Electronic supplementary information

Four coordination polymers constructed by a novel octacarboxylate functionalized calix[4]arene ligand: syntheses, structures, and photoluminescent property

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Table S1 Selected bond distances (Å) and angles (°) for **1**.

Zn(1)-O(24)	1.948(7)	Zn(1)-O(17)$^{\#1}$	1.958(5)
Zn(1)-O(6)$^{\#2}$	1.960(6)	Zn(1)-O(12)$^{\#3}$	1.987(5)
Zn(2)-O(15)	1.928(6)	Zn(2)-O(5)	2.004(6)
Zn(2)-O(9)$^{\#4}$	1.961(5)	Zn(2)-O(3)$^{\#5}$	2.114(12)
Zn(2)-O(1)$^{\#5}$	2.273(11)	Zn(3)-O(18)	1.965(5)
Zn(3)-O(19)	2.359(5)	Zn(3)-O(21)	1.981(6)
Zn(3)-O(12)$^{\#6}$	2.108(5)	Zn(3)-O(1W)	2.059(6)
Zn(3)-O(2W)	2.094(8)	O(24)-Zn(1)-O(17)$^{\#1}$	100.2(3)
O(24)-Zn(1)-O(6)$^{\#2}$	101.5(3)	O(17)$^{\#1}$-Zn(1)-O(6)$^{\#2}$	103.5(2)
O(24)-Zn(1)-O(12)$^{\#3}$	110.0(4)	O(17)$^{\#1}$-Zn(1)-O(12)$^{\#3}$	108.2(2)
O(6)$^{\#2}$-Zn(1)-O(12)$^{\#3}$	129.6(2)	O(15)-Zn(2)-O(9)$^{\#4}$	122.2(3)
O(15)-Zn(2)-O(5)	107.4(2)	O(15)-Zn(2)-O(3)$^{\#5}$	104.1(5)
O(9)$^{\#4}$-Zn(2)-O(5)	99.4(2)	O(9)$^{\#4}$-Zn(2)-O(3)$^{\#5}$	128.0(5)
O(5)-Zn(2)-O(3)$^{\#5}$	87.0(3)	O(15)-Zn(2)-O(2)$^{\#5}$	104.0(4)
O(9)$^{\#4}$-Zn(2)-O(2)$^{\#5}$	89.3(3)	O(5)-Zn(2)-O(2)$^{\#5}$	135.7(4)
O(3)$^{\#5}$-Zn(2)-O(2)$^{\#5}$	55.2(4)	O(18)-Zn(3)-O(21)	165.5(2)
O(18)-Zn(3)-O(1W)	93.8(3)	O(21)-Zn(3)-O(1W)	89.3(3)

O(18)-Zn(3)-O(2W)	88.1(3)	O(21)-Zn(3)-O(2W)	89.3(3)
O(1W)-Zn(3)-O(2W)	177.3(3)	O(18)-Zn(3)-O(12)$^{\#6}$	93.3(2)
O(21)-Zn(3)-O(12)$^{\#6}$	100.9(2)	O(1W)-Zn(3)-O(12)$^{\#6}$	87.8(2)
O(2W)-Zn(3)-O(12)$^{\#6}$	90.2(3)	O(18)-Zn(3)-O(19)	90.7(2)
O(21)-Zn(3)-O(19)	75.03(19)	O(1W)-Zn(3)-O(19)	92.8(2)
O(2W)-Zn(3)-O(19)	89.0(2)	O(12)$^{\#6}$-Zn(3)-O(19)	175.87(19)

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

Table S2 Selected bond distances (Å) and angles (°) for **2**.

Co(1)-O(5)	2.049(5)	Co(1)-O(9)	2.131(5)
Co(1)-O(13)	2.135(6)	Co(1)-O(3)$^{\#1}$	2.055(5)
Co(1)-O(11)$^{\#2}$	2.146(5)	Co(1)-O(3W)	2.119(7)
Co(2)-O(11)	2.119(5)	Co(2)-O(9)$^{\#1}$	2.089(5)
Co(2)-O(2)$^{\#3}$	2.066(6)	Co(2)-O(1W)	2.070(6)
Co(2)-O(2W)	2.153(6)	Co(2)-O(4W)	2.066(7)
O(5)-Co(1)-O(3)$^{\#1}$	173.9(2)	O(5)-Co(1)-O(3W)	96.5(3)
O(3)$^{\#1}$-Co(1)-O(3W)	85.6(3)	O(5)-Co(1)-O(9)	90.6(2)
O(3)$^{\#1}$-Co(1)-O(9)	88.3(2)	O(3W)-Co(1)-O(9)	169.0(3)
O(5)-Co(1)-O(13)	87.1(2)	O(3)$^{\#1}$-Co(1)-O(13)	87.2(2)
O(3W)-Co(1)-O(13)	88.3(3)	O(9)-Co(1)-O(13)	100.4(2)
O(5)-Co(1)-O(11)$^{\#2}$	95.7(2)	O(3)$^{\#1}$-Co(1)-O(11)$^{\#2}$	89.8(2)
O(3W)-Co(1)-O(11)$^{\#2}$	94.9(3)	O(9)-Co(1)-O(11)$^{\#2}$	76.0(2)
O(13)-Co(1)-O(11)$^{\#2}$	175.5(2)	O(2)$^{\#3}$-Co(2)-O(4W)	174.4(3)
O(2)$^{\#3}$-Co(2)-O(1W)	85.8(3)	O(4W)-Co(2)-O(1W)	93.2(3)
O(2)$^{\#3}$-Co(2)-O(9)$^{\#1}$	90.9(2)	O(4W)-Co(2)-O(9)$^{\#1}$	94.7(3)
O(1W)-Co(2)-O(9)$^{\#1}$	103.2(2)	O(2)$^{\#3}$-Co(2)-O(11)	93.3(2)
O(4W)-Co(2)-O(11)	87.7(3)	O(1W)-Co(2)-O(11)	178.8(3)
O(9)$^{\#1}$-Co(2)-O(11)	77.49(19)	O(2)$^{\#3}$-Co(2)-O(2W)	86.0(3)
O(4W)-Co(2)-O(2W)	88.4(3)	O(1W)-Co(2)-O(2W)	88.2(2)
O(9)$^{\#1}$-Co(2)-O(2W)	167.9(2)	O(11)-Co(2)-O(2W)	91.0(2)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x+1, -x+y+1, -z+4/3; $^{\#2}$ -x+1, -x+y, -z+4/3; $^{\#3}$ x, y+1, z; $^{\#4}$ y, x, -z+1; $^{\#5}$ x, y-1, z.

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

Ni(1)-O(6)	2.037(6)	Ni(1)-O(9)	2.101(7)
Ni(1)-O(13)	2.111(7)	Ni(1)-O(2)$^{\#1}$	2.040(7)
Ni(1)-O(12)$^{\#2}$	2.134(7)	Ni(1)-O(3W)	2.070(8)
Ni(2)-O(12)	2.086(7)	Ni(2)-O(9)$^{\#1}$	2.062(6)
Ni(2)-O(3)$^{\#3}$	2.038(8)	Ni(2)-O(1W)	2.054(7)
Ni(2)-O(2W)	2.114(7)	Ni(2)-O(4W)	2.050(9)
O(6)-Ni(1)-O(2)$^{\#1}$	173.9(3)	O(6)-Ni(1)-O(3W)	95.8(3)
O(2)$^{\#1}$-Ni(1)-O(3W)	85.4(3)	O(6)-Ni(1)-O(9)	90.8(3)
O(2)$^{\#1}$-Ni(1)-O(9)	89.0(3)	O(3W)-Ni(1)-O(9)	168.8(3)
O(6)-Ni(1)-O(13)	86.0(3)	O(2)$^{\#1}$-Ni(1)-O(13)	88.0(3)
O(3W)-Ni(1)-O(13)	89.3(3)	O(9)-Ni(1)-O(13)	100.2(3)
O(6)-Ni(1)-O(12)$^{\#2}$	95.5(3)	O(2)$^{\#1}$-Ni(1)-O(12)$^{\#2}$	90.4(3)
O(3W)-Ni(1)-O(12)$^{\#2}$	94.1(3)	O(9)-Ni(1)-O(12)$^{\#2}$	76.3(3)
O(13)-Ni(1)-O(12)$^{\#2}$	176.1(3)	O(3)$^{\#3}$-Ni(2)-O(4W)	174.2(3)
O(3)$^{\#3}$-Ni(2)-O(1W)	84.8(4)	O(4W)-Ni(2)-O(1W)	93.3(4)
O(3)$^{\#3}$-Ni(2)-O(9)$^{\#1}$	91.2(3)	O(4W)-Ni(2)-O(9)$^{\#1}$	94.6(3)
O(1W)-Ni(2)-O(9)$^{\#1}$	101.5(3)	O(3)$^{\#3}$-Ni(2)-O(12)	94.2(3)
O(4W)-Ni(2)-O(12)	87.7(3)	O(1W)-Ni(2)-O(12)	179.0(4)
O(9)$^{\#1}$-Ni(2)-O(12)	78.2(2)	O(3)$^{\#3}$-Ni(2)-O(2W)	85.8(3)
O(4W)-Ni(2)-O(2W)	88.6(4)	O(1W)-Ni(2)-O(2W)	88.4(3)
O(9)$^{\#1}$-Ni(2)-O(2W)	169.4(3)	O(12)-Ni(2)-O(2W)	91.9(3)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x+1, -x+y+1, -z+4/3; $^{\#2}$ -x+1, -x+y, -z+4/3; $^{\#3}$ x, y+1, z; $^{\#4}$ y, x, -z+1; $^{\#5}$ x, y-1, z.

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

Mn(1)-O(7)	2.332(5)	Mn(1)-O(8)	2.233(4)
Mn(1)-O(10)$^{\#1}$	2.098(4)	Mn(1)-O(16)$^{\#2}$	2.112(5)
Mn(1)-O(13)$^{\#3}$	2.142(5)	Mn(1)-O(23)$^{\#4}$	2.174(5)
Mn(2)-O(17)	2.085(6)	Mn(2)-O(19)	2.117(5)
Mn(2)-O(25)	2.160(5)	Mn(2)-O(6W)	2.205(5)
Mn(2)-O(23)$^{\#5}$	2.333(5)	Mn(2)-O(22)$^{\#5}$	2.355(6)
Mn(3)-O(5)	2.109(5)	Mn(3)-O(1W)	2.154(5)
Mn(3)-O(2W)	2.190(7)	Mn(3)-O(3W)	2.149(5)
Mn(3)-O(4W)	2.225(7)	Mn(3)-O(5W)	2.137(6)
O(10)$^{\#1}$-Mn(1)-O(16)$^{\#2}$	102.3(2)	O(10)$^{\#1}$-Mn(1)-O(13)$^{\#3}$	89.3(2)
O(16)$^{\#2}$-Mn(1)-O(13)$^{\#3}$	81.6(2)	O(10)$^{\#1}$-Mn(1)-O(23)$^{\#4}$	88.4(2)

O(16)$^{\#2}$-Mn(1)-O(23)$^{\#4}$	90.2(2)	O(13)$^{\#3}$-Mn(1)-O(23)$^{\#4}$	170.84(19)
O(10)$^{\#1}$-Mn(1)-O(8)	103.38(19)	O(16)$^{\#2}$-Mn(1)-O(8)	154.2(2)
O(13)$^{\#3}$-Mn(1)-O(8)	96.2(2)	O(23)$^{\#4}$-Mn(1)-O(8)	92.93(19)
O(10)$^{\#1}$-Mn(1)-O(7)	160.51(19)	O(16)$^{\#2}$-Mn(1)-O(7)	97.4(2)
O(13)$^{\#3}$-Mn(1)-O(7)	95.2(2)	O(23)$^{\#4}$-Mn(1)-O(7)	89.8(2)
O(8)-Mn(1)-O(7)	57.06(17)	O(17)-Mn(2)-O(19)	140.1(2)
O(17)-Mn(2)-O(25)	86.8(2)	O(19)-Mn(2)-O(25)	88.7(2)
O(17)-Mn(2)-O(6W)	87.2(2)	O(19)-Mn(2)-O(6W)	91.6(2)
O(25)-Mn(2)-O(6W)	170.2(2)	O(17)-Mn(2)-O(23)$^{\#5}$	85.79(18)
O(19)-Mn(2)-O(23)$^{\#5}$	134.07(18)	O(25)-Mn(2)-O(23)$^{\#5}$	95.03(19)
O(6W)-Mn(2)-O(23)$^{\#5}$	91.8(2)	O(17)-Mn(2)-O(22)$^{\#5}$	140.2(2)
O(19)-Mn(2)-O(22)$^{\#5}$	79.65(19)	O(25)-Mn(2)-O(22)$^{\#5}$	96.2(2)
O(6W)-Mn(2)-O(22)$^{\#5}$	93.6(2)	O(23)$^{\#5}$-Mn(2)-O(22)$^{\#5}$	54.43(18)
O(5)-Mn(3)-O(5W)	96.3(2)	O(5)-Mn(3)-O(3W)	91.5(2)
O(5W)-Mn(3)-O(3W)	171.8(2)	O(5)-Mn(3)-O(1W)	172.5(3)
O(5W)-Mn(3)-O(1W)	88.9(2)	O(3W)-Mn(3)-O(1W)	83.0(2)
O(5)-Mn(3)-O(2W)	91.2(3)	O(5W)-Mn(3)-O(2W)	89.8(3)
O(3W)-Mn(3)-O(2W)	92.4(2)	O(1W)-Mn(3)-O(2W)	93.8(2)
O(5)-Mn(3)-O(4W)	86.4(3)	O(5W)-Mn(3)-O(4W)	90.6(4)
O(3W)-Mn(3)-O(4W)	87.5(2)	O(1W)-Mn(3)-O(4W)	88.3(3)
O(2W)-Mn(3)-O(4W)	177.6(2)		

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ x+1, y, z; $^{\#2}$ x+1, y, z-1; $^{\#3}$ -x+1, -y, -z; $^{\#4}$ -x+1, -y+1, -z; $^{\#5}$ -x, -y+1, -z+1; $^{\#6}$ x-1, y, z; $^{\#7}$ x-1, y, z+1.

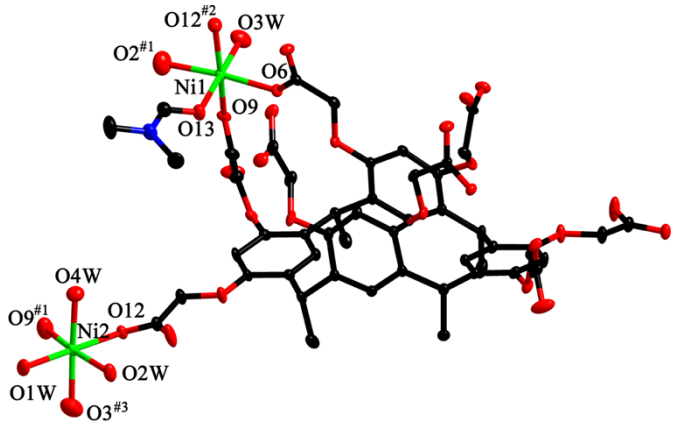

Fig. S1 Coordination spheres surrounding Ni(II) ions in **3**.

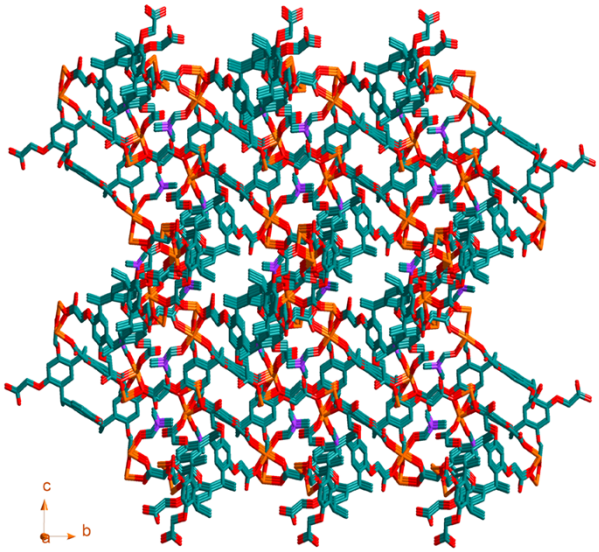

Fig. S2 View of the 3D frameworks of **2** and **3**.

Fig. S3 View of the 3D framework of **4**.

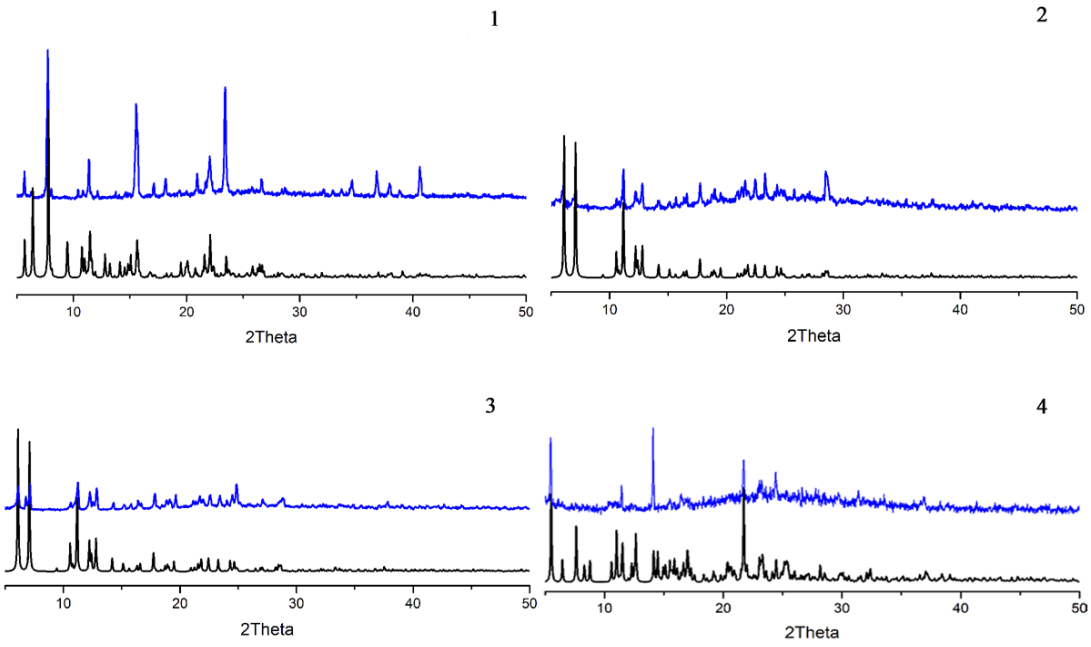

Fig. S4 The simulated (black) and experimental (blue) PXRD patterns for compounds **1-4**.

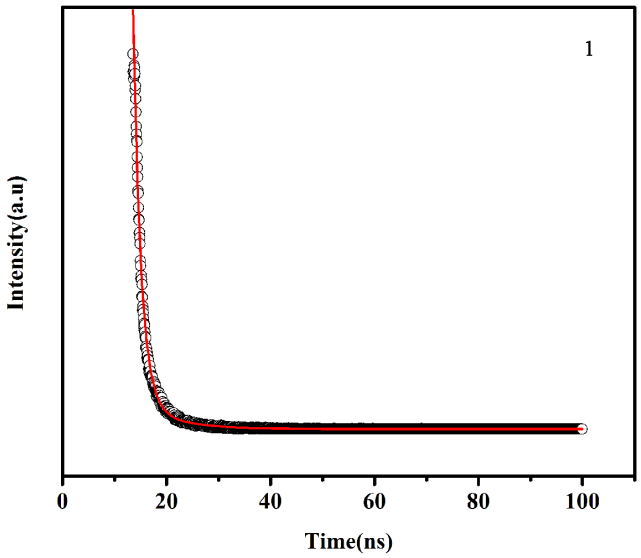

Fig. S5 Luminescence decay curve for compound **1** (the black circles represent experimental data, and the solid red line represent fitting result).

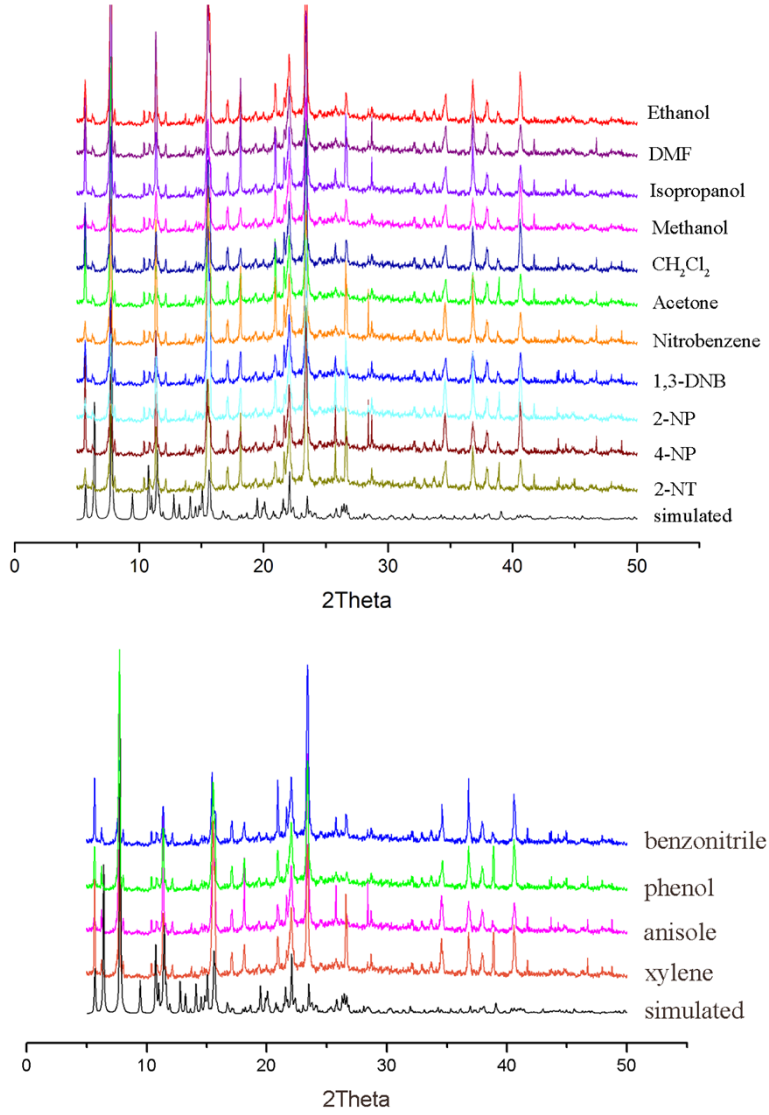

Fig. S6 PXRD patterns of **1** in various solvents and the simulated one.