Supporting Information

Construction of four low-dimensional NIR-luminescence-tunable Yb(III) complexes with two different dicarboxylates†

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Contents

Table S1. Crystal data and structure refinement of four compounds **1-4.**

	1	**2**	**3**	**4**
Chemical formula	$C_{12}H_{19}NO_{13}Yb$	$C_{12}H_{13}NO_{10}Yb$	$C_{13}H_{12}NO_{11}Yb$	$C_{26}H_{26}N_2O_{23}Yb_2$
M	558.32	504.27	531.28	1080.57
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a /Å	7.3918(12)	5.9187(6)	7.0405(10)	7.575(4)
b /Å	10.7892(18)	10.3360(11)	10.0943(14)	9.851(5)
c /Å	12.962(2)	14.5617(16)	12.0712(17)	12.196(6)
α /°	84.097(2)	101.2750(10)	104.103(2)	104.315(6)
β /°	81.426(2)	98.8080(10)	101.500(2)	106.679(6)
γ /°	86.601(2)	106.0300	105.459(2)	101.612(6)
V/Å^3	1015.8(3)	819.14(15)	769.20(19)	807.5(7)
Z	2	2	2	1
T /*K*	298(2)	298(2)	298(2)	298(2)
F(000)	544	484	510	520
D_{calcd} / g cm^{-3}	1.825	2.045	2.294	2.222
μ /mm^{-1}	4.665	5.760	6.145	5.858
λ /Å	0.71073	0.71073	0.71073	0.71073
R_{int}	0.0295	0.0204	0.0226	0.0277
data/restraint/parm	3581 / 15 / 254	2894 / 314 / 250	2857 / 0 / 240	2873 / 12 / 260
GOF	1.072	1.087	1.028	1.032
R_1 [$I = 2\sigma(I)$][a]	0.0593	0.0417	0.0388	0.0362
wR_2 [$I = 2\sigma(I)$][b]	0.1482	0.1092	0.0984	0.0809

[a] $R_1 = \Sigma||F_o| - |F_c||/|F_o|$, [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$, where $w = 1/[\sigma^2(F_o^2) + (aP)_2 + bP]$. $P = (F_o^2 + 2F_c^2)/3$.

Table S2. The selected bond lengths and angles for compounds **1-4.**

		1	
Yb(1)-O(7)	2.278(9)	O(7)-Yb(1)-O(4)	93.5(4)
Yb(1)-O(9)	2.279(11)	O(9)-Yb(1)-O(4)	152.3(4)
Yb(1)-O(2)#1	2.287(9)	O(2)#1-Yb(1)-O(4)	132.1(3)
Yb(1)-O(8)	2.287(9)	O(8)-Yb(1)-O(4)	94.6(4)
Yb(1)-O(5)#2	2.357(9)	O(5)#2-Yb(1)-O(4)	76.7(4)
Yb(1)-O(4)	2.368(10)	O(7)-Yb(1)-O(6)	140.6(3)
Yb(1)-O(6)	2.375(8)	O(9)-Yb(1)-O(6)	80.4(4)
Yb(1)-O(3)	2.412(9)	O(2)#1-Yb(1)-O(6)	136.9(3)
O(7)-Yb(1)-O(2)#1	75.8(3)	O(8)-Yb(1)-O(6)	71.0(3)
O(9)-Yb(1)-O(2)#1	75.5(4)	O(5)#2-Yb(1)-O(6)	68.5(3)
O(7)-Yb(1)-O(8)	148.3(3)	O(4)-Yb(1)-O(6)	78.4(3)
O(9)-Yb(1)-O(8)	95.1(5)	O(7)-Yb(1)-O(3)	80.0(3)
O(2)#1-Yb(1)-O(8)	76.1(3)	O(9)-Yb(1)-O(3)	153.4(3)
O(7)-Yb(1)-O(5)#2	72.1(3)	O(2)#1-Yb(1)-O(3)	77.9(3)
O(9)-Yb(1)-O(5)#2	79.2(4)	O(8)-Yb(1)-O(3)	80.2(4)
O(2)#1-Yb(1)-O(5)#2	138.1(3)	O(5)#2-Yb(1)-O(3)	121.1(3)
O(7)-Yb(1)-O(9)	91.7(4)	O(4)-Yb(1)-O(3)	54.1(3)
O(8)-Yb(1)-O(5)#2	139.5(3)	O(6)-Yb(1)-O(3)	121.6(3)
		2	
Yb(1)-O(1)#1	2.283(4)	O(1)#1-Yb(1)-O(5)	139.93(11)
Yb(1)-O(8)	2.344(3)	O(8)-Yb(1)-O(5)	68.63(10)
Yb(1)-O(2)#2	2.344(3)	O(2)#2-Yb(1)-O(5)	75.37(11)
Yb(1)-O(7)	2.355(3)	O(7)-Yb(1)-O(5)	75.48(11)
Yb(1)-O(6)#3	2.364(3)	O(6)#3-Yb(1)-O(5)	68.06(9)
Yb(1)-O(4	2.385(3)	O(4)-Yb(1)-O(5)	129.32(12)
Yb(1)-O(5)	2.398(2)	O(1)#1-Yb(1)-O(3)	78.52(10)
Yb(1)-O(3	2.415(2)	O(8)-Yb(1)-O(3)	137.43(10)
Yb(1)-O(1)#2	3.080(5)	O(2)#2-Yb(1)-O(3)	78.75(9)
O(2)-Yb(1)#2	2.344(3)	O(7)-Yb(1)-O(3)	130.16(10)
O(1)-Yb(1)#4	2.283(4)	O(6)#3-Yb(1)-O(3)	77.92(9)
O(1)-Yb(1)#2	3.080(5)	O(4)-Yb(1)-O(3)	54.26(10)

O(6)-Yb(1)#3	2.364(3)	O(5)-Yb(1)-O(3)	139.26(10)
O(1)#1-Yb(1)-O(8)	72.66(11)	O(1)#1-Yb(1)-C(11)	76.94(14)
O(1)#1-Yb(1)-O(2)#2	109.33(15)	O(8)-Yb(1)-C(11)	149.33(13)
O(8)-Yb(1)-O(2)#2	81.98(11)	O(2)#2-Yb(1)-C(11)	104.70(12)
O(1)#1-Yb(1)-O(7)	88.14(14)	O(7)-Yb(1)-C(11)	103.25(12)
O(8)-Yb(1)-O(7)	79.94(11)	O(6)#3-Yb(1)-C(11)	74.22(12)
O(2)#2-Yb(1)-O(7)	149.71(9)	O(4)-Yb(1)-C(11)	27.25(13)
O(1)#1-Yb(1)-O(6)#3	150.80(11)	O(5)-Yb(1)-C(11)	141.98(13)
O(8)-Yb(1)-O(6)#3	136.39(9)	O(3)-Yb(1)-C(11)	27.02(12)
O(2)#2-Yb(1)-O(6)#3	82.60(11)	O(1)#1-Yb(1)-O(1)#2	65.09(18)
O(7)-Yb(1)-O(6)#3	94.02(12)	O(8)-Yb(1)-O(1)#2	68.29(10)
O(1)#1-Yb(1)-O(4)	79.27(15)	O(2)#2-Yb(1)-O(1)#2	44.26(11)
O(8)-Yb(1)-O(4)	143.47(12)	O(7)-Yb(1)-O(1)#2	142.99(11)
O(2)#2-Yb(1)-O(4)	130.16(11)	O(6)#3-Yb(1)-O(1)#2	121.97(11)
O(7)-Yb(1)-O(4)	76.19(11)	O(4)-Yb(1)-O(1)#2	119.67(10)
O(6)#3-Yb(1)-O(4)	73.04(11)	O(5)-Yb(1)-O(1)#2	108.19(10)
		O(3)-Yb(1)-O(1)#2	71.42(9)
		3	
O(8)-Yb(1)#6	2.397(5)	O(4)-Yb(1)-O(8)#6	76.9(2)
O(6)-C(12)	1.241(9)	O(10)-Yb(1)-O(8)#6	103.2(2)
O(6)-Yb(1)#7	2.400(5)	O(9)-Yb(1)-O(8)#6	149.6(2)
O(9)-Yb(1)	2.388(5)	O(3)#8-Yb(1)-O(5)	121.40(18)
Yb(1)-O(3)#8	2.304(5)	O(4)-Yb(1)-O(5)	70.79(18)
Yb(1)-O(4)	2.321(5)	O(10)-Yb(1)-O(5)	136.79(19)
Yb(1)-O(10)	2.369(5)	O(9)-Yb(1)-O(5)	71.89(19)
Yb(1)-O(8)#6	2.397(5)	O(8)#6-Yb(1)-O(5)	83.97(18)
Yb(1)-O(5)	2.398(5)	O(3)#8-Yb(1)-O(6)#7	139.55(18)
Yb(1)-O(6)#7	2.400(5)	O(4)-Yb(1)-O(6)#7	130.96(18)
Yb(1)-O(7)	2.406(5)	O(10)-Yb(1)-O(6)#7	73.53(19)
O(4)-Yb(1)#8	2.297(6)	O(9)-Yb(1)-O(6)#7	79.8(2)
O(3)-Yb(1)#8	2.304(5)	O(8)#6-Yb(1)-O(6)#7	73.93(19)
O(8)-Yb(1)-O(6)	84.3(2)	O(5)-Yb(1)-O(6)#7	67.69(17)
O(3)#8-Yb(1)-O(4)	84.94(19)	O(3)#8-Yb(1)-O(7)	75.68(19)

O(3)#8-Yb(1)-O(10)	78.3(2)	O(4)-Yb(1)-O(7)	78.4(2)
O(4)-Yb(1)-O(10)	152.4(2)	O(10)-Yb(1)-O(7)	76.3(2)
O(3)#8-Yb(1)-O(9)	68.49(19)	O(9)-Yb(1)-O(7)	141.67(19)
O(4)-Yb(1)-O(9)	110.7(2)	O(8)#6-Yb(1)-O(7)	67.91(18)
O(10)-Yb(1)-O(9)	83.4(2)	O(5)-Yb(1)-O(7)	142.20(18)
O(3)#8-Yb(1)-O(8)#6	141.78(18)	O(6)#7-Yb(1)-O(7)	123.4(2)
		4	
Yb(1)-O(4)#8	2.272(5)	O(3)-Yb(1)-O(7)	139.40(16)
Yb(1)-O(1)	2.291(5)	O(4)#8-Yb(1)-O(5)	135.92(16)
Yb(1)-O(9)	2.312(5)	O(1)-Yb(1)-O(5)	73.45(16)
Yb(1)-O(3)	2.343(5)	O(9)-Yb(1)-O(5)	82.53(18)
Yb(1)-O(7)	2.352(5)	O(3)-Yb(1)-O(5)	139.05(16)
Yb(1)-O(5)	2.373(5)	O(7)-Yb(1)-O(5)	74.49(17)
Yb(1)-O(8)#9	2.395(5)	O(4)#8-Yb(1)-O(8)#9	82.21(18)
Yb(1)-O(6)#10	2.411(5)	O(1)-Yb(1)-O(8)#9	75.73(18)
O(4)-Yb(1)#8	2.272(5)	O(9)-Yb(1)-O(8)#9	143.33(17)
O(6)-Yb(1)#10	2.411(5)	O(3)-Yb(1)-O(8)#9	73.12(16)
O(8)-Yb(1)#9	2.395(5)	O(7)-Yb(1)-O(8)#9	67.97(15)
O(4)#8-Yb(1)-O(1)	150.32(17)	O(5)-Yb(1)-O(8)#9	121.45(17)
O(4)#8-Yb(1)-O(9)	99.5(2)	O(4)#8-Yb(1)-O(6)#10	70.62(16)
O(1)-Yb(1)-O(9)	87.04(19)	O(1)-Yb(1)-O(6)#10	138.44(17)
O(4)#8-Yb(1)-O(3)	80.40(17)	O(9)-Yb(1)-O(6)#0	73.85(18)
O(1)-Yb(1)-O(3)	74.39(17)	O(3)-Yb(1)-O(6)#0	129.37(17)
O(9)-Yb(1)-O(3)	71.12(17)	O(7)-Yb(1)-O(6)#10	77.88(17)
O(4)#8-Yb(1)-O(7)	83.3(2)	O(5)-Yb(1)-O(6)#10	67.79(16)
O(1)-Yb(1)-O(7)	105.95(18)	O(8)#9-Yb(1)-O(6)#10	138.42(17)
O(9)-Yb(1)-O(7)	148.69(17)		

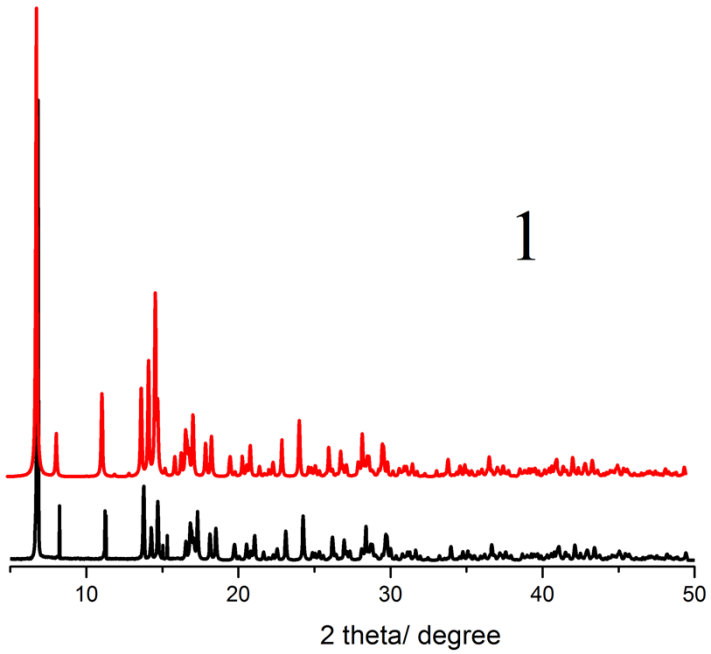
Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y+1,-z+1; #2 -x+1,-y+2,-z+1; #3 x+1,y,z; #4 -x+1,-y+2,-z+1; #5 -x+2,-y+3,-z+1; #6 -x,-y+1,-z+1; #7 -x+1,-y+2,-z+1; #8 -x+1,-y+1,-z; #9 -x,-y+1,-z; #10 -x,-y,-z.

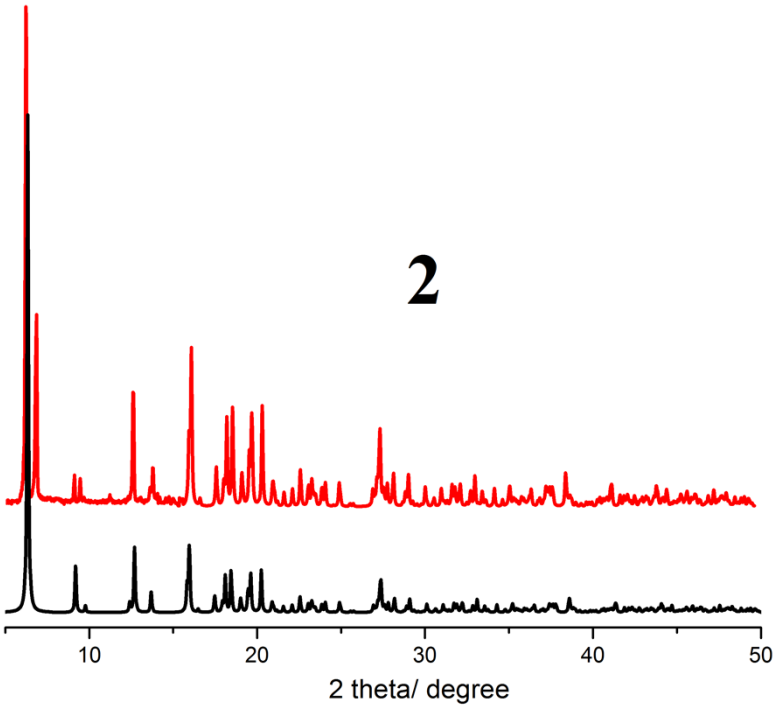
Table S3. Hydrogen bond parameters of compounds **1-4**.

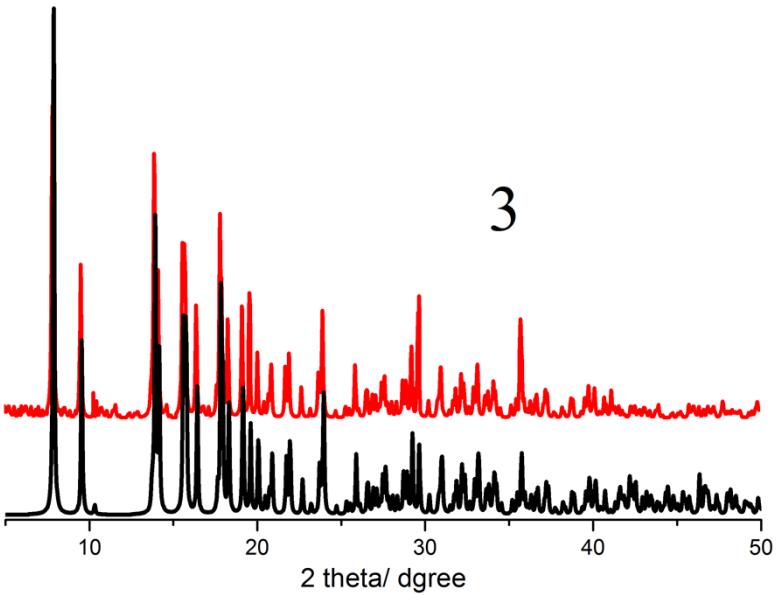
D-H···A	d (D-H) (Å)	d (H···A) (Å)	d (D···A) (Å)	∠ DHA (°)
		1		
O(7)-H(7A)...O(10)	0.85	1.92	2.732(14)	160.1
O(7)-H(7B)...O(1)#3	0.85	2.04	2.709(13)	134.3
O(8)-H(8A)...O(6)#4	0.85	2.31	2.754(13)	113.1
O(8)-H(8B)...O(1)#1	0.85	1.80	2.630(13)	165.3
O(9)-H(9A)...O(12)#5	0.86	2.00	2.72(2)	141.0
O(12)-H(12A)...O(4)#3	0.85	1.98	2.80(2)	163.2
O(13)-H(13B)...O(11)#5	0.85	2.01	2.71(3)	138.2
O(13)-H(13A)...O(11)#6	0.85	2.11	2.95(3)	165.9
O(10)-H(10A)...O(3)#1	0.98(19)	2.32(19)	2.989(16)	125(14)
O(11)-H(11A)...N(1)	0.85	2.00	2.822(16)	161.6
O(11)-H(11B)...O(9)#1	0.85	1.89	2.701(17)	159.9
		2		
O(7)-H(7B)…O(6) #6	0.85	2.05	2.867(9)	160.00
O(7)-H7C…O(10) #7	0.85	1.94	2.789(16)	167.00
O(8)-H(8B)…O(10)#8	0.85	2.55	3.231(16)	137.00
O(8)-H(8C)…O(3)#7	0.85	2.3700	3.168(4)	155.00
O(8)…H(8C)…O(3) #8	0.85	2.37	2.854(4)	116.00
		3		
O(11)-H(11A)...O(5)#12	0.85	2.12	2.9459)	163.00
O(10)-H(10A)...O(1)#11	0.85	2.01	2.850(9)	170.00
O(9)-H(9B)...O(11)#10	0.85	1.97	2.665(9)	138.00
O(9)-H(9A)...O(1)#11	0.85	2.31	3.009(9)	139.00
O(11)-H(11B)...O(8)	0.85	2.01	2.850(10)	170.00
C(3)-H(3)...O(4)	0.93	2.46	2.772(9)	100.00
C(3)-H(3) ... O(5)	0.93	2.26	3.168(9)	167.00
C(8)-H8(3) O(11)	0.93	2.58	3.274(10)	132.00
		4		
O(10)-H(10A)...O(11)	0.849(11)	2.19(8)	2.930(7)	146(12)
O(9)-H(9B)...O(12)#15	0.84	1.85	2.662(7)	161.1
O(10)-H(10B)...O(5)#16	0.84(10)	1.98(4)	2.799(8)	161(12)
O(12)-H(12A)...O(9)#15	0.850(10)	2.31(5)	3.059(9)	147(9)
O(12)-H(12B)...O(7)#14	0.849(10)	1.98(2)	2.824(8)	169(7)
N(1)-H(1)...O(2)#17	0.86	2.00	2.797(8)	154.6
O(9)-H(9A)...O(10)	0.92	1.86	2.720(8)	153.9

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y+1,-z+1; #2 -x+2,-y,-z+2; #3 x,y+1,z; #4 -x+2,-y+2,-z+1; #5 -x+1,-y+1,-z+1; #6 3-x,3-y,1-z; #7 1+x,1+y,z; #8 2-x,2-y,1-z; #9 -1+x,y,z; #10 -x,-y+2,-z+1; #11 -x+1,-y+2,-z+1; #12 x+1,y,z; #13 -x+1,-y+1,-z+1; #14 3-x,-y,-z; #15 -x+1,-y,-z;#16 x+1,y,z; #17 -x+1,-y+1,-z+1; #18 -x+2,-y+1,-z+1.

Figure S1



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10
20
30
40
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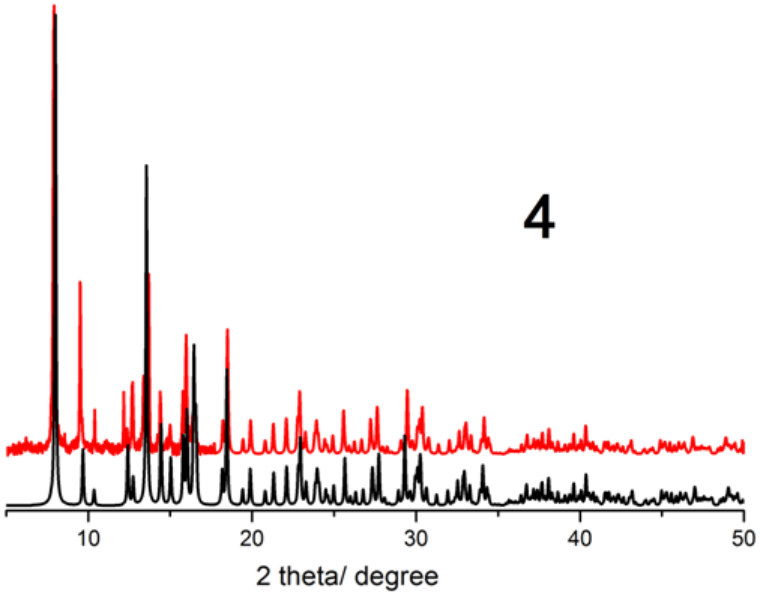
2 theta/ dgree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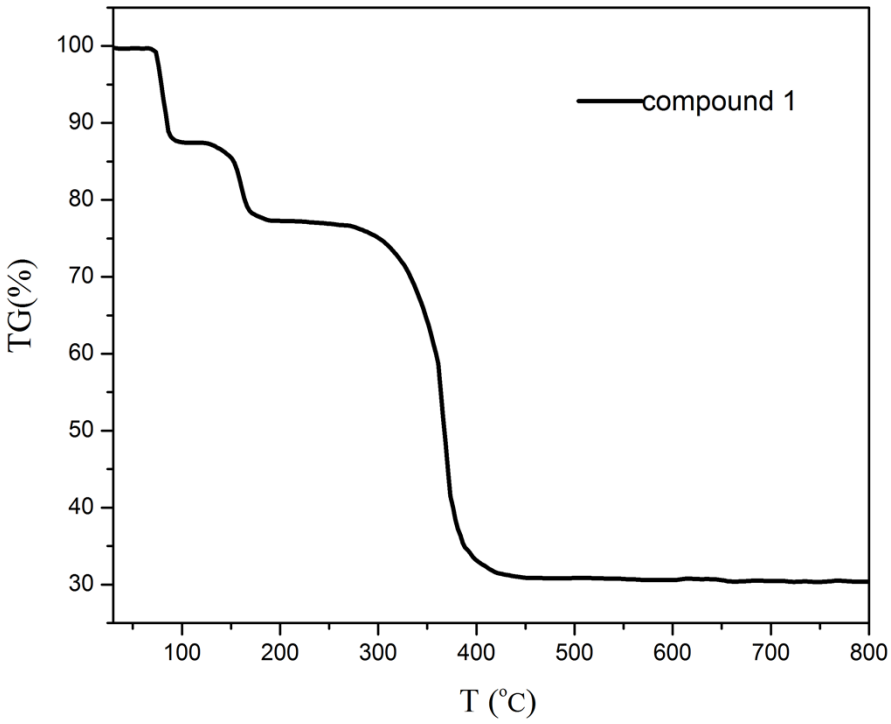
10
20
30
40
50
2 theta/ degree

Figure S2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T (°C)
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80
70
60
50
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30
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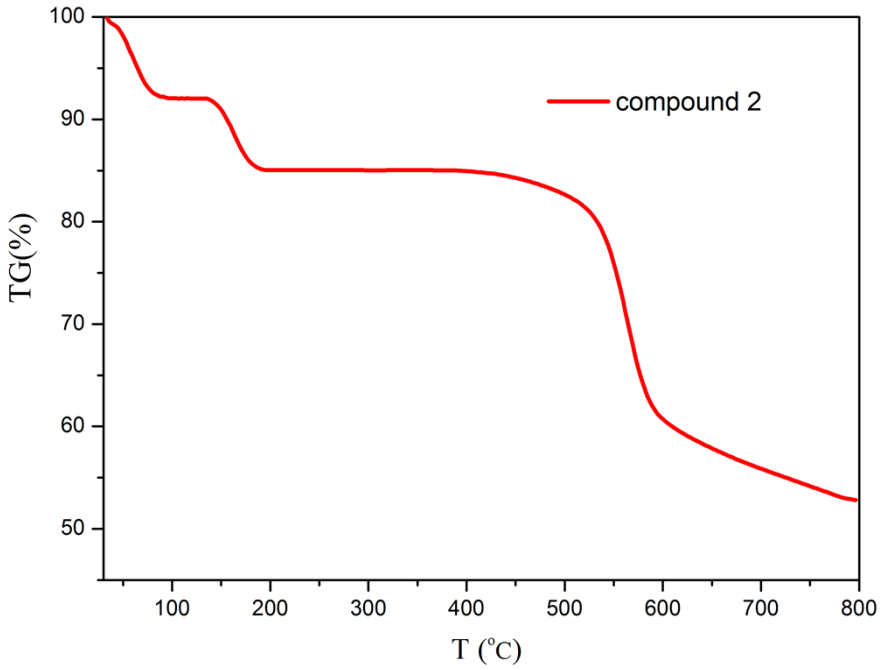
700
800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T (°C)
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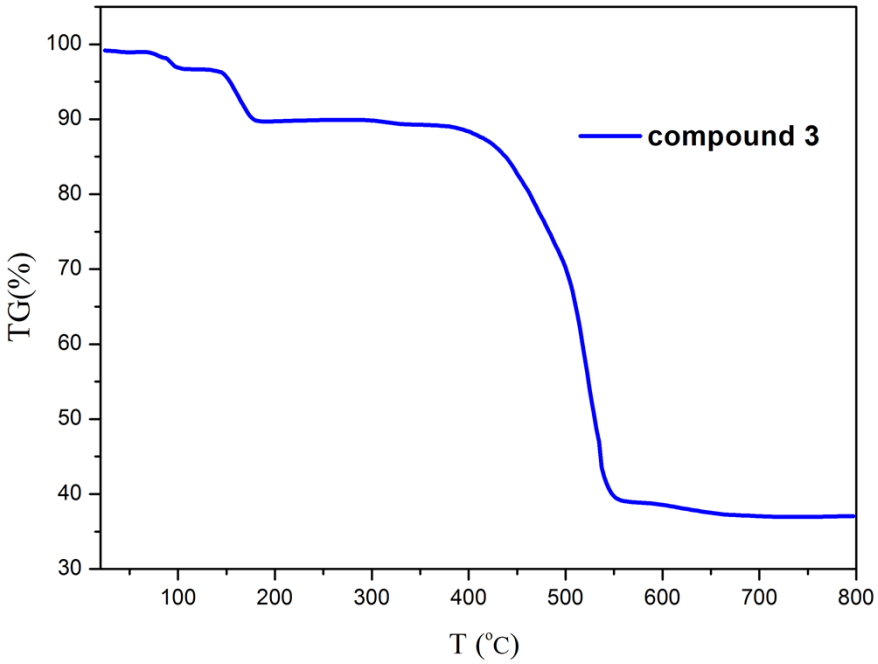
compound 3
TG(%)
T (°C)
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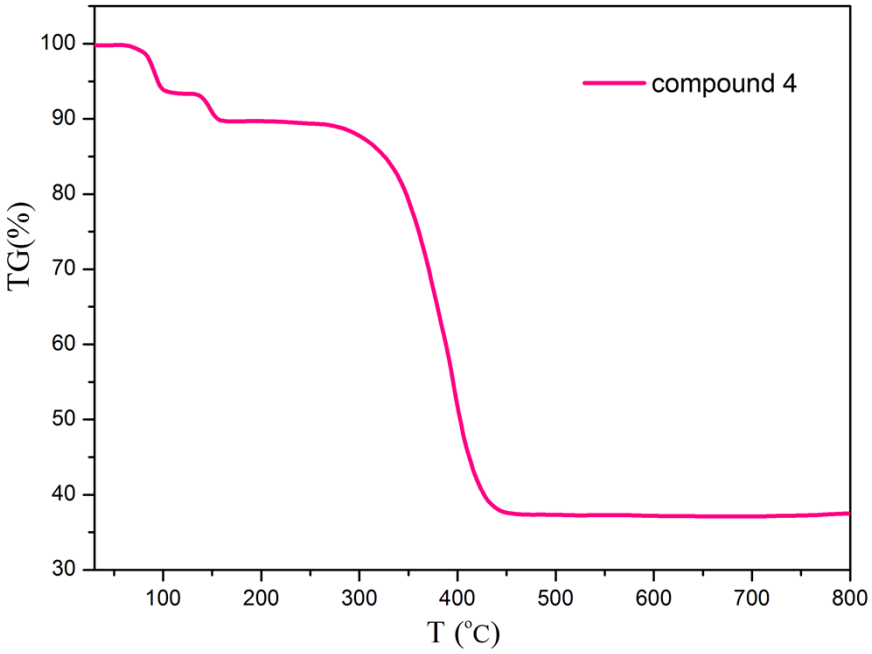
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TG(%)
T (°C)
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800

Figure S3.

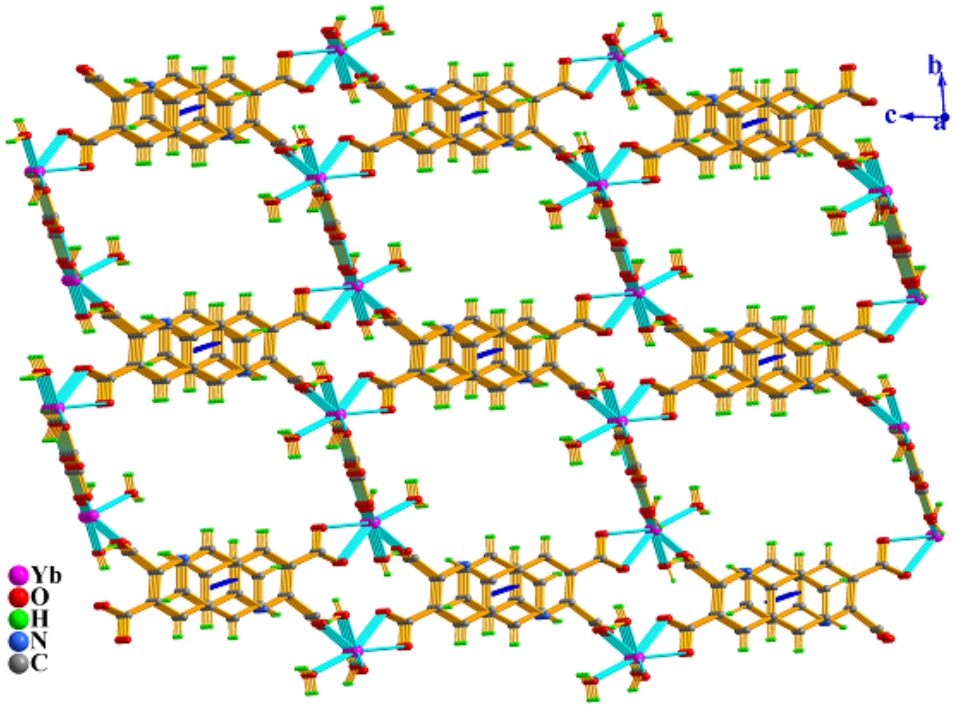

Figure S4.

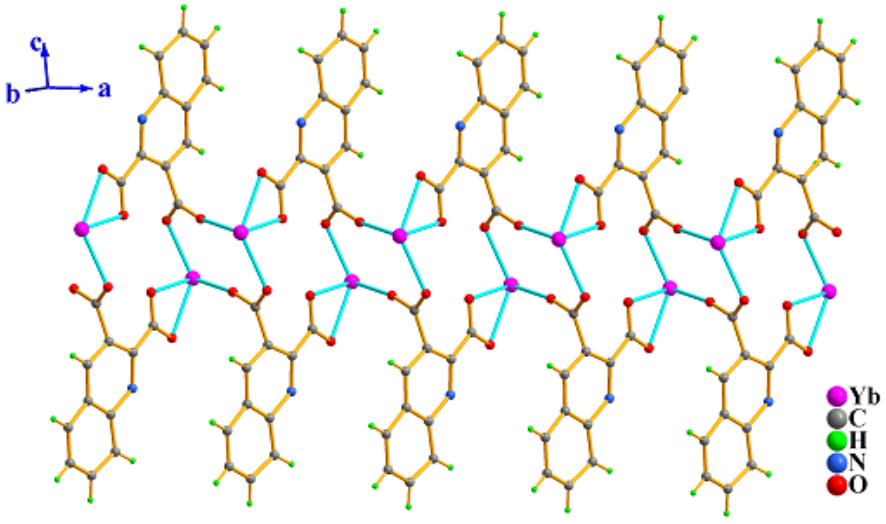

Figure S5.

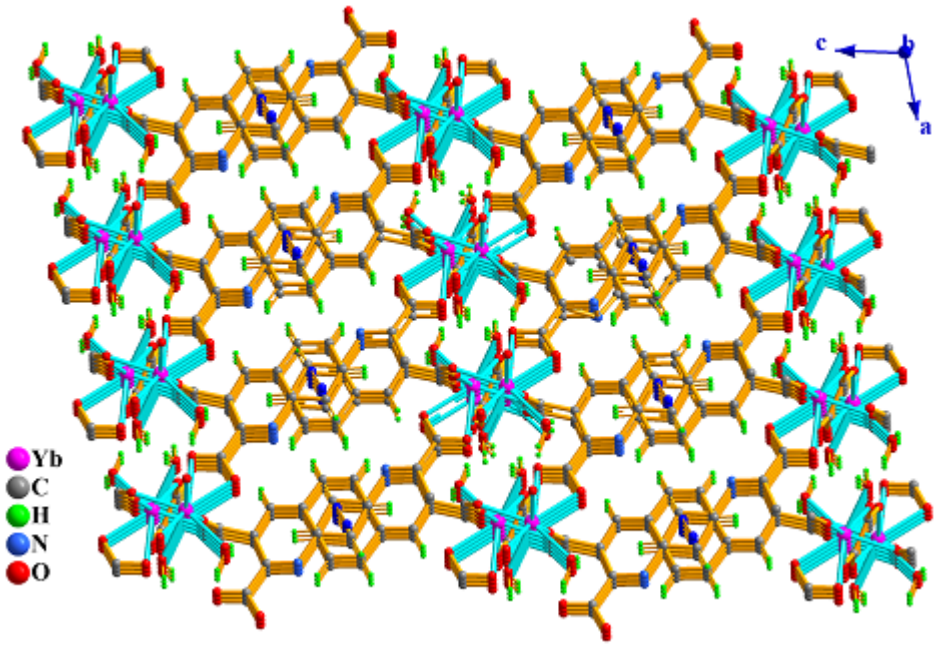

Figure S6.

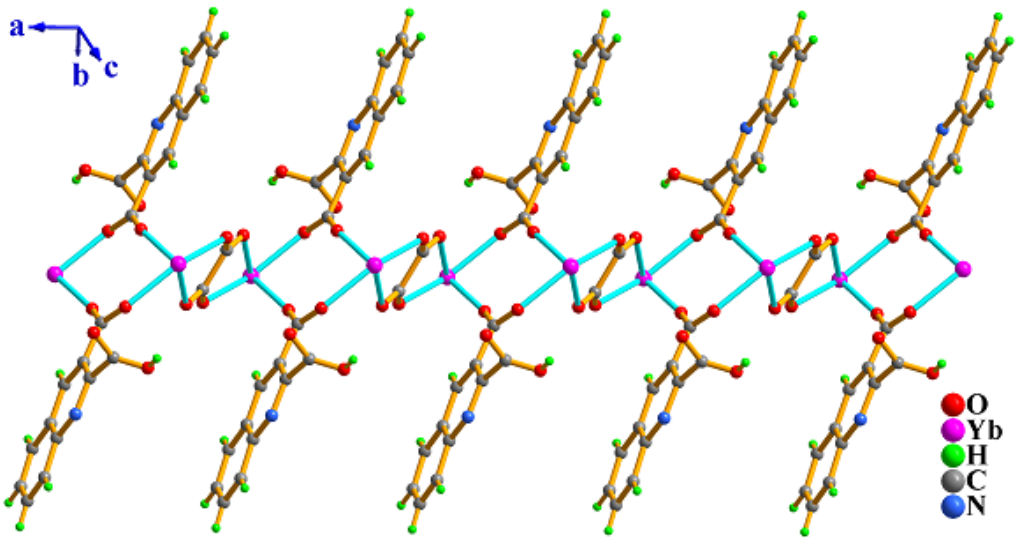

Figure S7.

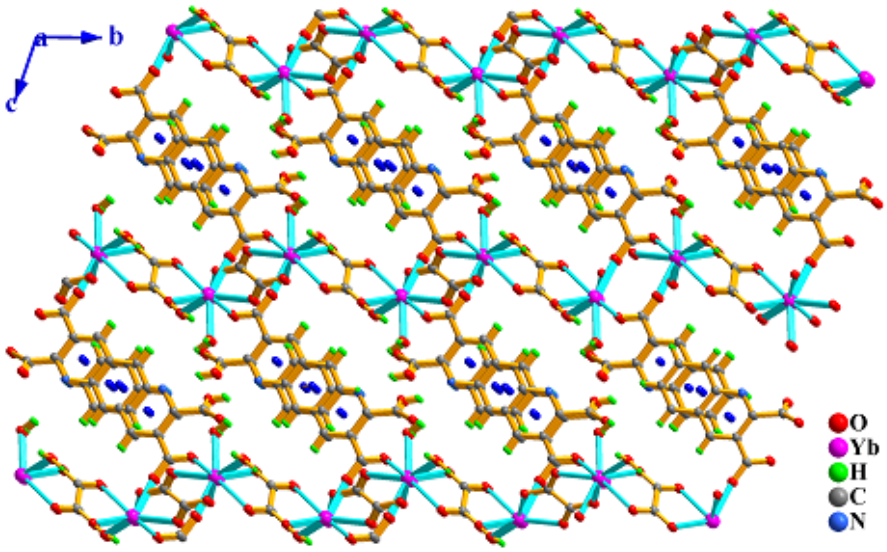

Figure S8.

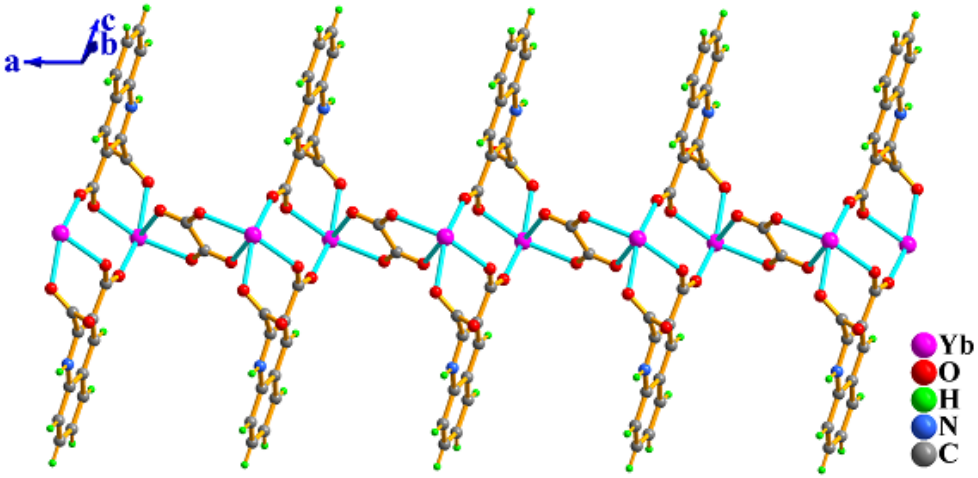

Figure S9.