Electronic Supplementary Material (ESI) for CrystEngComm.

Hydrothermal synthesis, crystal structures and photoluminescence properties of two mixed Eu^{3+} and Y^{3+} lanthanide metal-organic framework materials

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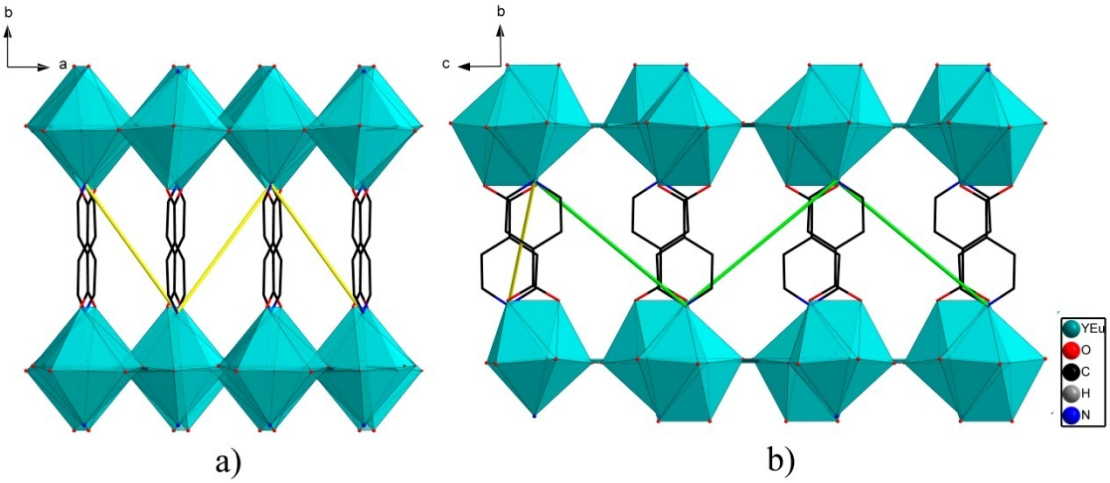

Fig. S1 a) View of the 3D structure of **2** along the c axis; Yellow line: the zigzag distribution of N atoms. b) View of the 3D structure of **2** along the a axis; Green line: the zigzag distribution of N atoms

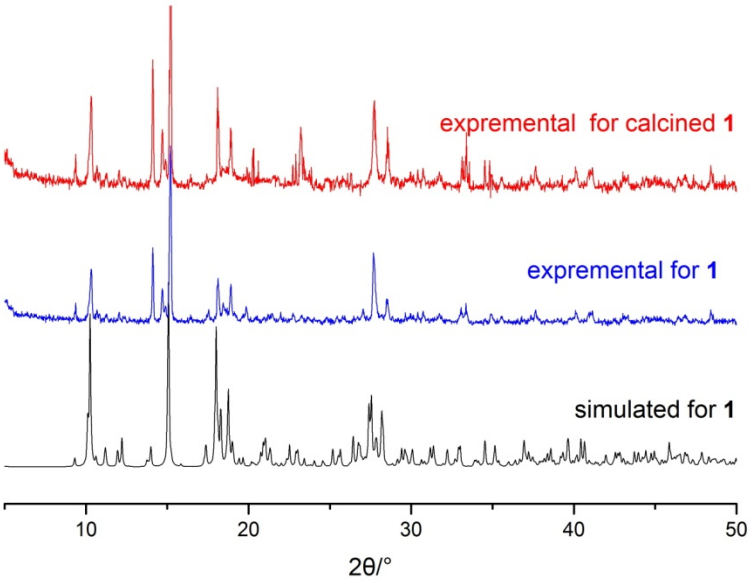

Fig. S2 The simulated and experimental powder X-ray diffraction patterns for compound **1** and **1** calcined at 200℃ for 2 hours.

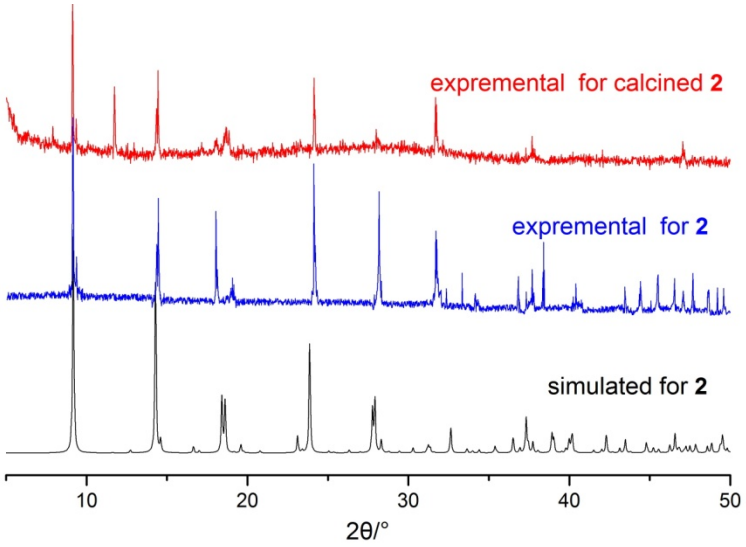

Fig. S3 The simulated and experimental powder X-ray diffraction patterns for compound **2** and **2** calcined at 200℃ for 2 hours.

Table. S1 EDX quantitative results for Eu/Y ratio of **1**

Element Line	*Weight %*	*Atom %*	*Formula*	*Compnd %*	*Norm. Compnd%*
Y L	50.90	63.93	Y	50.90	50.90
Eu L	49.10	36.07	Eu	49.10	49.10
Total	100.00	100.00		100.00	100.00

Table. S2 EDX quantitative results for Eu/Y ratio of **2**

Element Line	*Weight %*	*Atom %*	*Formula*	*Compnd %*	*Norm. Compnd%*
Y L	41.13	54.43	Y	41.13	41.13
Eu L	58.87	45.57	Eu	58.87	58.87
Total	100.00	100.00		100.00	100.00

Table. S3 Selected bonds distances (Å) and bond angles for **1**

Eu(1)-O(1)#1	2.272(3)	Eu(3)-O(18)	2.362(3)
Eu(1)-O(16)#1	2.302(3)	Eu(3)-O(6W)	2.370(3)
Eu(1)-O(10)	2.368(3)	Eu(3)-O(3W)	2.388(3)
Eu(1)-O(11)	2.398(3)	Eu(3)-O(9)	2.392(3)

Eu(1)-O(5W)	2.411(3)	Eu(3)-O(17)#4	2.430(3)
Eu(1)-O(5)	2.428(3)	Eu(3)-O(12)	2.455(3)
Eu(1)-O(2W)	2.431(3)	O(1)-Y(1)#5	2.272(3)
Eu(1)-O(7)	2.458(3)	O(1)-Eu(1)#5	2.272(3)
Eu(2)-O(3)	2.278(3)	O(4)-Y(2)#2	2.297(3)
Eu(2)-O(4)#2	2.297(3)	O(4)-Eu(2)#2	2.297(3)
Eu(2)-O(6)	2.381(3)	O(16)-Y(1)#5	2.302(3)
Eu(2)-O(20)	2.398(3)	O(16)-Eu(1)#5	2.302(3)
Eu(2)-O(4W)	2.406(3)	O(17)-Y(3)#4	2.430(3)
Eu(2)-O(1W)	2.422(3)	O(17)-Eu(3)#4	2.430(3)
Eu(2)-O(19)#3	2.428(3)	O(19)-Y(2)#3	2.428(3)
Eu(3)-O(2)	2.298(3)	O(19)-Eu(2)#3	2.428(3)
Eu(3)-O(15)	2.316(3)		

O(1)#1-Eu(1)-O(16)#1	103.71(13)	O(4W)-Eu(2)-O(1W)	130.51(11)
O(1)#1-Eu(1)-O(10)	140.72(11)	O(3)-Eu(2)-O(19)#3	143.35(10)
O(16)#1-Eu(1)-O(10)	78.82(11)	O(4)#2-Eu(2)-O(19)#3	76.11(12)
O(1)#1-Eu(1)-O(11)	151.54(11)	O(6)-Eu(2)-O(19)#3	80.65(10)
O(16)#1-Eu(1)-O(11)	79.87(12)	O(20)-Eu(2)-O(19)#3	67.16(9)
O(10)-Eu(1)-O(11)	67.71(10)	O(4W)-Eu(2)-O(19)#3	70.92(10)
O(1)#1-Eu(1)-O(5W)	70.85(12)	O(1W)-Eu(2)-O(19)#3	136.49(9)
O(16)#1-Eu(1)-O(5W)	78.71(12)	O(3)-Eu(2)-O(8)	82.53(11)
O(10)-Eu(1)-O(5W)	71.34(11)	O(4)#2-Eu(2)-O(8)	138.13(10)
O(11)-Eu(1)-O(5W)	136.58(11)	O(6)-Eu(2)-O(8)	66.59(10)
O(1)#1-Eu(1)-O(5)	87.61(12)	O(20)-Eu(2)-O(8)	73.57(10)
O(16)#1-Eu(1)-O(5)	139.71(11)	O(4W)-Eu(2)-O(8)	140.20(10)
O(10)-Eu(1)-O(5)	116.08(10)	O(1W)-Eu(2)-O(8)	70.04(10)
O(11)-Eu(1)-O(5)	73.20(10)	O(19)#3-Eu(2)-O(8)	120.80(11)
O(5W)-Eu(1)-O(5)	140.63(11)	O(2)-Eu(3)-O(15)	106.79(13)
O(1)#1-Eu(1)-O(2W)	77.48(11)	O(2)-Eu(3)-O(18)	134.47(10)
O(16)#1-Eu(1)-O(2W)	73.41(10)	O(15)-Eu(3)-O(18)	80.15(12)
O(10)-Eu(1)-O(2W)	137.88(10)	O(2)-Eu(3)-O(6W)	148.79(11)
O(11)-Eu(1)-O(2W)	76.61(10)	O(15)-Eu(3)-O(6W)	86.18(12)
O(5W)-Eu(1)-O(2W)	130.86(10)	O(18)-Eu(3)-O(6W)	74.85(10)
O(5)-Eu(1)-O(2W)	71.60(9)	O(2)-Eu(3)-O(3W)	77.70(11)
O(1)#1-Eu(1)-O(7)	81.76(11)	O(15)-Eu(3)-O(3W)	75.30(12)
O(16)#1-Eu(1)-O(7)	152.41(10)	O(18)-Eu(3)-O(3W)	144.66(11)
O(10)-Eu(1)-O(7)	80.23(10)	O(6W)-Eu(3)-O(3W)	78.48(11)
O(11)-Eu(1)-O(7)	108.33(10)	O(2)-Eu(3)-O(9)	78.25(12)
O(5W)-Eu(1)-O(7)	77.69(11)	O(15)-Eu(3)-O(9)	147.49(11)
O(5)-Eu(1)-O(7)	66.60(9)	O(18)-Eu(3)-O(9)	74.58(11)
O(2W)-Eu(1)-O(7)	133.72(10)	O(6W)-Eu(3)-O(9)	106.17(12)
O(3)-Eu(2)-O(4)#2	106.21(13)	O(3W)-Eu(3)-O(9)	136.00(11)
O(3)-Eu(2)-O(6)	84.67(12)	O(2)-Eu(3)-O(17)#4	70.98(10)
O(4)#2-Eu(2)-O(6)	153.09(11)	O(15)-Eu(3)-O(17)#4	72.78(11)

O(3)-Eu(2)-O(20)	149.31(11)	O(18)-Eu(3)-O(17)#4	68.51(9)
O(4)#2-Eu(2)-O(20)	80.76(11)	O(6W)-Eu(3)-O(17)#4	140.11(10)
O(6)-Eu(2)-O(20)	102.59(11)	O(3W)-Eu(3)-O(17)#4	125.52(10)
O(3)-Eu(2)-O(4W)	73.52(11)	O(9)-Eu(3)-O(17)#4	79.08(10)
O(4)#2-Eu(2)-O(4W)	79.99(11)	O(2)-Eu(3)-O(12)	76.04(10)
O(6)-Eu(2)-O(4W)	79.73(11)	O(15)-Eu(3)-O(12)	145.43(11)
O(20)-Eu(2)-O(4W)	136.90(10)	O(18)-Eu(3)-O(12)	123.21(10)
O(3)-Eu(2)-O(1W)	75.54(10)	O(6W)-Eu(3)-O(12)	77.54(10)
O(4)#2-Eu(2)-O(1W)	72.79(11)	O(3W)-Eu(3)-O(12)	71.70(10)
O(6)-Eu(2)-O(1W)	134.13(10)	O(9)-Eu(3)-O(12)	67.03(10)
O(20)-Eu(2)-O(1W)	78.35(10)	O(17)#4-Eu(3)-O(12)	136.57(10)

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z; #2 -x-1,-y,-z; #3 -x-2,-y,-z; #4 -x-2,-y-1,-z-1; #5 x-1,y,z

Table. S4 Selected bonds distances (Å) for **2**

Eu(1)-O(1H)#1	2.236(2)	Eu(1)-Eu(1)#1	3.9135(3)
Eu(1)-O(1H)	2.254(2)	O(1)-Y(1)#5	2.410(2)
Eu(1)-O(1)#2	2.410(2)	O(1)-Eu(1)#5	2.410(2)
Eu(1)-O(4)#3	2.425(2)	O(2)-Y(1)#5	2.426(3)
Eu(1)-O(2)#2	2.426(3)	O(2)-Eu(1)#5	2.426(3)
Eu(1)-O(3)	2.457(2)	O(3)-Y(1)#1	2.461(2)
Eu(1)-O(3)#4	2.461(2)	O(3)-Eu(1)#1	2.461(2)
Eu(1)-N(1)	2.575(3)	O(4)-Y(1)#6	2.425(2)
Eu(1)-Y(1)#1	3.9135(3)	O(4)-Eu(1)#6	2.425(2)
O(1H)#1-Eu(1)-O(1H)	145.37（5）	O(2)#2-Eu(1)-O(3)	74.26(8)
O(1H)#1-Eu(1)-O(1)#2	96.33(9)	O(1H)#1-Eu(1)-O(3)#4	142.45(7)
O(1H)-Eu(1)-O(1)#2	111.57(9)	O(1H)-Eu(1)-O(3)#4	66.43(7)
O(1H)#1-Eu(1)-O(4)#3	76.80(7)	O(1)#2-Eu(1)-O(3)#4	78.25(8)
O(1H)-Eu(1)-O(4)#3	129.37(7)	O(4)#3-Eu(1)-O(3)#4	65.93(6)
O(1)#2-Eu(1)-O(4)#3	74.07(8)	O(2)#2-Eu(1)-O(3)#4	110.01(8)
O(1H)#1-Eu(1)-O(2)#2	95.22(8)	O(3)-Eu(1)-O(3)#4	145.74(5)
O(1H)-Eu(1)-O(2)#2	85.78(8)	O(1H)#1-Eu(1)-N(1)	82.73(8)
O(1)#2-Eu(1)-O(2)#2	53.83(9)	O(1H)-Eu(1)-N(1)	80.93(8)
O(4)#3-Eu(1)-O(2)#2	126.28(8)	O(1)#2-Eu(1)-N(1)	153.61(9)
O(1H)#1-Eu(1)-O(3)	66.77(7)	O(4)#3-Eu(1)-N(1)	80.09(8)
O(1H)-Eu(1)-O(3)	80.39(7)	O(2)#2-Eu(1)-N(1)	152.54(9)
O(1)#2-Eu(1)-O(3)	124.12(8)	O(3)-Eu(1)-N(1)	79.87(8)
O(4)#3-Eu(1)-O(3)	140.16(6)	O(3)#4-Eu(1)-N(1)	86.49(7)

Symmetry transformations used to generate equivalent atoms:

#1 x+1/2,-y+1/2,-z+1； #2 -x+1/2,y+1/2,z； #3 -x+1/2,-y+1/2,z-1/2； #4 x-1/2,-y+1/2,-z+1； #5 -x+1/2,y-1/2,z； #6 -x+1/2,-y+1/2,z+1/2； #7 -x+1,y,-z+3/2

Table. S5 Hydrogen bonds in the title compound **1**

D—H…A	d(D--H)/Å	d(H--A)/Å	d(D--A)/Å	∠D—H…A/(°)
O1W--H1WA…N1	0.83(3)	1.84(3)	2.666(5)	169(3)
O1W--H1WB…O12	0.840(19)	2.128(19)	2.865(4)	146(3)
O2W--H2WA…N2	0.85(2)	1.84(2)	2.680(5)	170(2)
O2W--H2WB…O19	0.842(16)	2.122(19)	2.940(4)	164(4)
O3W--H3WA…O8	0.83(3)	2.00(3)	2.794(4)	161(3)
O3W--H3WB…O2W	0.83(3)	2.10(3)	2.889(5)	161(3)
O4W--H4WA…O5	0.85(3)	1.96(3)	2.801(4)	169(3)
O4W--H4WB…O1W	0.84(4)	2.14(4)	2.942(5)	160(3)
O5W--H5WA…O7W	0.84(3)	2.03(4)	2.670(9)	133(4)
O5W--H5WB…O17	0.85(3)	2.05(4)	2.871(5)	163(4)
O6W--H6WA…O7	0.83(3)	2.30(3)	3.116(4)	170(5)
O6W--H6WB…N3	0.84(2)	1.91(3)	2.717(6)	161(4)
O7W--H7WA…O9	0.881(16)	2.373(16)	2.888(9)	117.5(16)
O7W--H7WB…O9	0.89(4)	2.39(3)	2.888(9)	116(2)
O7W--H7WB…O18	0.89(4)	2.59(4)	3.350(11)	144(5)
C5--H5A…O11	0.93	2.58	3.349(5)	140.00

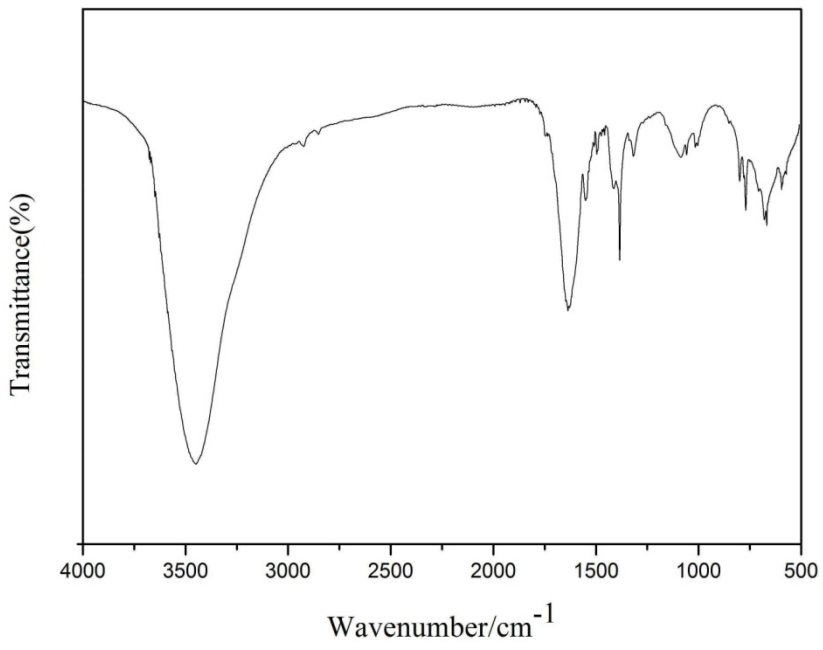

Fig. S4 The IR spectra of compound **1.**

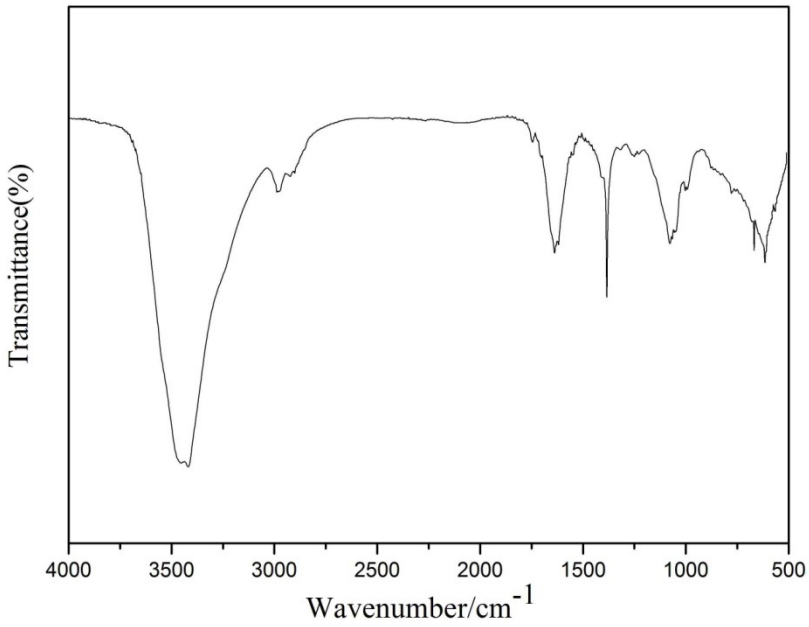

Fig. S5 The IR spectra of compound **2.**

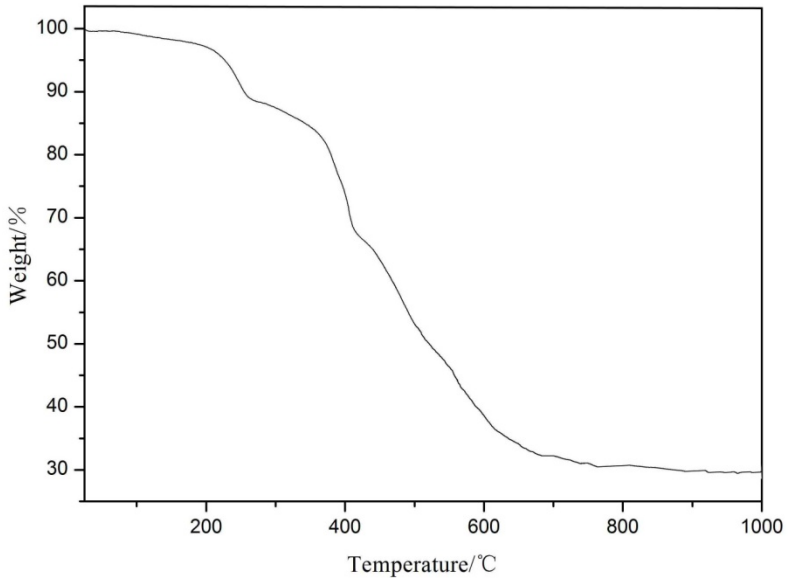

Fig. S6 The TG curve of compound **1**.

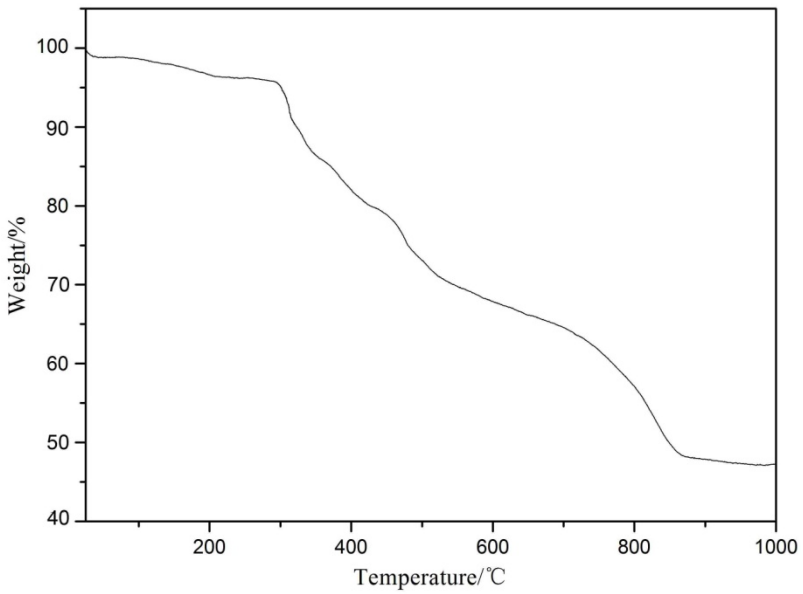

Fig. S7 The TG curve of compound **2**.