Supporting Information for

Three Metal-Organic Frameworks Based on the Semirigid V-shaped 5-(3-Amino-Tetrazole-5-Phenoxy)-Isophthalic Acid Ligand：Syntheses, Topological structures, and Properties

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Table S1. Selected bond lengths for compounds **1**–**3**.

1					
Cd(1)-O(2)	2.267(3)	Cd(1)-O(8)$^{\#1}$	2.275(3)	Cd(1)-O(3)$^{\#1}$	2.311(3)
Cd(1)-O(8)$^{\#2}$	2.375(3)	Cd(1)-O(4)$^{\#1}$	2.436(3)	Cd(1)-N(8)$^{\#3}$	2.503(4)
Cd(1)-O(1)	2.547(3)	Cd(2)-O(1)	2.231(3)	Cd(2)-O(9)$^{\#1}$	2.253(3)
Cd(2)-O(7)	2.275(3)	Cd(2)-O(4)$^{\#2}$	2.323(3)	Cd(2)-O(6)	2.357(3)
Cd(2)-N(9)$^{\#3}$	2.537(4)	O(2)-Cd(1)-O(3)$^{\#1}$	86.69(11)	O(8)$^{\#1}$-Cd(1)-O(3)$^{\#1}$	132.63(10)
O(2)-Cd(1)-O(8)$^{\#1}$	139.72(10)	O(8)$^{\#1}$-Cd(1)-O(8)$^{\#2}$	77.35(10)	O(3)$^{\#1}$-Cd(1)-O(8)$^{\#2}$	116.31(10)
O(2)-Cd(1)-O(8)$^{\#2}$	93.87(10)	O(8)$^{\#1}$-Cd(1)-O(4)$^{\#1}$	87.50(10)	O(3)$^{\#1}$-Cd(1)-O(4)$^{\#1}$	55.02(11)
O(2)-Cd(1)-O(4)$^{\#1}$	129.88(10)	O(2)-Cd(1)-N(8)$^{\#3}$	80.73(11)	O(8)$^{\#1}$-Cd(1)-N(8)$^{\#3}$	86.02(11)
O(8)$^{\#2}$-Cd(1)-O(4)$^{\#1}$	79.07(10)	O(8)$^{\#2}$-Cd(1)-N(8)$^{\#3}$	147.19(11)	O(4)$^{\#1}$-Cd(1)-N(8)$^{\#3}$	128.73(11)
O(3)$^{\#1}$-Cd(1)-N(8)$^{\#3}$	95.80(12)	O(8)$^{\#1}$-Cd(1)-O(1)	85.42(10)	O(3)$^{\#1}$-Cd(1)-O(1)	139.54(10)
O(2)-Cd(1)-O(1)	54.31(10)	O(4)$^{\#1}$-Cd(1)-O(1)	159.34(10)	N(8)$^{\#3}$-Cd(1)-O(1)	70.09(11)
O(8)$^{\#2}$-Cd(1)-O(1)	80.45(10)	O(1)-Cd(2)-O(7)	96.94(10)	O(9)$^{\#1}$-Cd(2)-O(7)	139.25(10)
O(1)-Cd(2)-O(9)$^{\#1}$	123.63(10)	O(9)$^{\#1}$-Cd(2)-O(4)$^{\#2}$	90.41(11)	O(7)-Cd(2)-O(4)$^{\#2}$	102.15(11)
O(1)-Cd(2)-O(4)$^{\#2}$	78.93(10)	O(9)$^{\#1}$-Cd(2)-O(6)	82.64(10)	O(7)-Cd(2)-O(6)	56.95(10)
O(1)-Cd(2)-O(6)	153.72(10)	O(1)-Cd(2)-N(9)$^{\#3}$	75.86(11)	O(9)$^{\#1}$-Cd(2)-N(9)$^{\#3}$	81.99(12)
O(4)$^{\#2}$-Cd(2)-O(6)	102.21(11)	O(4)$^{\#2}$-Cd(2)-N(9)$^{\#3}$	143.33(10)	O(6)-Cd(2)-N(9)$^{\#3}$	112.18(11)
O(7)-Cd(2)-N(9)$^{\#3}$	106.93(11)	O(4)$^{\#2}$-Cd(2)-N(9)$^{\#3}$	143.33(10)	O(6)-Cd(2)-N(9)$^{\#3}$	112.18(11)
Symmetry transformations used to generate equivalent atoms:					
#1 x+1, y, z; #2 -x+2, -y+1, -z+2; #3 -x+3/2, y+1/2, -z+3/2					
2					
Cu(1)-O(11)	1.878(3)	Cu(1)-O(2)	1.931(2)	Cu(1)-O(4)$^{\#1}$	2.008(3)
Cu(1)-O(3)$^{\#1}$	2.035(3)	Cu(1)-O(12)$^{\#2}$	2.338(3)	Cu(2)-O(11)	1.894(3)
Cu(2)-O(12)	1.934(2)	Cu(2)-O(8)$^{\#1}$	1.962(3)	Cu(2)-O(1)	1.973(3)
Cu(2)-N(8)$^{\#3}$	2.361(4)	Cu(3)-O(12)	1.925(2)	Cu(3)-O(9)$^{\#1}$	1.929(2)
Cu(3)-O(7)	2.013(2)	Cu(3)-O(6)	2.021(3)	O(11)-Cu(1)-O(2)	97.59(12)
O(11)-Cu(1)-O(4)$^{\#1}$	96.51(11)	O(2)-Cu(1)-O(4)$^{\#1}$	159.39(12)	O(11)-Cu(1)-O(3)$^{\#1}$	159.36(12)
O(2)-Cu(1)-O(3)$^{\#1}$	98.39(11)	O(4)$^{\#1}$-Cu(1)-O(3)$^{\#1}$	64.85(11)	O(11)-Cu(1)-O(12)$^{\#2}$	99.37(12)
O(2)-Cu(1)-O(12)$^{\#2}$	103.52(11)	O(4)$^{\#1}$-Cu(1)-O(12)$^{\#2}$	88.89(11)	O(3)$^{\#1}$-Cu(1)-O(12)$^{\#2}$	89.49(11)
O(11)-Cu(2)-O(12)	172.87(12)	O(11)-Cu(2)-O(8)$^{\#1}$	87.01(12)	O(12)-Cu(2)-O(8)$^{\#1}$	91.61(11)
O(11)-Cu(2)-O(1)	92.21(11)	O(12)-Cu(2)-O(1)	88.58(11)	O(8)$^{\#1}$-Cu(2)-O(1)	175.13(12)
O(11)-Cu(2)-N(8)$^{\#3}$	99.39(14)	O(12)-Cu(2)-N(8)$^{\#3}$	87.67(12)	O(8)$^{\#1}$-Cu(2)-N(8)$^{\#3}$	93.09(13)
O(1)-Cu(2)-N(8)$^{\#3}$	91.78(13)	O(12)-Cu(3)-O(9)$^{\#1}$	99.41(11)	O(12)-Cu(3)-O(7)	97.77(11)
O(9)$^{\#1}$-Cu(3)-O(7)	161.51(11)	O(12)-Cu(3)-O(6)	159.42(11)	O(9)$^{\#1}$-Cu(3)-O(6)	96.81(10)

O(7)-Cu(3)-O(6)	64.96(10)				

Symmetry transformations used to generate equivalent atoms:

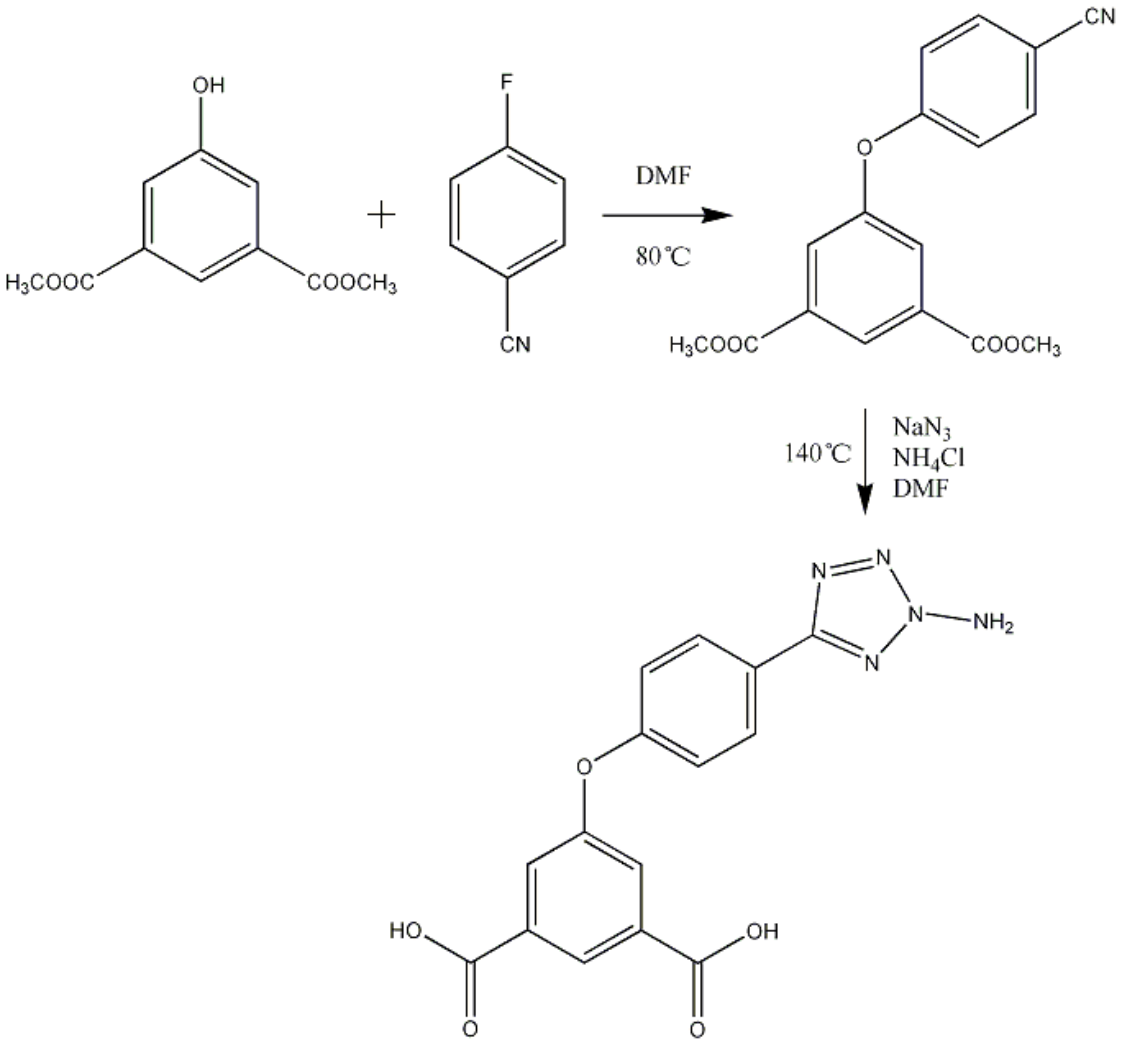
#1 x+1, y, z; #2 -x+1, -y+1, -z+1; #3 -x, -y+1, -z

3

Mn(1)-O(9)$^{\#1}$	2.104(3)	Mn(1)-O(9)$^{\#2}$	2.104(3)	Mn(1)-O(13)$^{\#3}$	2.138(3)
Mn(1)-O(13)$^{\#4}$	2.138(3)	Mn(1)-O(1)$^{\#5}$	2.289(3)	Mn(1)-O(1)	2.289(3)
Mn(2)-O(8)$^{\#2}$	2.122(3)	Mn(2)-O(14)$^{\#4}$	2.124(3)	Mn(2)-O(16)	2.168(4)
Mn(2)-O(7)	2.192(3)	Mn(2)-O(1)	2.210(3)	Mn(3)-O(12)$^{\#3}$	2.088(3)
Mn(3)-O(12)	2.088(3)	Mn(3)-O(4)$^{\#6}$	2.189(3)	Mn(3)-O(4)$^{\#7}$	2.189(3)
Mn(3)-O(6)$^{\#3}$	2.296(3)	Mn(3)-O(6)	2.296(3)	Mn(4)-O(11)	2.113(3)
Mn(4)-O(3)$^{\#6}$	2.163(3)	Mn(4)-O(17)	2.174(3)	Mn(4)-O(2)	2.223(3)
Mn(4)-O(6)	2.229(3)	O(9)$^{\#1}$-Mn(1)-O(9)$^{\#2}$	180.0(2)	O(9)$^{\#1}$-Mn(1)-O(13)$^{\#3}$	92.59(13)
O(9)$^{\#2}$-Mn(1)-O(13)$^{\#3}$	87.41(13)	O(9)$^{\#1}$-Mn(1)-O(13)$^{\#4}$	87.41(13)	O(9)$^{\#2}$-Mn(1)-O(13)$^{\#4}$	92.59(13)
O(13)$^{\#3}$-Mn(1)-O(13)$^{\#4}$	180.000(1)	O(9)$^{\#1}$-Mn(1)-O(1)$^{\#5}$	85.08(12)	O(9)$^{\#2}$-Mn(1)-O(1)$^{\#5}$	94.92(12)
O(13)$^{\#3}$-Mn(1)-O(1)$^{\#5}$	88.06(11)	O(13)$^{\#4}$-Mn(1)-O(1)$^{\#5}$	91.94(11)	O(9)$^{\#1}$-Mn(1)-O(1)	94.92(12)
O(9)$^{\#2}$-Mn(1)-O(1)	85.08(12)	O(13)$^{\#3}$-Mn(1)-O(1)	91.94(11)	O(13)$^{\#4}$-Mn(1)-O(1)	88.06(11)
O(1)$^{\#5}$-Mn(1)-O(1)	180.00(13)	O(8)$^{\#2}$-Mn(2)-O(14)$^{\#4}$	95.09(14)	O(8)$^{\#2}$-Mn(2)-O(16)	117.11(17)
O(14)$^{\#4}$-Mn(2)-O(16)	81.19(14)	O(8)$^{\#2}$-Mn(2)-O(7)	91.40(12)	O(14)$^{\#4}$-Mn(2)-O(7)	164.17(13)
O(16)-Mn(2)-O(7)	83.00(14)	O(8)$^{\#2}$-Mn(2)-O(1)	110.22(13)	O(14)$^{\#4}$-Mn(2)-O(1)	95.15(13)
O(16)-Mn(2)-O(1)	132.68(15)	O(7)-Mn(2)-O(1)	96.12(11)	O(12)$^{\#3}$-Mn(3)-O(12)	180.00(10)
O(12)$^{\#3}$-Mn(3)-O(4)$^{\#6}$	88.38(12)	O(12)-Mn(3)-O(4)$^{\#6}$	91.62(12)	O(12)$^{\#3}$-Mn(3)-O(4)$^{\#7}$	91.62(12)
O(12)-Mn(3)-O(4)$^{\#7}$	88.38(12)	O(4)$^{\#6}$-Mn(3)-O(4)$^{\#7}$	180.00(18)	O(12)$^{\#3}$-Mn(3)-O(6)$^{\#3}$	90.16(11)
O(12)-Mn(3)-O(6)$^{\#3}$	89.84(11)	O(4)$^{\#6}$-Mn(3)-O(6)$^{\#3}$	103.65(12)	O(4)$^{\#7}$-Mn(3)-O(6)$^{\#3}$	76.35(11)
O(12)$^{\#3}$-Mn(3)-O(6)	89.84(11)	O(12)-Mn(3)-O(6)	90.16(11)	O(4)$^{\#6}$-Mn(3)-O(6)	76.35(11)
O(4)$^{\#7}$-Mn(3)-O(6)	103.65(11)	O(6)$^{\#3}$-Mn(3)-O(6)	180.0	O(11)-Mn(4)-O(3)$^{\#6}$	95.68(13)
O(11)-Mn(4)-O(17)	82.54(12)	O(3)$^{\#6}$-Mn(4)-O(17)	103.27(14)	O(11)-Mn(4)-O(2)	164.72(12)
O(3)$^{\#6}$-Mn(4)-O(2)	90.41(11)	O(17)-Mn(4)-O(2)	82.43(12)	O(11)-Mn(4)-O(6)	92.36(12)
O(3)$^{\#6}$-Mn(4)-O(6)	122.49(12)	O(17)-Mn(4)-O(6)	134.24(12)	O(2)-Mn(4)-O(6)	96.17(11)

Symmetry transformations used to generate equivalent atoms:

#1 x+1/2, -y+3/2, z+1/2; #2 -x, y, -z+1/2; #3 -x+1/2, -y+3/2, -z; #4 x, y, z+1; #5 -x+1/2, -y+3/2, -z+1; #6 -x+1, y, -z+1/2; #7 x-1/2, -y+3/2, z-1/2



5-(3-amino-tetrazole-5-phenoxy)-isophthalic acid (H_2atpia).

Scheme S1. Synthesis of H_2atpia.

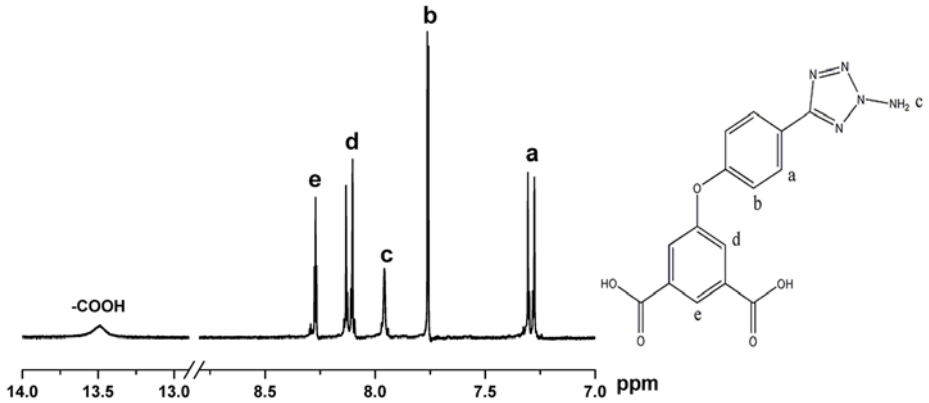


Fig. S1. ^{1}H-NMR spectrum of H_2atpia in DMSO-d_6.

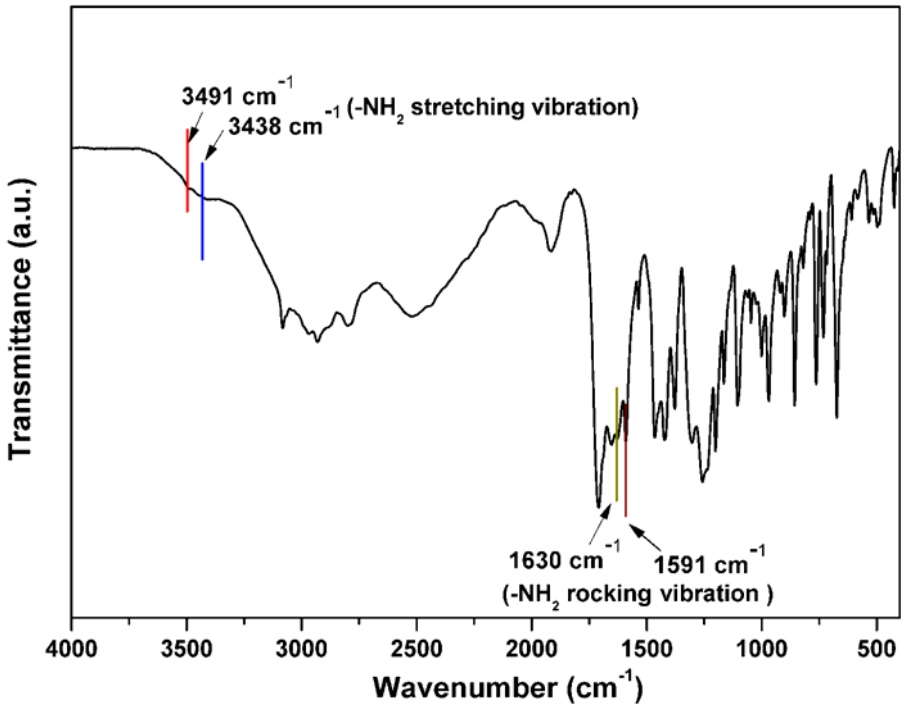


Fig. S2. IR Spectra of H_2atpia ligand.

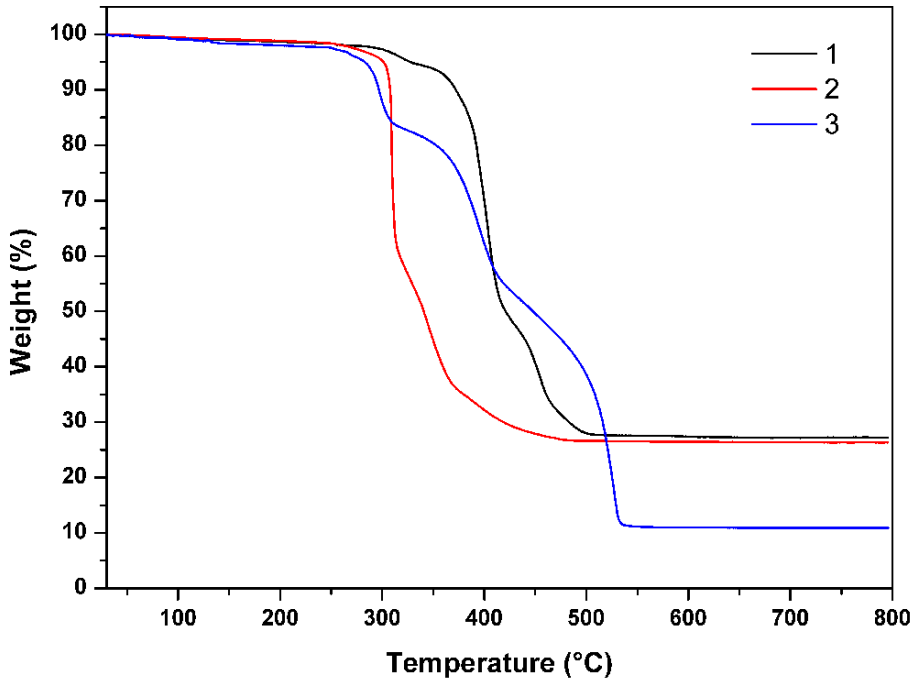


Fig. S3. TGA plot of compounds **1**–**3**.

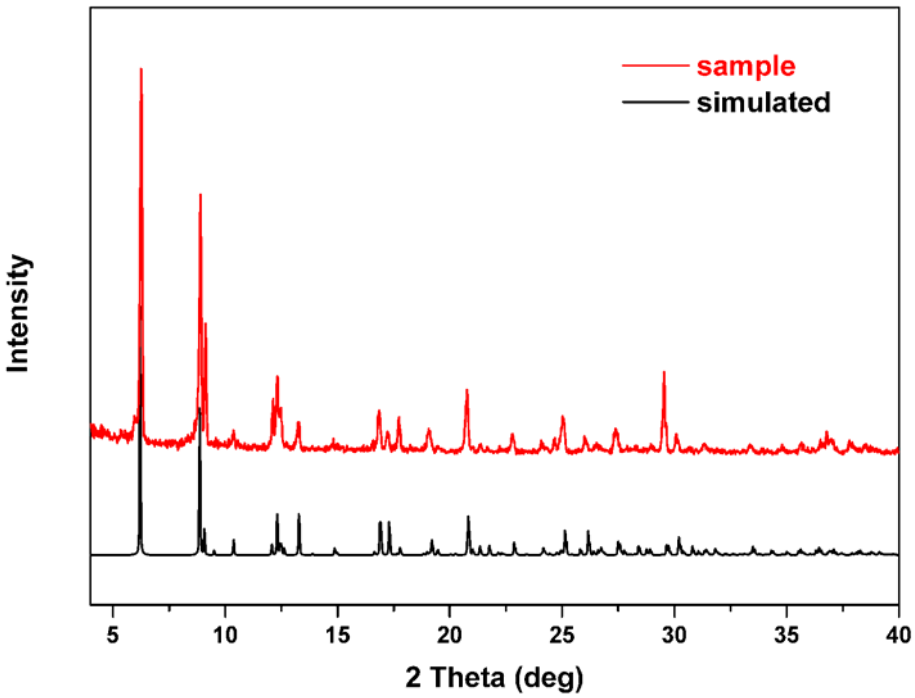


Fig. S4. The PXRD data of **1** showing good agreement with the simulated one for as-synthesized sample.

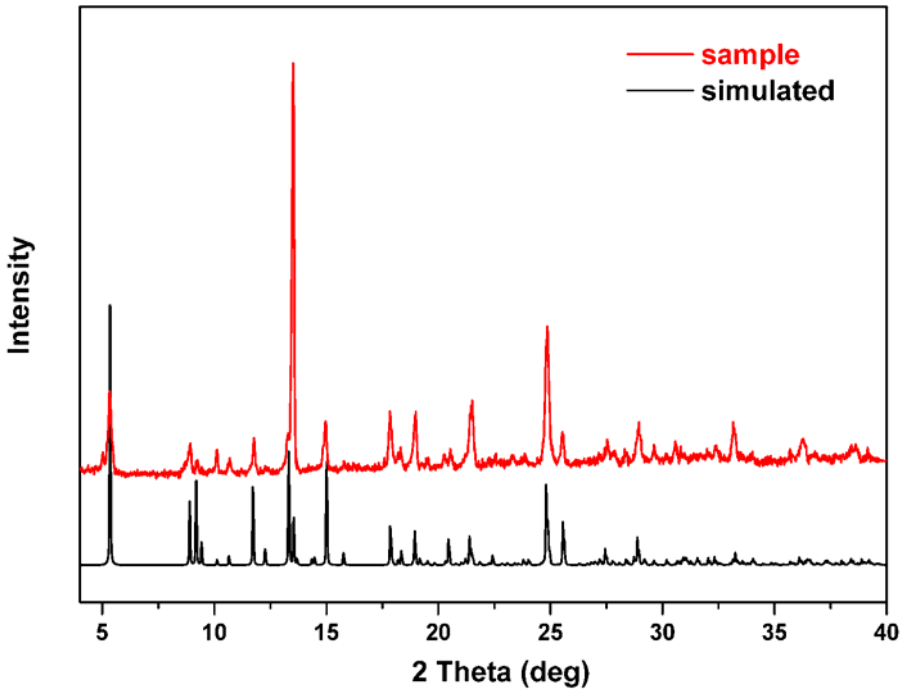


Fig. S5. The PXRD data of **2** showing good agreement with the simulated one for as-synthesized sample.

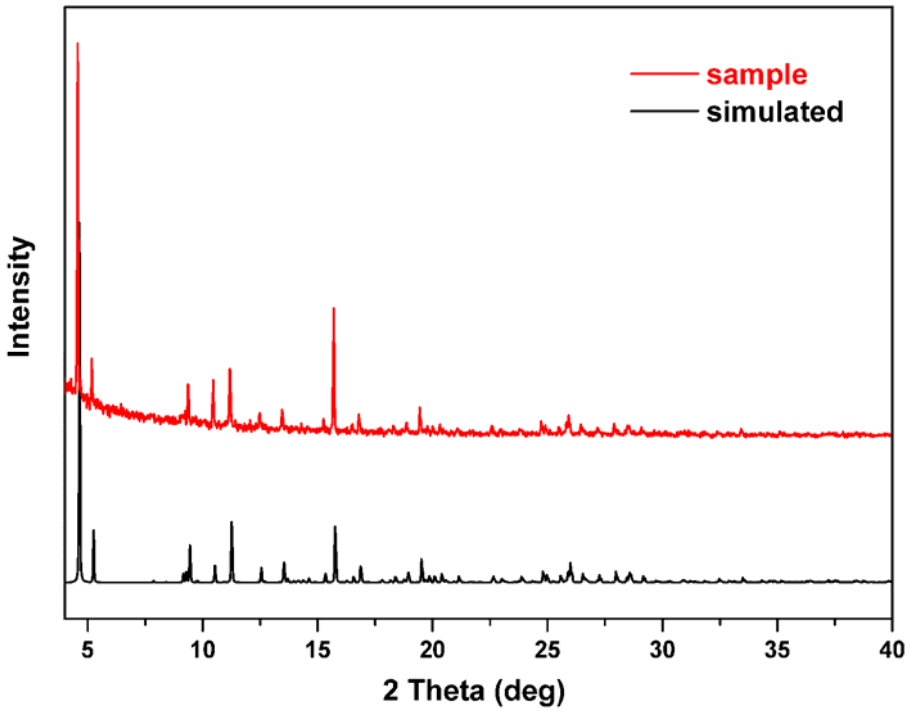


Fig. S6. The PXRD data of **3** showing good agreement with the simulated one for as-synthesized sample.

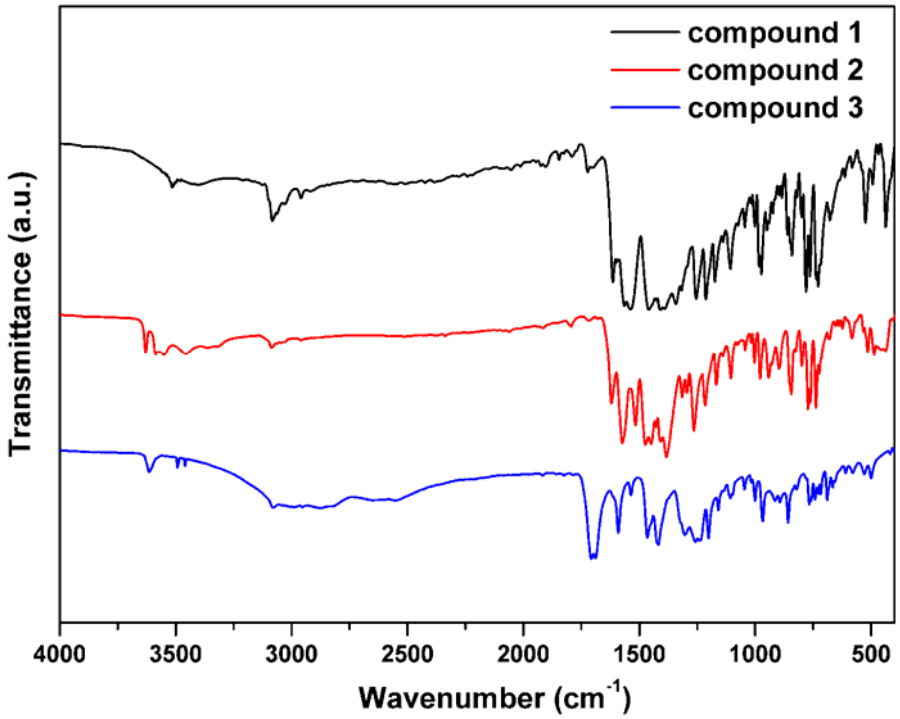


Fig. S7. IR Spectra of compound **1-3**.