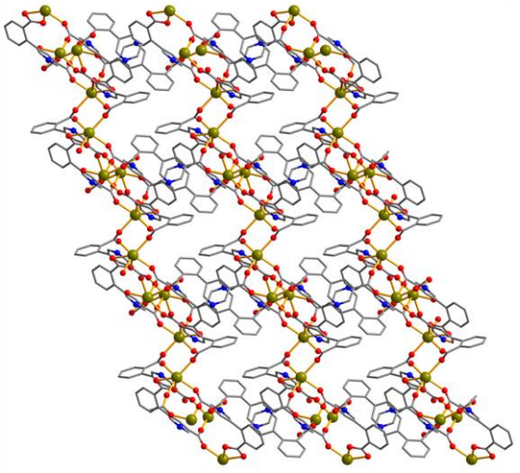

Fig. S6 View of the 3D framework along the *b*-axis in **6**. The hydrogen atoms water molecules are omitted for clarity.

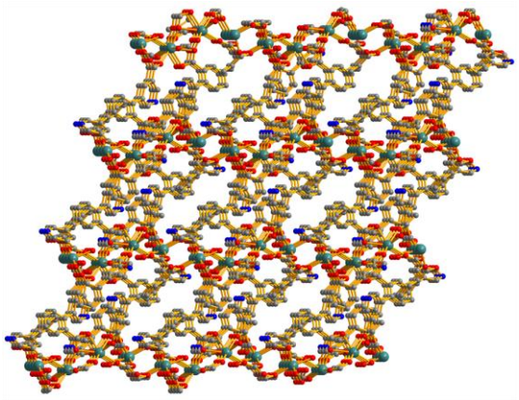

Fig. S7 A perspective of 3D framework in **9** along the *bc* plane.

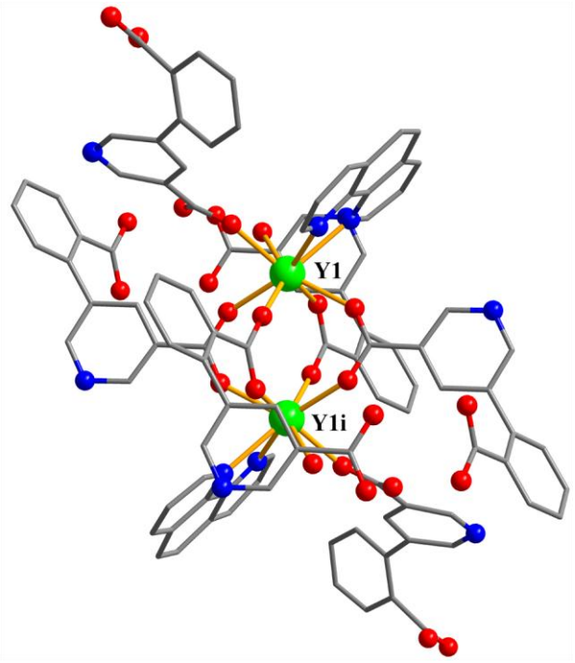

Fig. S8 $Y1_2$ dinuclear unit in **10**. The hydrogen atoms are omitted for clarity. Symmetry code: i = –*x*, –*y* + 2, –*z* + 1.

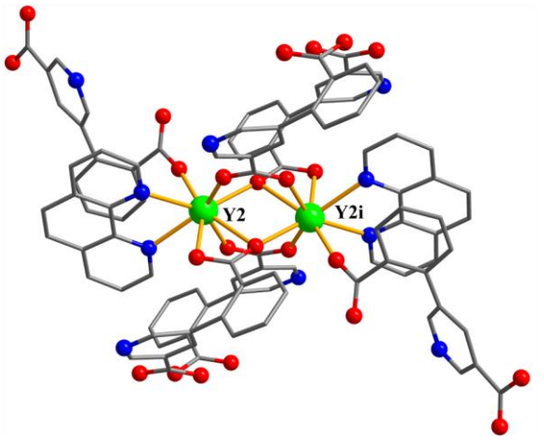

Fig. S9 $Y2_2$ dinuclear unit. The hydrogen atoms are omitted for clarity. Symmetry code: i = –*x*, –*y* + 1, –*z*.

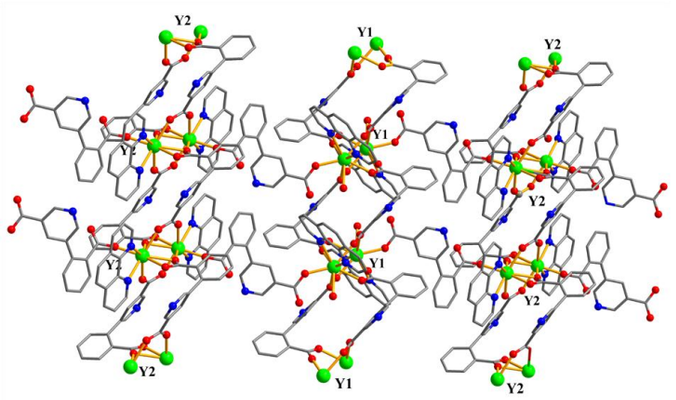

Fig. S10 A perspective of 2D layer along the *ac* plane. The hydrogen atoms are omitted for clarity.

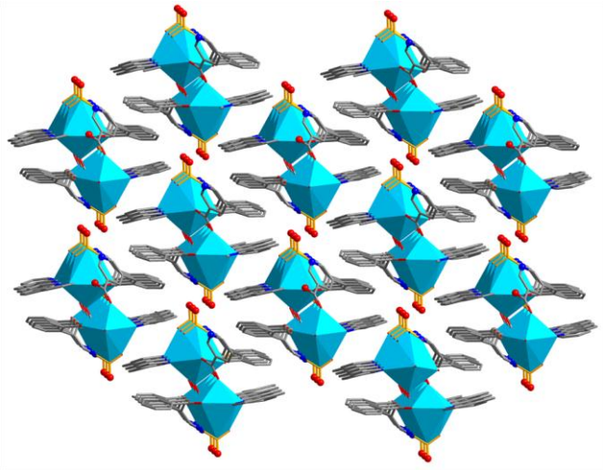

Fig. S11 A perspective of 3D framework in **11** along the *ac* plane. The hydrogen atoms are omitted for clarity.

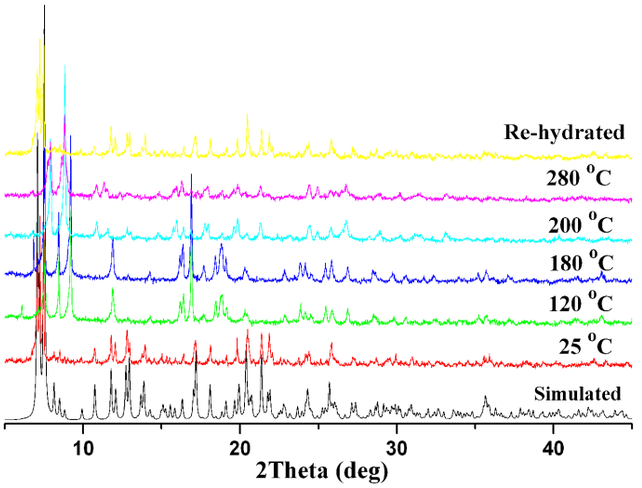

Fig. S12 Results of the temperature-dependent powder XRD study of compound **6**.

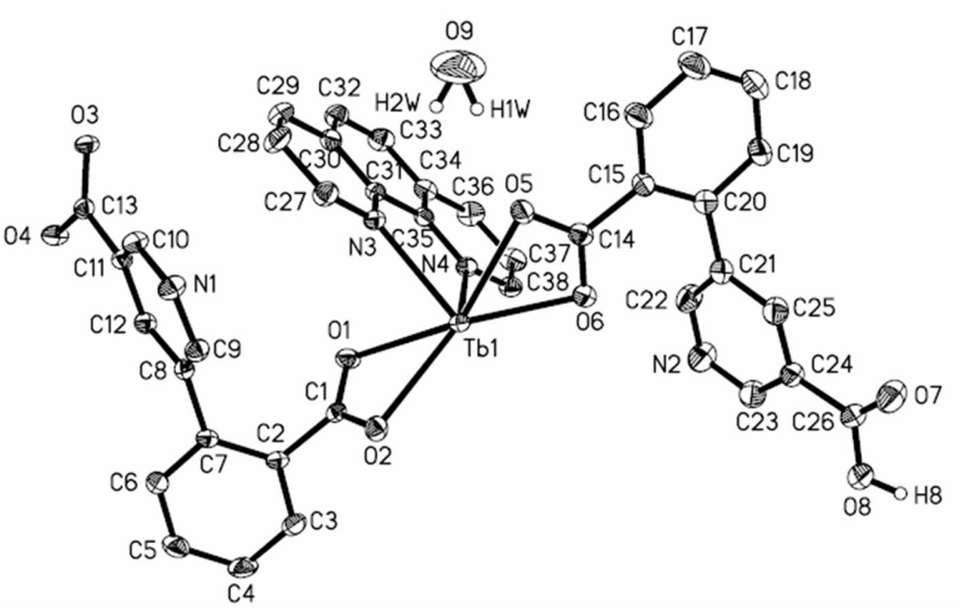

Fig. S13 Drawing of the asymmetric unit of complex **2** (H atoms were omitted for clarity except those bond to O atoms.)

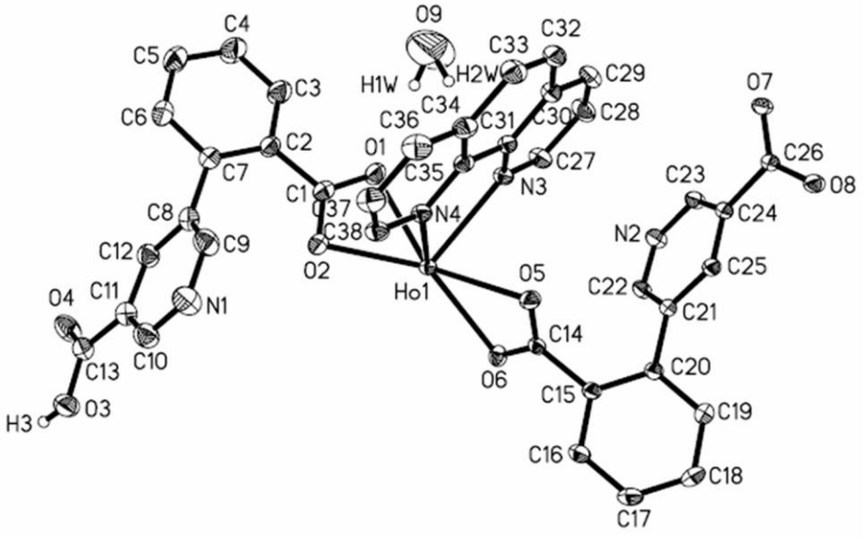

Fig. S14 Drawing of the asymmetric unit of complex **3** (H atoms were omitted for clarity except those bond to O atoms.)

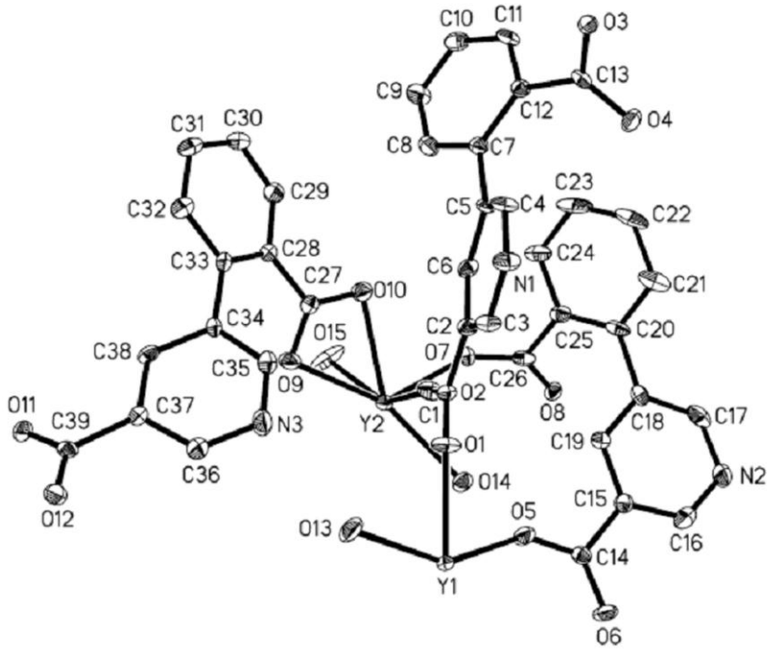

Fig. S15 Drawing of the asymmetric unit of complex **5** (H atoms were omitted for clarity.)

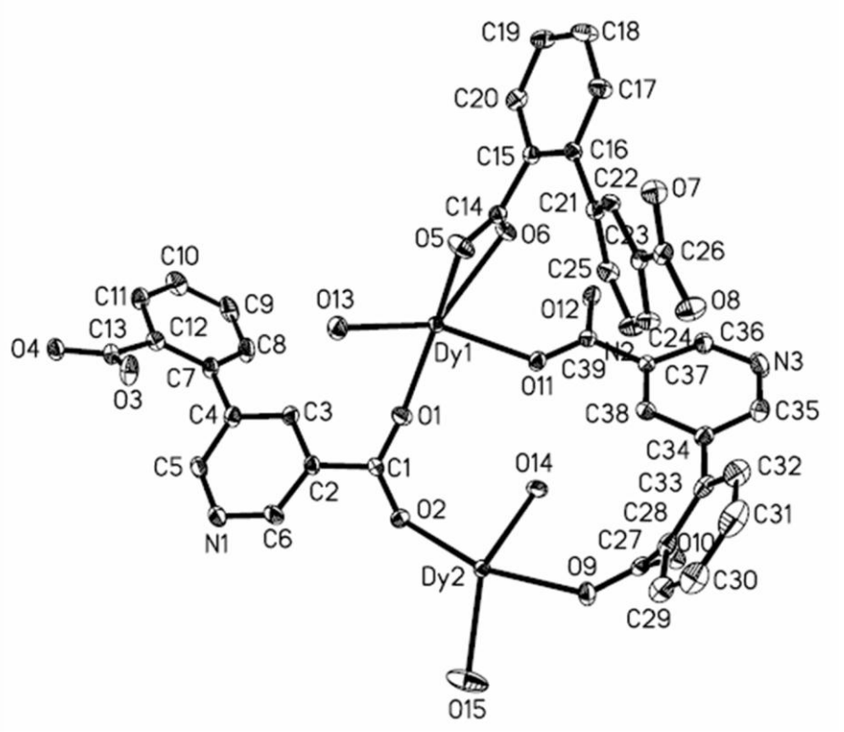

Fig. S16 Drawing of the asymmetric unit of complex **7** (H atoms were omitted for clarity.)

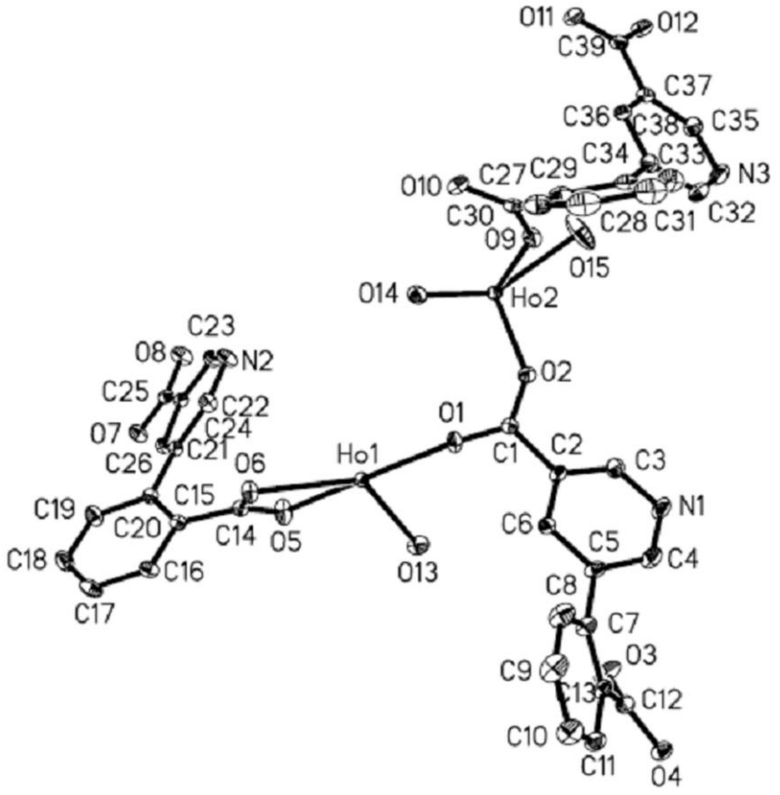

Fig. S17 Drawing of the asymmetric unit of complex **8** (H atoms were omitted for clarity.)

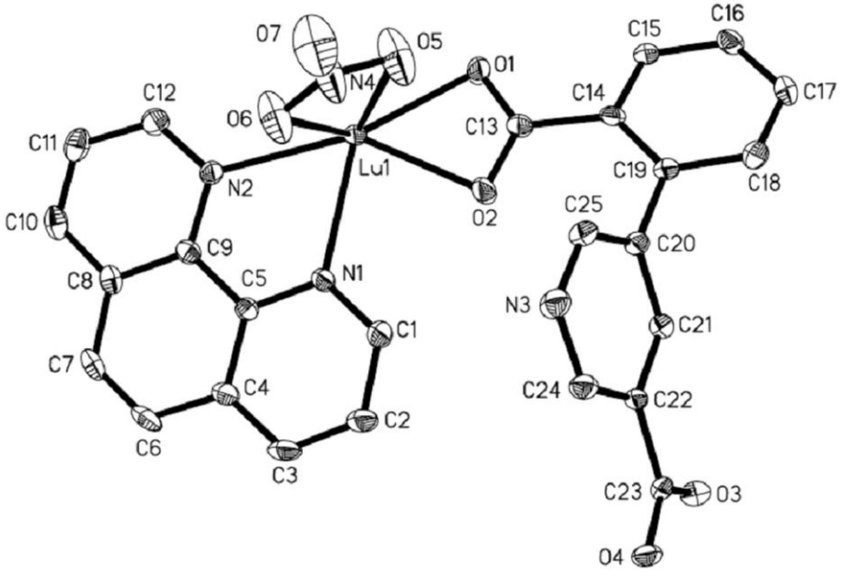

Fig. S18 Drawing of the asymmetric unit of complex **12** (H atoms were omitted for clarity.)