Electronic Supplementary Information for

Effects of template molecules on the structures and luminescence intensities of a series of porous Tb-MOFs based on 2-nitroterephthalate ligand

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RSC advances

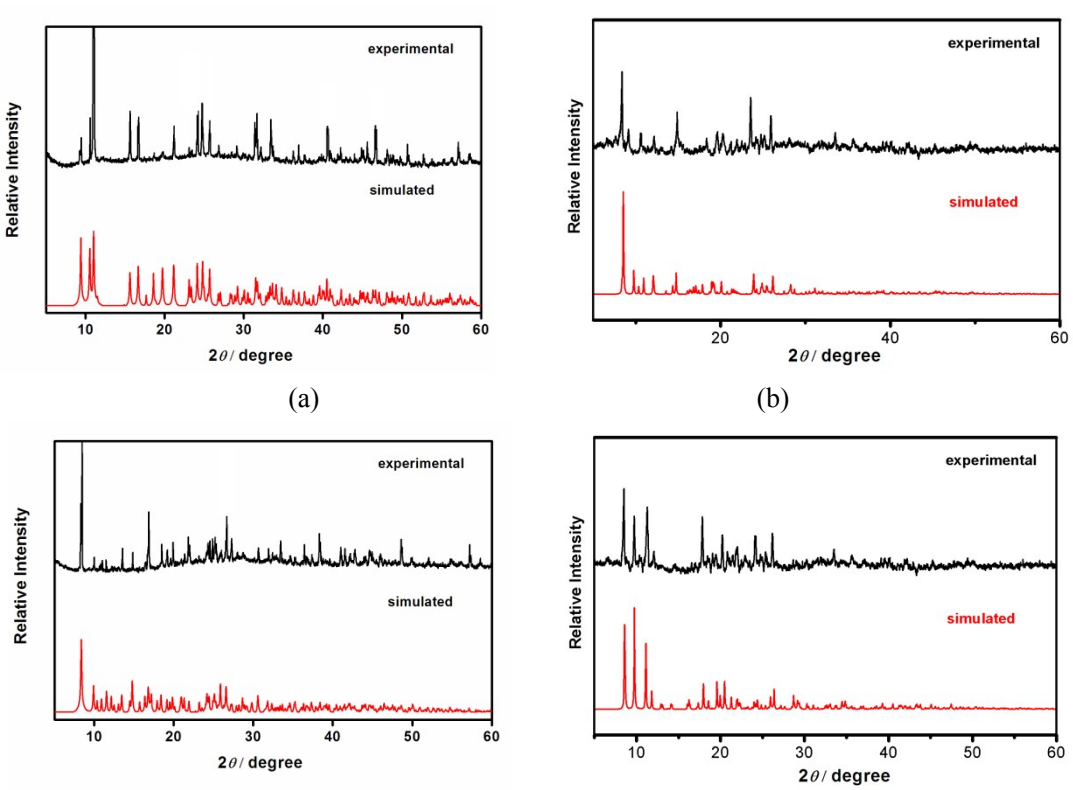


Fig. S1 The PXRD patterns for complexes **1**(a),**2**(b),**3**(c) and **4(**d).

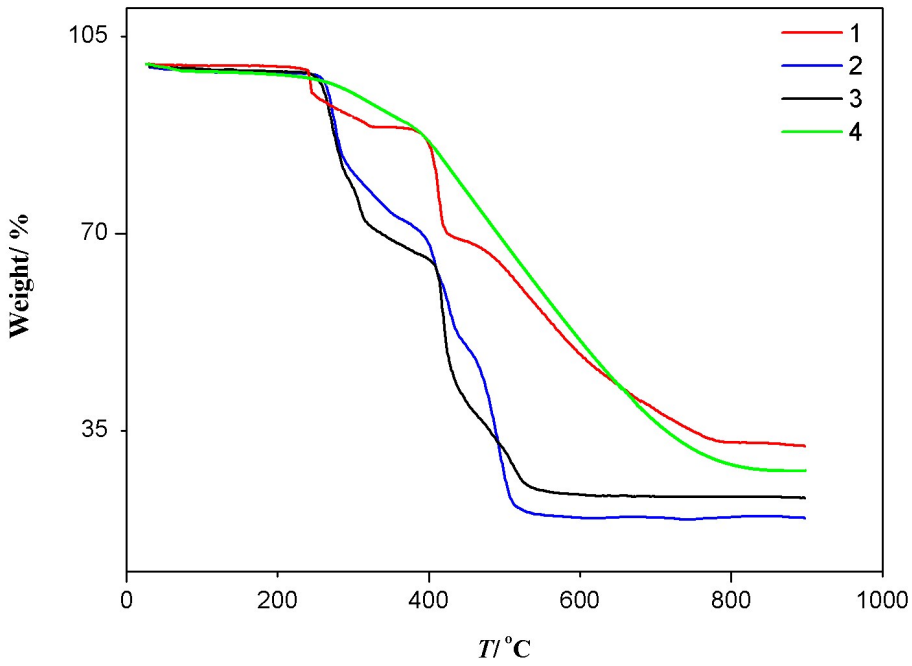


Fig. S2 The thermo-gravimetric curves for complexes **1-4**

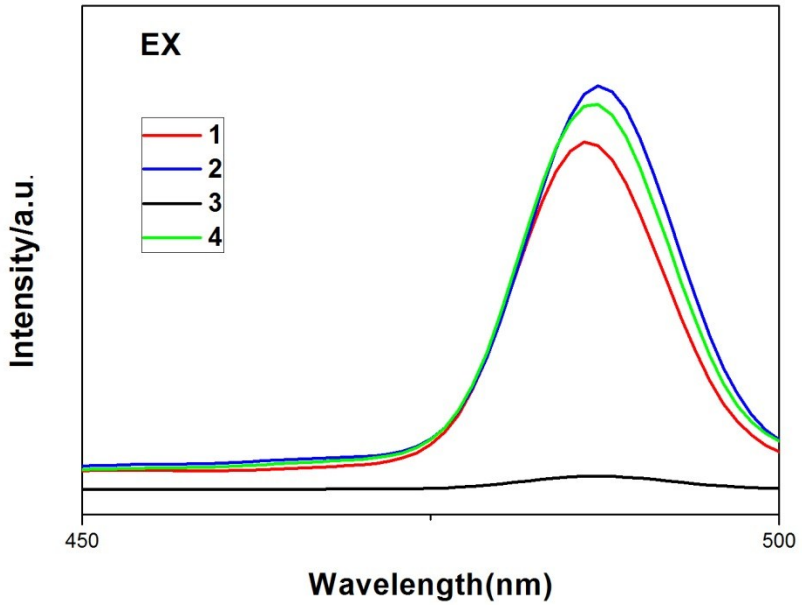
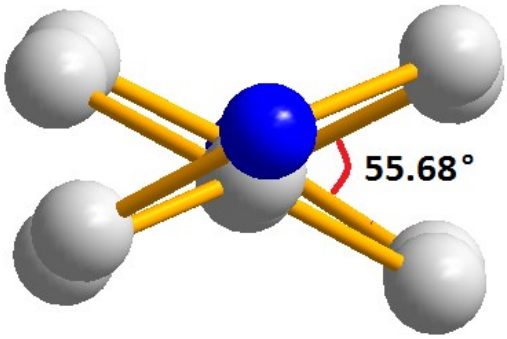
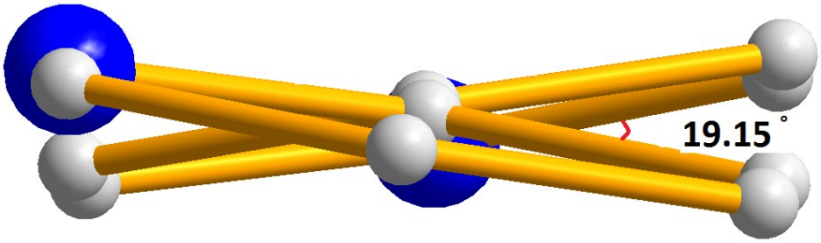


Fig.S3 The excitation spectra of complexes **1**-**4**.



(a)



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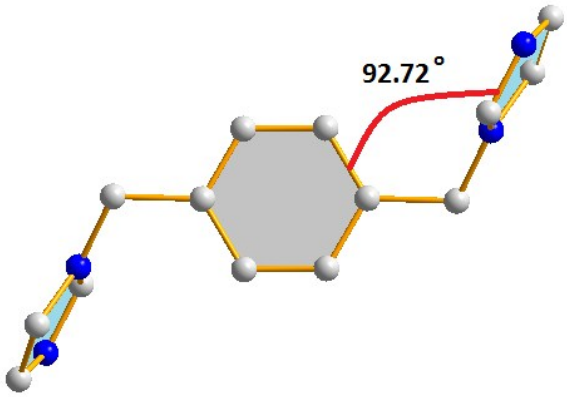

(c)

Fig.S4 The dihedral angles of guests: 4,4'-bipy(a), 2,4-bipy(b) and 1,4-bbi(c) in complexes **2-4**.

Table S1 Selected bond lengths (Å) and angles (°) for complex **1**

Tb(1)-O(1)#1	2.292(2)	Tb(1)-O(11)	2.373(3)
Tb(1)-O(2)#2	2.317(2)	Tb(1)-O(10)#4	2.388(2)
Tb(1)-O(7)	2.324(2)	Tb(1)-O(4)	2.473(3)
Tb(1)-O(3)#3	2.336(3)	Tb(1)-O(3)	2.601(3)
O(1)#1-Tb(1)-O(2)#2	86.99(9)	O(11)-Tb(1)-O(10)#4	70.30(10)
O(1)#1-Tb(1)-O(7)	99.78(9)	O(1)#1-Tb(1)-O(4)	157.37(11)
O(2)#2-Tb(1)-O(7)	74.15(9)	O(2)#2-Tb(1)-O(4)	80.71(9)
O(1)#1-Tb(1)-O(3)#3	77.35(10)	O(7)-Tb(1)-O(4)	95.06(10)
O(2)#2-Tb(1)-O(3)#3	142.51(9)	O(3)#3-Tb(1)-O(4)	123.28(9)
O(7)-Tb(1)-O(3)#3	75.27(9)	O(11)-Tb(1)-O(4)	75.70(11)
O(1)#1-Tb(1)-O(11)	82.93(11)	O(10)#4-Tb(1)-O(4)	79.47(10)
O(2)#2-Tb(1)-O(11)	75.89(11)	O(1)#1-Tb(1)-O(3)	150.67(10)
O(7)-Tb(1)-O(11)	149.71(10)	O(2)#2-Tb(1)-O(3)	117.75(8)
O(3)#3-Tb(1)-O(11)	133.98(10)	O(7)-Tb(1)-O(3)	74.53(8)
O(1)#1-Tb(1)-O(10)#4	100.43(10)	O(3)#3-Tb(1)-O(3)	73.37(9)
O(2)#2-Tb(1)-O(10)#4	144.04(10)	O(11)-Tb(1)-O(3)	116.71(9)
O(7)-Tb(1)-O(10)#4	137.23(10)	O(10)#4-Tb(1)-O(3)	69.44(9)
O(3)#3-Tb(1)-O(10)#4	73.00(9)	O(4)-Tb(1)-O(3)	50.56(9)

Symmetry transformations used to generate equivalent atoms: #1: 0.5+*x*, 1.5−*y*, −0.5+*z*; #2: 0.5−*x*, 0.5+*y*, 0.5−*z*; #3:1−*x*, *y*, 0.5−*z*; #4 :*x*, −1+*y*, *z*.

Table S2 Selected bond lengths (Å) and angles (°) for complex **2**

Tb(1)-O(6)#1	2.304(2)	Tb(1)-O(1)	2.443(2)
Tb(1)-O(1W)	2.390(2)	Tb(1)-O(7)	2.471(2)

Tb(1)-O(8)	2.391(3)	Tb(1)-O(12)#3	2.512(2)
Tb(1)-O(2)#2	2.400(2)	Tb(1)-O(2)	2.638(2)
Tb(1)-O(11)#3	2.427(3)		
O(6)#1-Tb(1)-O(1W)	83.28(9)	O(11)#3-Tb(1)-O(7)	78.78(9)
O(6)#1-Tb(1)-O(8)	75.36(10)	O(1)-Tb(1)-O(7)	149.77(9)
O(1W)-Tb(1)-O(8)	73.26(8)	O(6)#1-Tb(1)-O(12)#3	77.01(9)
O(6)#1-Tb(1)-O(2)#2	155.74(9)	O(1W)-Tb(1)-O(12)#3	153.74(9)
O(1W)-Tb(1)-O(2)#2	81.88(8)	O(8)-Tb(1)-O(12)#3	117.23(8)
O(8)-Tb(1)-O(2)#2	82.03(9)	O(2)#2-Tb(1)-O(12)#3	122.17(8)
O(6)#1-Tb(1)-O(11)#3	129.48(9)	O(11)#3-Tb(1)-O(12)#3	52.67(8)
O(1W)-Tb(1)-O(11)#3	141.53(8)	O(1)-Tb(1)-O(12)#3	78.17(9)
O(8)-Tb(1)-O(11)#3	128.38(9)	O(7)-Tb(1)-O(12)#3	71.74(9)
O(2)#2-Tb(1)-O(11)#3	72.22(8)	O(6)#1-Tb(1)-O(2)	126.25(8)
O(6)#1-Tb(1)-O(1)	79.50(9)	O(1W)-Tb(1)-O(2)	71.36(8)
O(1W)-Tb(1)-O(1)	81.34(9)	O(8)-Tb(1)-O(2)	134.79(8)
O(8)-Tb(1)-O(1)	145.92(10)	O(2)#2-Tb(1)-O(2)	66.00(9)
O(2)#2-Tb(1)-O(1)	116.85(8)	O(11)#3-Tb(1)-O(2)	72.29(8)
O(11)#3-Tb(1)-O(1)	85.51(9)	O(1)-Tb(1)-O(2)	50.92(7)
O(6)#1-Tb(1)-O(7)	90.75(9)	O(7)-Tb(1)-O(2)	142.38(8)
O(1W)-Tb(1)-O(7)	126.21(9)	O(12)#3-Tb(1)-O(2)	106.90(8)
O(8)-Tb(1)-O(7)	53.68(8)	O(2)#2-Tb(1)-O(7)	82.74(8)

Symmetry transformations used to generate equivalent atoms: #1:1.5−*x*, 0.5+*y*, 0.5−*z*; #2:2−*x*, 1−*y*, −*z*; #3: 1.5−*x*, −0.5+*y*, −0.5−*z*.

Table S3 Selected bond lengths (Å) and angles (°) for complex **3**

Tb(1)-O(12)#1	2.2778(16)	Tb(1)-O(7)	2.4461(18)
Tb(1)-O(8)#2	2.3715(17)	Tb(1)-O(5)#3	2.4598(18)
Tb(1)-O(1W)	2.3961(17)	Tb(1)-O(2)	2.5481(18)
Tb(1)-O(1)	2.4095(17)	Tb(1)-O(8)	2.6714(18)
Tb(1)-O(6)#3	2.4455(18)		
O(12)#1-Tb(1)-O(8)#2	155.05(6)	O(1)-Tb(1)-O(5)#3	125.47(7)
O(12)#1-Tb(1)-O(1W)	83.13(6)	O(6)#3-Tb(1)-O(5)#3	53.02(6)
O(8)#2-Tb(1)-O(1W)	78.43(6)	O(7)-Tb(1)-O(5)#3	148.47(7)
O(12)#1-Tb(1)-O(1)	130.41(6)	O(12)#1-Tb(1)-O(2)	78.23(6)
O(8)#2-Tb(1)-O(1)	73.24(6)	O(8)#2-Tb(1)-O(2)	123.53(6)
O(1W)-Tb(1)-O(1)	141.45(6)	O(1W)-Tb(1)-O(2)	155.93(6)
O(12)#1-Tb(1)-O(6)#3	94.68(7)	O(1)-Tb(1)-O(2)	52.47(6)
O(8)#2-Tb(1)-O(6)#3	83.17(6)	O(6)#3-Tb(1)-O(2)	70.53(6)
O(1W)-Tb(1)-O(6)#3	126.59(6)	O(7)-Tb(1)-O(2)	78.13(7)
O(1)-Tb(1)-O(6)#3	75.50(6)	O(5)#3-Tb(1)-O(2)	114.26(6)
O(12)#1-Tb(1)-O(7)	78.79(6)	O(12)#1-Tb(1)-O(8)	123.74(6)
O(8)#2-Tb(1)-O(7)	115.21(6)	O(8)#2-Tb(1)-O(8)	65.12(6)
O(1W)-Tb(1)-O(7)	83.44(7)	O(1W)-Tb(1)-O(8)	70.64(6)
O(1)-Tb(1)-O(7)	85.50(7)	O(1)-Tb(1)-O(8)	73.94(6)

O(6)#3-Tb(1)-O(7)	148.66(7)	O(6)#3-Tb(1)-O(8)	140.92(6)
O(12)#1-Tb(1)-O(5)#3	75.96(7)	O(7)-Tb(1)-O(8)	50.18(6)
O(8)#2-Tb(1)-O(5)#3	83.11(6)	O(5)#3-Tb(1)-O(8)	136.85(6)
O(1W)-Tb(1)-O(5)#3	75.12(6)	O(2)-Tb(1)-O(8)	107.66(6)

Symmetry transformations used to generate equivalent atoms: #1: −1.5−*x*, −0.5+*y*, 1.5−*z*; #2 −*x*, 1−*y*, 1−*z*; #3 −0.5+*x*, −0.5+*y*, −1.5+*z*.

Table S4 Selected bond lengths (Å) and angles (°) for complex **4**

Tb(1)-O(6)	2.338(5)	Tb(1)-O(16)	2.428(6)
Tb(1)-O(10)	2.339(5)	Tb(1)-O(8)#1	2.471(6)
Tb(1)-O(11)	2.355(5)	Tb(1)-O(3)	2.505(5)
Tb(1)-O(4)	2.371(5)	Tb(1)-O(6)#1	2.724(6)
Tb(1)-O(15)	2.406(5)		
O(6)-Tb(1)-O(10)	75.73(16)	O(15)-Tb(1)-O(8)#1	145.23(18)
O(6)-Tb(1)-O(11)	71.88(16)	O(16)-Tb(1)-O(8)#1	78.0(2)
O(10)-Tb(1)-O(11)	132.91(19)	O(6)-Tb(1)-O(3)	77.8(2)
O(6)-Tb(1)-O(4)	143.03(17)	O(10)-Tb(1)-O(3)	78.04(18)
O(10)-Tb(1)-O(4)	141.23(18)	O(11)-Tb(1)-O(3)	125.55(17)
O(11)-Tb(1)-O(4)	76.83(18)	O(4)-Tb(1)-O(3)	106.02(19)
O(6)-Tb(1)-O(15)	82.10(19)	O(15)-Tb(1)-O(3)	52.7(2)
O(10)-Tb(1)-O(15)	129.26(18)	O(16)-Tb(1)-O(3)	72.9(2)
O(11)-Tb(1)-O(15)	78.75(19)	O(8)#1-Tb(1)-O(3)	149.15(18)
O(4)-Tb(1)-O(15)	72.82(18)	O(6)-Tb(1)-O(6)#1	72.2(2)
O(6)-Tb(1)-O(16)	140.58(18)	O(10)-Tb(1)-O(6)#1	67.61(15)
O(10)-Tb(1)-O(16)	72.80(19)	O(11)-Tb(1)-O(6)#1	70.48(15)
O(11)-Tb(1)-O(16)	147.44(18)	O(4)-Tb(1)-O(6)#1	115.01(16)
O(4)-Tb(1)-O(16)	71.9(2)	O(15)-Tb(1)-O(6)#1	144.63(18)
O(15)-Tb(1)-O(16)	100.0(2)	O(16)-Tb(1)-O(6)#1	115.30(18)
O(6)-Tb(1)-O(8)#1	121.6(2)	O(8)#1-Tb(1)-O(6)#1	49.38(18)
O(10)-Tb(1)-O(8)#1	83.85(17)	O(3)-Tb(1)-O(6)#1	138.74(17)
O(11)-Tb(1)-O(8)#1	84.93(17)	O(4)-Tb(1)-O(8)#1	73.67(18)

Symmetry transformations used to generate equivalent atoms: #1 :1−*x*, 1−*y*, −*z*.