Electronic supplementary information (ESI)

Four novel topological frameworks based on 4,4'-(hexafluoroisopropylidene)diphthalic acid and 1,1'-(1,4-butanediyl)bis(imidazole) ligand

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Table S1. Selected bond distances (Å) and angles (^{o}) for **1**.

Cd(1)-N(5)	2.230(3)	Cd(1)-O(3)$^{\#1}$	2.417(3)
Cd(1)-N(1)	2.287(3)	Cd(1)-O(3W)	2.421(3)
Cd(1)-O(2)	2.365(2)	Cd(1)-O(1)	2.591(2)
N(5)-Cd(1)-N(1)	100.55(10)	N(5)-Cd(1)-O(1)	85.33(9)
N(5)-Cd(1)-O(2)	138.09(8)	N(1)-Cd(1)-O(1)	105.11(9)
N(1)-Cd(1)-O(2)	89.31(9)	O(2)-Cd(1)-O(1)	52.86(7)
N(5)-Cd(1)-O(3)$^{\#1}$	129.10(9)	O(3)$^{\#1}$-Cd(1)-O(1)	143.12(8)
N(1)-Cd(1)-O(3)$^{\#1}$	83.41(9)	O(3W)-Cd(1)-O(1)	79.32(9)
O(2)-Cd(1)-O(3)$^{\#1}$	92.26(8)	N(5)-Cd(1)-O(4)$^{\#1}$	80.00(9)
N(5)-Cd(1)-O(3W)	97.45(9)	N(1)-Cd(1)-O(4)$^{\#1}$	107.17(10)
N(1)-Cd(1)-O(3W)	161.73(9)	O(2)-Cd(1)-O(4)$^{\#1}$	135.80(8)
O(2)-Cd(1)-O(3W)	79.24(8)	O(3)#1-Cd(1)-O(4)$^{\#1}$	51.24(8)
O(3)$^{\#1}$-Cd(1)-O(3W)	82.88(8)	O(3W)-Cd(1)-O(4)$^{\#1}$	72.94(9)
O(1)-Cd(1)-O(4)$^{\#1}$	146.43(9)		

Symmetry codes for **1**: #1 = -x + 1, -y + 1, -z.

Table S2. Selected bond distances (Å) and angles (^{o}) for **2**.

Cd(1)-O(5)$^{\#1}$	2.263(3)	Cd(2)-O(7)$^{\#3}$	2.268(3)
Cd(1)-N(1)	2.276(4)	Cd(2)-O(4)$^{\#4}$	2.280(3)
Cd(1)-O(8)$^{\#3}$	2.281(3)	Cd(2)-O(1W)	2.296(4)
Cd(1)-O(6)$^{\#2}$	2.304(3)	Cd(2)-O(6)$^{\#2}$	2.342(3)
Cd(1)-O(3)	2.328(3)	Cd(2)-O(2W)	2.377(4)
Cd(1)-O(1)	2.362(3)	Cd(2)-O(1)	2.383(4)
O(5)$^{\#1}$-Cd(1)-N(1)	94.72(10)	O(5)$^{\#1}$-Cd(1)-O(8)$^{\#3}$	85.93(10)
N(1)-Cd(1)-O(8)$^{\#3}$	91.34(11)	O(5)$^{\#1}$-Cd(1)-O(6)$^{\#2}$	98.36(9)
N(1)-Cd(1)-O(6)$^{\#2}$	165.99(10)	O(8)$^{\#3}$-Cd(1)-O(6)$^{\#2}$	84.61(10)
O(5)$^{\#1}$-Cd(1)-O(3)	109.65(10)	N(1)-Cd(1)-O(3)	88.05(11)
(8)$^{\#2}$-Cd(1)-O(3)	164.41(8)	O(6)$^{\#2}$-Cd(1)-O(1)	76.57(11)
O(6)$^{\#2}$-Cd(1)-O(3)	92.26(10)	O(3)-Cd(1)-O(1)	81.00(11)
O(5)$^{\#1}$-Cd(1)-O(1)	168.58(10)	O(7)$^{\#3}$-Cd(2)-O(4)$^{\#4}$	92.73(10)
N(1)-Cd(1)-O(1)	89.66(12)	O(7)$^{\#3}$-Cd(2)-O(1W)	92.85(11)
O(8)$^{\#3}$-Cd(1)-O(1)	83.42(11)	O(4)$^{\#4}$-Cd(2)-O(1W)	84.71(10)
O(7)$^{\#3}$-Cd(2)-O(6)$^{\#2}$	85.83(9)	O(6)$^{\#2}$-Cd(2)-O(2W)	82.67(9)

O(4)$^{\#4}$-Cd(2)-O(6)$^{\#2}$	164.39(10)	O(7)$^{\#3}$-Cd(2)-O(1)	85.79(12)
O(1W)-Cd(2)-O(6)$^{\#2}$	110.88(10)	O(4)$^{\#4}$-Cd(2)-O(1)	88.91(10)
O(7)$^{\#3}$-Cd(2)-O(2W)	158.60(10)	O(1W)-Cd(2)-O(1)	173.41(9)
O(4)$^{\#4}$-Cd(2)-O(2W)	103.10(11)	O(6)$^{\#2}$-Cd(2)-O(1)	75.48(9)
O(1W)-Cd(2)-O(2W)	74.65(12)	O(2W)-Cd(2)-O(1)	108.53(13)

Symmetry codes for **2**: #1 = x, y - 1, z; #2 = -x, -y + 2, -z + 1; #3 = x - 1, y - 1, z; #4 = x - 1, y, z.

Table S3. Selected bond distances (Å) and angles (°) for **3**.

|			
Mn(1)-O(7)$^{\#2}$	2.113(2)	Mn(2)-O(5)$^{\#1}$	2.131(2)
Mn(1)-O(6)$^{\#1}$	2.1541(19)	Mn(2)-O(2)$^{\#4}$	2.195(2)
Mn(1)-O(1)	2.192(2)	Mn(2)-O(2W)	2.204(3)
Mn(1)-N(1)	2.219(3)	Mn(2)-O(1W)	2.228(3)
Mn(1)-O(3)	2.250(2)	Mn(2)-O(3)	2.240(2)
Mn(1)-O(8)$^{\#3}$	2.270(2)	Mn(2)-O(8)$^{\#3}$	2.259(2)
O(7)$^{\#2}$-Mn(1)-O(6)$^{\#1}$	89.38(9)	N(1)-Mn(1)-O(8)$^{\#3}$	168.92(9)
O(7)$^{\#2}$-Mn(1)-O(1)	100.97(8)	O(3)-Mn(1)-O(8)$^{\#3}$	74.50(8)
O(6)$^{\#1}$-Mn(1)-O(1)	169.33(8)	O(5)$^{\#1}$-Mn(2)-O(2)$^{\#4}$	91.18(9)
O(7)$^{\#2}$-Mn(1)-N(1)	92.40(10)	O(5)$^{\#1}$-Mn(2)-O(2W)	165.65(9)
O(6)$^{\#1}$-Mn(1)-N(1)	88.47(9)	O(2)$^{\#4}$-Mn(2)-O(2W)	97.62(9)
O(1)-Mn(1)-N(1)	88.48(9)	O(5)$^{\#1}$-Mn(2)-O(1W)	90.80(9)
O(7)$^{\#2}$-Mn(1)-O(3)	171.74(8)	O(2)$^{\#4}$-Mn(2)-O(1W)	84.76(9)
O(6)$^{\#1}$-Mn(1)-O(3)	88.11(9)	O(2W)-Mn(2)-O(1W)	78.80(10)
O(1)-Mn(1)-O(3)	82.00(8)	O(5)$^{\#1}$-Mn(2)-O(3)	91.67(9)
N(1)-Mn(1)-O(3)	95.39(10)	O(2)$^{\#4}$-Mn(2)-O(3)	87.37(8)
O(7)$^{\#2}$-Mn(1)-O(8)$^{\#3}$	97.50(8)	O(2W)-Mn(2)-O(3)	100.01(10)
O(6)$^{\#1}$-Mn(1)-O(8)$^{\#3}$	86.68(8)	O(1W)-Mn(2)-O(3)	171.80(9)
O(1)-Mn(1)-O(8)$^{\#3}$	94.48(8)	O(5)$^{\#1}$-Mn(2)-O(8)$^{\#3}$	88.19(8)
O(2)$^{\#4}$-Mn(2)-O(8)$^{\#3}$	162.24(8)	O(1W)-Mn(2)-O(8)$^{\#3}$	112.99(8)
O(2W)-Mn(2)-O(8)$^{\#3}$	86.85(9)	O(3)-Mn(2)-O(8)$^{\#3}$	74.91(8)

Symmetry codes for **3**: #1 = x - 1, y - 1, z; #2 = x, y - 1, z; #3 = -x + 2, -y + 1, -z + 1; #4 = x - 1, y, z; #5 = -x + 2, -y + 1, -z.

**Table S4**. Selected bond distances (Å) and angles (°) for **4**.

Zn(1)-O(3)$^{\#1}$	1.966(3)	Zn(2)-O(5)$^{\#4}$	1.940(4)
Zn(1)-O(8)$^{\#2}$	1.975(4)	Zn(2)-N(4)$^{\#3}$	1.983(4)
Zn(1)-N(1)	1.986(5)	Zn(2)-N(5)	1.989(4)

Zn(1)-O(2)	2.006(3)	Zn(2)-O(1)	2.004(4)
O(3)$^{#1}$-Zn(1)-O(8)$^{#2}$	104.86(16)	O(5)$^{#4}$-Zn(2)-N(4)$^{#3}$	116.3(2)
O(3)$^{#1}$-Zn(1)-N(1)	115.34(18)	O(5)$^{#4}$-Zn(2)-N(5)	124.8(2)
O(8)$^{#2}$-Zn(1)-N(1)	107.35(18)	N(4)$^{#3}$-Zn(2)-N(5)	110.3(2)
O(3)$^{#1}$-Zn(1)-O(2)	104.63(15)	O(5)$^{#4}$-Zn(2)-O(1)	95.60(18)
O(8)$^{#2}$-Zn(1)-O(2)	102.54(15)	N(4)$^{#3}$-Zn(2)-O(1)	111.83(17)
N(1)-Zn(1)-O(2)	120.41(18)	N(5)-Zn(2)-O(1)	93.05(17)

Symmetry codes for **4**: #1 = -x, -y, -z + 1; #2 = -x + 1,-y, -z + 1; #3 = -x, y - 1/2, - z + 3/2; #4 = -x + 1, y + 1/2, -z + 1.5.
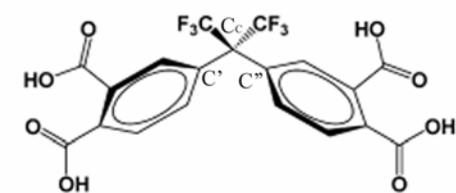
(I)
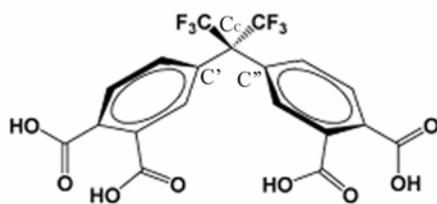
(II)
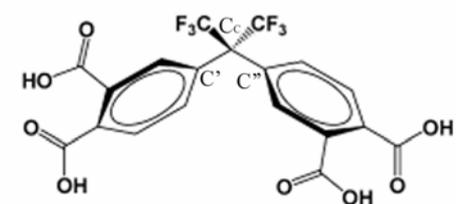
(III)

Scheme S1. The three configurations of H$_4$hfpdpt.
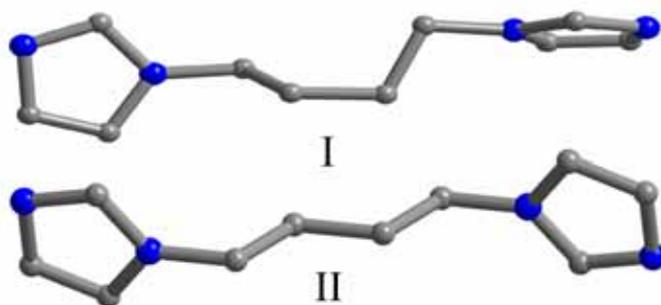
Fig. S1. The two coordination modes of biim-4 ligand.
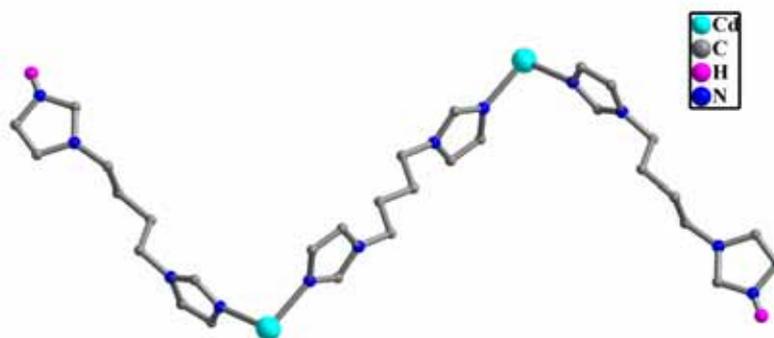
Fig. S2. View of the discrete segment based on the biim-4 ligands and the Cd(II) ions in **1**.
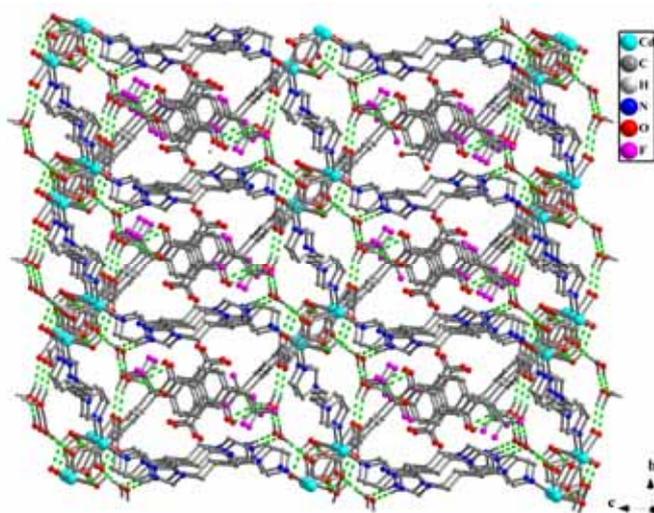

Fig. S3. The 3D supramolecular framework of **1**.

**Fig. S4.** Coordination mode of the biim-4 ligand in **2**.
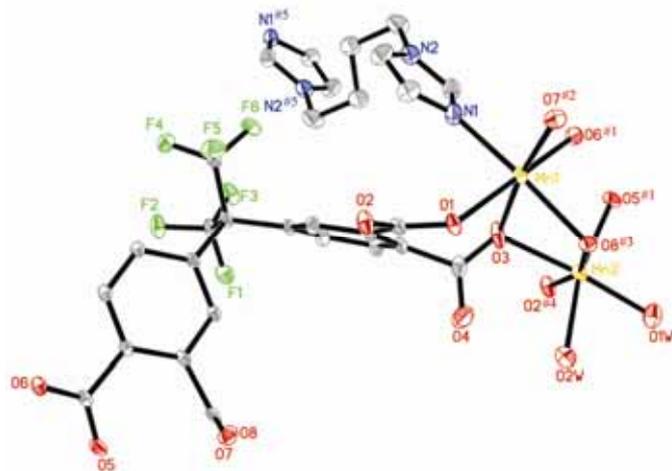
Fig. S5. Coordination environment of the Mn(II) ions in **3** and water molecules have been omitted for clarity (30% probability displacement ellipsoids). Symmetry code: #1 = x - 1, y - 1, z; #2 = x, y - 1, z; #3 = -x + 2, -y + 1, -z + 1; #4 = x - 1, y, z; #5 = -x + 2, -y + 1, -z.
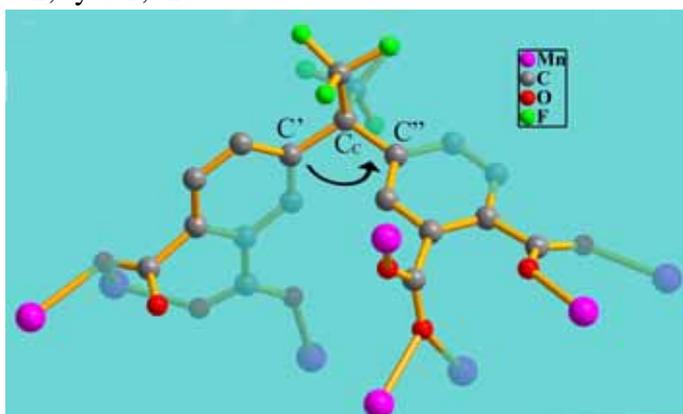
Fig. S6. Coordination mode of the L anion in **3**.
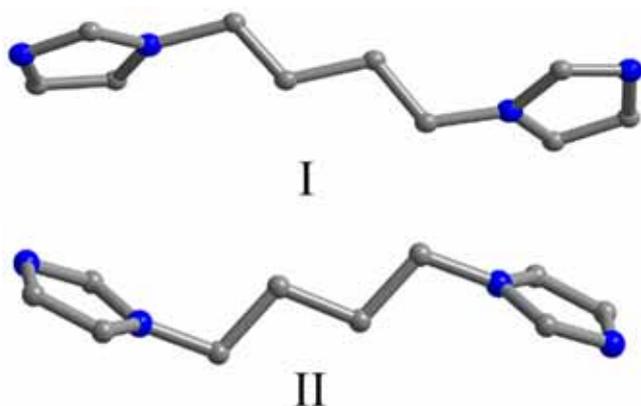
Fig. S7. Coordination modes of the biim-4 ligands in **4**.
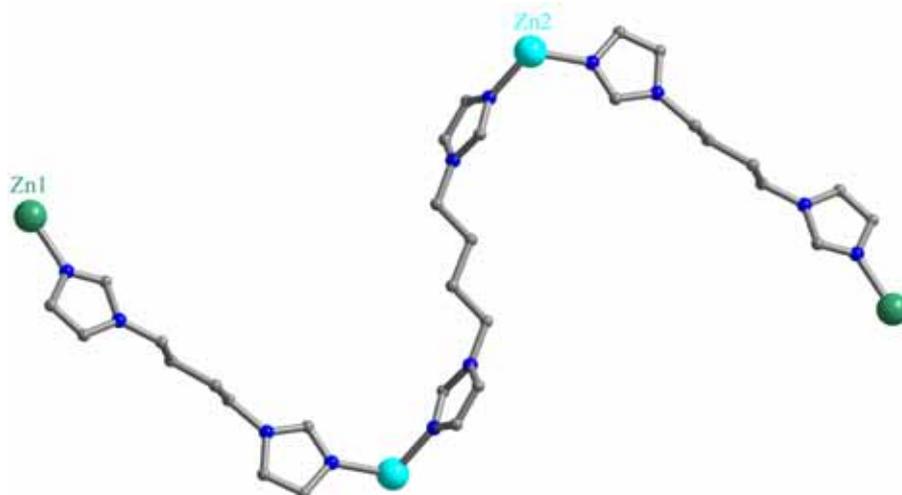
Fig. S8. View of the discrete segment based on the biim-4 ligands and the Cd(II) ions in **4**.
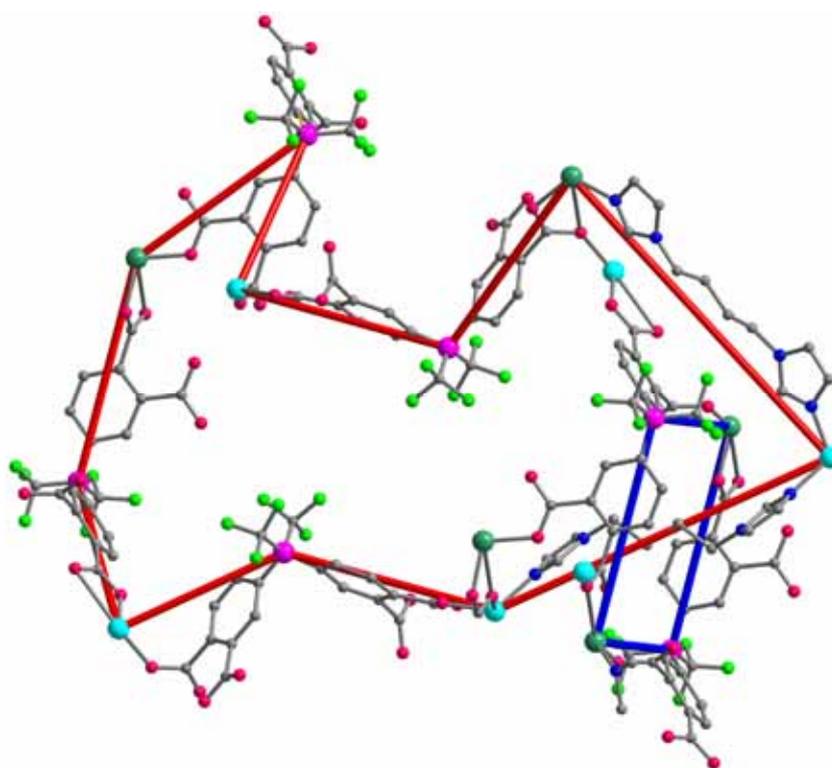
Fig. S9. A schematic illustration of the shortest four-membered circuits passed through by rods of biim-4 ligands of the ten-membered ring in **4**.
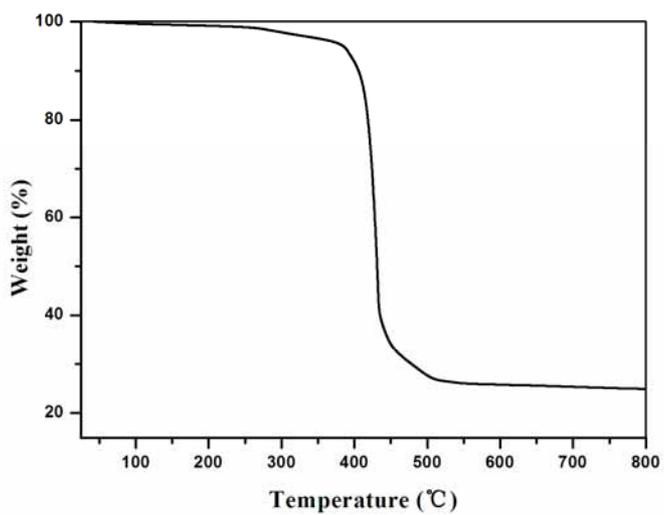
**Fig. S10**. TGA curve of **1**.
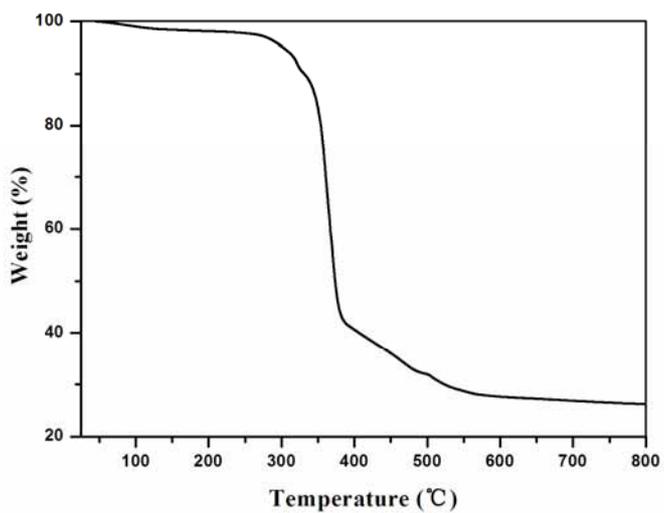
**Fig. S11**. TGA curve of **2**.
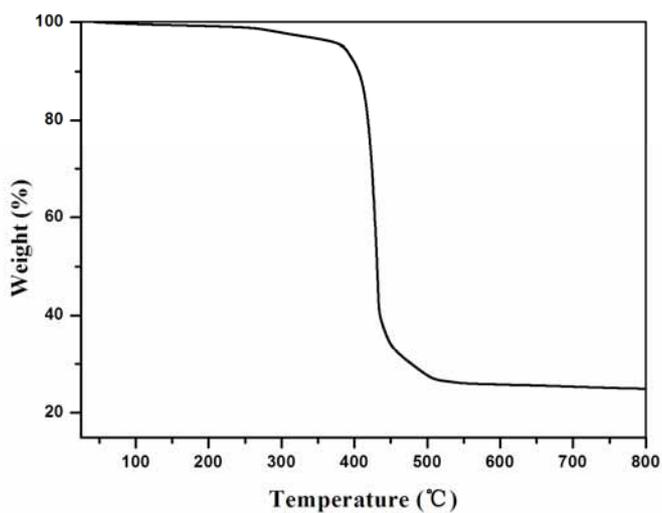
Fig. S12. TGA curve of **4**.
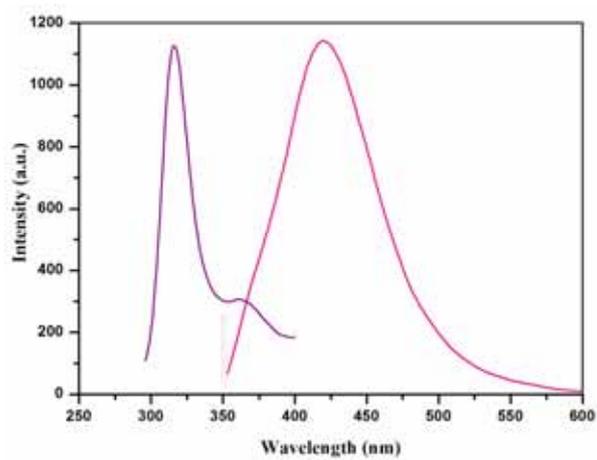

Fig. S13. Emission and the excitation spectra of **1**.
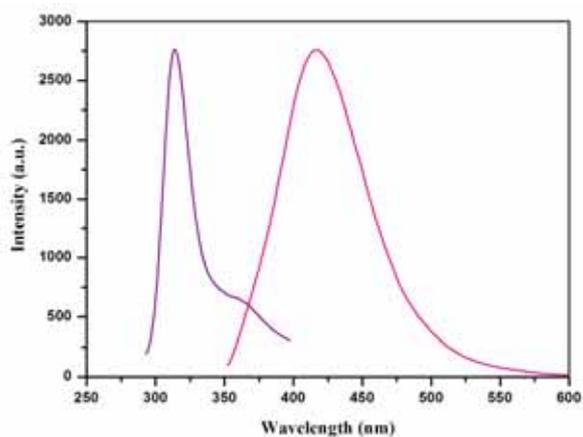

Fig. S14. Emission and the excitation spectra of **2**.
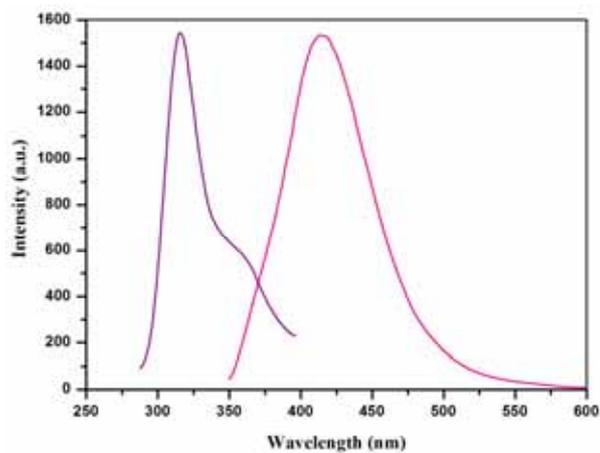
**Fig. S15.** Emission and the excitation spectra of **4**.

Equation	y = A1*exp(-x/t1) + y0	
Adj. R-Square	0.9911	
	Value	Standard Error
y0	-0.00545	1.28775E-4
A1	9.47747E-4	2.5765E-5
t1	1.68789E-8	9.63696E-11

(a)

Equation	y = A1*exp(-x/t1) + y0	
Adj. R-Square	0.9906	
	Value	Standard Error
y0	-0.00669	1.0065E-4
A1	4.12585E-4	1.27402E-5
t1	1.49056E-8	8.51368E-11
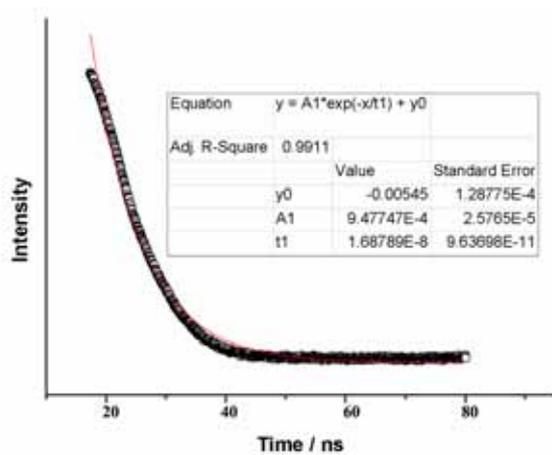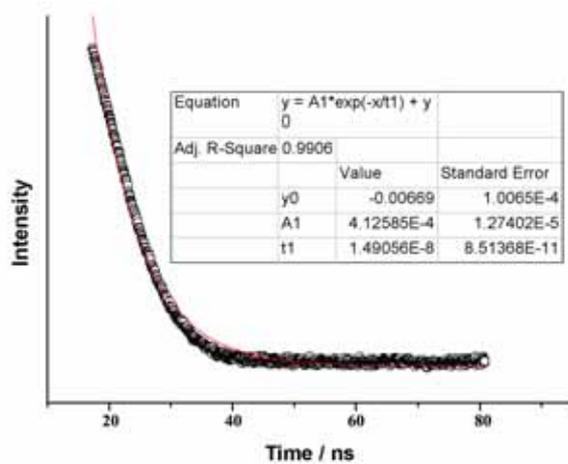
(b)
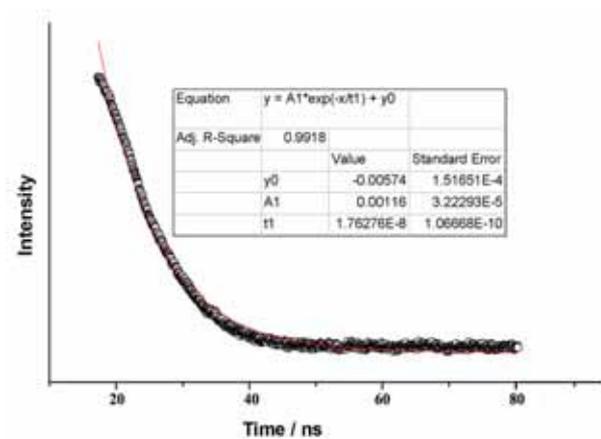
(c)

Fig. S16. Luminescent decay for **1** (λ_{em} = 420 nm) (a), **2** (λ_{em} = 417 nm) (b) and **4** (λ_{em} = 416 nm) (c).