

Supporting information for

**Assembly of a series of d¹⁰ Coordination Polymers of Pamoic Acid
through Mixed-Ligand Synthetic Strategy:
Syntheses, Structures and Fluorescent Properties**

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Changhui Zhou^a, Dacheng Li^a, Junfeng Bai^{b*}

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Table S1. Selected bond lengths and angles of compounds **1-8**.

1			
Zn(1)-O(1)	1.919(2)	Zn(1)-O(4)#1	1.946(2)
Zn(1)-N(1)#2	2.027(3)	Zn(1)-N(2)	2.034(3)
O(1)-Zn(1)-O(4)#1	123.19(10)	O(1)-Zn(1)-N(1)#2	116.53(11)
O(4)#1-Zn(1)-N(1)#2	100.29(12)	O(1)-Zn(1)-N(2)	96.27(12)
O(4)#1-Zn(1)-N(2)	117.09(12)	N(1)#2-Zn(1)-N(2)	102.48(12)
2			
Cd(1)-O(1)#1	2.314(4)	Cd(1)-O(7)	2.316(4)
Cd(1)-O(1)	2.314(4)	Cd(1)-N(1)	2.347(6)
O(1)#1-Cd(1)-O(1)	175.7(2)	O(1)#1-Cd(1)-O(7)#1	86.15(16)
O(1)-Cd(1)-O(7)#1	96.84(16)	O(7)-Cd(1)-N(1)#1	88.1(2)
O(1)-Cd(1)-O(7)	86.15(16)	O(7)#1-Cd(1)-O(7)	91.4(2)
O(1)#1-Cd(1)-N(1)	97.45(18)	O(1)-Cd(1)-N(1)	79.67(18)
O(7)#1-Cd(1)-N(1)	88.1(2)	O(7)-Cd(1)-N(1)	165.64(17)
N(1)#1-Cd(1)-N(1)	95.9(3)		
3			
Zn(1)-O(1)	1.929(3)	Zn(1)-O(4)#1	1.972(4)
Zn(1)-N(1)	2.021(5)		
O(1)-Zn(1)-O(4)#1	102.02(16)	O(1)-Zn(1)-N(4)#2	127.61(18)
O(4)#1-Zn(1)-N(4)#2	111.1(2)	O(1)-Zn(1)-N(1)	106.42(18)
O(4)#1-Zn(1)-N(1)	103.45(17)	N(4)#2-Zn(1)-N(1)	103.9(2)
4			
Cd(1)-N(3)	2.235(5)	Cd(1)-N(1)	2.253(6)
Cd(1)-O(7)	2.310(5)	Cd(1)-O(1)	2.314(4)
Cd(1)-O(5)#1	2.319(4)	Cd(1)-O(4)#1	2.437(5)
N(3)-Cd(1)-O(7)	115.7(2)	N(3)-Cd(1)-N(1)	95.7(2)
N(3)-Cd(1)-O(1)	97.33(16)	N(1)-Cd(1)-O(7)	77.5(2)
O(7)-Cd(1)-O(1)	82.06(16)	N(1)-Cd(1)-O(1)	159.07(19)
N(1)-Cd(1)-O(5)#1	108.0(2)	N(3)-Cd(1)-O(5)#1	85.87(18)
O(1)-Cd(1)-O(5)#1	89.25(15)	O(7)-Cd(1)-O(5)#1	157.51(19)
N(1)-Cd(1)-O(4)#1	89.1(2)	N(3)-Cd(1)-O(4)#1	139.54(16)
O(1)-Cd(1)-O(4)#1	91.51(16)	O(7)-Cd(1)-O(4)#1	104.57(19)
5			
Cd(1)-N(5)	2.287(5)	Cd(1)-O(2)#1	2.293(4)
Cd(1)-N(1)	2.305(5)	Cd(1)-O(4)#2	2.334(4)
Cd(1)-Cl(1)	2.5423(14)	Cd(1)-O(5)#2	2.555(4)
Cd(2)-N(4)#2	2.226(6)	Cd(2)-N(4)#3	2.226(6)
Cd(2)-Cl(1)#1	2.7649(14)	Cd(2)-Cl(1)	2.7649(14)

Cd(2)-O(1)	2.381(4)	Cd(2)-O(1)#1	2.7649(14)
N(5)-Cd(1)-O(2)#1	87.96(18)	N(5)-Cd(1)-N(1)	92.43(18)
O(2)#1-Cd(1)-N(1)	163.66(16)	N(5)-Cd(1)-O(4)#2	148.00(17)
O(2)#1-Cd(1)-O(4)#2	76.66(16)	N(1)-Cd(1)-O(4)#2	94.86(16)
N(5)-Cd(1)-Cl(1)	105.81(15)	O(2)#1-Cd(1)-Cl(1)	100.58(11)
N(1)-Cd(1)-Cl(1)	95.03(14)	O(4)#2-Cd(1)-Cl(1)	104.52(11)
N(5)-Cd(1)-O(5)#2	95.44(17)	O(2)#1-Cd(1)-O(5)#2	76.45(14)
N(1)-Cd(1)-O(5)#2	87.26(16)	O(4)#2-Cd(1)-O(5)#2	53.96(13)
N(5)-Cd(1)-O(5)#2	95.44(17)	O(2)#1-Cd(1)-O(5)#2	76.45(14)
N(1)-Cd(1)-O(5)#2	87.26(16)	O(4)#2-Cd(1)-O(5)#2	53.96(13)
Cl(1)-Cd(1)-O(5)#2	158.48(10)	N(5)-Cd(1)-C(13)#2	121.19(19)
O(2)#1-Cd(1)-C(13)#2	70.31(16)	N(1)-Cd(1)-C(13)#2	95.75(17)
N(4)#3-Cd(2)-O(1)	89.92(18)	N(4)#2-Cd(2)-O(1)#1	89.92(18)
N(4)#3-Cd(2)-O(1)#1	90.08(18)	N(4)#2-Cd(2)-Cl(1)	90.42(15)
N(4)#3-Cd(2)-Cl(1)	89.58(15)	O(1)-Cd(2)-Cl(1)	78.57(10)
O(1)#1-Cd(2)-Cl(1)	101.43(10)	N(4)#3-Cd(2)-Cl(1)#1	90.42(15)
N(4)#2-Cd(2)-Cl(1)#1	89.58(15)	O(1)-Cd(2)-Cl(1)#1	101.43(10)
O(1)#1-Cd(2)-Cl(1)#1	78.57(10)	Cd(1)-Cl(1)-Cd(2)	102.65(5)

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Zn(1)-O(1)	1.992(4)	Zn(1)-N(1)	2.011(5)
Zn(1)-N(6)	1.996(4)	Zn(1)-O(14)	2.013(3)
Zn(2)-O(7)	1.975(4)	Zn(2)-O(4)	1.961(4)
Zn(2)-N(3)#1	1.969(4)	Zn(2)-N(7)#2	1.950(5)
Zn(3)-O(7)	1.975(4)	Zn(3)-N(8)#4	1.912(8)
Zn(3)-N(2)	2.022(8)	Zn(3)-O(10) #3	2.098(8)
O(1)-Zn(1)-N(1)	105.18(17)	O(1)-Zn(1)-N(6)	106.81(17)
N(1)-Zn(1)-N(6)	105.57(19)	O(1)-Zn(1)-O(14)	132.74(15)
N(1)-Zn(1)-O(14)	98.48(17)	N(6)-Zn(1)-O(14)	105.26(16)
N(7)#2-Zn(2)-O(4)	101.29(19)	N(7)#2-Zn(2)-N(3)	111.84(18)
O(4)-Zn(2)-N(3)#1	105.57(19)	N(7)#2-Zn(2)-O(7)	101.22(19)
O(4)-Zn(2)-O(7)	105.05(19)	N(3)#1-Zn(2)-O(7)	118.4(2)
O(16)-Zn(3)-N(8)#4	119.8(2)	O(16)-Zn(3)-N(2)	111.84(18)
N(8)#4-Zn(3)-N(2)	101.29(19)	O(16)-Zn(3)-O(10)#3	110.22(19)
N(8)#4-Zn(3)-O(10)#3	105.05(19)	N(2)-Zn(3)-O(10)#3	118.4(2)

7

Cd(1)-N(3)#1	2.214(13)	Cd(1)-O(1)	2.217(12)
Cd(1)-N(2)#2	2.244(12)	Cd(1)-N(1)	2.345(13)
Cd(1)-O(4)	2.467(15)	Cd(1)-O(2)	2.805(14)
N(3)#1-Cd(1)-O(1)	105.3(5)	N(3)#1-Cd(1)-N(2)#2	109.8(5)
O(1)-Cd(1)-N(2)#2	142.2(5)	N(3)#1-Cd(1)-N(1)	96.2(5)

O(1)-Cd(1)-N(1)	88.7(5)	N(2)#2-Cd(1)-N(1)	101.1(5)
N(3)#1-Cd(1)-O(4)	94.8(6)	O(1)-Cd(1)-O(4)	81.3(5)
N(2)#2-Cd(1)-O(4)	82.0(5)	N(1)-Cd(1)-O(4)	166.8(5)
N(3)#1-Cd(1)-O(2)	155.6(5)	O(1)-Cd(1)-O(2)	50.4(5)
N(2)#2-Cd(1)-O(2)	93.4(4)	N(1)-Cd(1)-O(2)	86.5(5)
O(4)-Cd(1)-O(2)	80.5(5)		

8

Cd(1)-N(1)	2.246(5)	Cd(1)-N(8)#2	2.285(5)
Cd(1)-O(1)	2.288(4)	Cd(1)-O(7)	2.313(4)
Cd(1)-O(13)	2.449(4)	Cd(1)-O(8)	2.619(4)
Cd(2)-N(5)	2.255(5)	Cd(2)-N(4)#3	2.256(5)
Cd(2)-O(4)	2.326(4)	Cd(2)-O(11)#4	2.393(4)
Cd(2)-O(14)	2.424(5)	Cd(2)-O(10)#4	2.552(5)
Cd(2)-O(3)	2.599(4)	N(1)-Cd(1)-N(8)#2	105.13(17)
N(1)-Cd(1)-O(1)	128.14(16)	N(8)#2-Cd(1)-O(1)	90.46(15)
N(1)-Cd(1)-O(7)	86.86(17)	N(8)#2-Cd(1)-O(7)	94.19(16)
O(1)-Cd(1)-O(7)	141.94(16)	N(1)-Cd(1)-O(13)	89.08(17)
N(8)#2-Cd(1)-O(13)	165.34(16)	O(1)-Cd(1)-O(13)	77.66(15)
O(7)-Cd(1)-O(13)	90.10(15)	N(1)-Cd(1)-O(8)	138.41(16)
N(8)#2-Cd(1)-O(8)	86.87(15)	O(1)-Cd(1)-O(8)	90.53(14)
O(7)-Cd(1)-O(8)	52.17(14)	O(13)-Cd(1)-O(8)	84.71(14)
N(5)-Cd(2)-N(4)#3	168.22(18)	N(5)-Cd(2)-O(4)	87.62(16)
N(4)#3-Cd(2)-O(4)	100.29(15)	N(5)-Cd(2)-O(11)#4	94.16(16)
N(4)#3-Cd(2)-O(11)#4	86.18(16)	O(4)-Cd(2)-O(11)#4	136.19(17)
N(5)-Cd(2)-O(14)	80.77(18)	N(4)#3-Cd(2)-O(14)	87.46(18)
O(4)-Cd(2)-O(14)	133.34(19)	O(11)#4-Cd(2)-O(14)	89.9(2)
N(5)-Cd(2)-O(10)#4	90.89(16)	N(4)#3-Cd(2)-O(10)#4	98.59(16)
O(4)-Cd(2)-O(10)#4	83.73(15)	O(11)#4-Cd(2)-O(10)#4	52.50(16)
O(14)-Cd(2)-O(10)#4	140.96(19)	N(5)-Cd(2)-O(3)	95.01(16)
N(4)#3-Cd(2)-O(3)	83.26(15)	O(4)-Cd(2)-O(3)	52.09(14)
O(11)#4-Cd(2)-O(3)	167.99(15)	O(14)-Cd(2)-O(3)	83.96(19)
O(10)#4-Cd(2)-O(3)	134.96(14)		

Symmetry codes: **1**, #1, x+1,y,z, #2, x,-y-1/2,z+1/2, #3, x,-y-1/2,z-1/2, #4, x-1,y,z; **2**, #1, -x,y,-z+1/2; **3**, #1, x+1/2,-y+1/2,z+1/2, #2, -x+1/2,y-1/2,-z+5/2, #3, x-1/2,-y+1/2,z-1/2; #4, -x+1/2,y+1/2,-z+5/2; **4**, #1, -x+2,-y,-z+2, #2, -x+1,-y+1,-z+3, #3, -x,-y,-z+2; **5**, #1, -x+1,-y+1,-z+1, #2, -x+1/2,y+1/2,-z+1/2, #3, x+1/2,-y+1/2,z+1/2, #4, -x+1/2,y-1/2,-z+1/2, #5, -x+2,-y+1,-z; **6**, #1, 1/2-x, 1/2-y, -z; #2, x, 1-y, -1/2+z; #3, 1-x, y, 1/2-z; #4, 1/2-x, -1/2+y, -1/2-z.; **7**, #1, -x+1/2,y-1/2,-z+1/2, #2, x,-y+2,z+1/2, #3, x,-y+2,z-1/2, #4, -x+1/2,y+1/2,-z+1/2, #5, -x,y,-z+1/2; **8**, #1, x-1,y,z-1, #2, x-2,-y+1/2,z-1/2, #3, -x,-y+1,-z+1, #4, x+1,y,z+1, #5, x+2,-y+1/2,z+1/2.

Figure S1. View of the two mirror-related conformations of PA ligand in compound 3.

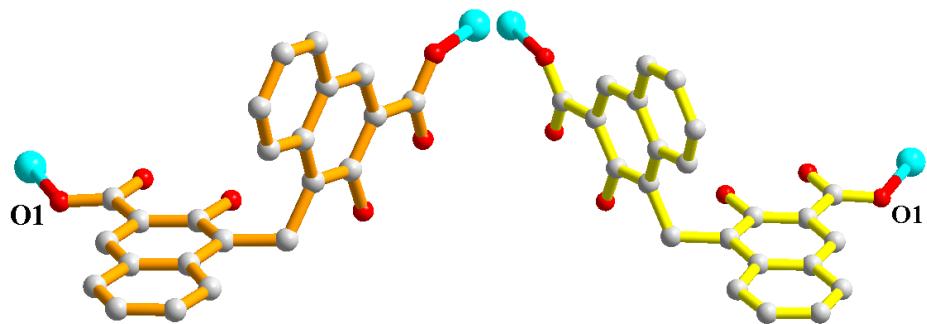


Figure S2. Perspective View of the 3D supramolecular structure of compound 4, showing the AB packing mode of adjacent 2D→3D layers.

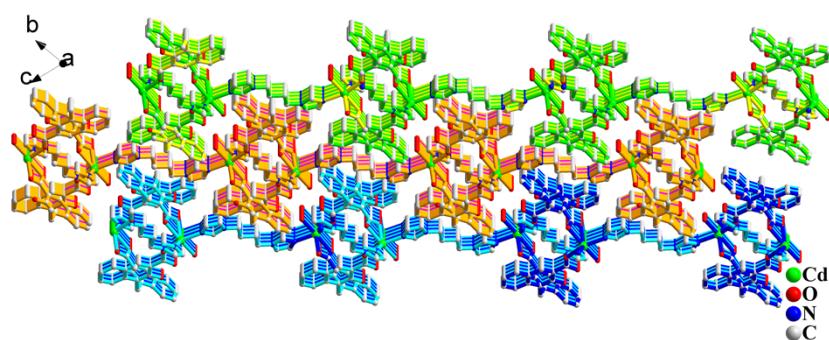


Figure S3. (a) and (b) View of pores along a and c axis in compound 7, showing the environment of the pore.

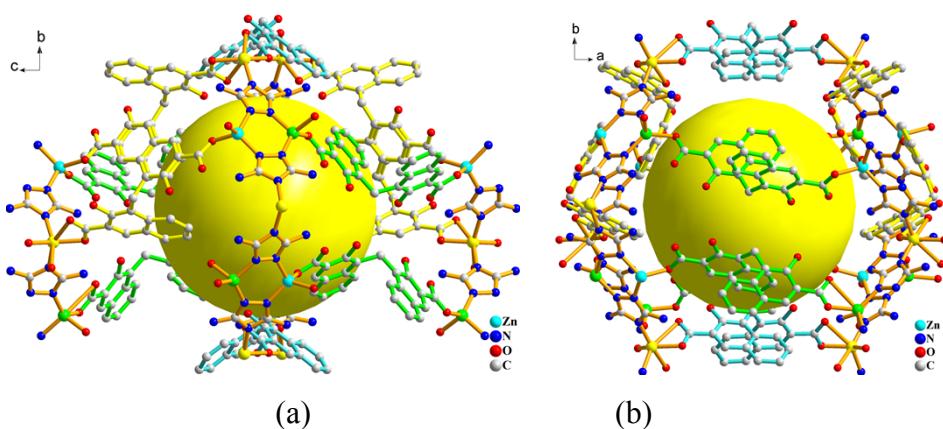
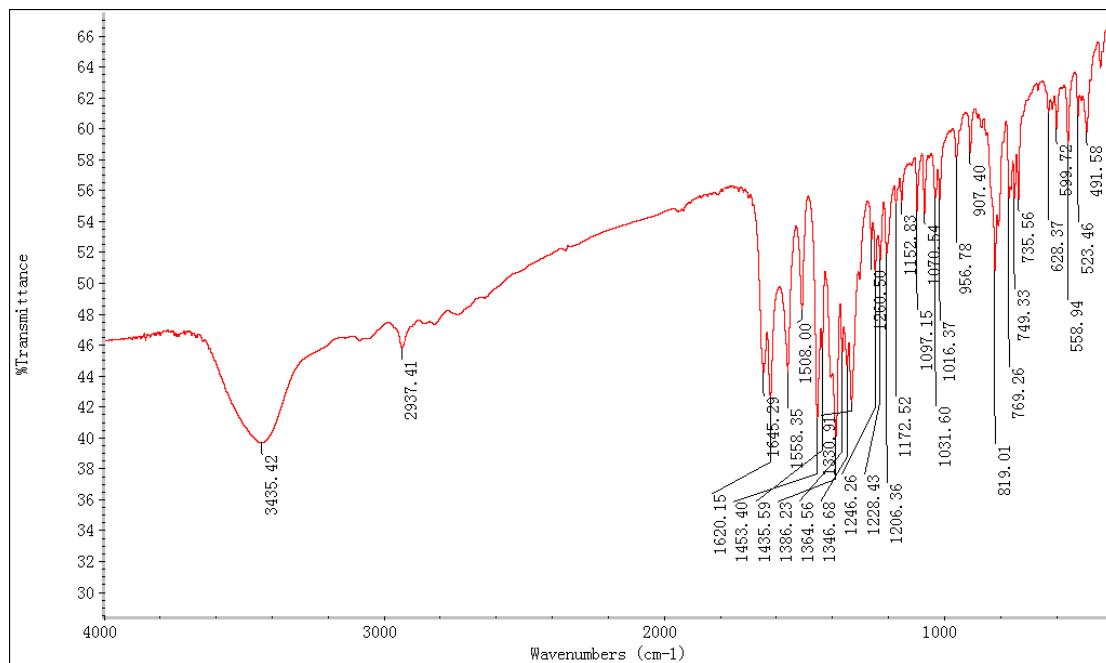
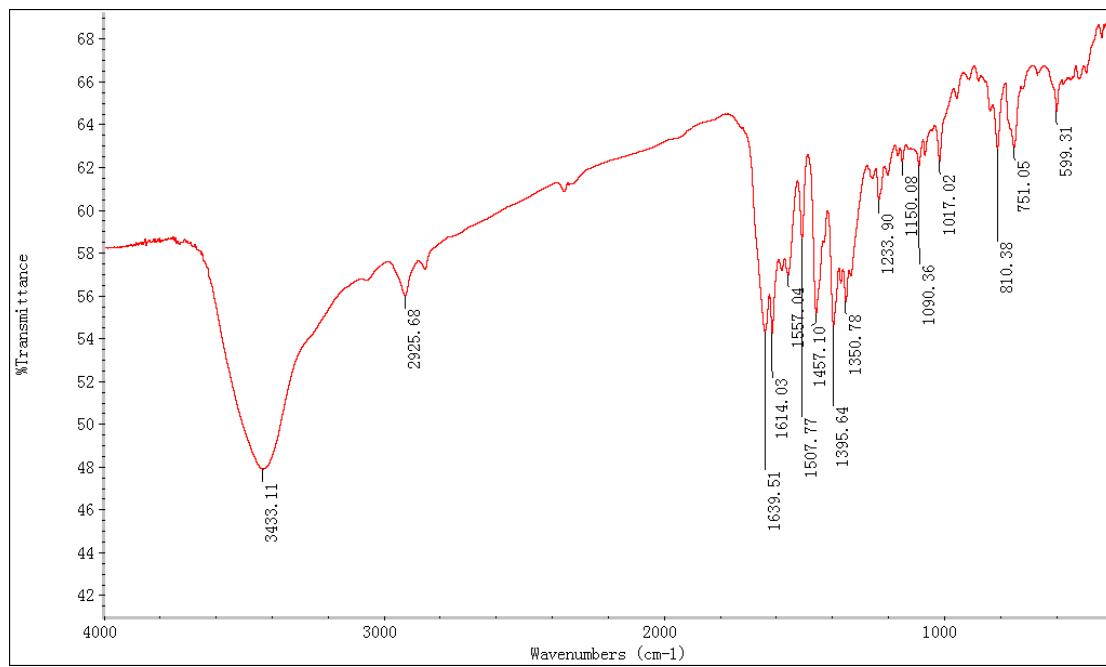


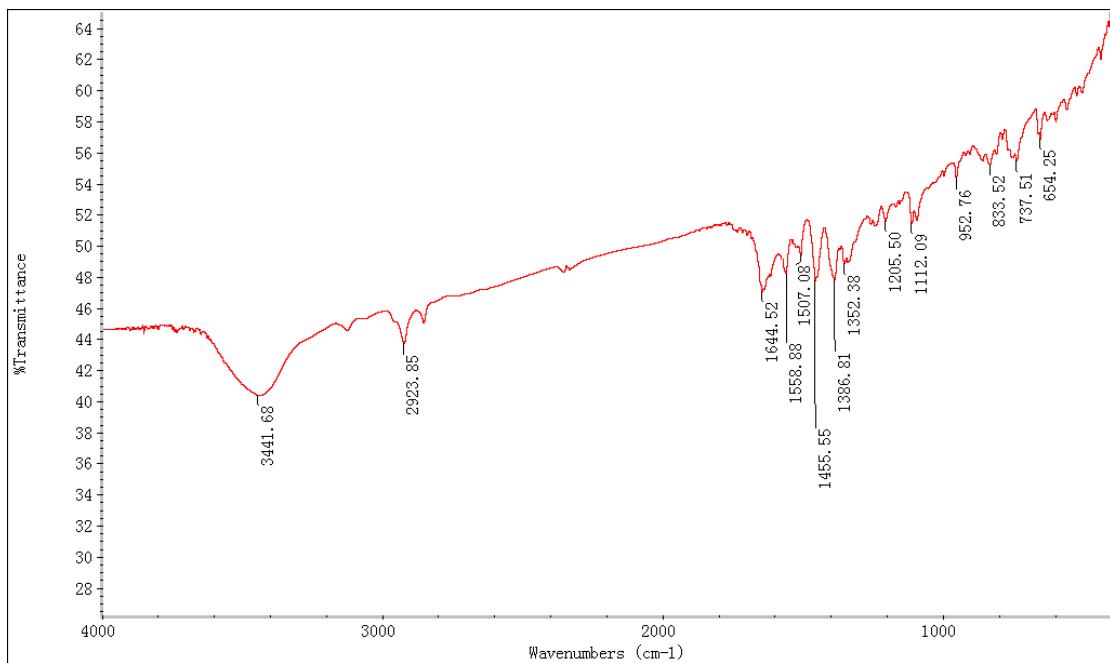
Figure S4. IR spectra of compounds 1-8.



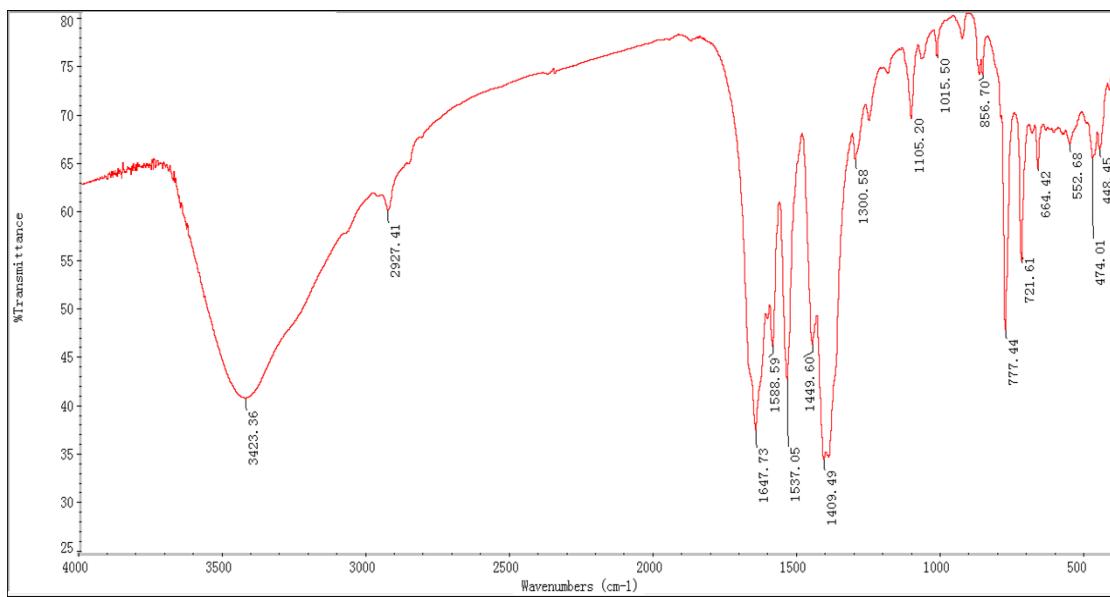
Compound 1



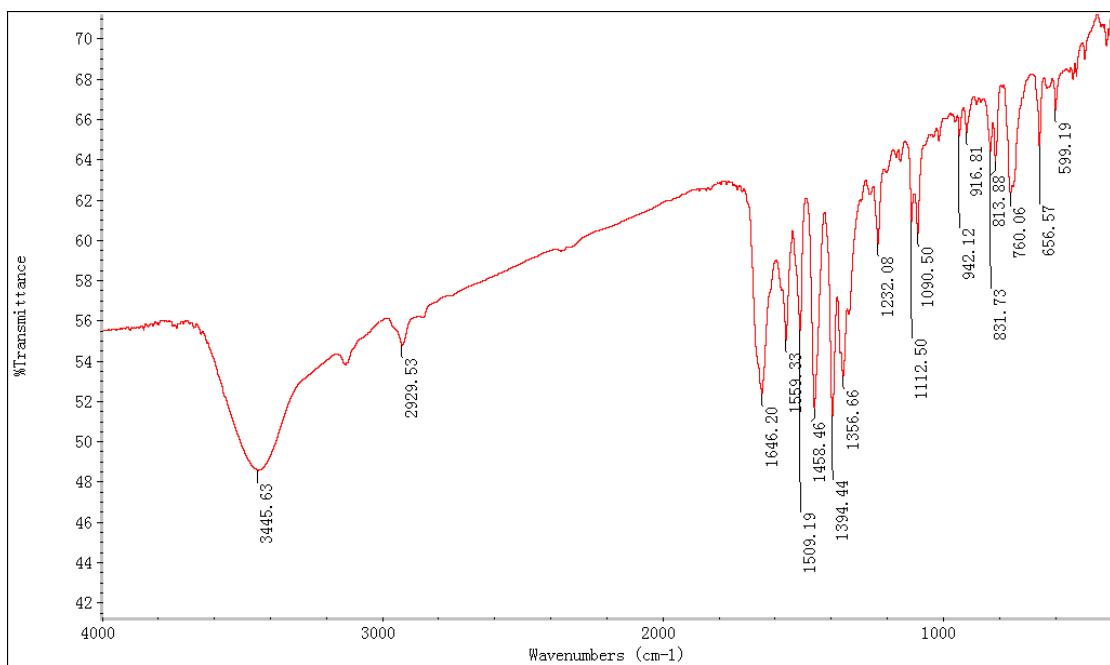
Compound 2



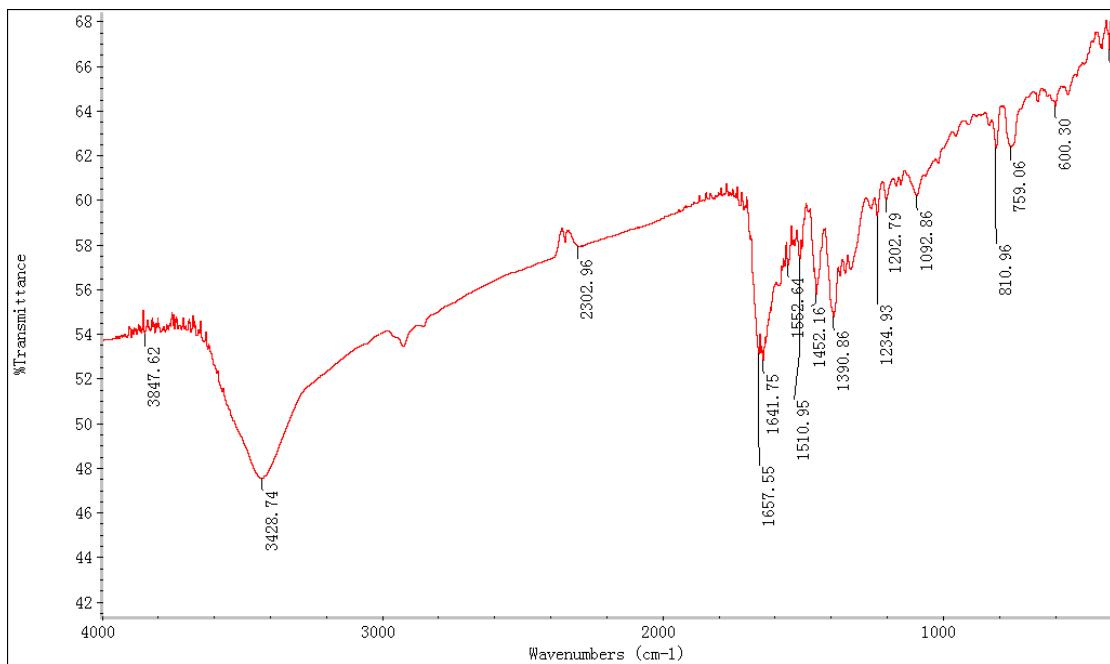
Compound 3



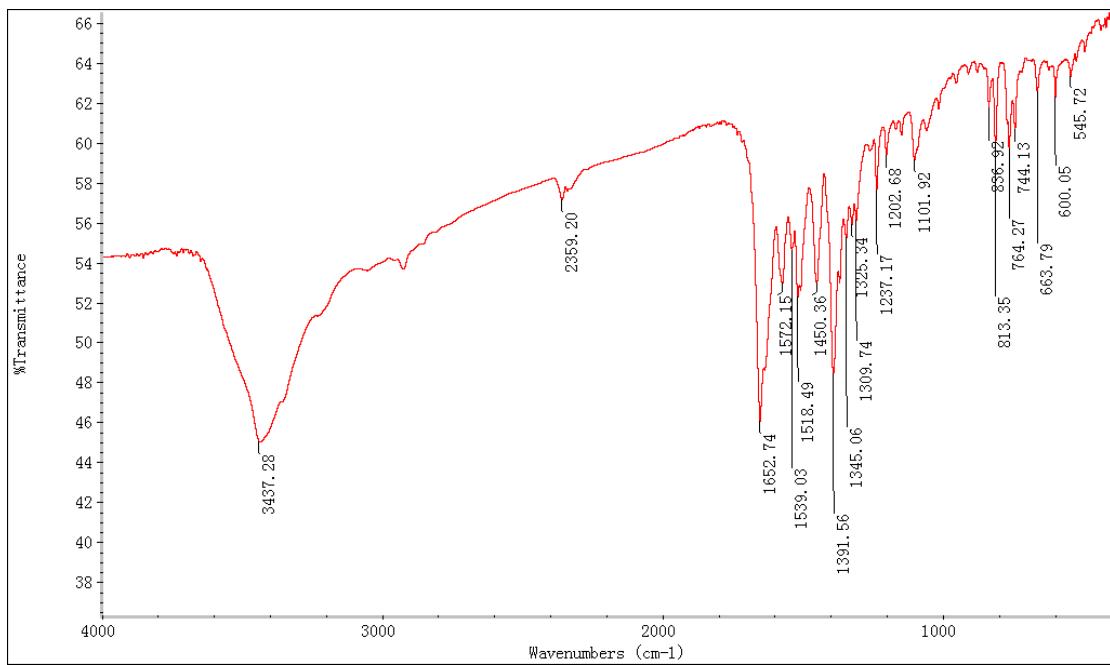
Compound 4



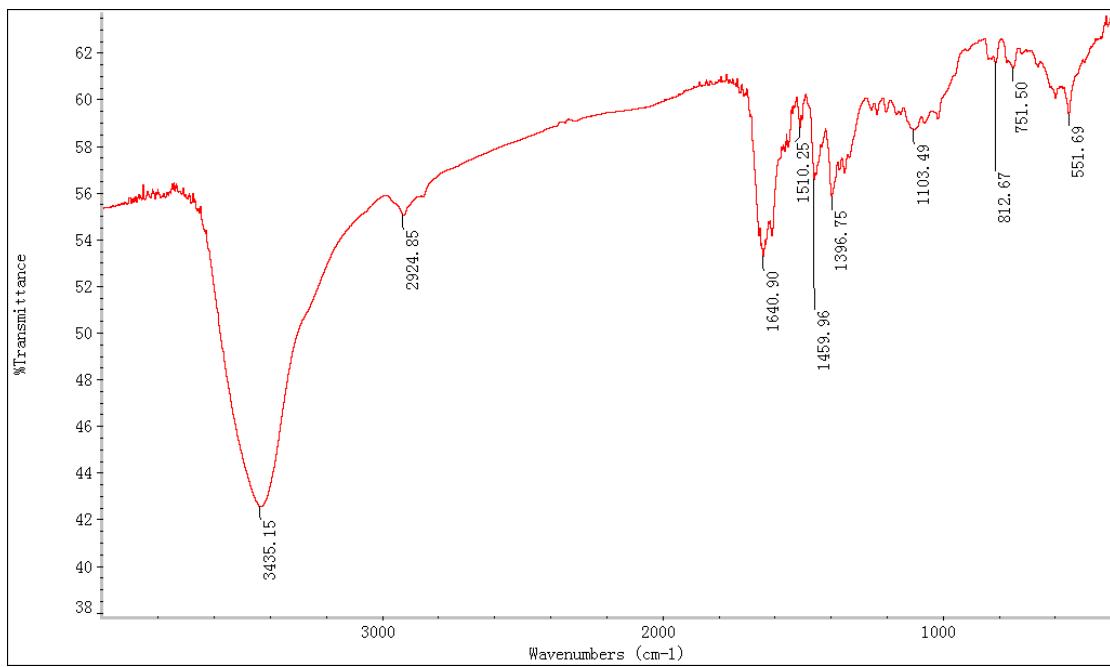
Compound 5



Compound 6

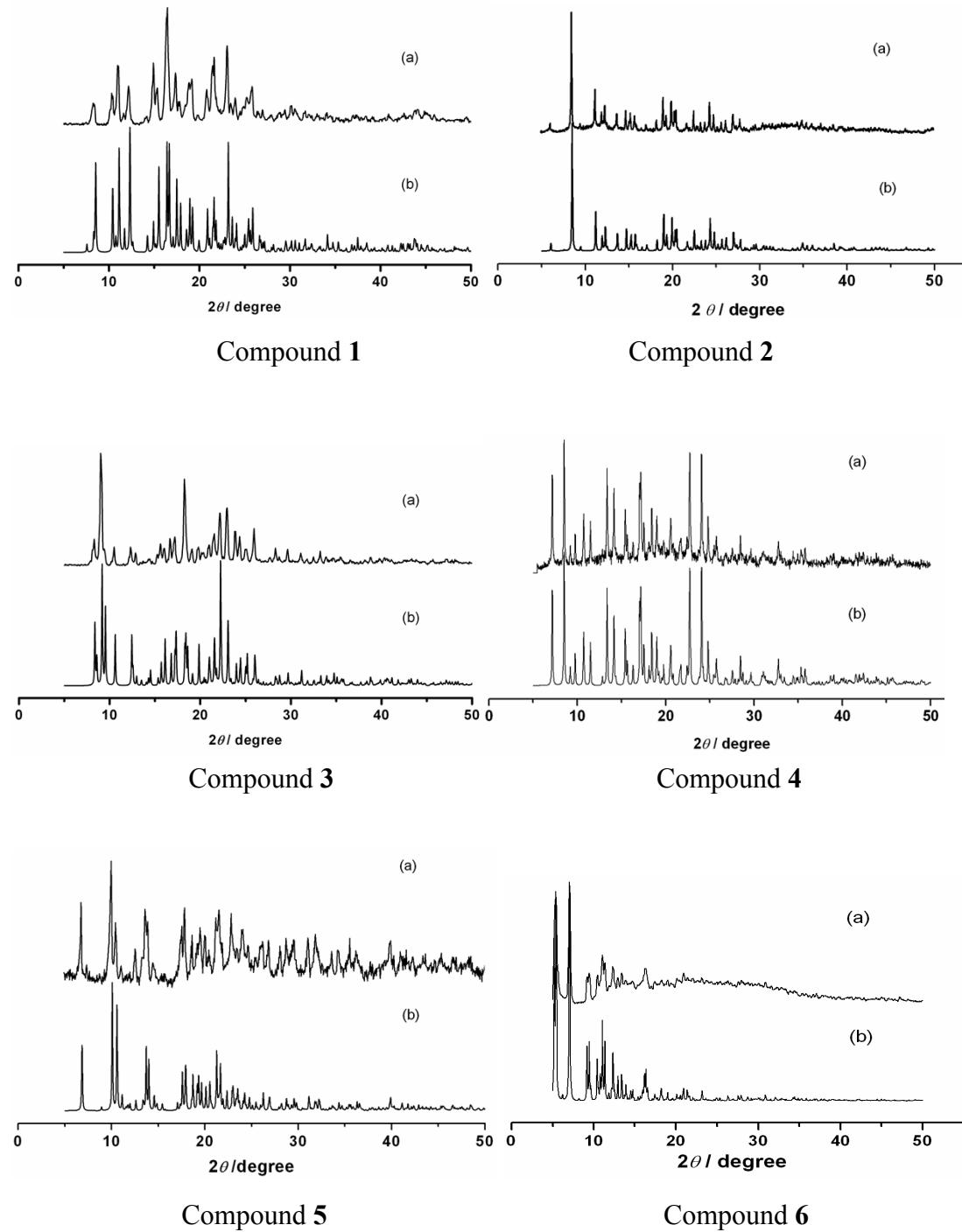


Compound 7



Compound 8

Figure S5. Powder XRD spectra of compounds **1-8** in the solid state at room temperature. (a) as-synthesized; (b) simulated.



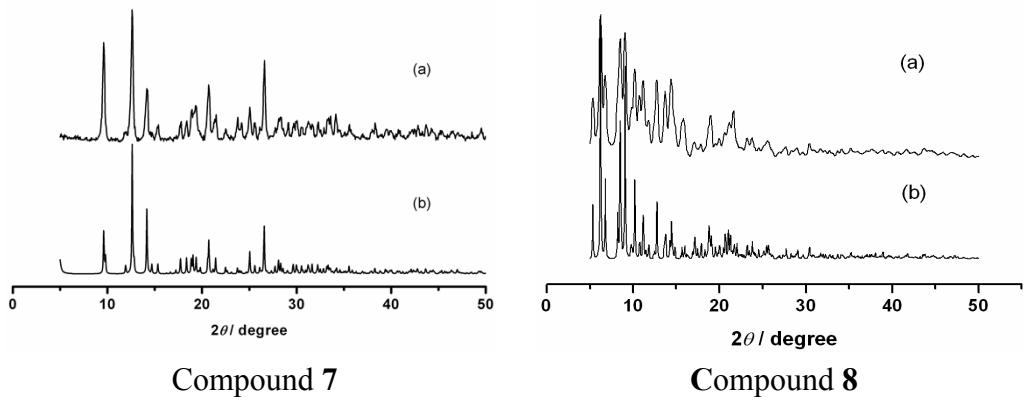


Figure S6 TG data of compounds 1-8.

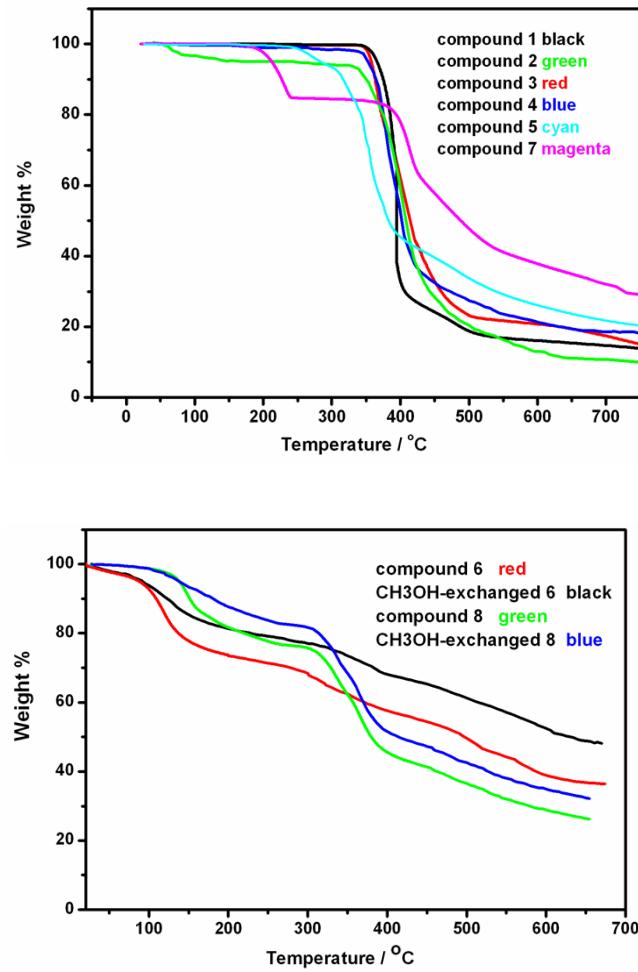


Figure S7. PXRD data of compounds **6** (a) and **8** (b) after immersed in different solvents.

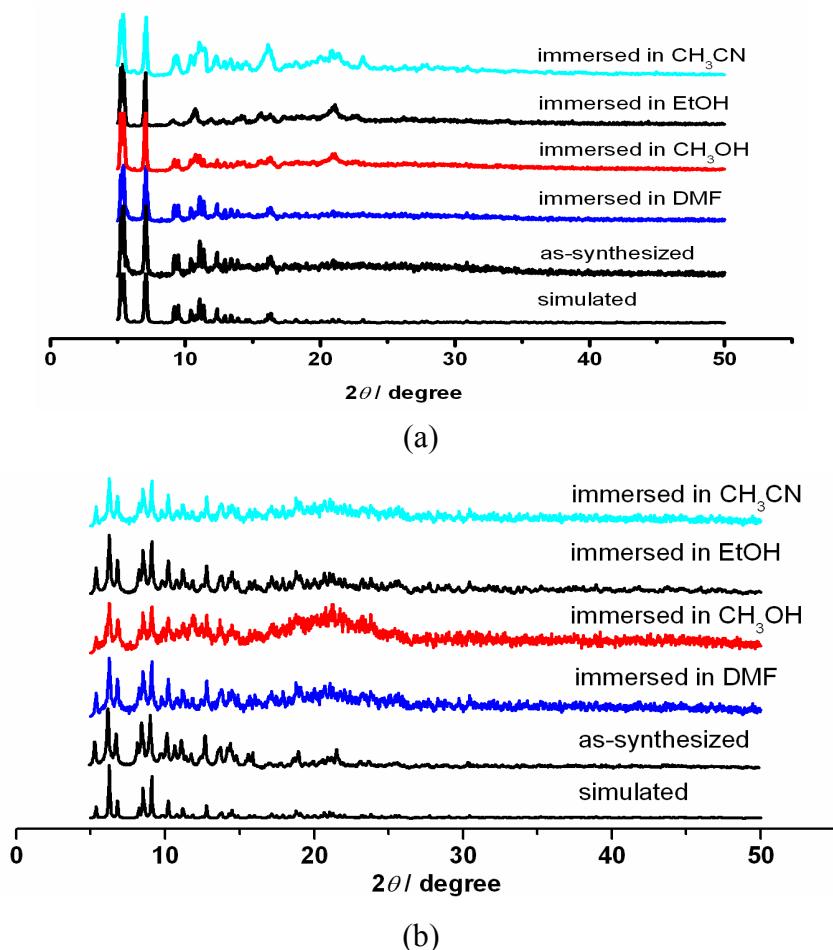


Figure S8. Fluorescent spectra of the ligands at room temperature.

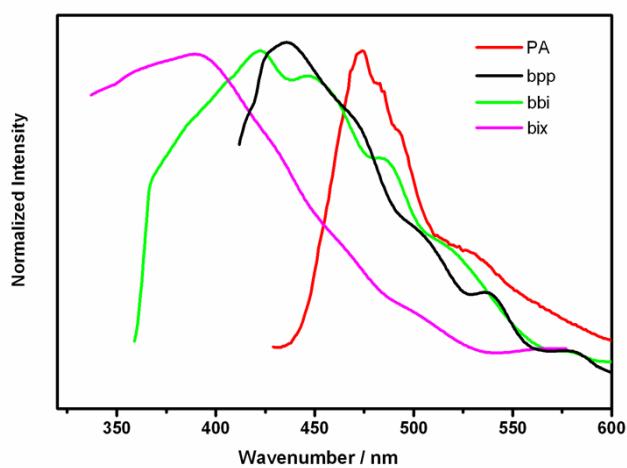


Figure S9. Concentration-dependent photoluminescence of compounds **6** (a and b) and **8** (c and d) by the addition of different amounts of NB in MeOH.

