Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information

In situ hydrothermal syntheses of five new cadmium(II) coordination polymers based on 3-(1H-tetrazol-5-yl)benzoate ligand

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Table S1. Selected Angles (°) for Compounds **1**–**5.**

Compound **1**[(a)]			
N(13)-Cd(1)-O(5)	118.6(3)	N(13)-Cd(1)-N(2)#1	93.7(3)
O(5)-Cd(1)-N(2)#1	135.9(3)	N(13)-Cd(1)-O(8)	85.4(3)
O(5)-Cd(1)-O(8)	132.2(3)	N(2)#1-Cd(1)-O(8)	75.3(3)
N(13)-Cd(1)-O(7)	135.1(3)	O(5)-Cd(1)-O(7)	84.7(3)
N(2)#1-Cd(1)-O(7)	92.9(3)	O(8)-Cd(1)-O(7)	53.7(3)
N(13)-Cd(1)-O(6)	148.7(3)	O(5)-Cd(1)-O(6)	54.4(2)
N(2)#1-Cd(1)-O(6)	82.1(3)	O(8)-Cd(1)-O(6)	122.7(2)
O(7)-Cd(1)-O(6)	76.2(3)	N(9)-Cd(2)-O(3W)	86.7(5)
N(9)-Cd(2)-N(3)#1	174.4(3)	O(3W)-Cd(2)-N(3)#1	97.3(5)
N(9)-Cd(2)-O(8)	94.7(3)	O(3W)-Cd(2)-O(8)	178.3(5)
N(3)#1-Cd(2)-O(8)	81.3(3)	N(9)-Cd(2)-N(14)	95.2(3)
O(3W)-Cd(2)-N(14)	98.6(5)	N(3)#1-Cd(2)-N(14)	88.1(3)
O(8)-Cd(2)-N(14)	80.5(3)	N(9)-Cd(2)-O(10)#2	85.4(3)
O(3W)-Cd(2)-O(10)#2	80.9(5)	N(3)#1-Cd(2)-O(10)#2	91.3(3)
O(8)-Cd(2)-O(10)#2	100.0(3)	N(14)-Cd(2)-O(10)#2	179.2(3)
N(11)#3-Cd(3)-O(6)	94.8(3)	N(11)#3-Cd(3)-N(1)#1	157.8(3)

O(6)-Cd(3)-N(1)#1	92.0(3)	N(11)#3-Cd(3)-N(7)#4	80.6(3)
O(6)-Cd(3)-N(7)#4	147.5(3)	N(1)#1-Cd(3)-N(7)#4	82.3(3)
N(11)#3-Cd(3)-O(12)#1	105.2(3)	O(6)-Cd(3)-O(12)#1	80.5(3)
N(1)#1-Cd(3)-O(12)#1	96.8(3)	N(7)#4-Cd(3)-O(12)#1	131.9(3)
N(11)#3-Cd(3)-O(11)#1	79.2(3)	O(6)-Cd(3)-O(11)#1	128.7(3)
N(1)#1-Cd(3)-O(11)#1	112.5(3)	N(7)#4-Cd(3)-O(11)#1	82.3(3)
O(12)#1-Cd(3)-O(11)#1	53.4(3)	N(6)#5-Cd(4)-O(11)	86.5(3)
N(6)#5-Cd(4)-O(9)	148.6(3)	O(11)-Cd(4)-O(9)	108.9(3)
N(6)#5-Cd(4)-O(10)	148.4(3)	O(11)-Cd(4)-O(10)	105.7(3)
O(9)-Cd(4)-O(10)	54.8(3)	N(6)#5-Cd(4)-O(4W)	77.6(4)
O(11)-Cd(4)-O(4W)	148.0(4)	O(9)-Cd(4)-O(4W)	75.2(3)
O(10)-Cd(4)-O(4W)	102.2(4)	N(6)#5-Cd(4)-N(10)#6	83.2(3)
O(11)-Cd(4)-N(10)#6	73.0(3)	O(9)-Cd(4)-N(10)#6	126.9(3)
O(10)-Cd(4)-N(10)#6	73.2(3)	O(4W)-Cd(4)-N(10)#6	131.0(4)
N(6)#5-Cd(4)-O(5)	90.1(3)	O(11)-Cd(4)-O(5)	72.1(3)
O(9)-Cd(4)-O(5)	70.1(2)	O(10)-Cd(4)-O(5)	121.2(2)
O(4W)-Cd(4)-O(5)	80.2(4)	N(10)#6-Cd(4)-O(5)	144.8(3)
Compound **2**[(b)]			
N(6)#1-Cd(1)-O(1)	103.00(11)	O(1)-Cd(1)-N(4)	80.04(10)
O(1)-Cd(1)-N(2)	89.82(11)	O(1)-Cd(1)-N(3)	146.50(9)
O(1)-Cd(1)-N(1)	127.93(9)	N(4)-Cd(1)-O(2)	132.60(8)
N(3)-Cd(1)-O(2)	160.25(8)	N(2)-Cd(1)-O(2)	90.27(11)
N(1)-Cd(1)-O(2)	79.54(8)	N(6)#1-Cd(1)-O(2)	92.20(12)
O(1)-Cd(1)-O(2)	52.64(8)	N(6)#1-Cd(1)-N(2)	165.52(9)
N(6)#1-Cd(1)-N(4)	96.44(11)	N(6)#1-Cd(1)-N(1)	97.53(9)
N(2)-Cd(1)-N(4)	92.35(10)	N(2)-Cd(1)-N(1)	68.90(9)
N(6)#1-Cd(1)-N(3)	86.99(12)	N(1)-Cd(1)-N(4)	144.19(9)
N(2)-Cd(1)-N(3)	85.88(11)	N(1)-Cd(1)-N(3)	81.01(9)
N(4)-Cd(1)-N(3)	66.99(10)		

Compound **3**[c]			
O(1)-Cd(1)-N(4)#1	116.57(12)	O(1)-Cd(1)-N(2)	139.67(11)
N(4)#1-Cd(1)-N(2)	86.92(10)	O(1)-Cd(1)-N(5)#2	88.42(10)
N(4)#1-Cd(1)-N(5)#2	86.86(9)	N(2)-Cd(1)-N(5)#2	127.25(10)
O(1)-Cd(1)-N(1)	99.88(13)	N(4)#1-Cd(1)-N(1)	141.99(11)
N(2)-Cd(1)-N(1)	70.47(11)	N(5)#2-Cd(1)-N(1)	83.56(10)
O(1)-Cd(1)-O(2)	53.87(9)	N(4)#1-Cd(1)-O(2)	105.18(11)
N(2)-Cd(1)-O(2)	89.79(10)	N(5)#2-Cd(1)-O(2)	142.06(9)
N(1)-Cd(1)-O(2)	104.87(12)		
Compound **4**[d]			
O(8)#1-Cd(1)-N(10)	103.57(11)	O(8)#1-Cd(1)-N(4)#2	86.38(12)
N(10)-Cd(1)-N(4)#2	97.36(11)	O(8)#1-Cd(1)-N(6)	84.52(12)
N(10)-Cd(1)-N(6)	94.85(11)	N(4)#2-Cd(1)-N(6)	166.19(11)
O(8)#1-Cd(1)-O(2)#3	159.29(11)	N(10)-Cd(1)-O(2)#3	96.73(10)
N(4)#2-Cd(1)-O(2)#3	87.00(11)	N(6)-Cd(1)-O(2)#3	97.96(11)
O(8)#1-Cd(1)-O(3)#3	105.37(10)	N(10)-Cd(1)-O(3)#3	150.47(10)
N(4)#2-Cd(1)-O(3)#3	90.23(10)	N(6)-Cd(1)-O(3)#3	82.23(10)
O(2)#3-Cd(1)-O(3)#3	55.05(9)	O(6)#4-Cd(2)-N(5)	138.84(11)
O(6)#4-Cd(2)-O(4)#3	140.48(10)	N(5)-Cd(2)-O(4)#3	80.24(11)
O(6)#4-Cd(2)-N(1)	86.06(11)	N(5)-Cd(2)-N(1)	106.92(11)
O(4)#3-Cd(2)-N(1)	86.46(11)	O(6)#4-Cd(2)-N(9)#5	88.67(11)
N(5)-Cd(2)-N(9)#5	91.09(11)	O(4)#4-Cd(2)-N(9)#5	83.99(11)
N(1)-Cd(2)-N(9)#5	157.87(10)	O(6)#4-Cd(2)-O(7)#4	53.48(10)
N(5)-Cd(2)-O(7)#4	87.15(10)	O(4)#3-Cd(2)-O(7)#4	164.68(10)
N(1)-Cd(2)-O(7)#4	88.95(11)	N(9)#5-Cd(2)-O(7)#4	105.05(11)
O(6)#4-Cd(2)-O(5)#3	88.19(9)	N(5)-Cd(2)-O(5)#3	132.36(10)
O(4)#3-Cd(2)-O(5)#3	52.32(9)	N(1)-Cd(2)-O(5)#3	77.43(9)
N(9)#5-Cd(2)-O(5)#3	80.94(9)	O(7)#4-Cd(2)-O(5)#3	140.35(9)
O(9)#1-Cd(3)-O(5)#3	164.69(11)	O(9)#1-Cd(3)-O(3)#3	95.56(10)

O(5)#3-Cd(3)-O(3)#3	99.13(9)	O(9)#1-Cd(3)-O(1)	83.05(13)
O(5)#3-Cd(3)-O(1)	81.99(12)	O(3)#3-Cd(3)-O(1)	175.82(12)
O(9)#1-Cd(3)-N(2)	100.20(11)	O(5)#3-Cd(3)-N(2)	82.97(10)
O(3)#3-Cd(3)-N(2)	94.43(10)	O(1)-Cd(3)-N(2)	89.70(13)
O(9)#1-Cd(3)-N(7)	88.48(11)	O(5)#3-Cd(3)-N(7)	89.03(10)
O(3)#3-Cd(3)-N(7)	83.16(10)	O(1)-Cd(3)-N(7)	92.85(14)
N(2)-Cd(3)-N(7)	171.19(10)		
Compound **5**[(e)]			
O(3)-Cd(1)-N(7)#1	111.23(11)	O(3)-Cd(1)-N(6)#2	86.76(12)
N(7)#1-Cd(1)-N(6)#2	141.01(12)	O(3)-Cd(1)-O(4)#3	162.91(11)
N(7)#1-Cd(1)-O(4)#3	79.73(12)	N(6)#2-Cd(1)-O(4)#3	92.45(12)
O(3)-Cd(1)-O(2)	79.56(14)	N(7)#1-Cd(1)-O(2)	132.32(13)
N(6)#2-Cd(1)-O(2)	83.60(12)	O(4)#3-Cd(1)-O(2)	83.38(13)
O(3)-Cd(1)-O(4)#4	73.67(11)	N(7)#1-Cd(1)-O(4)#4	76.97(11)
N(6)#2-Cd(1)-O(4)#4	75.53(11)	O(4)#3-Cd(1)-O(4)#4	122.64(7)
O(2)-Cd(1)-O(4)#4	146.68(14)	O(3)-Cd(1)-O(1)	86.11(12)
N(7)#1-Cd(1)-O(1)	80.49(11)	N(6)#2-Cd(1)-O(1)	136.81(11)
O(4)#3-Cd(1)-O(1)	82.80(11)	O(2)-Cd(1)-O(1)	53.22(10)
O(4)#4-Cd(1)-O(1)	141.42(10)		

Symmetry codes: (a) #1: $-x + 5/2, y + 1/2, -z + 1/2$; #2: $-x + 3/2, y + 1/2, -z + 1/2$; #3: $x + 1, y, z$; #4: $x + 1/2, -y + 3/2, z - 1/2$; #5: $-x + 2, -y + 1, -z + 1$; #6: $-x + 3/2, y - 1/2, -z + 1/2$. (b) #1: $-x + 1/2, y + 1/2, z$. (c) #1: $x - 1/2, -y + 1/2, z - 1/2$; #2: $-x + 1/2, -y + 1/2, -z + 1$. (d) #1: $x, -y + 5/2, z - 1/2$; #2: $-x + 2, -y + 2, -z + 1$; #3: $x, -y + 3/2, z + 1/2$; #4: $x, y, z - 1$; #5: $-x + 1, -y + 2, -z + 1$. (e) #1: $x - 1/2, -y + 1/2, z$; #2: $-x + 3/2, y + 1/2, z + 1/2$; #3: $x + 1/2, -y + 1/2, z - 1$; #4: $-x + 1/2, y + 1/2, z - 1/2$.

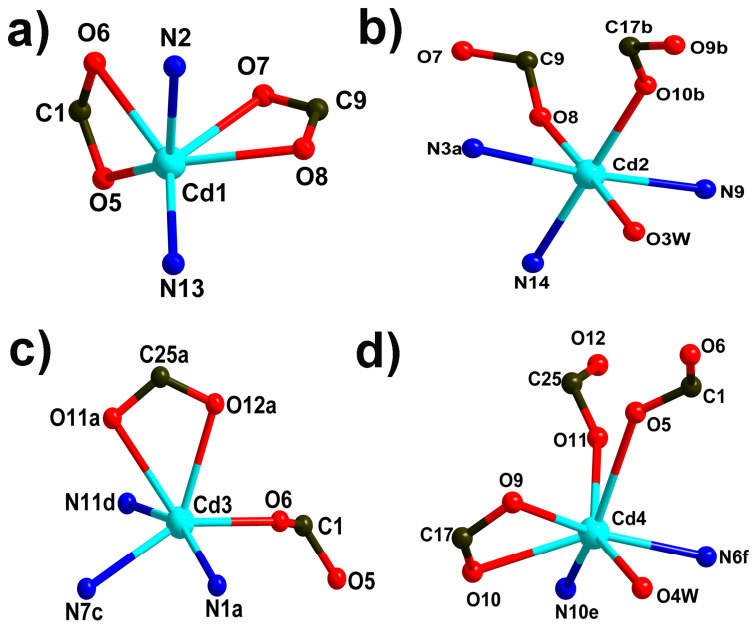


Figure S1. View of the coordination environment of Cd(II) ions in compound **1**. Symmetry code: a: 2.5 - *x*, 0.5 + *y*, 0.5 – *z*; b: 1.5 – *x*, 0.5 + *y*, 0.5 – *z*; c: 0.5 + *x*, 1.5 – *y*, -0.5 + *z*; d: 1 + *x*, *y*, *z*; e: 1.5 – *x*, -0.5 + *y*, 0.5 – *z*; f: 2 – *x*, 1 – *y*, 1 – *z*.

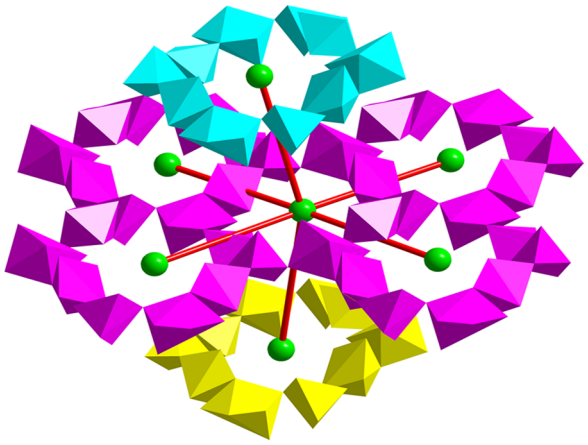


Figure S2. View of a six-connected node in compound **1**.

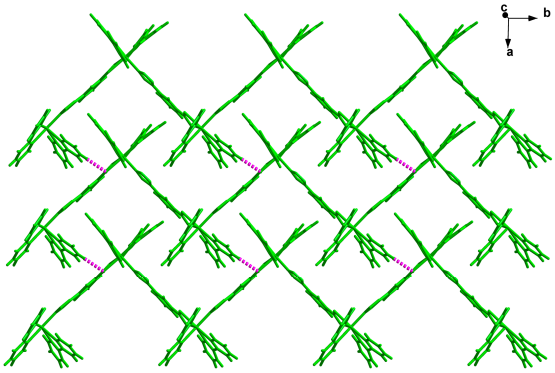
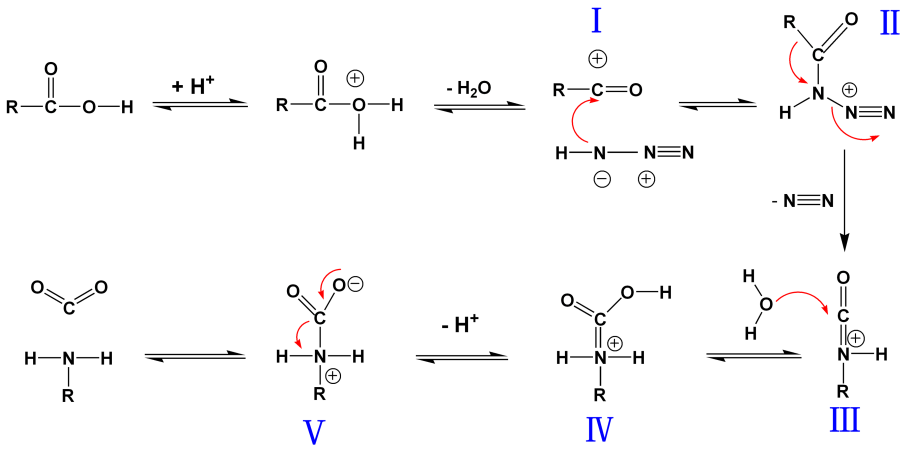


Figure S3. View of the 2D supramolecular framework of compound **2** formed by hydrogen bonding.



Scheme S1. The mechanism of the Schmidt reaction.

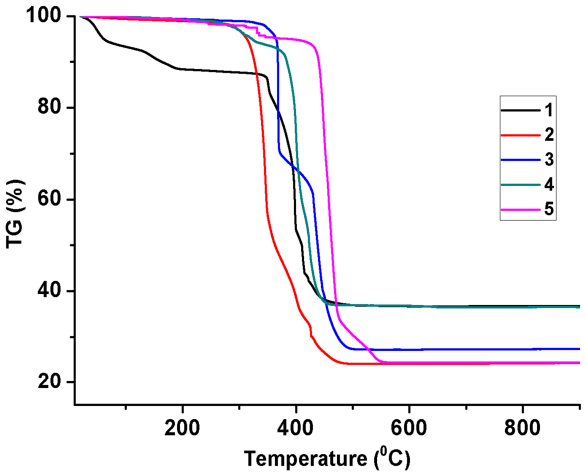


Fig. S4 The TGA curves of compounds **1-5.**

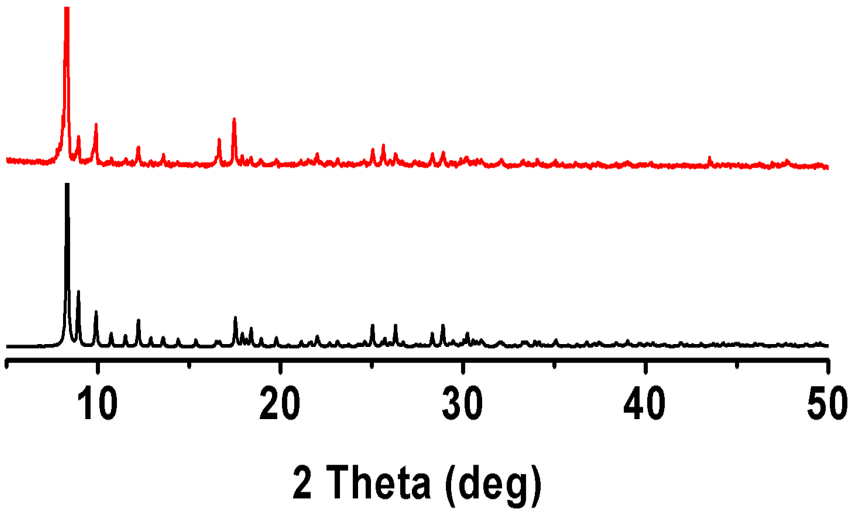


Fig S5. PXRD patterns simulated based on the X-ray single crystal diffraction data of **1** (bottom), for as-synthesized **1** (top).

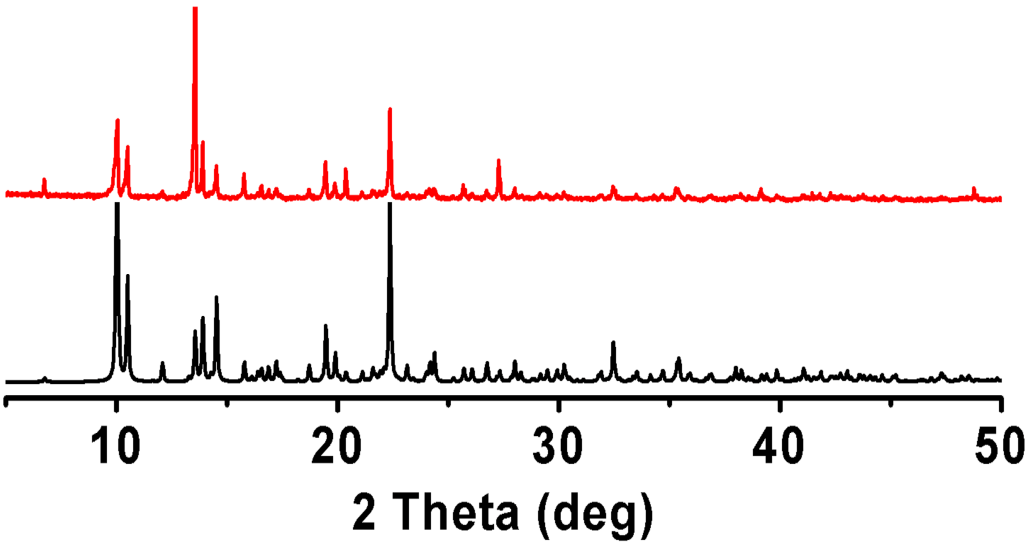


Fig S6. PXRD patterns simulated based on the X-ray single crystal diffraction data of **2** (bottom), for as-synthesized **2** (top).

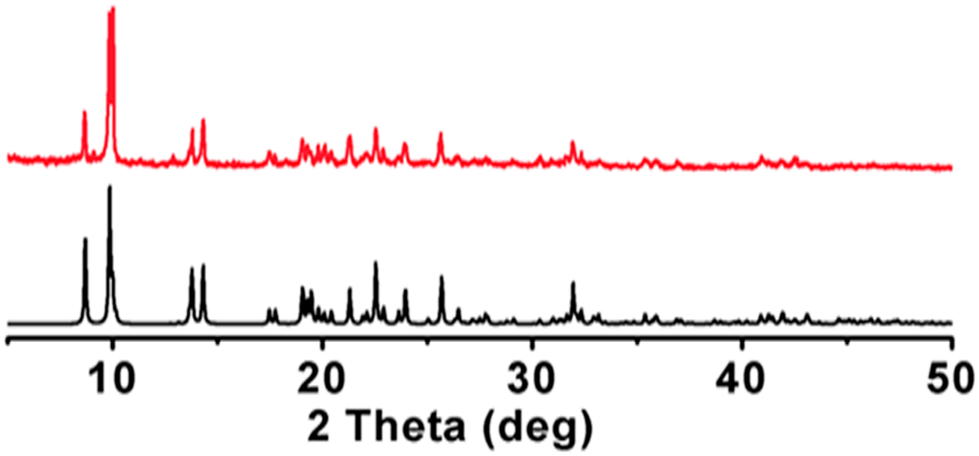


Fig S7. PXRD patterns simulated based on the X-ray single crystal diffraction data of **3** (bottom), for as-synthesized **3** (top).

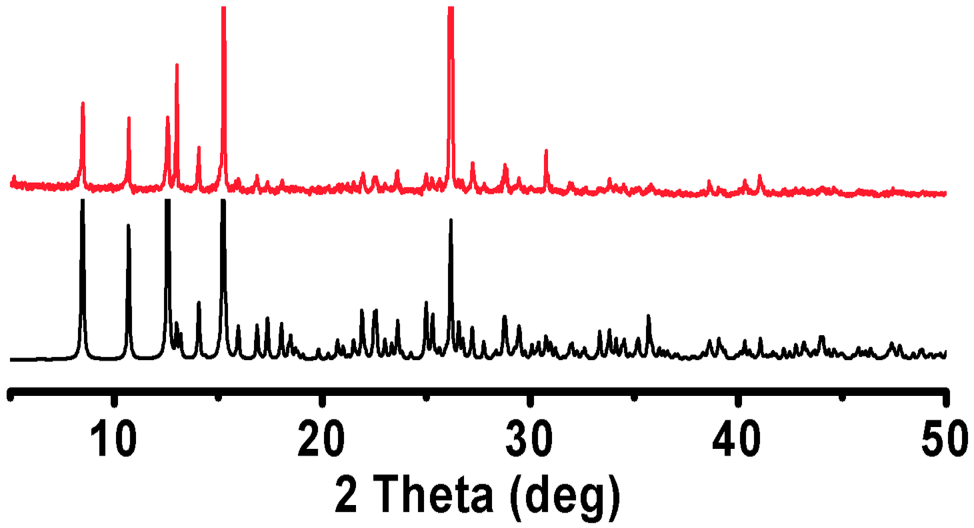


Fig S8. PXRD patterns simulated based on the X-ray single crystal diffraction data of **4** (bottom), for as-synthesized **4** (top).

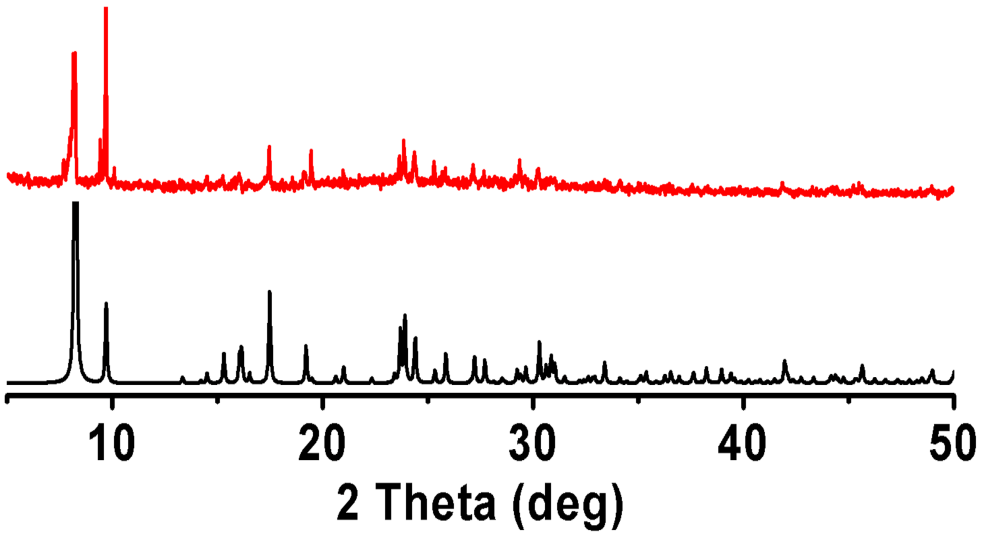


Fig S9. PXRD patterns simulated based on the X-ray single crystal diffraction data of **5** (bottom), for as-synthesized **5** (top).

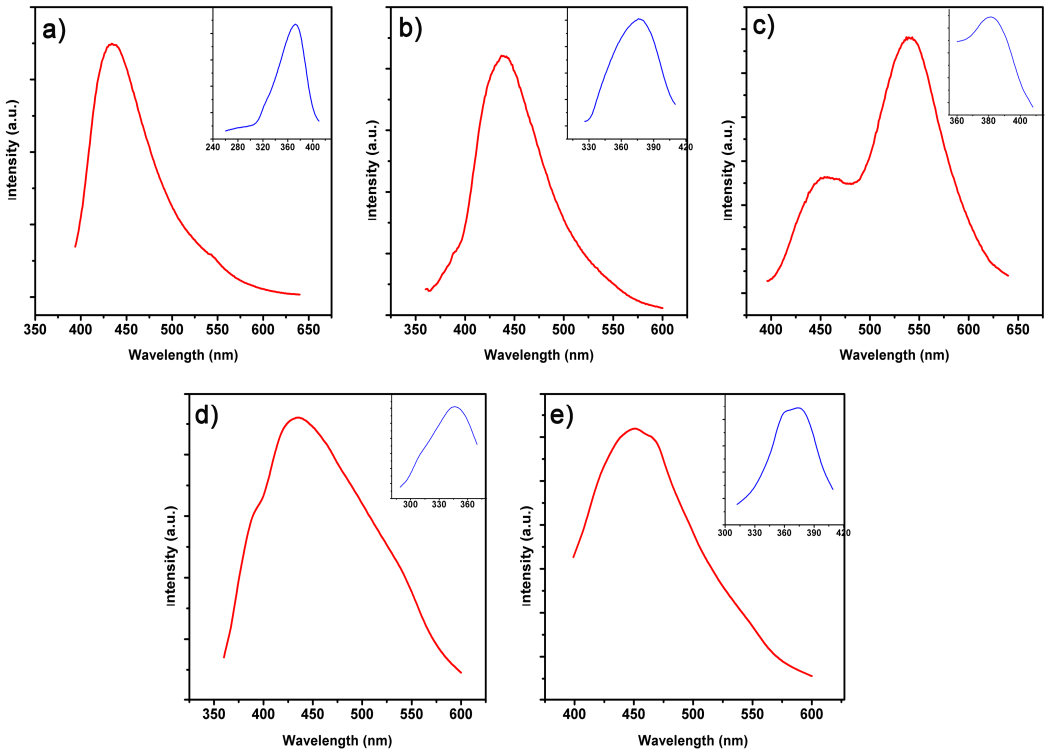


Fig. S10 Solid state emission-excitation spectra of compounds **1** (a), **2** (b), **3** (c), **4** (d), **5** (e) at room temperature. The red and blue lines are the emission and excitation spectra of **1**-**5**, respectively.