Supporting Information

Magnetic Properties and Photoluminescence of Lanthanide Coordination Polymers Constructed with Conformation-Flexible Cyclohexane-Tetracarboxylate Ligands

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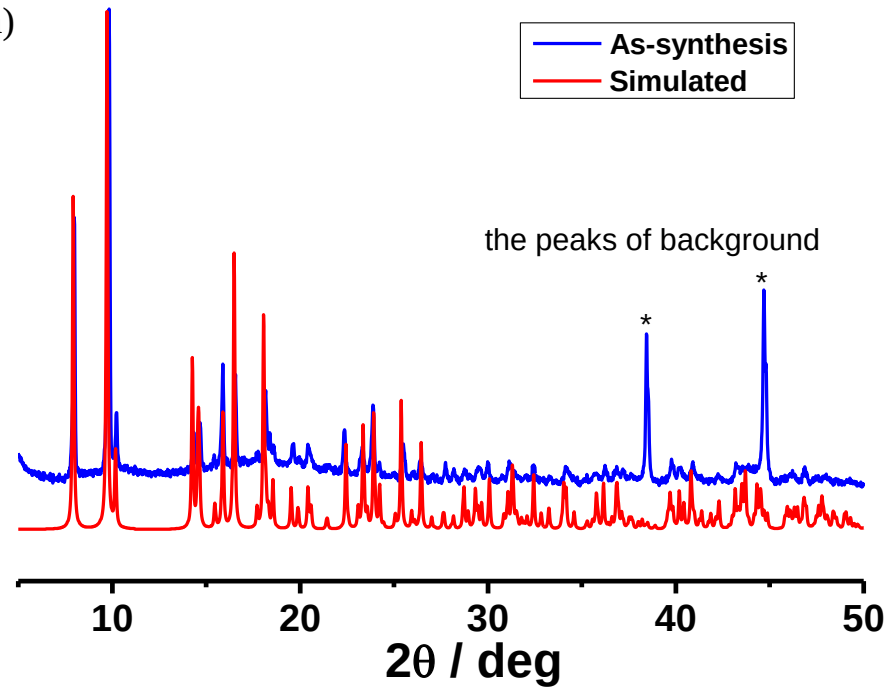
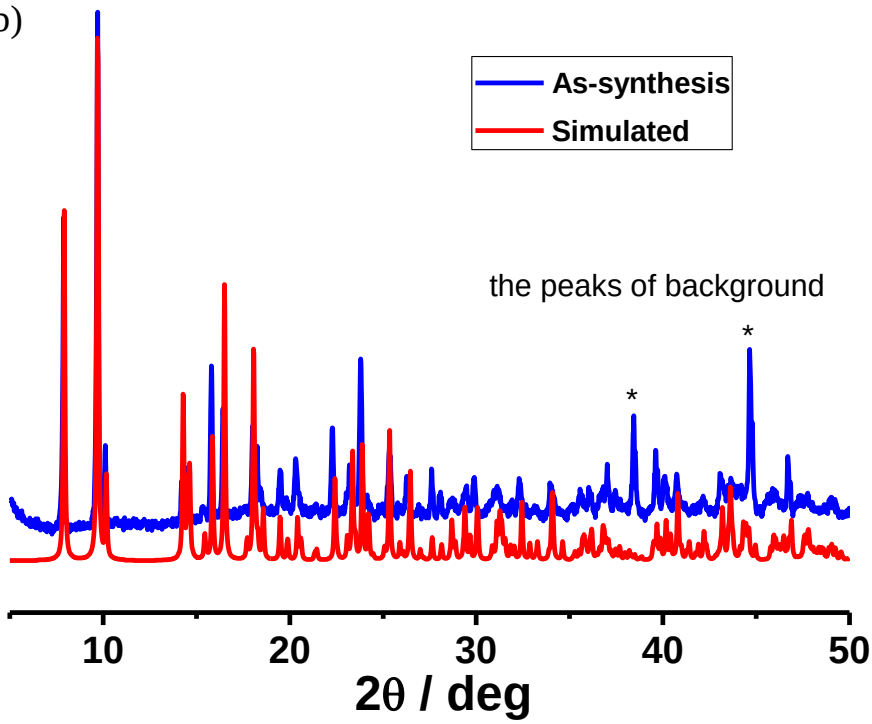
(a)


As-synthesis
Simulated
the peaks of background
*
*
10
20
30
40
50
2θ / deg

(b)


As-synthesis
Simulated
the peaks of background
*
*
10
20
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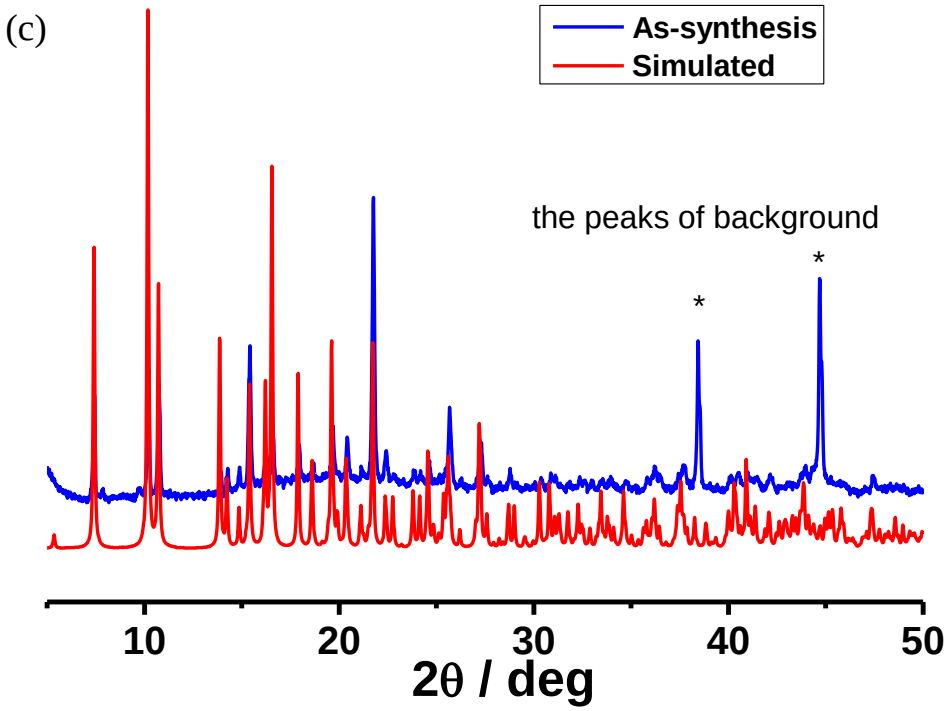
40
50
2θ / deg



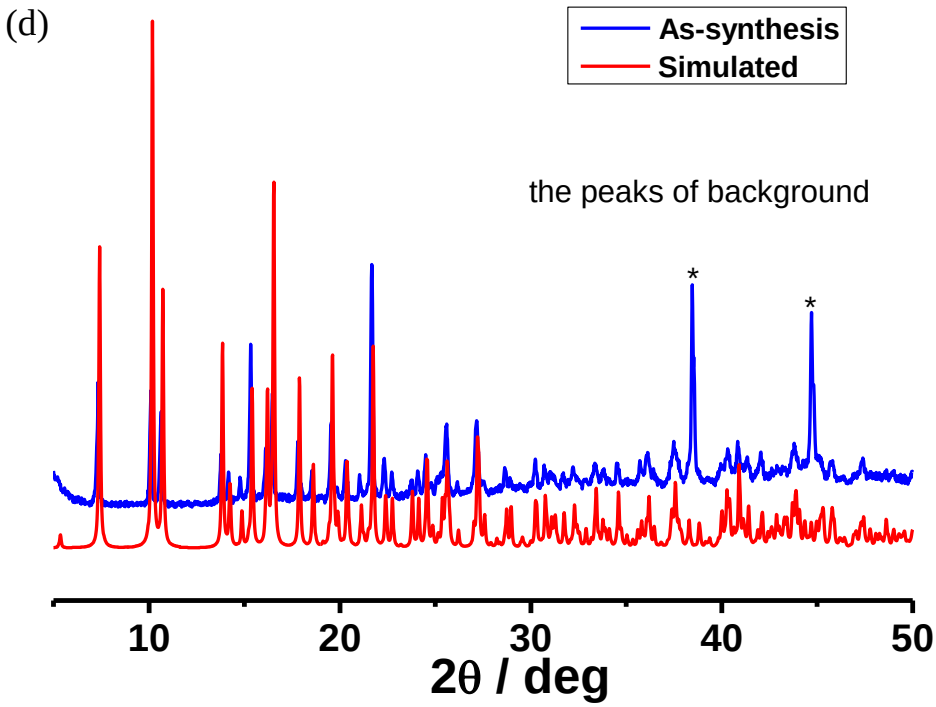


Figure S1. The experimental and simulated PXRD data for **1**(a), **2**(b)**, 3**(c) and **4**(d).

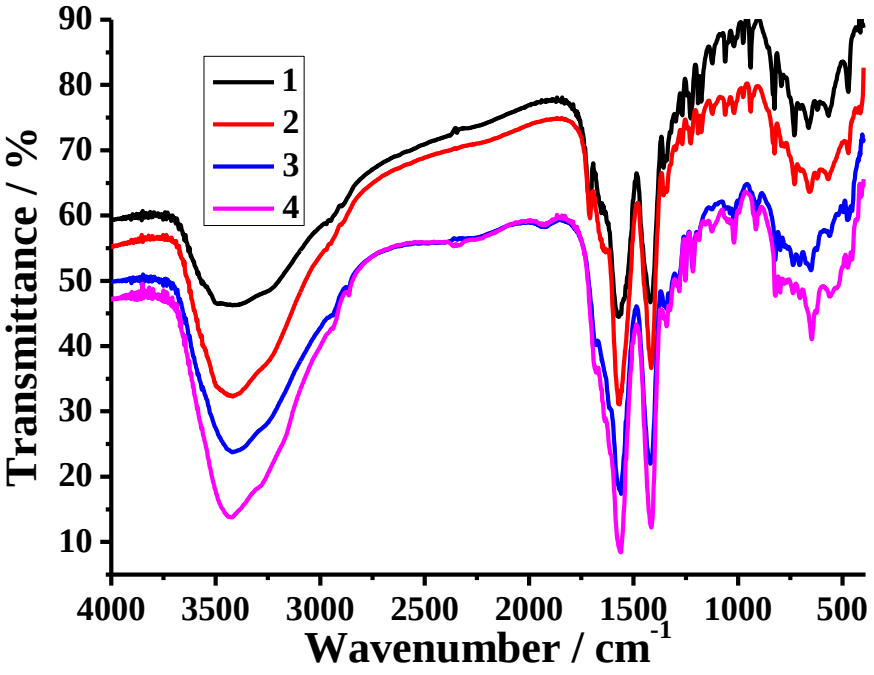
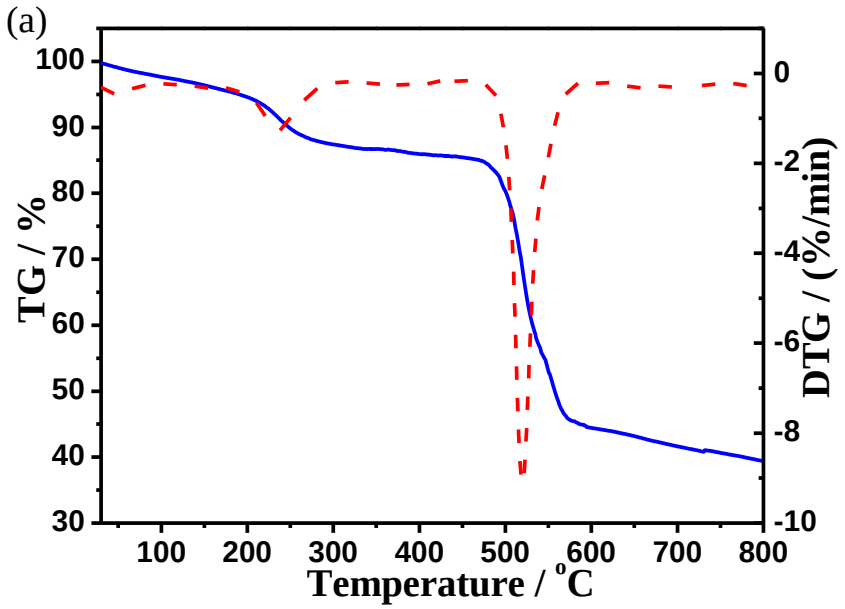
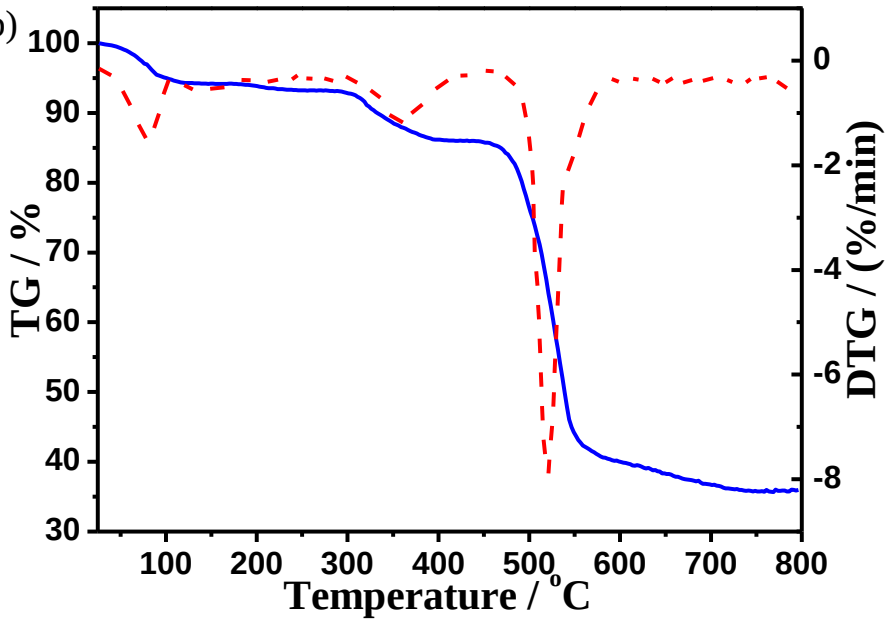


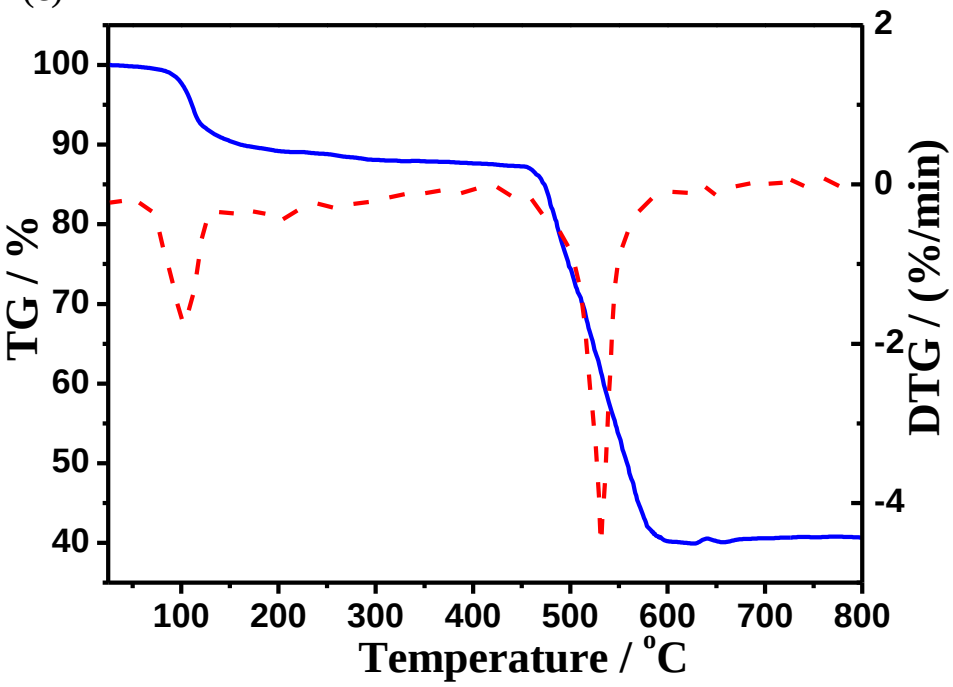
Figure S2. IR spectra for **1-4**.



(b)


100
90
80
70
60
50
40
30
TG / %
0
-2
-4
-6
-8
DTG / (%/min)
100
200
300
400
500
600
700
800
Temperature / °C

(c)


100
90
80
70
60
50
40
TG / %
2
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-2
-4
DTG / (%/min)
100
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400
500
600
700
800
Temperature / °C

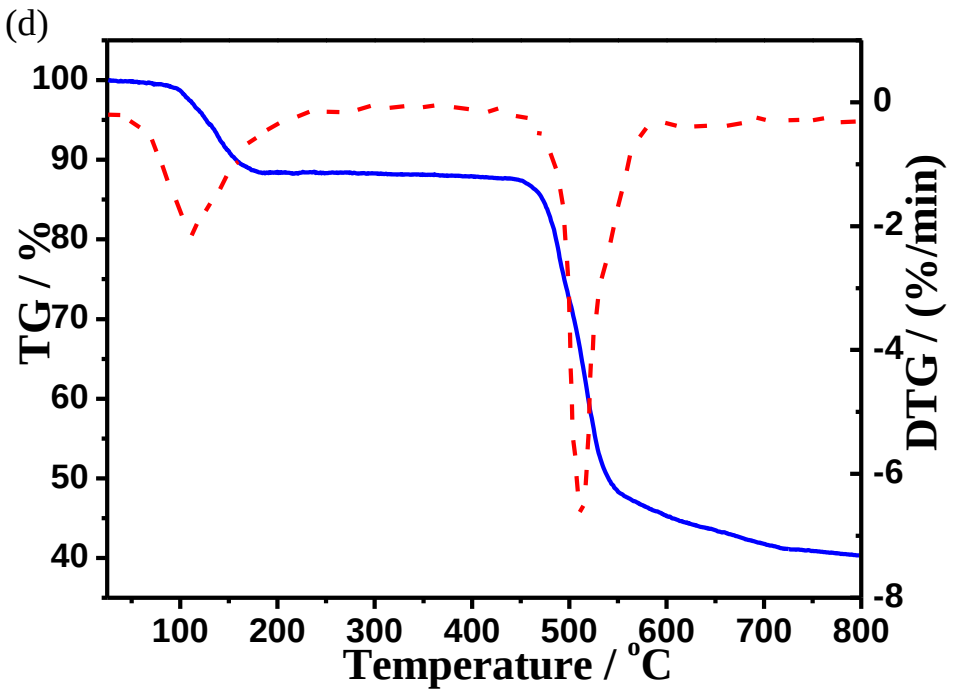


Figure S3. Themogravimetric analysis data of **1** (a), **2** (b), **3** (c) and **4** (d)

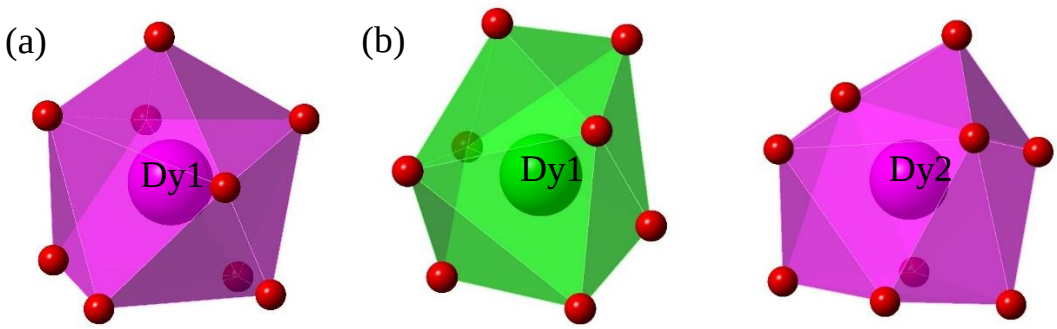
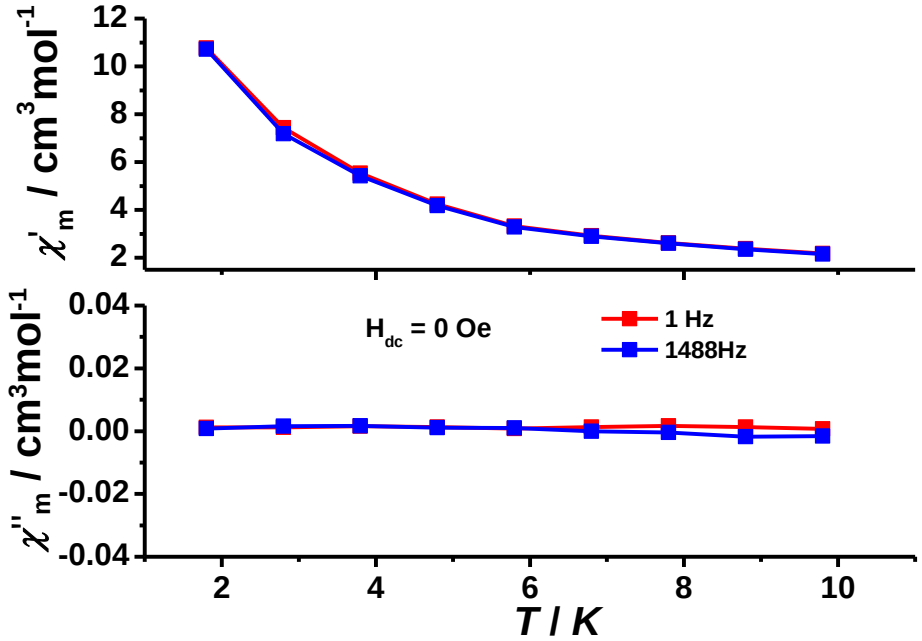


Figure S4. Polyhedral view of lanthanide atoms in **1** (a) and **3** (b).

(a)



(b)

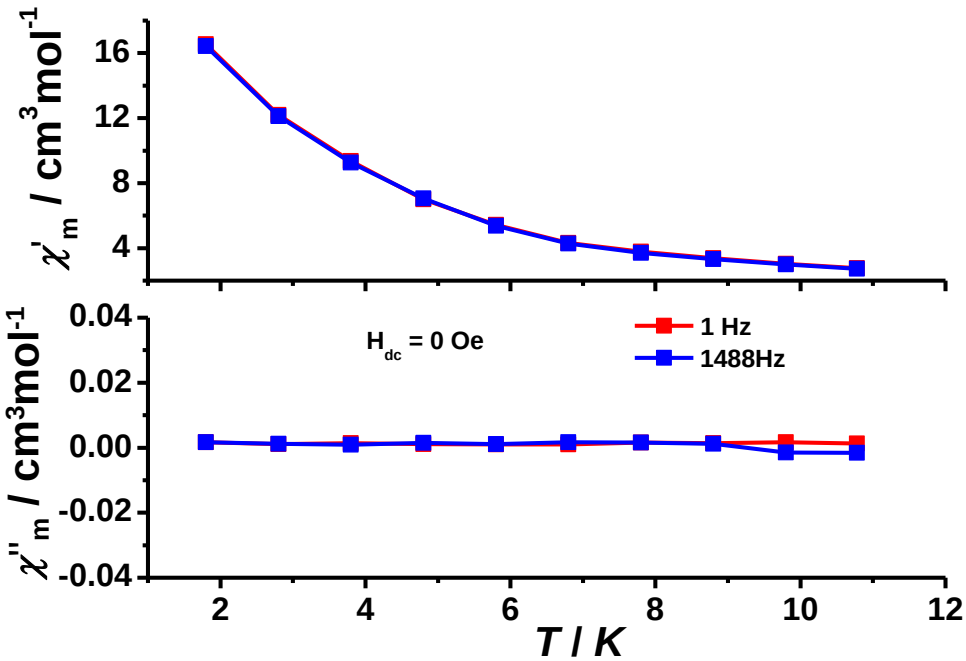


Figure S5. Temperature dependence of the in-phase (χ') and out-of-phase (χ'') susceptibilities for **1** (c) and **3** (d) in the absence of dc field. The solid lines are guidelines only.

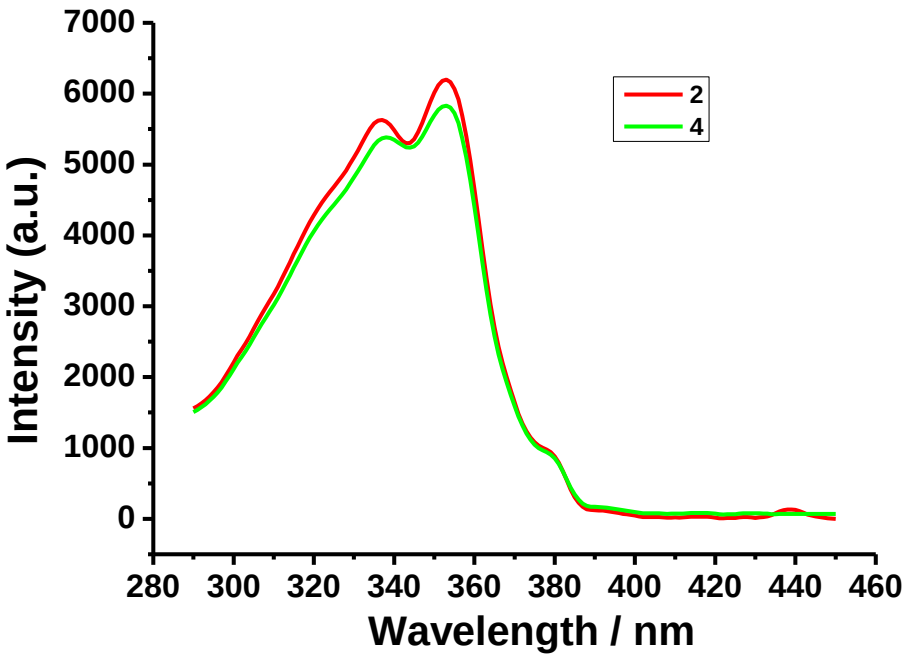


Figure S6. Solid state excitation spectra of complexes **2** and **4**.

Table S1 The free energies of the conformations and Δ*G* values compared with conformation **I**.

	Gas phase		Solvate in Water	
	a.u.	kcal mol^{-1}(Δ*G*)	a.u.	kcal mol^{-1}(Δ*G*)
I	-989.964446	0	-990.007046	0
II	-989.987394	-14.4001	-990.026199	-12.0187
III	-989.983688	-12.0745	-990.025561	-11.6183
IV	-989.976385	-7.49184	-990.016613	-6.0034

Table S2. Selected Bond Lengths (Å) and Angles (deg) for complexes **1-4**.

1			
Dy(1)-O(1*a*)	2.345(7)	Dy(1)-O(3*c*)	2.425(6)
Dy(1)-O(1W)	2.360(7)	Dy(1)-O(8*b*)	2.444(7)
Dy(1)-O(2W)	2.380(6)	Dy(1)-O(4*c*)	2.477(7)
Dy(1)-O(2)	2.384(7)	Dy(1)-O(1)	2.686(7)
Dy(1)-O(7*b*)	2.396(6)		
O(1*a*)-Dy(1)-O(1W)	154.8(2)	O(2)-Dy(1)-O(8*b*)	145.1(2)
O(1*a*)-Dy(1)-O(2W)	78.4(2)	O(7*b*)-Dy(1)-O(8*b*)	54.0(2)
O(1W)-Dy(1)-O(2W)	82.3(2)	O(3*c*)-Dy(1)-O(8*b*)	77.3(2)
O(1*a*)-Dy(1)-O(2)	118.6(2)	O(1*a*)-Dy(1)-O(4*c*)	126.8(2)
O(1W)-Dy(1)-O(2)	70.6(2)	O(1W)-Dy(1)-O(4*c*)	77.9(2)
O(2W)-Dy(1)-O(2)	74.5(2)	O(2W)-Dy(1)-O(4*c*)	144.5(2)

O(1*a*)-Dy(1)-O(7*b*)	80.8(2)	O(2)-Dy(1)-O(4*c*)	71.2(2)
O(1W)-Dy(1)-O(7*b*)	78.3(2)	O(7*b*)-Dy(1)-O(4*c*)	129.2(2)
O(2W)-Dy(1)-O(7*b*)	73.7(2)	O(3*c*)-Dy(1)-O(4*c*)	52.5(2)
O(2)-Dy(1)-O(7*b*)	137.8(2)	O(8*b*)-Dy(1)-O(4*c*)	79.8(2)
O(1*a*)-Dy(1)-O(3*c*)	74.5(2)	O(1*a*)-Dy(1)-O(1)	69.3(2)
O(1W)-Dy(1)-O(3*c*)	129.3(2)	O(1W)-Dy(1)-O(1)	120.8(2)
O(2W)-Dy(1)-O(3*c*)	144.5(2)	O(2W)-Dy(1)-O(1)	74.9(2)
O(2)-Dy(1)-O(3*c*)	99.0(2)	O(2)-Dy(1)-O(1)	50.9(2)
O(7*b*)-Dy(1)-O(3*c*)	122.9(2)	O(7*b*)-Dy(1)-O(1)	140.1(2)
O(1*a*)-Dy(1)-O(8*b*)	94.2(2)	O(3*c*)-Dy(1)-O(1)	74.4(2)
O(1W)-Dy(1)-O(8*b*)	84.9(2)	O(8*b*)-Dy(1)-O(1)	150.1(2)
O(2W)-Dy(1)-O(8*b*)	127.6(2)	O(4*c*)-Dy(1)-O(1)	90.4(2)
		2	
Tb(1)-O(1W)	2.332(4)	Tb(1)-O(2)	2.452(5)
Tb(1)-O(4*a*)	2.371(4)	Tb(1)-O(6*c*)	2.453(5)
Tb(1)-O(2W)	2.382(5)	Tb(1)-O(1)	2.489(4)
Tb(1)-O(3*b*)	2.391(5)	Tb(1)-O(4*b*)	2.674(5)
Tb(1)-O(5*c*)	2.412(4)		
O(1W)-Tb(1)-O(4*a*)	155.08(15)	O(3*b*)-Tb(1)-O(6*c*)	145.16(14)
O(1W)-Tb(1)-O(2W)	81.15(15)	O(5*c*)-Tb(1)-O(6*c*)	53.61(16)
O(4*a*)-Tb(1)-O(2W)	78.83(15)	O(2)-Tb(1)-O(6*c*)	77.14(15)
O(1W)-Tb(1)-O(3*b*)	69.41(16)	O(1W)-Tb(1)-O(1)	78.30(15)
O(4*a*)-Tb(1)-O(3*b*)	118.69(15)	O(4*a*)-Tb(1)-O(1)	126.34(15)
O(2W)-Tb(1)-O(3*b*)	75.08(15)	O(2W)-Tb(1)-O(1)	144.72(15)
O(1W)-Tb(1)-O(5*c*)	79.17(15)	O(3*b*)-Tb(1)-O(1)	70.96(17)
O(4*a*)-Tb(1)-O(5*c*)	80.93(14)	O(5*c*)-Tb(1)-O(1)	129.45(16)
O(2W)-Tb(1)-O(5*c*)	73.15(16)	O(2)-Tb(1)-O(1)	52.43(13)
O(3*b*)-Tb(1)-O(5*c*)	138.03(18)	O(6*c*)-Tb(1)-O(1)	80.22(15)
O(1W)-Tb(1)-O(2)	129.73(14)	O(1W)-Tb(1)-O(4*b*)	119.22(15)
O(4*a*)-Tb(1)-O(2)	74.15(14)	O(4*a*)-Tb(1)-O(4*b*)	69.62(15)
O(2W)-Tb(1)-O(2)	145.25(14)	O(2W)-Tb(1)-O(4*b*)	75.71(14)
O(3*b*)-Tb(1)-O(2)	99.21(16)	O(3*b*)-Tb(1)-O(4*b*)	50.60(14)
O(5*c*)-Tb(1)-O(2)	122.45(17)	O(5*c*)-Tb(1)-O(4*b*)	140.50(14)
O(1W)-Tb(1)-O(6*c*)	86.20(16)	O(2)-Tb(1)-O(4*b*)	74.66(15)
O(4*a*)-Tb(1)-O(6*c*)	93.97(15)	O(6*c*)-Tb(1)-O(4*b*)	150.33(15)
O(2W)-Tb(1)-O(6*c*)	126.70(14)	O(1)-Tb(1)-O(4*b*)	89.77(14)
		3	
Dy(1)-O(4*a*)	2.232(5)	Dy(2)-O(7*c*)	2.320(4)
Dy(1)-O(3*b*)	2.332(4)	Dy(2)-O(4W)	2.334(4)
Dy(1)-O(1W)	2.358(3)	Dy(2)-O(3W)	2.336(3)
Dy(1)-O(2W)	2.360(5)	Dy(2)-O(13)	2.352(4)
Dy(1)-O(9)	2.378(4)	Dy(2)-O(8)	2.363(4)
Dy(1)-O(1)	2.410(3)	Dy(2)-O(5*b*)	2.415(4)
Dy(1)-O(10)	2.484(4)	Dy(2)-O(14)	2.473(4)

Dy(1)-O(2)	2.542(4)	Dy(2)-O(6*b*)	2.601(4)
		Dy(2)-O(7)	2.848(4)
O(4*a*)-Dy(1)-O(3*b*)	108.60(17)	O(4W)-Dy(2)-O(13)	86.51(16)
O(4*a*)-Dy(1)-O(1W)	75.51(14)	O(3W)-Dy(2)-O(13)	129.58(13)
O(3*b*)-Dy(1)-O(1W)	76.95(13)	O(7*c*)-Dy(2)-O(8)	118.07(14)
O(4*a*)-Dy(1)-O(2W)	160.22(16)	O(4W)-Dy(2)-O(8)	74.93(15)
O(3*b*)-Dy(1)-O(2W)	81.77(17)	O(3W)-Dy(2)-O(8)	78.63(14)
O(1W)-Dy(1)-O(2W)	91.12(13)	O(13)-Dy(2)-O(8)	146.03(14)
O(4*a*)-Dy(1)-O(9)	86.31(17)	O(7*c*)-Dy(2)-O(5*b*)	78.05(13)
O(3*b*)-Dy(1)-O(9)	152.21(14)	O(4W)-Dy(2)-O(5*b*)	123.15(13)
O(1W)-Dy(1)-O(9)	130.40(12)	O(3W)-Dy(2)-O(5*b*)	142.14(13)
O(2W)-Dy(1)-O(9)	91.67(17)	O(13)-Dy(2)-O(5*b*)	78.27(13)
O(4*a*)-Dy(1)-O(1)	125.64(15)	O(8)-Dy(2)-O(5*b*)	88.29(15)
O(3*b*)-Dy(1)-O(1)	75.97(14)	O(7*c*)-Dy(2)-O(14)	89.36(14)
O(1W)-Dy(1)-O(1)	150.06(13)	O(4W)-Dy(2)-O(14)	70.11(14)
O(2W)-Dy(1)-O(1)	72.58(14)	O(3W)-Dy(2)-O(14)	77.21(12)
O(9)-Dy(1)-O(1)	76.30(14)	O(13)-Dy(2)-O(14)	53.84(12)
O(4*a*)-Dy(1)-O(10)	88.13(16)	O(8)-Dy(2)-O(14)	137.87(15)
O(3*b*)-Dy(1)-O(10)	146.51(16)	O(5*b*)-Dy(2)-O(14)	130.62(13)
O(1W)-Dy(1)-O(10)	79.70(11)	O(7*c*)-Dy(2)-O(6*b*)	129.30(13)
O(2W)-Dy(1)-O(10)	74.99(15)	O(4W)-Dy(2)-O(6*b*)	71.78(13)
O(9)-Dy(1)-O(10)	53.55(13)	O(3W)-Dy(2)-O(6*b*)	146.30(14)
O(1)-Dy(1)-O(10)	118.10(13)	O(13)-Dy(2)-O(6*b*)	76.81(13)
O(4*a*)-Dy(1)-O(2)	75.01(14)	O(8)-Dy(2)-O(6*b*)	70.49(13)
O(3*b*)-Dy(1)-O(2)	79.49(15)	O(5*b*)-Dy(2)-O(6*b*)	51.50(14)
O(1W)-Dy(1)-O(2)	133.58(12)	O(14)-Dy(2)-O(6*b*)	117.82(13)
O(2W)-Dy(1)-O(2)	124.23(13)	O(7*c*)-Dy(2)-O(7)	70.20(14)
O(9)-Dy(1)-O(2)	82.13(13)	O(4W)-Dy(2)-O(7)	122.13(14)
O(1)-Dy(1)-O(2)	52.02(13)	O(3W)-Dy(2)-O(7)	72.92(12)
O(10)-Dy(1)-O(2)	133.70(13)	O(13)-Dy(2)-O(7)	146.74(14)
O(7*c*)-Dy(2)-O(4W)	156.94(12)	O(8)-Dy(2)-O(7)	48.30(14)
O(7*c*)-Dy(2)-O(3W)	77.27(14)	O(5*b*)-Dy(2)-O(7)	71.92(11)
O(4W)-Dy(2)-O(3W)	87.70(14)	O(14)-Dy(2)-O(7)	146.74(11)
O(7*c*)-Dy(2)-O(13)	89.71(15)	O(6*b*)-Dy(2)-O(7)	95.29(12)
		4	
Tb(1)-O(2*a*)	2.239(4)	Tb(2)-O(6*c*)	2.330(4)
Tb(1)-O(1)	2.341(5)	Tb(2)-O(3W)	2.351(4)
Tb(1)-O(2W)	2.365(4)	Tb(2)-O(4W)	2.361(4)
Tb(1)-O(1W)	2.376(4)	Tb(2)-O(13)	2.361(4)
Tb(1)-O(9)	2.385(4)	Tb(2)-O(5*b*)	2.381(4)
Tb(1)-O(4*b*)	2.414(4)	Tb(2)-O(7)	2.413(4)
Tb(1)-O(10)	2.482(4)	Tb(2)-O(14)	2.483(4)
Tb(1)-O(3*b*)	2.545(4)	Tb(2)-O(8)	2.609(4)
		Tb(2)-O(6*b*)	2.801(4)

O(2*a*)-Tb(1)-O(1)	108.58(18)	O(3W)-Tb(2)-O(13)	128.81(15)
O(2*a*)-Tb(1)-O(2W)	75.19(16)	O(4W)-Tb(2)-O(13)	86.55(16)
O(1)-Tb(1)-O(2W)	77.13(17)	O(6*c*)-Tb(2)-O(5*b*)	118.13(14)
O(2*a*)-Tb(1)-O(1W)	161.01(17)	O(3W)-Tb(2)-O(5*b*)	78.92(16)
O(1)-Tb(1)-O(1W)	80.91(17)	O(4W)-Tb(2)-O(5*b*)	74.11(15)
O(2W)-Tb(1)-O(1W)	91.58(16)	O(13)-Tb(2)-O(5*b*)	145.97(15)
O(2*a*)-Tb(1)-O(9)	86.73(17)	O(6*c*)-Tb(2)-O(7)	78.01(14)
O(1)-Tb(1)-O(9)	152.24(17)	O(3W)-Tb(2)-O(7)	142.83(14)
O(2W)-Tb(1)-O(9)	130.12(15)	O(4W)-Tb(2)-O(7)	123.16(14)
O(1W)-Tb(1)-O(9)	91.79(17)	O(13)-Tb(2)-O(7)	78.01(14)
O(2*a*)-Tb(1)-O(4*b*)	125.48(15)	O(5*b*)-Tb(2)-O(7)	89.34(16)
O(1)-Tb(1)-O(4*b*)	75.83(16)	O(6*c*)-Tb(2)-O(14)	89.93(14)
O(2W)-Tb(1)-O(4*b*)	150.29(15)	O(3W)-Tb(2)-O(14)	76.81(14)
O(1W)-Tb(1)-O(4*b*)	72.22(14)	O(4W)-Tb(2)-O(14)	70.03(14)
O(9)-Tb(1)-O(4*b*)	76.43(15)	O(13)-Tb(2)-O(14)	53.51(13)
O(2*a*)-Tb(1)-O(10)	88.53(18)	O(5*b*)-Tb(2)-O(14)	137.10(15)
O(1)-Tb(1)-O(10)	146.47(16)	O(7)-Tb(2)-O(14)	130.09(14)
O(2W)-Tb(1)-O(10)	79.94(15)	O(6*c*)-Tb(2)-O(8)	129.32(13)
O(1W)-Tb(1)-O(10)	75.58(16)	O(3W)-Tb(2)-O(8)	146.79(14)
O(9)-Tb(1)-O(10)	53.06(14)	O(4W)-Tb(2)-O(8)	71.82(13)
O(4*b*)-Tb(1)-O(10)	117.92(14)	O(13)-Tb(2)-O(8)	76.87(14)
O(2*a*)-Tb(1)-O(3*b*)	74.80(15)	O(5*b*)-Tb(2)-O(8)	70.65(14)
O(1)-Tb(1)-O(3*b*)	79.79(15)	O(7)-Tb(2)-O(8)	51.49(13)
O(2W)-Tb(1)-O(3*b*)	133.49(14)	O(14)-Tb(2)-O(8)	117.54(13)
O(1W)-Tb(1)-O(3*b*)	123.78(14)	O(6*c*)-Tb(2)-O(6*b*)	69.54(14)
O(9)-Tb(1)-O(3*b*)	82.29(14)	O(3W)-Tb(2)-O(6*b*)	73.74(13)
O(4*b*)-Tb(1)-O(3*b*)	51.96(13)	O(4W)-Tb(2)-O(6*b*)	122.29(14)
O(10)-Tb(1)-O(3*b*)	133.38(14)	O(13)-Tb(2)-O(6*b*)	146.54(13)
O(6*c*)-Tb(2)-O(3W)	76.91(14)	O(5*b*)-Tb(2)-O(6*b*)	49.16(13)
O(6*c*)-Tb(2)-O(4W)	157.14(14)	O(7)-Tb(2)-O(6*b*)	71.99(13)
O(3W)-Tb(2)-O(4W)	87.54(14)	O(14)-Tb(2)-O(6*b*)	147.13(12)
O(6*c*)-Tb(2)-O(13)	90.23(15)	O(8)-Tb(2)-O(6*b*)	95.21(12)

Symmetry codes:

For **1**: *a* -x+1, -y+1, -z+2; *b* x, -y+1, z-1/2; *c* x, y-1, z.

For **2**: *a* -x+1, -y+1, -z; *b* x, y-1, z; *c* x, -y+1, z+1/2.

For **3**: *a* -x, -y+1, -z+1; *b* x+1, y, z; *c* -x+1, -y+2, -z.

For **4**: *a* -x, -y+1, -z; *b* x+1, y, z; *c* -x-1, -y, -z+1.

Table S3. Hydrogen-bond parameters for complexes **1**-**4**.

D-H ··A	d(D-H)	d(H ··A)	d(D ··A)	<(DHA)
		1		
O(6)-H(6O) ··O(4*b*)	0.82	1.91	2.727(10)	174.5
O(1W)-H(1WA) ··O(3W)	0.85	2.13	2.720(10)	125.9

O(1W)-H(1WB) ··O(3W*c*)	0.85	2.07	2.795(10)	143.6
O(2W)-H(2WA) ··O(8*d*)	0.85	2.08	2.827(10)	146.2
O(2W)-H(2WB) ··O(4W)	0.85	2.47	3.319(6)	172.8
O(3W)-H(3WA) ··O(8*b*)	0.85	2.19	2.851(10)	134.6
O(3W)-H(3WB) ··O(4*c*)	0.85	2.49	3.043(10)	123.5
O(4W)-H(4WA) ··O(7*a*)	0.85	2.09	2.941(9)	180.0
2				
O(8)-H(8O) ··O(1*b*)	0.85	1.88	2.729(6)	174.8
O(1W)-H(1WA) ··O(3W)	0.85	2.24	2.840(6)	128.1
O(1W)-H(1WB) ··O(3W*c*)	0.85	2.01	2.742(7)	143.0
O(2W)-H(2WA) ··O(2*d*)	0.85	1.89	2.701(6)	159.1
O(2W)-H(2WB) ··O(6*e*)	0.85	2.03	2.809(7)	151.5
O(3W)-H(3WA) ··O(6*f*)	0.85	1.99	2.832(6)	172.1
O(3W)-H(3WB) ··O(7*a*)	0.85	1.93	2.772(6)	171.3
O(4W)-H(4W) ··O(5)	0.85	2.10	2.947(7)	173.5
3				
O(16)-H(16) ··O(1*c*)	0.98	1.57	2.507(5)	158.5
O(1W)-H(1WA) ··O(9*b*)	0.82	1.93	2.632(6)	143.3
O(1W)-H(1WB) ··O(2*h*)	0.85	1.98	2.805(5)	164.7
O(2W)-H(2WA) ··O(15*c*)	0.82	2.17	2.934(5)	155.9
O(2W)-H(2WB) ··O(5W)	0.87	1.91	2.723(7)	156.7
O(3W)-H(3WA) ··O(5*f*)	0.82	1.94	2.732(6)	163.7
O(3W)-H(3WB) ··O(13*d*)	0.85	1.85	2.670(6)	161.0
O(4W)-H(4WA) ··O(11*e*)	0.82	1.93	2.711(6)	159.7
O(4W)-H(4WB) ··O(15*a*)	0.86	1.98	2.792(6)	155.6
O(5W)-H(5WA) ··O(6*g*)	0.85	2.25	2.992(7)	145.3
O(5W)-H(5WB) ··O(11*b*)	0.85	2.10	2.938(6)	166.3
O(6W)-H(6WA) ··O(3*b*)	0.85	2.51	3.361(16)	179.5
4				
O(11)-H(11C) ··O(8*g*)	0.84	1.89	2.724(6)	169.0
O(15)-H(15A) ··O(4*c*)	0.84	1.67	2.500(6)	168.8
O(1W)-H(1WA) ··O(16*h*)	0.85	2.12	2.927(6)	159.3
O(1W)-H(1WB) ··O(5W)	0.85	2.13	2.720(7)	126.6
O(2W)-H(2WA) ··O(9*d*)	0.85	1.88	2.630(6)	146.2
O(2W)-H(2WB) ··O(3*f*)	0.85	1.99	2.785(6)	155.2
O(3W)-H(3WA) ··O(7*h*)	0.85	1.91	2.732(6)	161.7
O(3W)-H(3WB) ··O(13*b*)	0.85	1.90	2.660(6)	148.0
O(4W)-H(4WA) ··O(12*e*)	0.85	1.89	2.706(6)	160.2
O(4W)-H(4WB) ··O(16*a*)	0.85	2.24	2.765(6)	119.6
O(5W)-H(5WA) ··O(8*g*)	0.85	2.14	2.986(7)	172.8
O(5W)-H(5WB) ··O(12*d*)	0.85	2.10	2.941(7)	170.3
O(6W)-H(6WA) ··O(1*h*)	0.85	2.46	3.304(18)	169.6
O(6W)-H(6WB) ··O(3W)	0.85	2.33	3.06(2)	144.7

Symmetry codes:

For **1**: *a* -x+1, -y+1, -z+2; *b* -x+3/2, y-1/2, -z+5/2; *c* -x+3/2, -y+3/2, -z+2; *d* x, -y+2, z-1/2.
For **2**: *a* x, -y+1, z+1/2; *b* -x+1/2, y+1/2, -z-1/2; *c* -x+1/2, -y-1/2, -z; *d* -x+1, -y, -z; *e* x, -y, z+1/2; *f* -x+1/2, y-1/2, -z-1/2.
For **3**: *a* -x+1, -y+3, -z; *b* x+1, y, z; *c* -x+1, -y+2, -z; *d* x-1, y, z; *e* x, y+1, z; *f* -x, -y+2, -z; *g*: x+1, y-1, z; *h* -x+1, -y+1, -z+1.
For **4**: *a* -x, -y-1, -z+1; *b* x+1, y, z; *c* -x-1, -y, -z+1; *d* x, y-1, z; *e* -x+1, -y+2, -z; *f* -x-1, -y+1, -z; *g* x, y+1, z; *h* -x, -y, -z+1.