

Solvent-Induced Synthesis of Cobalt(II) Coordination Polymers Based on a Rigid Ligand and Flexible Carboxylic Acid Ligands: Syntheses, Structures and Magnetic Properties

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Table S1. Selected Bond Distances and Angles for (1).

Co(1)-O(1)	2.089(2)	Co(1)-O(2)	2.104(2)
Co(1)-N(1) ^{#2}	2.1480(17)	Co(1)-N(1) ^{#1}	2.1480(17)
Co(1)-N(3) ^{#3}	2.1492(18)	Co(1)-N(3)	2.1492(18)
O(1)-Co(1)-O(2)	180.000(1)	O(1)-Co(1)-N(1) ^{#2}	91.33(5)
O(2)-Co(1)-N(1) ^{#2}	88.67(5)	O(1)-Co(1)-N(1) ^{#1}	91.33(5)
O(2)-Co(1)-N(1) ^{#1}	88.67(5)	N(1) ^{#2} -Co(1)-N(1) ^{#1}	177.35(10)
O(1)-Co(1)-N(3) ^{#3}	88.59(4)	O(2)-Co(1)-N(3) ^{#3}	91.41(4)
N(1) ^{#2} -Co(1)-N(3) ^{#3}	90.16(7)	N(1) ^{#1} -Co(1)-N(3) ^{#3}	89.90(7)
O(1)-Co(1)-N(3)	88.59(4)	O(2)-Co(1)-N(3)	91.41(4)
N(1) ^{#2} -Co(1)-N(3)	89.90(7)	N(1) ^{#1} -Co(1)-N(3)	90.16(7)
N(3) ^{#3} -Co(1)-N(3)	177.19(9)		

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

Table S2. Selected Bond Distances and Angles for (2).

Co(1)-O(5) ^{#1}	1.965(2)	Co(1)-O(2)	1.966(2)
Co(1)-N(4)	1.997(3)	Co(1)-N(3)	2.016(3)
O(5) ^{#1} -Co(1)-O(2)	100.75(10)	O(5) ^{#1} -Co(1)-N(4)	112.10(11)
O(2)-Co(1)-N(4)	112.42(10)	O(5) ^{#1} -Co(1)-N(3)	101.67(10)
O(2)-Co(1)-N(3)	111.77(10)	N(4)-Co(1)-N(3)	116.48(11)

Symmetry codes: #1 = $-x + 2, y - 1/2, -z + 3/2$.

Table S3. Selected Bond Distances and Angles for (3).

Co(1)-O(3) ^{#1}	2.0196(14)	Co(1)-O(1)	2.0209(15)
Co(1)-N(1)	2.0567(16)	Co(1)-O(4) ^{#2}	2.0615(14)
Co(1)-O(2) ^{#3}	2.1169(14)		
O(3) ^{#1} -Co(1)-O(1)	93.63(7)	O(3) ^{#1} -Co(1)-N(1)	103.78(6)
O(1)-Co(1)-N(1)	106.09(7)	O(3) ^{#1} -Co(1)-O(4) ^{#2}	161.01(6)
O(1)-Co(1)-O(4) ^{#2}	86.64(6)	N(1)-Co(1)-O(4) ^{#2}	94.34(6)
O(3) ^{#1} -Co(1)-O(2) ^{#3}	87.38(6)	O(1)-Co(1)-O(2) ^{#3}	160.99(7)
N(1)-Co(1)-O(2) ^{#3}	92.05(6)	O(4) ^{#2} -Co(1)-O(2) ^{#3}	86.33(6)
O(3) ^{#1} -Co(1)-Co(1) ^{#3}	82.19(5)	O(1)-Co(1)-Co(1) ^{#3}	92.33(5)
N(1)-Co(1)-Co(1) ^{#3}	160.04(5)	O(4) ^{#2} -Co(1)-Co(1) ^{#3}	78.83(4)
O(2) ^{#3} -Co(1)-Co(1) ^{#3}	68.98(5)		

Symmetry codes: #1 = $x, -y + 1, 1/2 + z$; #2 = $1 - x, y - 1, -z + 3/2$; #3: $-x + 1, -y, z + 2$.

Table S4. Selected Bond Distances and Angles for (4).

Co(1)-O(2)	2.047(3)	Co(1)-N(3) ^{#1}	2.099(4)
Co(1)-O(4) ^{#2}	2.101(4)	Co(1)-O(3) ^{#3}	2.105(4)
Co(1)-N(1)	2.118(5)		
O(2)-Co(1)-N(3) ^{#1}	88.85(16)	O(2)-Co(1)-O(4) ^{#2}	93.31(17)
N(3) ^{#1} -Co(1)-O(4) ^{#2}	88.29(17)	O(2)-Co(1)-O(3) ^{#3}	131.64(18)
N(3) ^{#1} -Co(1)-O(3) ^{#3}	87.60(17)	O(4) ^{#2} -Co(1)-O(3) ^{#3}	134.72(15)
O(2)-Co(1)-N(1)	87.45(16)	N(3) ^{#1} -Co(1)-N(1)	175.73(16)
O(4) ^{#2} -Co(1)-N(1)	89.79(17)	O(3) ^{#3} -Co(1)-N(1)	96.45(18)

Symmetry codes: #1 = $x - 1/2, -y + 1/2, z - 1/2$, #2 = $-x, y, -z + 1/2$, #3 = $x + 1/2, -y + 1/2, z - 1/2$

Table S5. Selected Bond Distances and Angles for (5).

Co(1)-N(3)	2.063(2)	Co(1)-O(3)	2.070(2)
Co(1)-N(4) ^{#3}	2.076(2)	Co(1)-O(5)	2.147(2)
Co(1)-O(6)	2.219(2)	Co(1)-O(2)	2.237(2)
N(3)-Co(1)-O(3)	98.12(9)	N(3)-Co(1)-N(4) ^{#3}	94.48(10)
O(3)-Co(1)-N(4) ^{#3}	95.77(9)	N(3)-Co(1)-O(5)	91.97(9)
O(3)-Co(1)-O(5)	163.66(10)	N(4) ^{#3} -Co(1)-O(5)	96.23(10)
N(3)-Co(1)-O(6)	150.85(9)	O(3)-Co(1)-O(6)	109.29(9)
N(4) ^{#3} -Co(1)-O(6)	92.51(9)	O(5)-Co(1)-O(6)	59.12(8)
N(3)-Co(1)-O(2)	92.77(9)	O(3)-Co(1)-O(2)	60.30(8)
N(4) ^{#3} -Co(1)-O(2)	155.78(9)	O(5)-Co(1)-O(2)	106.60(10)
O(6)-Co(1)-O(2)	92.33(8)		

Symmetry codes: #1 = $-x + 1, y, -z + 1/2$

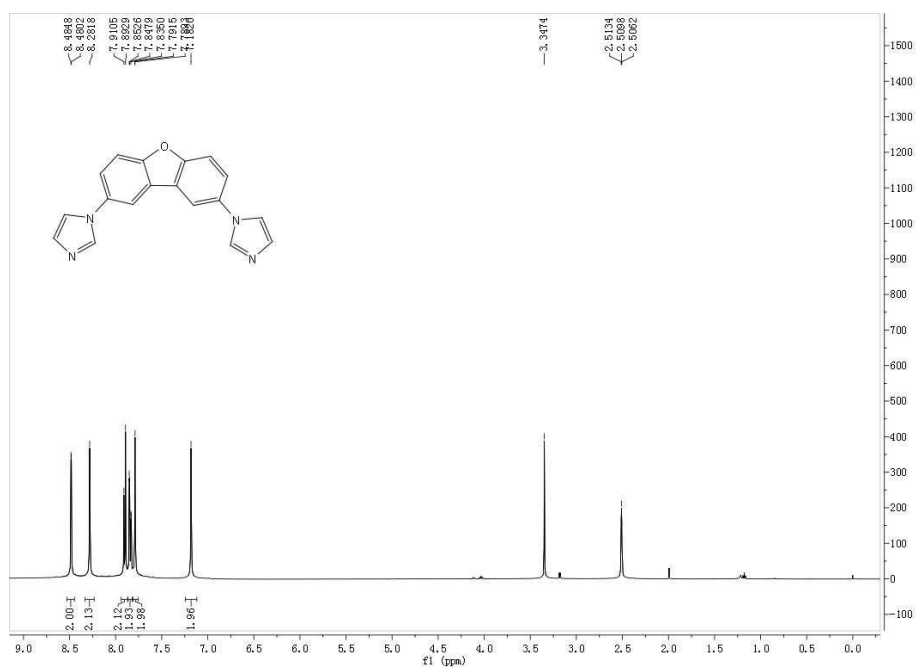


Figure S1. ¹H NMR spectra of L.

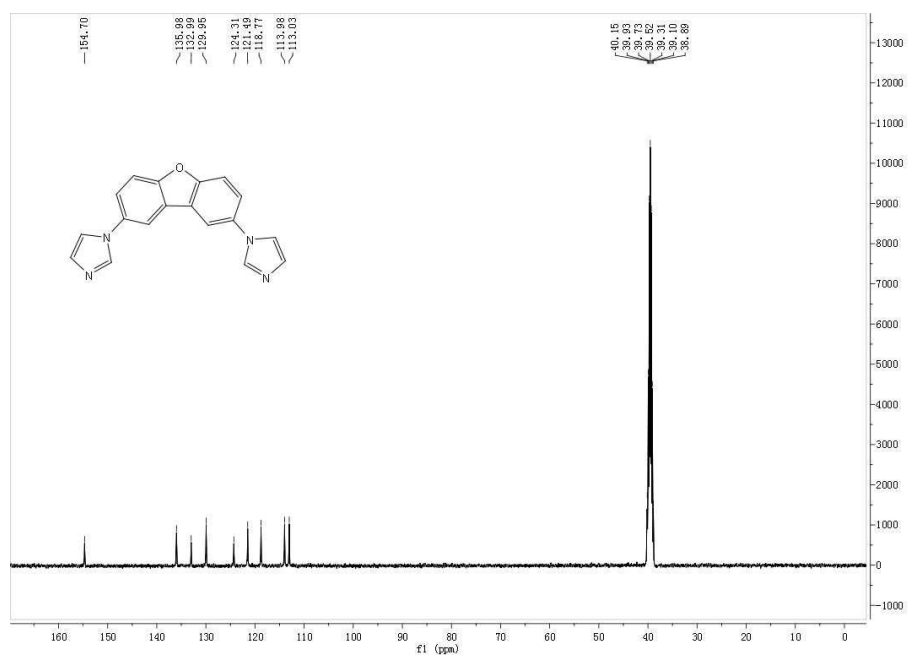


Figure S2. ¹³C NMR spectra of L.

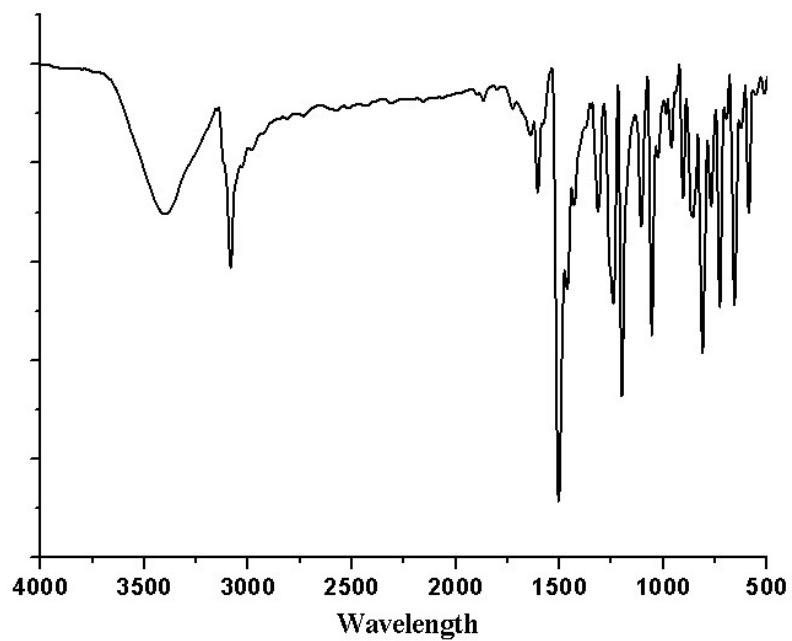
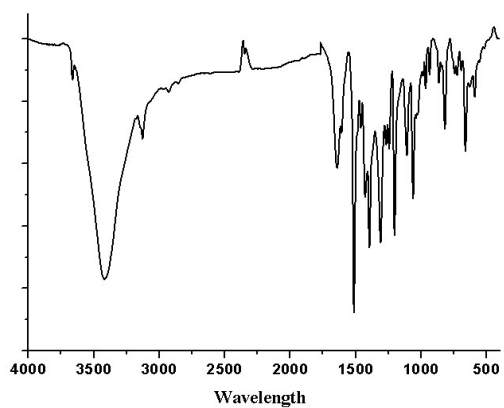
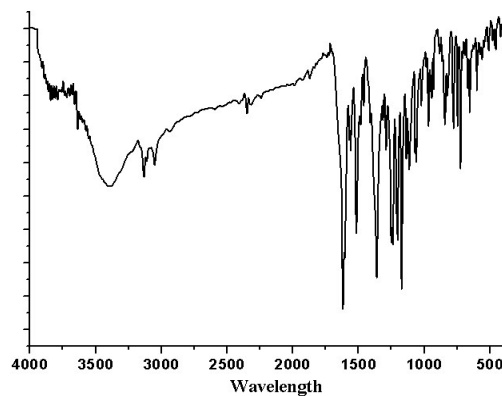


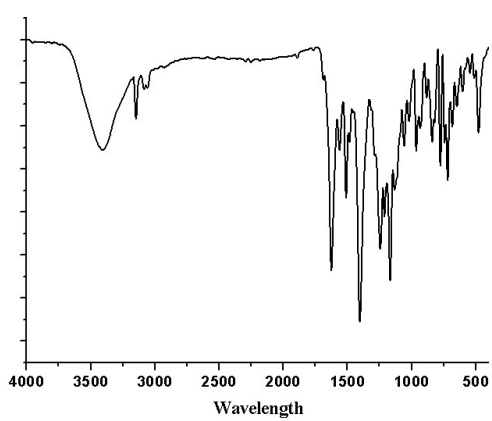
Figure S3. IR spectra of L.



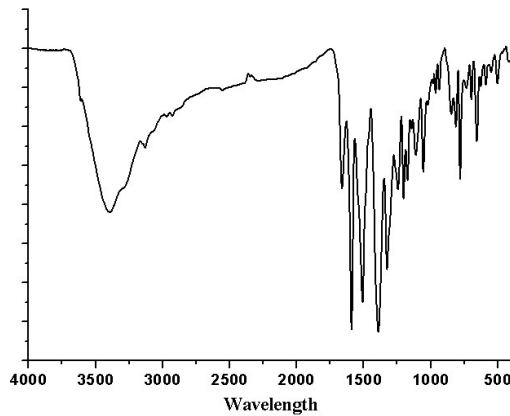
(1)



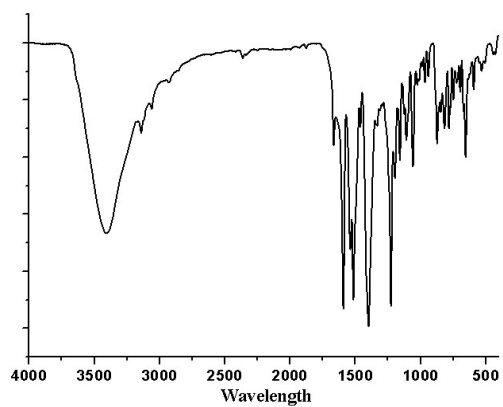
(2)



(3)



(4)



(5)

Figure S4. IR spectra of complex 1-5.

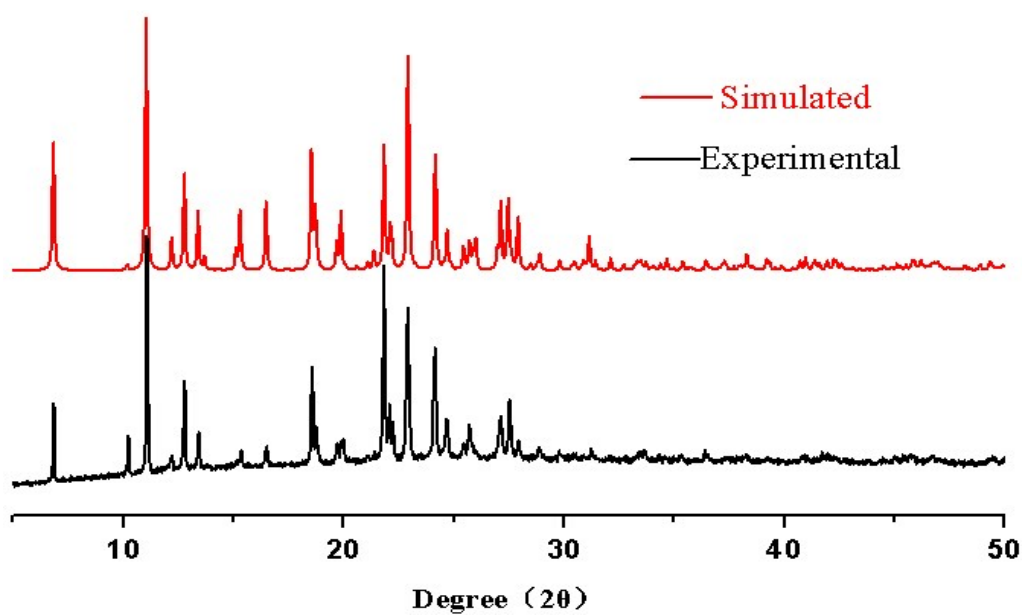


Figure S5. Powder X-ray diffraction patterns of complex 1

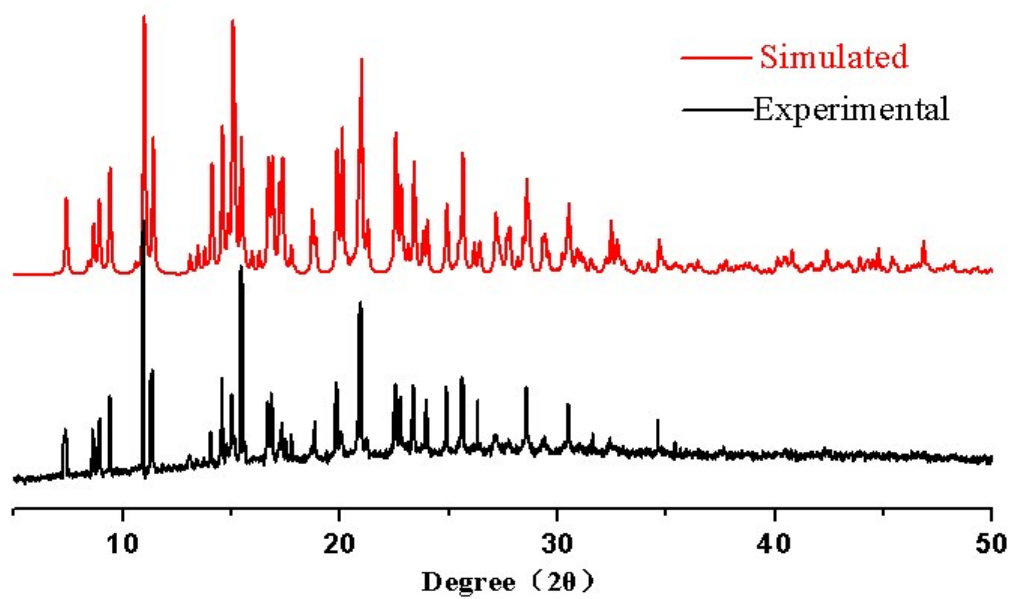


Figure S6. Powder X-ray diffraction patterns of complex 2

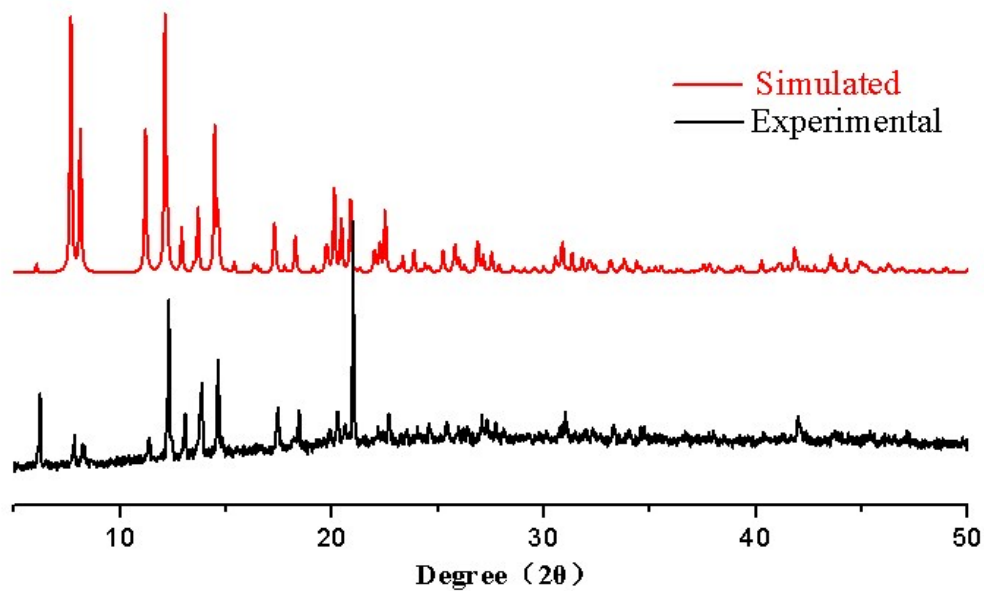


Figure S7. Powder X-ray diffraction patterns of complex 3

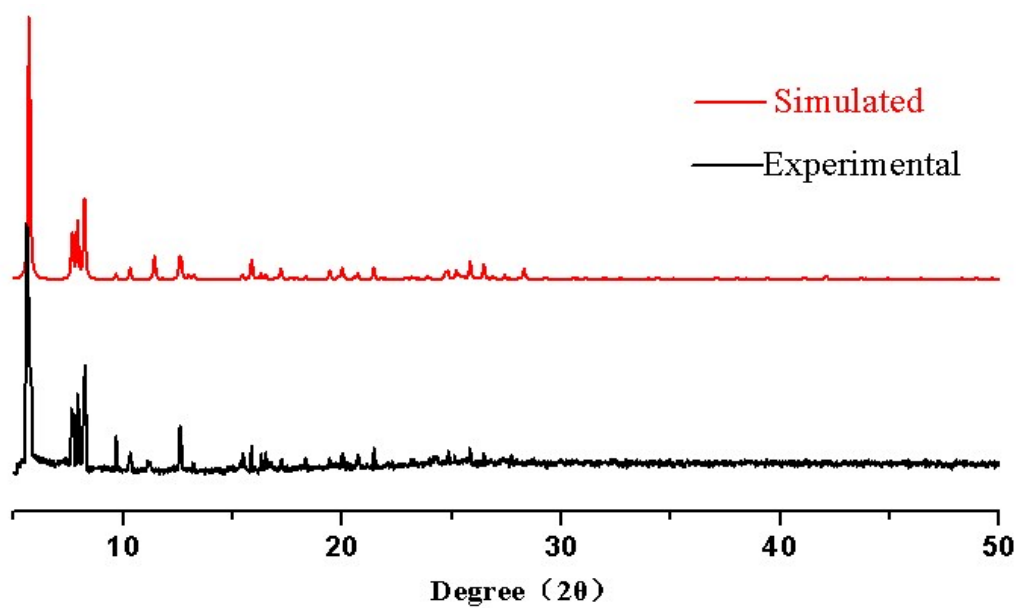


Figure S8. Powder X-ray diffraction patterns of complex 4

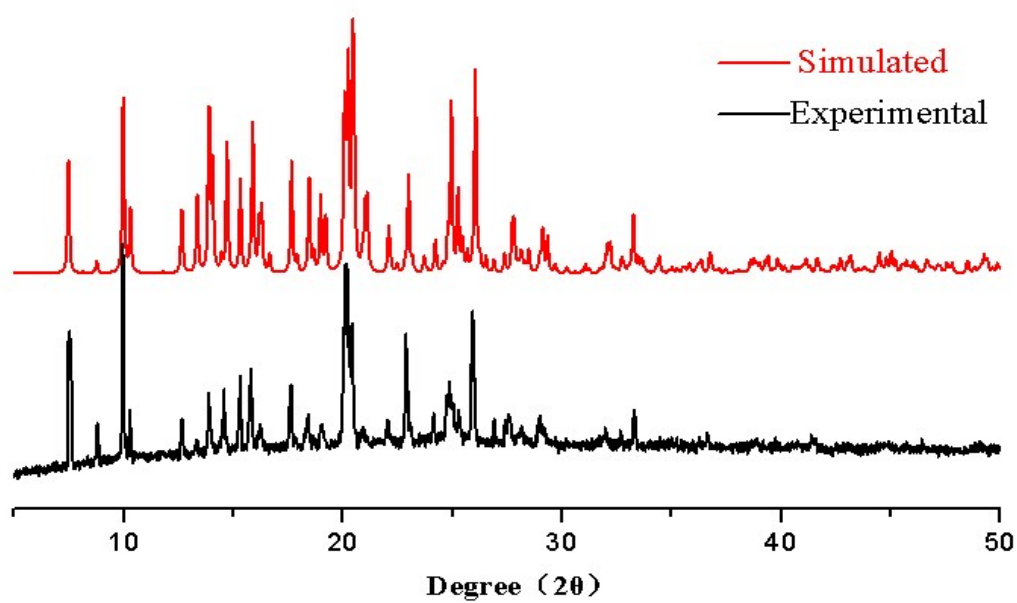


Figure S9. Powder X-ray diffraction patterns of complex 5