Five 8-Hydroxyquinolinate-Based Coordination Polymers with Tunable Structures and Photoluminescent Properties for Sensing Nitroaromatics

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1.1. Table S1. Crystal data and structure refinement for complexes **1**-**5**.

Complex	**1**	**2**	**3**	**4**	**5**
formula	$C_{120}H_{84}N_{18}O_6Zn_3$	$C_{42}H_{36}N_6O_4Zn$	$C_{40}H_{28}N_6O_2Zn$	$C_{40}H_{28}N_6O_2Cd$	$C_{60}H_{42}Cd_2N_9O_3$
fw	2070.224	754.16	690.05	737.08	1161.82
Temperature (K)	173(2)	173(2)	141(2)	296(2) K	296(2) K
cryst syst	monoclinic	monoclinic	orthorhombic	orthorhombic	rhombohedral
space group	$P2_1/n$	$P2_1/c$	*P*bca	*P*bca	*R*-3
a (Å)	14.440(3)	12.9164(17)	9.168(3)	9.0309(8)	30.7574(16)
b (Å)	23.641(4)	10.2951(14)	17.701(7)	17.7660(15)	30.7574(16)
c (Å)	15.858(3)	14.240(2)	19.845(8)	20.1395(18)	12.1006(12)
α(deg)	90	90	90	90	90
β(deg)	109.184(5)	113.820(3)	90	90	90
γ(deg)	90	90	90	90	120
V(Å^3)	5113.2	1732.3(4)	3220(2)	3231.0(5)	9913.7(12)
Z	2	2	4	4	6
D_c (g·cm^{-3})	1.345	1.344	1.423	1.515	1.168
F(000)	2136	725	1424	1496	3822
μ (mm^{-1})	0.765	0.755	0.810	0.723	0.700
reflns/unique	20936/8952	9981/3948	13398/3639	15611/2837	20753/5015
R_{int}	0.0753	0.0290	0.0382	0.0459	0.0284
data/restraints/ params	8952/18/689	3948/0/244	3639/0/224	2837/0/224	5015/0/262
GOF on F^2	0.947	1.095	1.033	1.073	1.051
R_1, wR_2 ($I > 2\sigma(I)$)	0.0680, 0.1643	0.0407, 0.0948	0.0363, 0.1052	0.0821, 0.2069	0.0278, 0.0815
R_1, wR_2 (all data)	0.1340, 0.1942	0.0521, 0.1001	0.0619, 0.1215	0.1045, 0.2338	0.0354, 0.0854
largest diff. peak and hole (e·Å^{-3})	0.738, -0.369	0.502, -0.424	0.307, -0.274	0.608, -3.882	0.872, -0.312

1.2. Table S2 Selected Bond lengths [Å] and angles [º] for **1**.

Zn(1)-O(1)#1	2.033(3)
Zn(1)-O(1)	2.033(3)
Zn(1)-N(1)	2.221(4)
Zn(1)-N(1)#1	2.221(4)
Zn(1)-N(9)#2	2.246(4)
Zn(1)-N(9)#3	2.246(4)
Zn(2)-O(2)	1.931(3)
Zn(2)-O(3)	1.961(4)
Zn(2)-N(2)	2.087(5)
Zn(2)-N(7)	2.167(4)
Zn(2)-N(4)	2.261(5)
O(1)#1-Zn(1)-O(1)	180.00(8)
O(1)#1-Zn(1)-N(1)	101.99(15)
O(1)-Zn(1)-N(1)	78.01(15)
O(1)#1-Zn(1)-N(1)#1	78.00(15)
O(1)-Zn(1)-N(1)#1	102.00(15)
N(1)-Zn(1)-N(1)#1	180.0
O(1)#1-Zn(1)-N(9)#2	91.65(14)
O(1)-Zn(1)-N(9)#2	88.35(14)
N(1)-Zn(1)-N(9)#2	86.57(15)
N(1)#1-Zn(1)-N(9)#2	93.43(15)
O(1)#1-Zn(1)-N(9)#3	88.35(14)
O(1)-Zn(1)-N(9)#3	91.65(14)
N(1)-Zn(1)-N(9)#3	93.43(15)
N(1)#1-Zn(1)-N(9)#3	86.57(15)
N(9)#2-Zn(1)-N(9)#3	179.999(1)
O(2)-Zn(2)-O(3)	137.21(17)
O(2)-Zn(2)-N(2)	116.16(19)
O(3)-Zn(2)-N(2)	106.61(18)
O(2)-Zn(2)-N(7)	97.81(15)
O(3)-Zn(2)-N(7)	80.03(16)
N(2)-Zn(2)-N(7)	93.83(19)
O(2)-Zn(2)-N(4)	78.66(16)
O(3)-Zn(2)-N(4)	98.76(16)
N(2)-Zn(2)-N(4)	92.7(2)
N(7)-Zn(2)-N(4)	173.47(19)
C(8)-O(1)-Zn(1)	115.2(3)
C(28)-O(2)-Zn(2)	119.1(3)
C(48)-O(3)-Zn(2)	116.5(3)
C(1)-N(1)-Zn(1)	132.3(4)

C(9)-N(1)-Zn(1)	108.7(3)
C(15)-N(2)-Zn(2)	127.3(4)
C(11)-N(2)-Zn(2)	115.8(4)
C(21)-N(4)-Zn(2)	134.4(5)
C(29)-N(4)-Zn(2)	107.5(3)
C(41)-N(7)-Zn(2)	130.9(4)
C(49)-N(7)-Zn(2)	109.1(3)
C(56)-N(9)-Zn(1)#4	122.7(3)
C(60)-N(9)-Zn(1)#4	121.4(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x, -y+1, -z+1 #2 x-1, y, z #3 -x+1, -y+1, -z+1
#4 x+1, y, z #5 -x+2, -y, -z+2

1.3. Table S3 Selected Bond lengths [Å] and angles [º] for **2**.

Zn(1)-O(1)	2.0199(18)
Zn(1)-O(1)#1	2.0200(18)
Zn(1)-N(3)#2	2.222(2)
Zn(1)-N(3)#3	2.222(2)
Zn(1)-N(1)#1	2.243(2)
Zn(1)-N(1)	2.243(2)
O(1)-Zn(1)-O(1)#1	180.00(9)
O(1)-Zn(1)-N(3)#2	89.86(8)
O(1)#1-Zn(1)-N(3)#2	90.14(8)
O(1)-Zn(1)-N(3)#3	90.14(8)
O(1)#1-Zn(1)-N(3)#3	89.86(8)
N(3)#2-Zn(1)-N(3)#3	180.0
O(1)-Zn(1)-N(1)#1	101.73(8)
O(1)#1-Zn(1)-N(1)#1	78.27(8)
N(3)#2-Zn(1)-N(1)#1	92.92(9)
N(3)#3-Zn(1)-N(1)#1	87.08(9)
O(1)-Zn(1)-N(1)	78.27(8)
O(1)#1-Zn(1)-N(1)	101.73(8)
N(3)#2-Zn(1)-N(1)	87.08(9)
N(3)#3-Zn(1)-N(1)	92.92(9)
N(1)#1-Zn(1)-N(1)	180.00(8)
C(7)-O(1)-Zn(1)	116.17(16)
C(2)-N(1)-Zn(1)	131.8(2)
C(6)-N(1)-Zn(1)	108.08(16)
C(19)-N(3)-Zn(1)#4	118.69(19)
C(18)-N(3)-Zn(1)#4	124.59(18)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1, -y+1, -z #2 -x+1, y-1/2, -z-1/2
#3 x, -y+3/2, z+1/2 #4 -x+1, y+1/2, -z-1/2

1.4. Table S4 Selected Bond lengths [Å] and angles [º] for **3**.

Zn(1)-O(1)#1	2.0001(14)
Zn(1)-O(1)	2.0002(14)
Zn(1)-N(1)	2.2438(18)
Zn(1)-N(1)#1	2.2438(18)
Zn(1)-N(3)#2	2.297(2)
Zn(1)-N(3)#3	2.297(2)
N(3)-Zn(1)#4	2.297(2)
O(1)#1-Zn(1)-O(1)	180.0
O(1)#1-Zn(1)-N(1)	101.31(6)
O(1)-Zn(1)-N(1)	78.69(6)
O(1)#1-Zn(1)-N(1)#1	78.69(6)
O(1)-Zn(1)-N(1)#1	101.31(6)
N(1)-Zn(1)-N(1)#1	180.0
O(1)#1-Zn(1)-N(3)#2	89.47(7)
O(1)-Zn(1)-N(3)#2	90.53(7)
N(1)-Zn(1)-N(3)#2	87.00(7)
N(1)#1-Zn(1)-N(3)#2	93.00(7)
O(1)#1-Zn(1)-N(3)#3	90.53(7)
O(1)-Zn(1)-N(3)#3	89.47(7)
N(1)-Zn(1)-N(3)#3	93.00(7)
N(1)#1-Zn(1)-N(3)#3	87.00(7)
N(3)#2-Zn(1)-N(3)#3	180.00(6)
C(7)-O(1)-Zn(1)	117.16(13)
C(2)-N(1)-Zn(1)	132.13(15)
C(6)-N(1)-Zn(1)	108.38(13)
C(19)-N(3)-Zn(1)#4	122.85(15)
C(20)-N(3)-Zn(1)#4	120.05(15)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1, -y, -z+1 #2 -x+1/2, y-1/2, z
#3 x+1/2, -y+1/2, -z+1 #4 x-1/2, -y+1/2, -z+1

1.5. Table S5 Selected Bond lengths [Å] and angles [º] for **4**.

Cd(1)-O(1)	2.058(3)
Cd(1)-O(1)#1	2.058(3)
Cd(1)-N(1)#1	2.275(4)

Cd(1)-N(1)	2.275(4)
Cd(1)-N(3)#2	2.335(4)
Cd(1)-N(3)#3	2.335(4)
O(1)-Cd(1)-O(1)#1	179.998(1)
O(1)-Cd(1)-N(1)#1	102.98(13)
O(1)#1-Cd(1)-N(1)#1	77.02(13)
O(1)-Cd(1)-N(1)	77.02(13)
O(1)#1-Cd(1)-N(1)	102.98(13)
N(1)#1-Cd(1)-N(1)	179.999(1)
O(1)-Cd(1)-N(3)#2	90.45(13)
O(1)#1-Cd(1)-N(3)#2	89.55(13)
N(1)#1-Cd(1)-N(3)#2	93.49(14)
N(1)-Cd(1)-N(3)#2	86.51(14)
O(1)-Cd(1)-N(3)#3	89.55(13)
O(1)#1-Cd(1)-N(3)#3	90.45(13)
N(1)#1-Cd(1)-N(3)#3	86.50(14)
N(1)-Cd(1)-N(3)#3	93.49(14)
N(3)#2-Cd(1)-N(3)#3	179.999(1)
C(7)-O(1)-Cd(1)	117.2(3)
C(2)-N(1)-Cd(1)	131.0(3)
C(6)-N(1)-Cd(1)	109.6(3)
C(19)-N(3)-Cd(1)#4	123.9(3)
C(20)-N(3)-Cd(1)#4	119.0(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1, -y, -z+1 #2 -x+1/2, y-1/2, z
#3 x+1/2, -y+1/2, -z+1 #4 x-1/2, -y+1/2, -z+1

1.6. Table S6 Selected Bond lengths [Å] and angles [º] for **5**.

Cd(1)-O(1)#1	2.211(3)
Cd(1)-O(1)	2.211(3)
Cd(1)-N(3)#2	2.374(4)
Cd(1)-N(3)#3	2.374(4)
Cd(1)-N(1)	2.380(4)
Cd(1)-N(1)#1	2.380(4)
Cd(2)-N(2)#5	2.383(3)
Cd(2)-N(2)#6	2.383(3)
Cd(2)-N(2)	2.383(3)
Cd(2)-N(2)#7	2.383(3)
Cd(2)-N(2)#8	2.383(3)
N(3)-Cd(1)#9	2.374(4)

O(1)#1-Cd(1)-O(1)	180.0
O(1)#1-Cd(1)-N(3)#2	88.09(14)
O(1)-Cd(1)-N(3)#2	91.91(14)
O(1)#1-Cd(1)-N(3)#3	91.90(14)
O(1)-Cd(1)-N(3)#3	88.10(14)
N(3)#2-Cd(1)-N(3)#3	180.0
O(1)#1-Cd(1)-N(1)	107.55(11)
O(1)-Cd(1)-N(1)	72.46(11)
N(3)#2-Cd(1)-N(1)	91.75(15)
N(3)#3-Cd(1)-N(1)	88.25(15)
O(1)#1-Cd(1)-N(1)#1	72.45(11)
O(1)-Cd(1)-N(1)#1	107.55(11)
N(3)#2-Cd(1)-N(1)#1	88.25(15)
N(3)#3-Cd(1)-N(1)#1	91.75(15)
N(1)-Cd(1)-N(1)#1	180.0
C(7)-O(1)-Cd(1)	116.1(2)
C(2)-N(1)-Cd(1)	128.1(3)
C(6)-N(1)-Cd(1)	110.8(3)
N(2)#4-Cd(2)-N(2)#5	180.0
N(2)#4-Cd(2)-N(2)#6	93.93(12)
N(2)#5-Cd(2)-N(2)#6	86.07(12)
N(2)#4-Cd(2)-N(2)	86.07(12)
N(2)#5-Cd(2)-N(2)	93.93(12)
N(2)#6-Cd(2)-N(2)	86.08(12)
N(2)#4-Cd(2)-N(2)#7	93.93(12)
N(2)#5-Cd(2)-N(2)#7	86.07(12)
N(2)#6-Cd(2)-N(2)#7	93.92(12)
N(2)-Cd(2)-N(2)#7	180.0
N(2)#4-Cd(2)-N(2)#8	86.07(12)
N(2)#5-Cd(2)-N(2)#8	93.93(12)
N(2)#6-Cd(2)-N(2)#8	180.0
N(2)-Cd(2)-N(2)#8	93.93(12)
N(2)#7-Cd(2)-N(2)#8	86.07(12)
C(14)-N(2)-Cd(2)	125.6(3)
C(13)-N(2)-Cd(2)	118.1(3)
C(19)-N(3)-Cd(1)#9	124.9(4)
C(18)-N(3)-Cd(1)#9	118.6(4)

Symmetry transformations used to generate equivalent atoms:

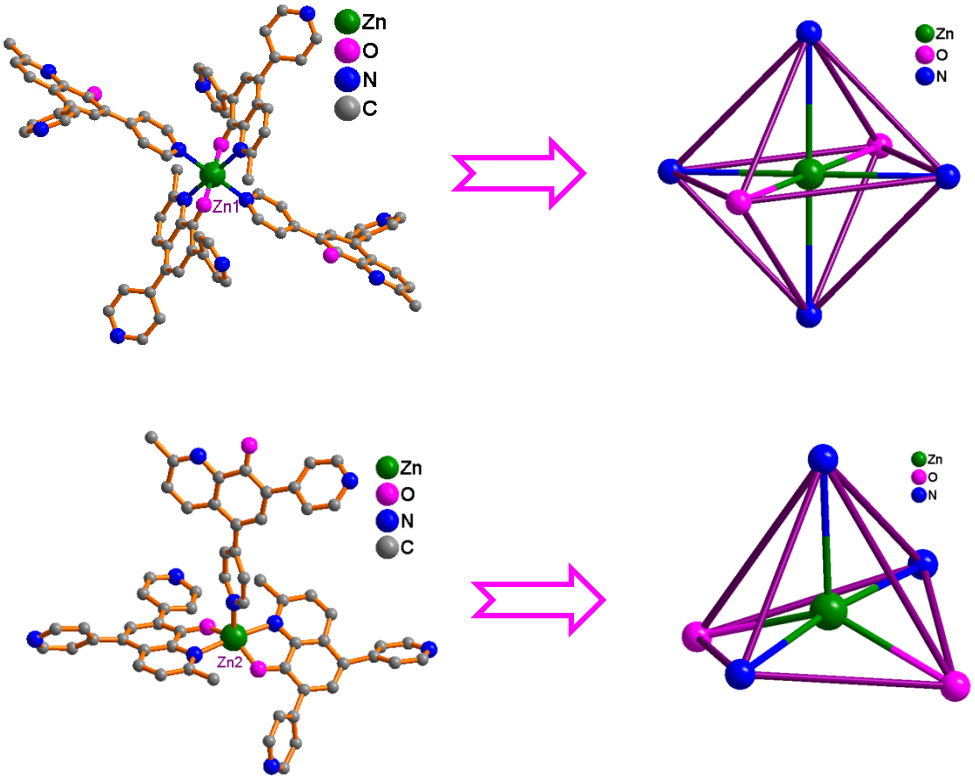
#1 -x-1/3, -y+1/3, -z+1/3 #2 -y-1/3, x-y+1/3, z-2/3

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

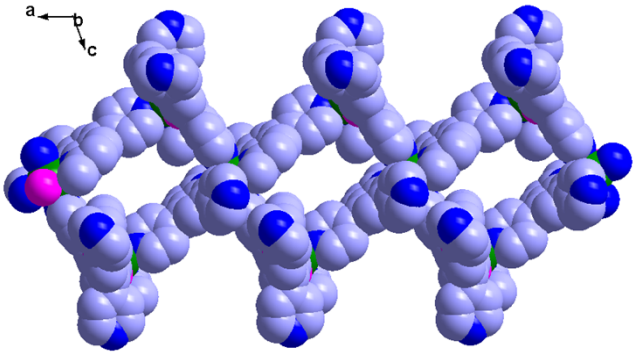
#6 x-y, x, -z #7 -x, -y, -z #8 -x+y, -x, z

#9 -x+y-2/3, -x-1/3, z+2/3

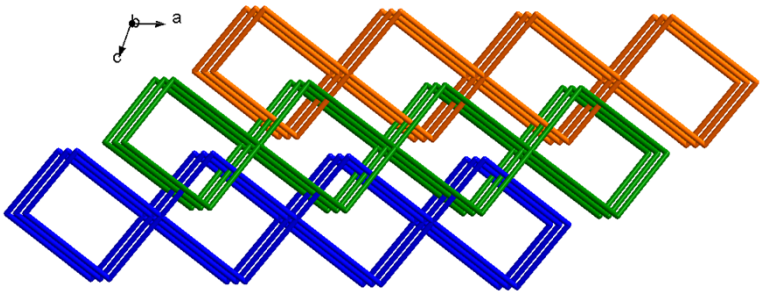
2.1. **Fig. S1** The coordination geometries of Zn1 and Zn2 in **1**



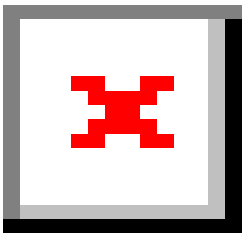
2.2. **Fig. S2** The space-filling mode of 1D infinite chain in **1** along the *a*-axis



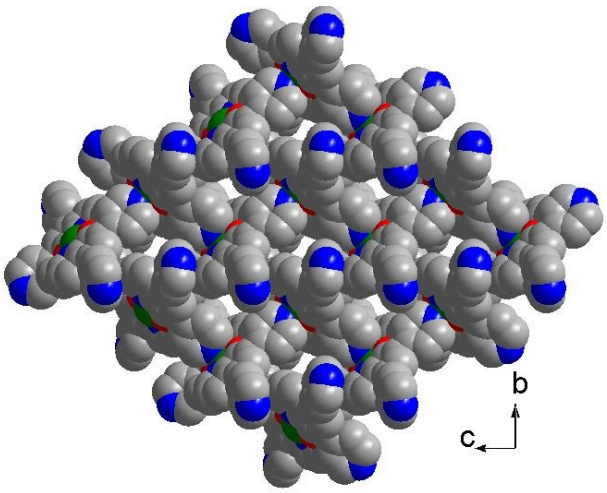
2.3. **Fig. S3** Schematic view showing 3-fold interpenetration in complex **1**.



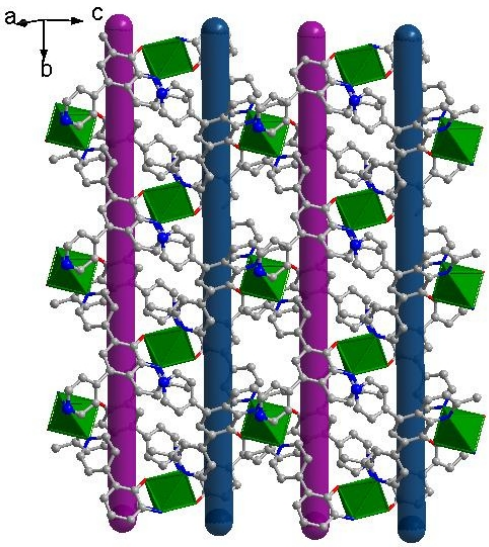
3.1. **Fig. S4** The adjacen layers are connected via nonclassical C-H···N hydrogen bonds in **2**.



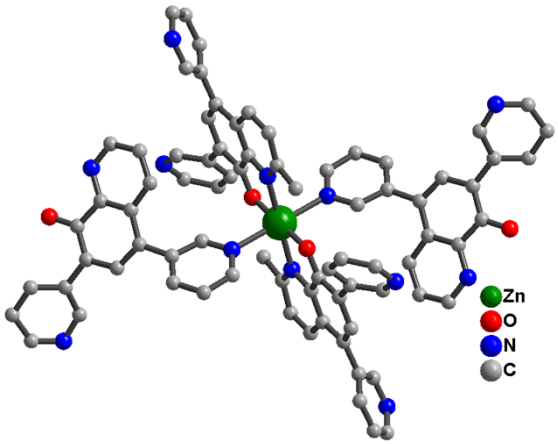
3.2. **Fig. S5** The space-filling mode of 3D network in **2**.



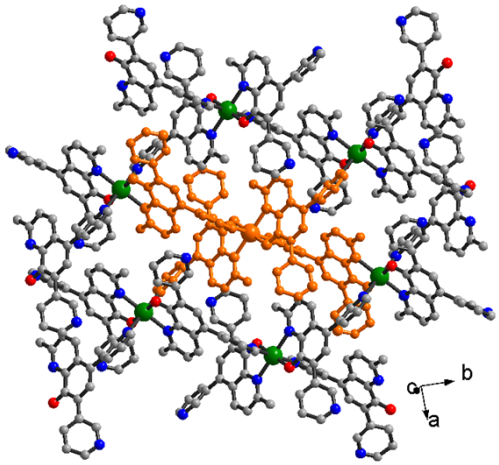
3.3. **Fig. S6** 2D layer structure of **2** containing *meso*-helical chains (*P*+*M*).



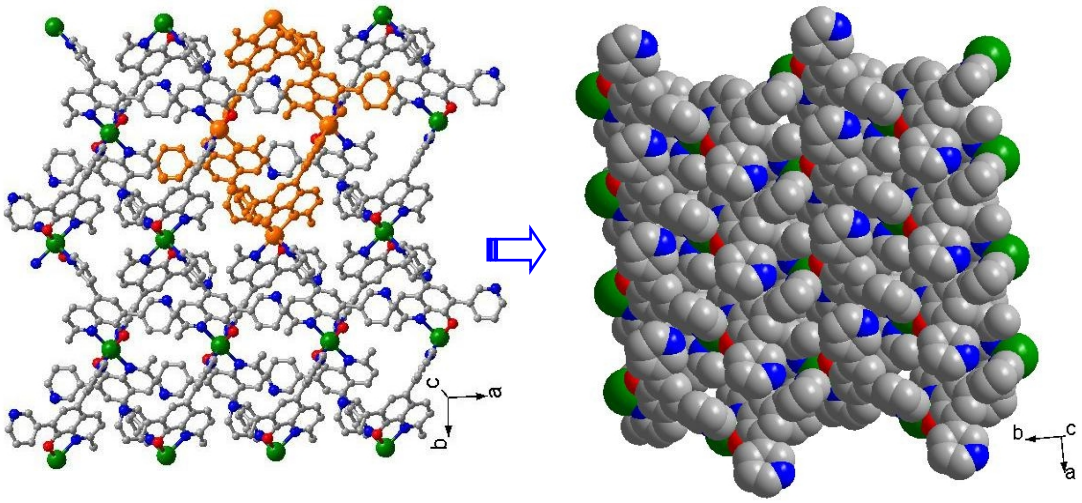
4.1. **Fig. S7** View of the coordination geometries of Zn(II) atoms in **3**.



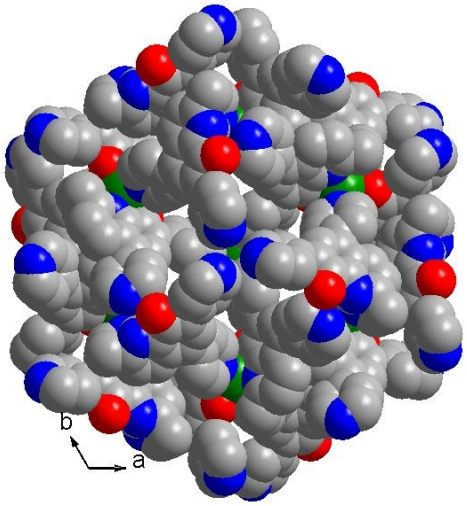
4.2. **Fig. S8** The 2D polymeric network of **3**.



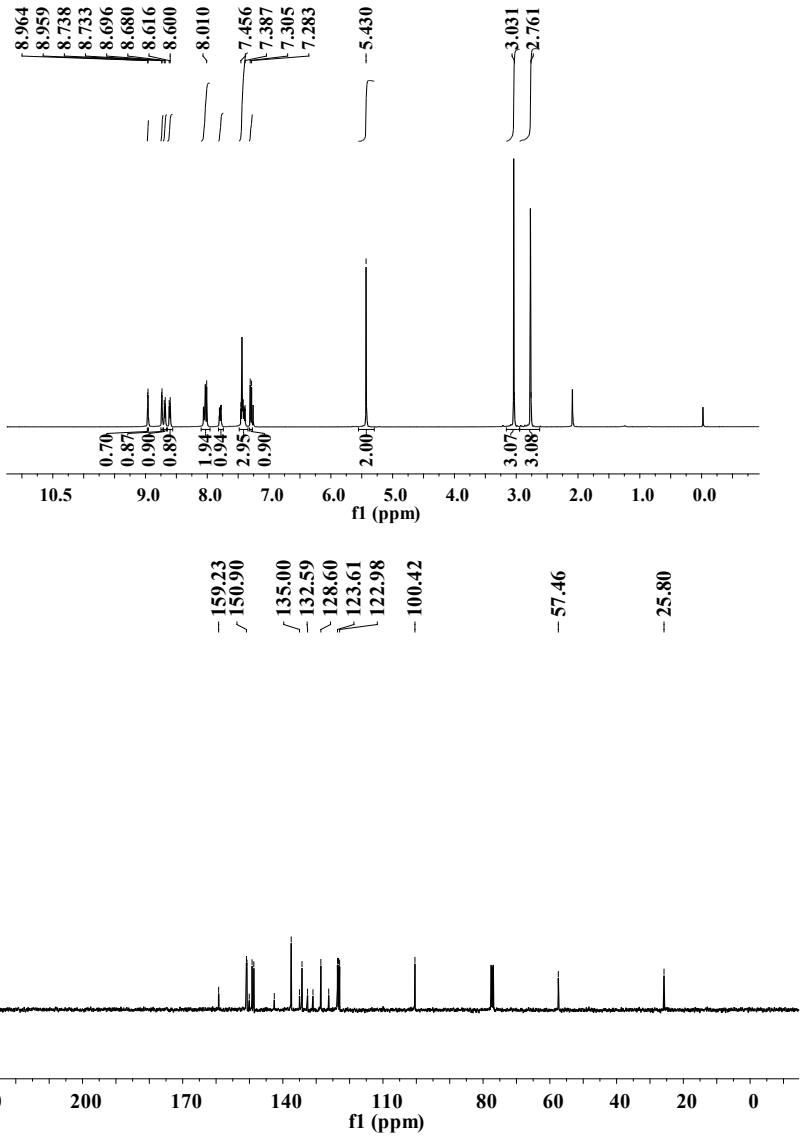
5. **Fig. S9** The 2D polymeric network of **4**.



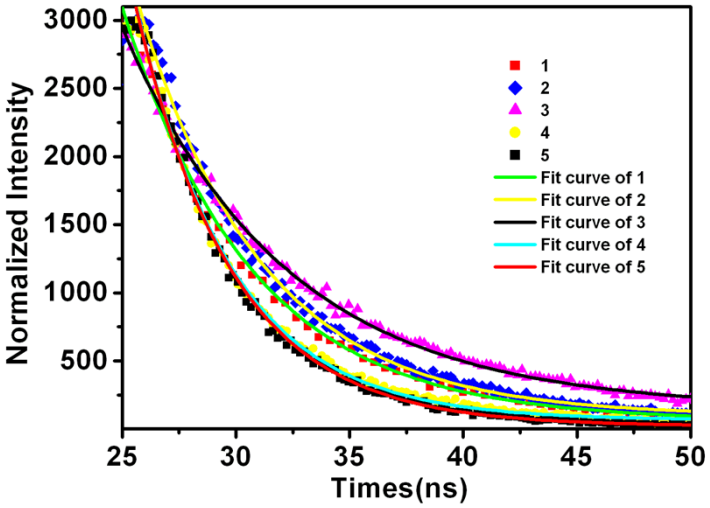
6. **Fig. S10** The space-filling mode of 3D network in **5**.



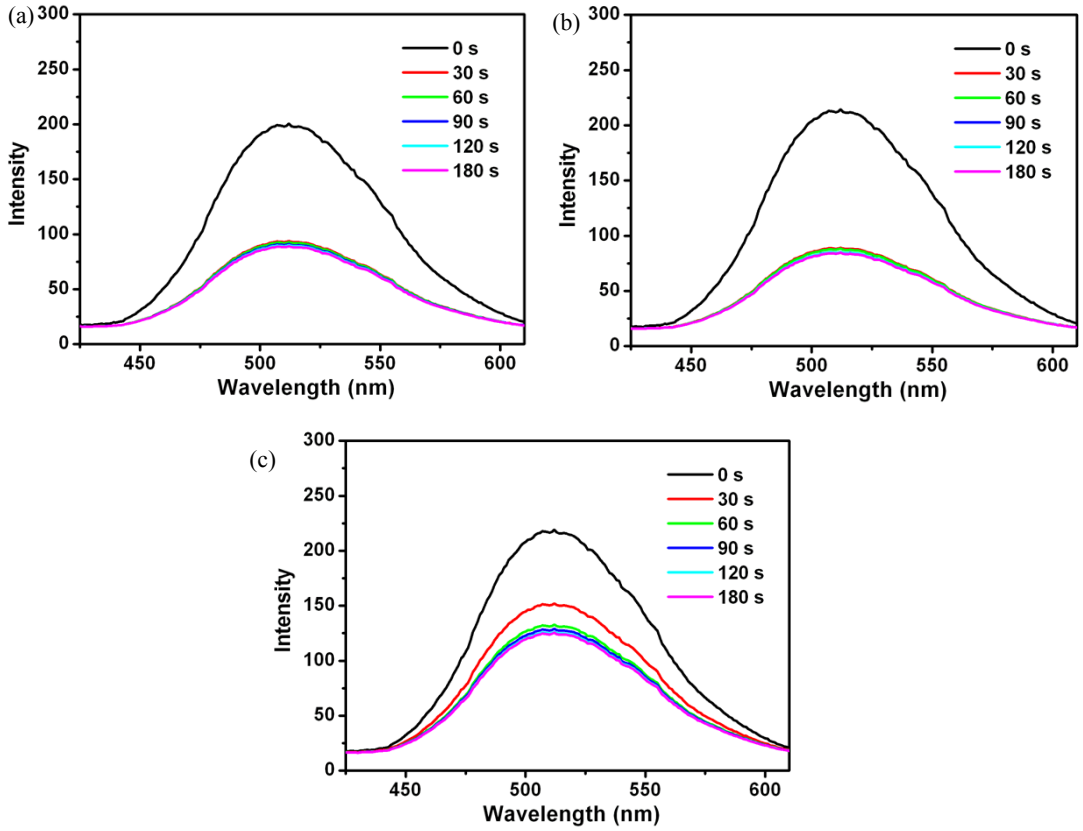
7. **Fig. S11** ^{1}H and ^{13}C NMR spectra of the ligand L_2-MOM.



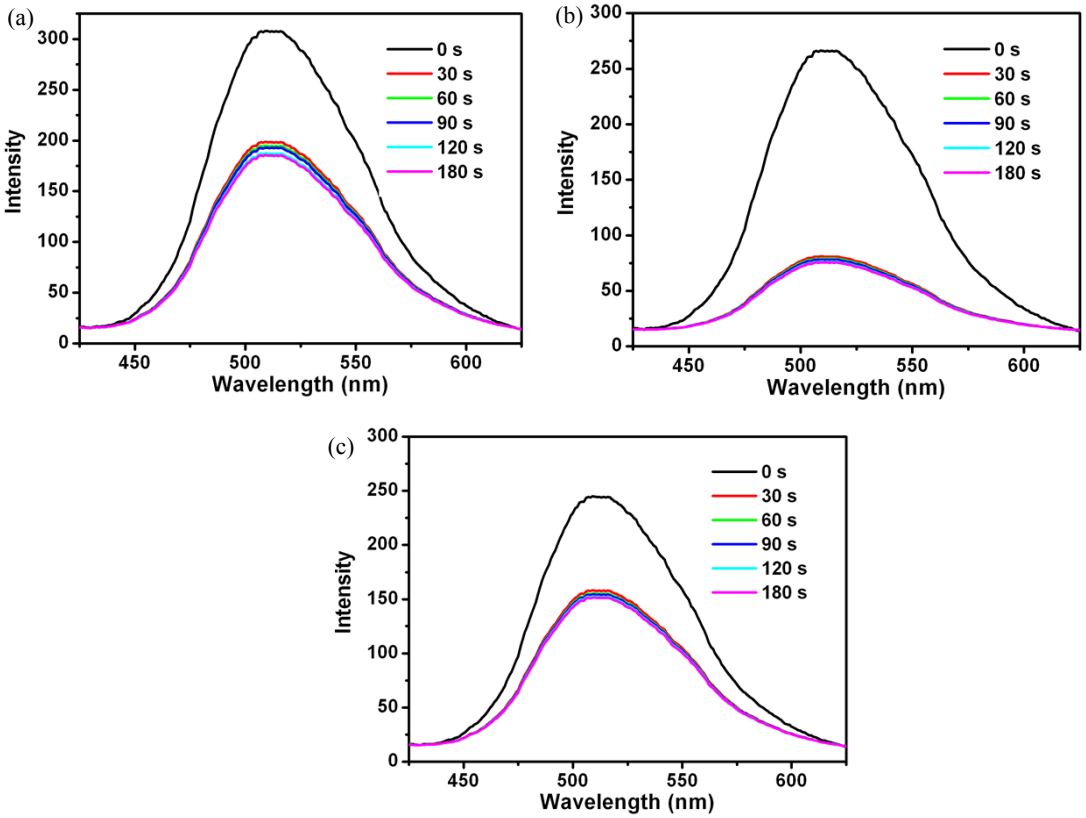
8. **Fig. S12** Fluorescence decay curves of coordination polymers **1-5** in the solid state.



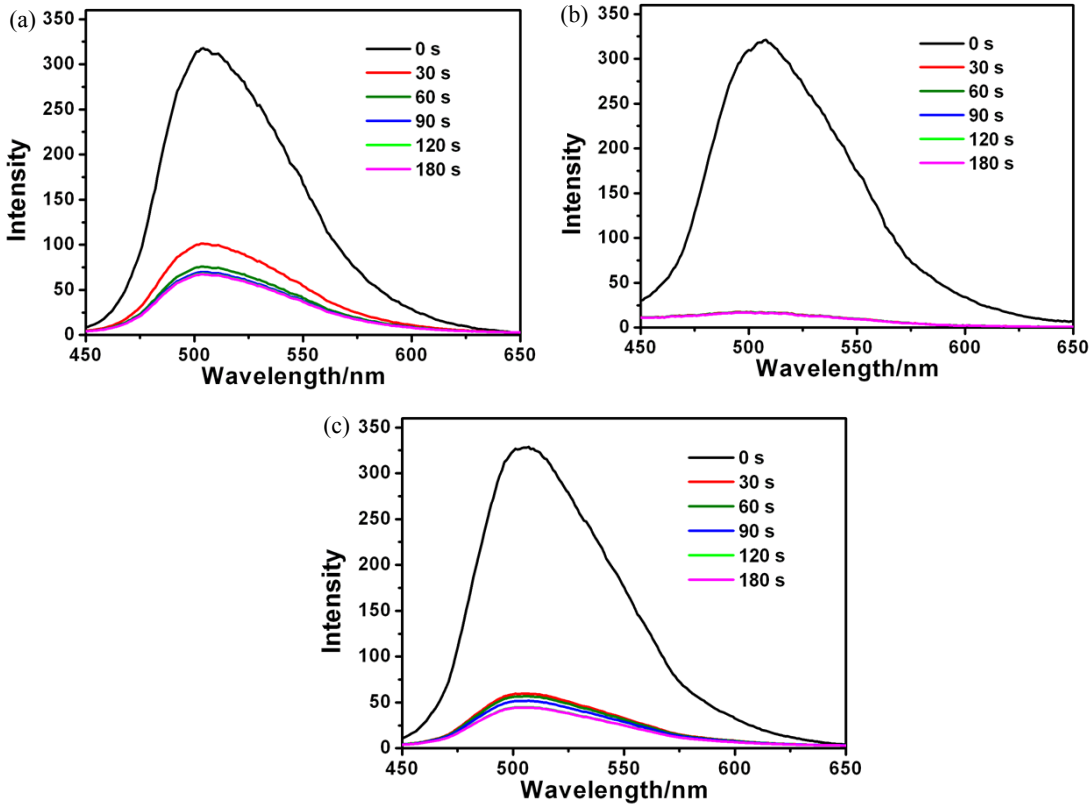
9. **Fig. S13** Fluorescence quench response of **1** upon exposure to NB (a), 2-NT (b) and 3-NT (c) vapour at the specified exposure times.



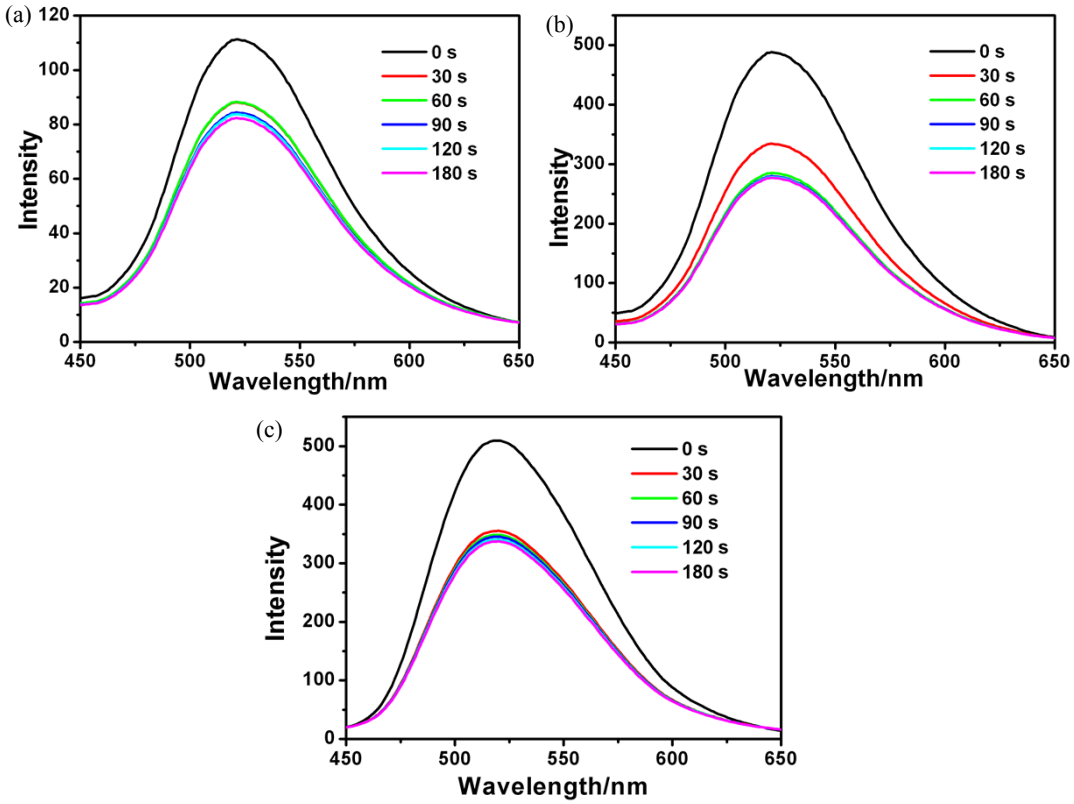
10. **Fig. S14** Fluorescence quench response of **2** upon exposure to NB (a), 2-NT (b) and 3-NT (c) vapour at the specified exposure times.



11. **Fig. S15** Fluorescence quench response of **3** upon exposure to NB (a), 2-NT (b) and 3-NT (c) vapour at the specified exposure times.



12. **Fig. S16** Fluorescence quench response of **4** upon exposure to NB (a), 2-NT (b) and 3-NT (c) vapour at the specified exposure times.



13. **Fig. S17** Fluorescence quench response of **5** upon exposure to NB (a), 2-NT (b) and 3-NT (c) vapour at the specified exposure times.