Supplementary Materials

Syntheses, Structures, and Photoluminescent Properties of a Series of Zinc(II)-3-amino-1,2,4-triazolate Coordination Polymers Constructed by Varying Carboxylate Anions

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Table S1 Selected bond distances (Å) and angles (°) for complexes **1-5**.

Compound 1					
Zn(1)-N(2)#1	1.996(7)	N(1)-C(2)	1.363(12)	N(2)-Zn(1)#4	1.996(7)
Zn(1)-O(1)	2.020(10)	N(4)-C(2)	1.344(13)	N(3)-Zn(1)#3	2.023(7)
Zn(1)-N(3)#2	2.023(7)	C(2)-N(3)	1.324(12)	N(3)-N(2)	1.392(10)
Zn(1)-N(1)	2.032(7)	C(4)-C(5)	1.33(2)	C(1)-N(2)	1.315(11)
O(1)-C(3)	1.224(15)	C(4)-C(9)	1.357(19)	N(1)-C(1)	1.338(12)
N(2)#1-Zn(1)-O(1)	131.2(4)	N(2)#1-Zn(1)-N(3)#2	106.4(3)	O(1)-Zn(1)-N(3)#2	94.2(4)
N(2)#1-Zn(1)-N(1)	109.3(3)	O(1)-Zn(1)-N(1)	105.6(4)	N(3)#2-Zn(1)-N(1)	107.2(3)
C(3)-O(1)-Zn(1)	104.3(10)	C(1)-N(1)-C(2)	103.6(8)	C(1)-N(1)-Zn(1)	127.5(6)
N(3)-C(2)-N(4)	123.9(9)	C(5)-C(4)-C(9)	119.1(15)	O(1)-C(3)-O(2)	120.3(15)
Symmetry codes: #1 x+1/2,-y+1/2,-z+1 #2 -x+1/2,y-1/2,z #3 -x+1/2,y+1/2,z #4 x-1/2,-y+1/2,-z+1					
Compound 2					
Zn(1)-O(1)	1.947(5)	Zn(1)-N(2)#1	1.984(5)	Zn(1)-N(4)#2	2.031(5)
Zn(1)-N(1)	2.031(5)	O(2)-C(3)	1.226(10)	O(1)-C(3)	1.226(10)
C(4)-C(5)	1.366(10)	N(2)-C(2)	1.332(8)	N(2)-N(1)	1.390(7)
N(2)-Zn(1)#1	1.984(5)	C(2)-N(4)	1.351(7)	C(2)-N(3)	1.355(8)
N(4)-Zn(1)#4	2.031(5)	C(1)-N(4)	1.337(7)	C(1)-N(1)	1.308(8)
O(1)-Zn(1)-N(2)#1	132.2(2)	O(1)-Zn(1)-N(4)#2	108.1(2)	N(2)#1-Zn(1)-N(4)#2	108.4(2)
O(1)-Zn(1)-N(1)	96.8(2)	N(2)#1-Zn(1)-N(1)	105.80(19)	N(4)#2-Zn(1)-N(1)	100.5(2)
C(3)-O(1)-Zn(1)	108.9(5)	C(5)-C(4)-C(6)#3	118.8(7)	O(2)-C(3)-O(1)	122.2(7)
C(2)-N(2)-Zn(1)#1	132.2(4)	C(2)-N(2)-N(1)	105.5(5)	N(1)-N(2)-Zn(1)#1	118.6(4)
Symmetry codes: #1 -x+2,-y,-z+1 #2 -y+1,x-1/2,-z+1 #3 -x+3/2,y,-z+3/2 #4 y+1/2,-x+1,-z+1					
Compound 3					
C(1)-N(1)	1.323(8)	C(1)-N(2)	1.357(9)	C(3)-N(5)	1.346(8)
C(3)-N(8)	1.351(8)	C(3)-N(7)	1.374(8)	C(4)-N(6)	1.324(8)
C(4)-N(7)	1.368(8)	C(5)-O(2)	1.232(9)	C(5)-O(1)	1.298(8)
Zn(2)-O(4)#5	2.004(5)	Zn(2)-N(2)#6	2.048(5)	C(12)-O(3)	1.220(9)
C(12)-O(4)	1.301(9)	C(2)-N(4)	1.301(9)	C(2)-N(3)	1.362(9)
N(5)-N(6)	1.412(8)	N(5)-Zn(2)	2.001(5)	N(4)-N(1)	1.401(7)
N(1)-Zn(1)	1.977(5)	N(2)-Zn(2)#1	2.048(5)	N(7)-Zn(1)#2	2.029(5)
O(1)-Zn(1)	1.960(5)	O(4)-Zn(2)#3	2.004(5)	Zn(1)-N(7)#4	2.029(5)
O(1)-Zn(1)-N(1)	121.2(2)	O(1)-Zn(1)-N(7)#4	98.9(2)	N(1)-Zn(1)-N(7)#4	110.0(2)
O(1)-Zn(1)-N(6)	102.9(2)	N(1)-Zn(1)-N(6)	110.5(2)	N(7)#4-Zn(1)-N(6)	113.0(2)
N(5)-Zn(2)-O(4)#5	124.1(2)	N(5)-Zn(2)-N(4)	109.8(2)	O(4)#5-Zn(2)-N(4)	95.2(2)
N(5)-Zn(2)-N(2)#6	116.2(2)	O(4)#5-Zn(2)-N(2)#6	99.9(2)	N(4)-Zn(2)-N(2)#6	109.3(2)
C(1)-N(1)-Zn(1)	131.1(5)	N(4)-N(1)-Zn(1)	123.4(4)	C(5)-O(1)-Zn(1)	111.3(5)
N(1)-N(4)-Zn(2)	124.3(4)	C(3)-N(5)-Zn(2)	130.0(5)	O(3)-C(12)-O(4)	122.0(7)
Symmetry codes: #1 -x+2,y-1/2,-z+1/2 #2 -x+1,y+1/2,-z+1/2 #3 x-1,-y+1/2,z-1/2 #4 -x+1,y-1/2,-z+1/2 #5 x+1,-y+1/2,z+1/2 #6 -x+2,y+1/2,-z+1/2					
Compound 4					
Zn(3)-O(1)	1.984(3)	Zn(3)-N(2)	1.998(4)	Zn(3)-N(5)	2.000(4)
Zn(3)-O(7)	2.075(4)	Zn(2)-N(6)	1.991(4)	Zn(2)-N(3)	1.999(4)
Zn(2)-O(11)#1	2.002(3)	Zn(2)-O(2W)	2.005(2)	Zn(1)-O(5)#2	1.918(3)
Zn(1)-O(8)#3	1.940(3)	Zn(1)-N(1)	1.979(3)	Zn(1)-O(1W)	2.0023(19)
Zn(4)-O(4)#4	1.910(3)	Zn(4)-O(9)#5	1.920(3)	Zn(4)-N(7)	1.977(4)
Zn(4)-O(3W)	2.0090(19)	N(3)-C(2)	1.332(5)	N(3)-N(2)	1.396(5)
C(5)-O(2)	1.254(5)	C(5)-O(1)	1.264(5)	C(5)-C(6)	1.490(6)

N(7)-C(3)	1.343(6)	N(7)-C(4)	1.352(5)	N(6)-C(3)	1.312(6)
N(6)-N(5)	1.390(5)	O(11)-Zn(2)#1	2.002(3)	O(8)-Zn(1)#3	1.940(3)
O(5)-Zn(1)#6	1.918(3)	O(4)-Zn(4)#7	1.910(3)	O(9)-Zn(4)#5	1.920(3)
O(1)-Zn(3)-N(2)	137.81(15)	O(1)-Zn(3)-N(5)	102.46(14)	N(2)-Zn(3)-N(5)	107.64(15)
O(1)-Zn(3)-O(7)	95.99(14)	N(2)-Zn(3)-O(7)	107.43(15)	N(5)-Zn(3)-O(7)	99.14(14)
N(6)-Zn(2)-N(3)	107.47(16)	N(6)-Zn(2)-O(11)#1	136.37(16)	N(3)-Zn(2)-O(11)#1	101.52(14)
N(6)-Zn(2)-O(2W)	106.26(13)	N(3)-Zn(2)-O(2W)	99.50(13)	O(11)#1-Zn(2)-O(2W)	100.14(13)
O(5)#2-Zn(1)-O(8)#3	95.11(14)	O(5)#2-Zn(1)-N(1)	127.57(15)	O(8)#3-Zn(1)-N(1)	123.13(14)
O(5)#2-Zn(1)-O(1W)	104.53(12)	O(8)#3-Zn(1)-O(1W)	103.74(12)	N(1)-Zn(1)-O(1W)	99.72(12)
O(4)#4-Zn(4)-O(9)#5	94.12(15)	O(4)#4-Zn(4)-N(7)	128.09(16)	O(9)#5-Zn(4)-N(7)	124.69(16)
Symmetry codes: #1 -x,-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 #5 -x+1/2,-y-1/2,-z+1 #6 x+1/2,y-1/2,z #7 x+1/2,y+1/2,z					
Compound 5					
Zn(1)-O(4)#1	1.966(7)	C(5)-C(6)#5	1.379(12)	Zn(1)-N(3)#3	1.973(7)
Zn(1)-N(3)	1.973(7)	Zn(2)-N(1)	2.000(7)	Zn(2)-N(2)#4	2.031(6)
Zn(2)-O(3)	2.148(8)	Zn(2)-O(1)	2.175(7)	Zn(2)-O(2)	2.228(7)
Zn(2)-O(1W)	2.276(6)	C(3)-O(2)	1.250(12)	C(3)-O(1)	1.253(12)
C(3)-C(4)	1.498(13)	C(6)-C(7)#6	1.507(13)	N(1)-C(2)	1.336(11)
C(7)-C(6)#6	1.507(13)	N(2)-Zn(2)#4	2.031(6)	O(4)-Zn(1)#2	1.966(7)
O(4)#1-Zn(1)-O(4)#2	103.4(4)	O(4)#1-Zn(1)-N(3)#3	117.2(3)	O(4)#2-Zn(1)-N(3)#3	104.0(3)
O(4)#1-Zn(1)-N(3)	104.0(3)	O(4)#2-Zn(1)-N(3)	117.2(3)	N(3)#3-Zn(1)-N(3)	111.3(4)
N(1)-Zn(2)-N(2)#4	107.1(3)	N(1)-Zn(2)-O(3)	103.5(3)	N(2)#4-Zn(2)-O(3)	93.2(3)
N(1)-Zn(2)-O(1)	99.3(3)	N(2)#4-Zn(2)-O(1)	152.0(3)	O(3)-Zn(2)-O(1)	89.7(3)
N(1)-Zn(2)-O(2)	157.3(3)	N(2)#4-Zn(2)-O(2)	93.3(2)	O(3)-Zn(2)-O(2)	84.9(3)
O(1)-Zn(2)-O(2)	91.8(2)	O(2)-C(3)-O(1)	120.7(9)	N(2)-C(1)-N(3)	112.6(8)
Symmetry codes: #1 x,-y,z-1/2 #2 -x+2,-y,-z+1 #3 -x+2,y,-z+1/2 #4 -x+3/2,-y+1/2,-z+1 #5 -x,-y,-z+1 #6 -x+1,-y,-z+1					

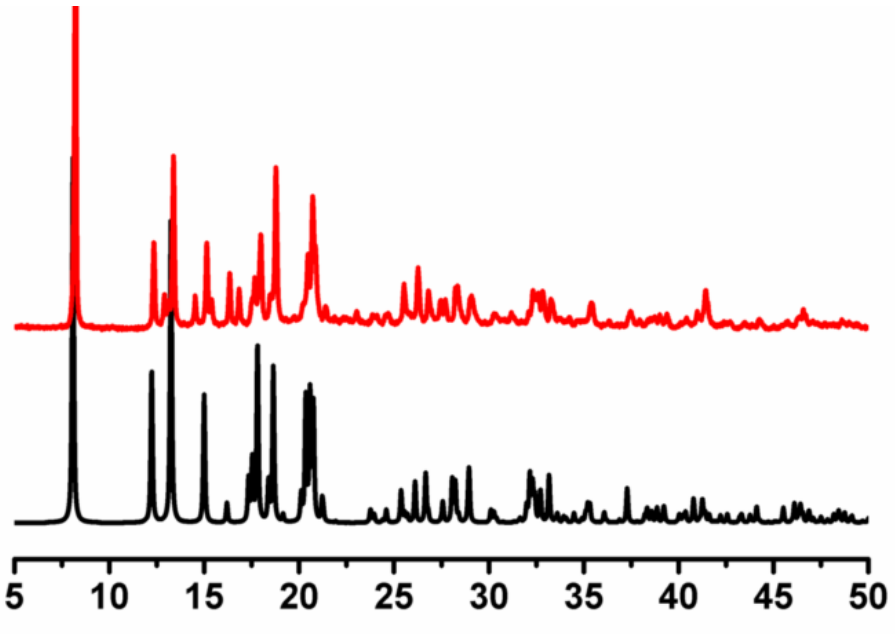

Fig. S1. Powder X-ray diffraction data for compounds **1.** black: simulated, red: measured.

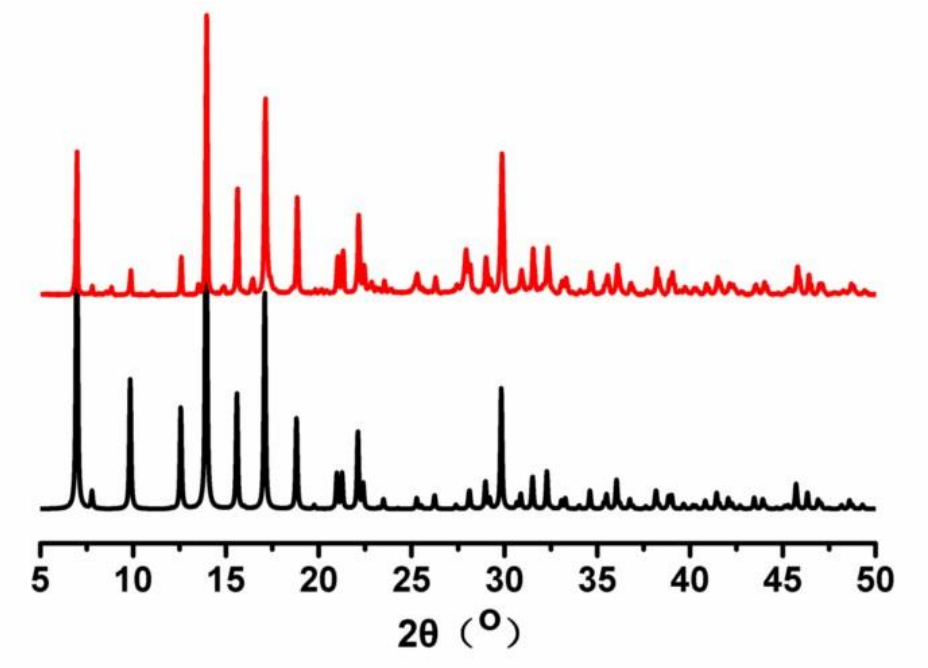

Fig. S2. Powder X-ray diffraction data for compounds **2.** black: simulated, red: measured.

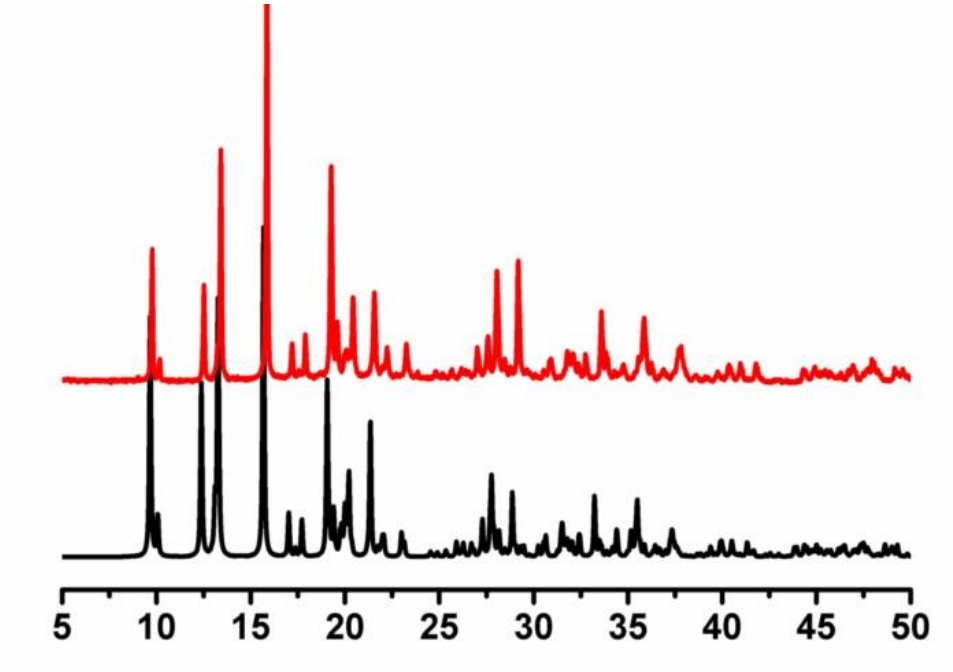

Fig. S3. Powder X-ray diffraction data for compounds **3.** black: simulated, red: measured.

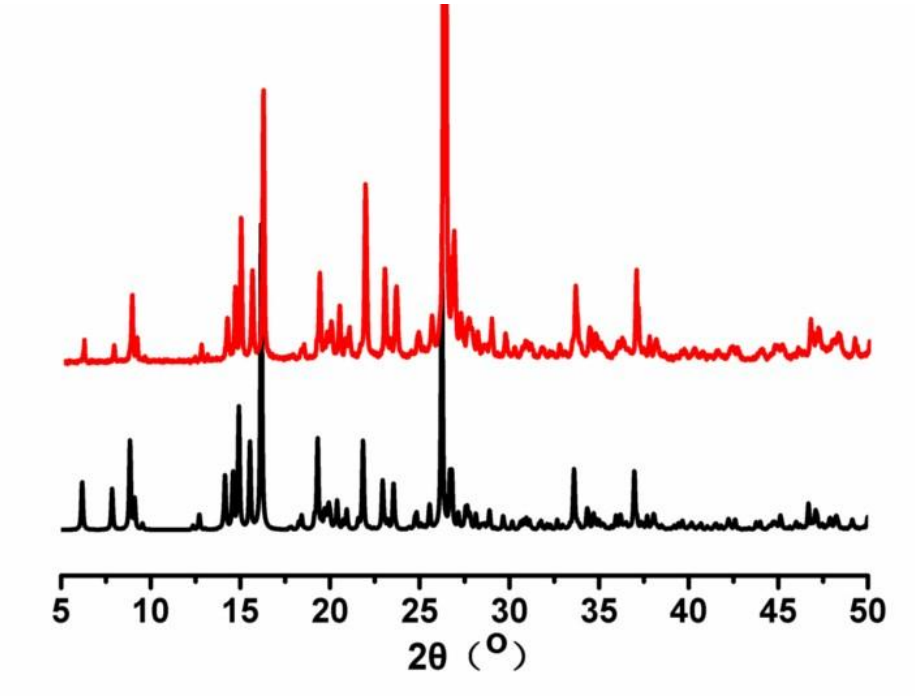

Fig. S4. Powder X-ray diffraction data for compounds **4.** black: simulated, red: measured.

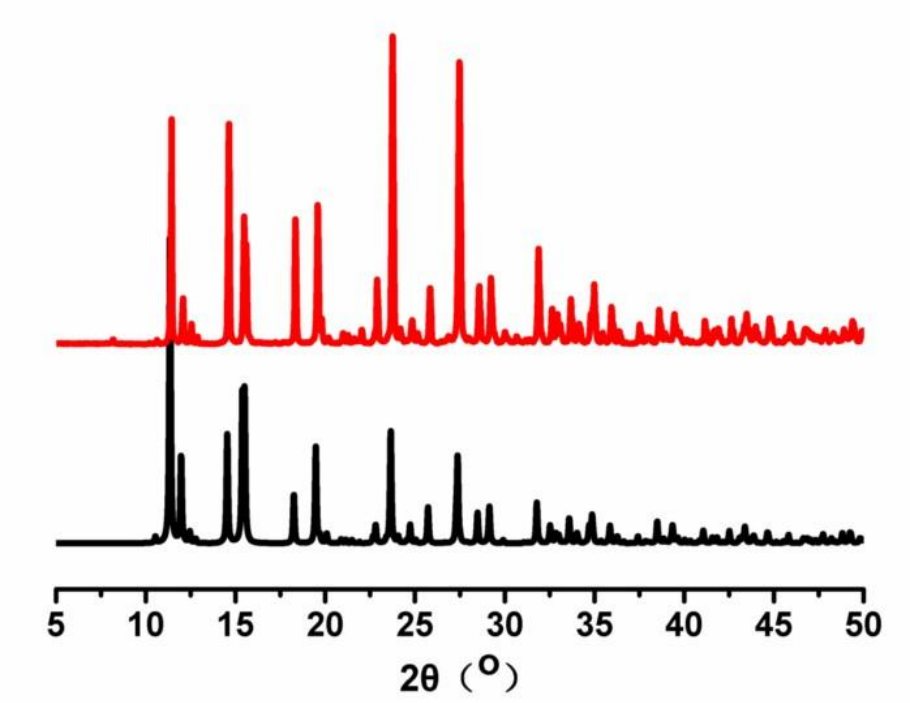

Fig. S5. Powder X-ray diffraction data for compounds **5.** black: simulated, red: measured.

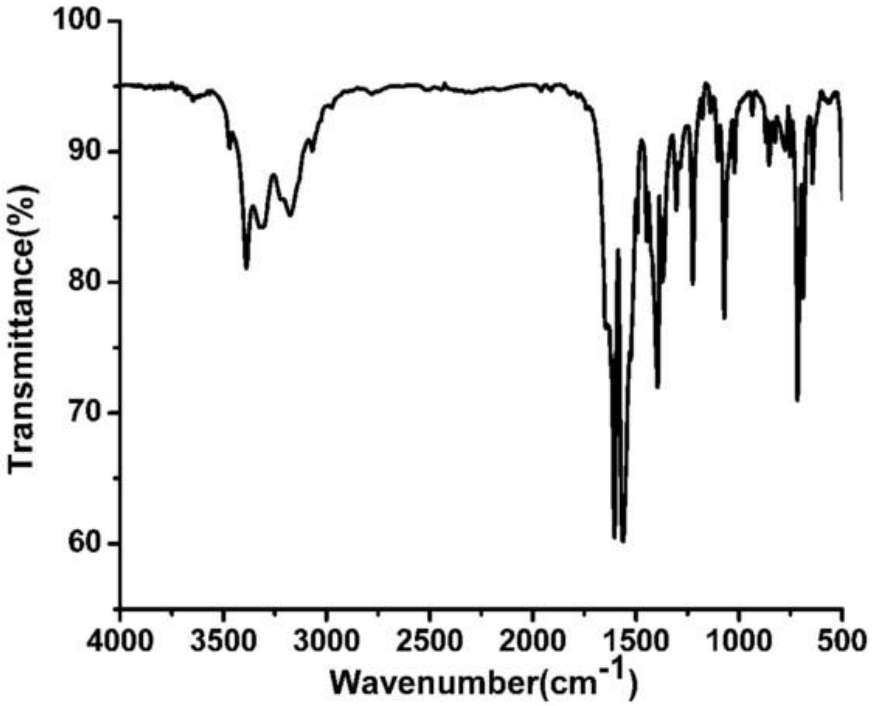

Fig. S6. IR spectra of compound **1**.

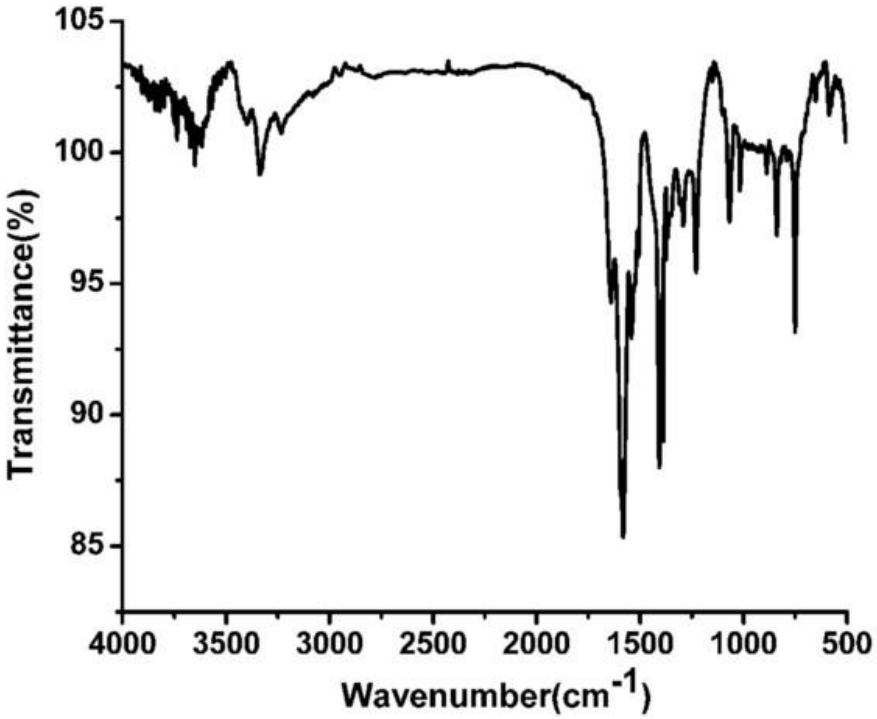

Fig. S7. IR spectra of compound **2**.

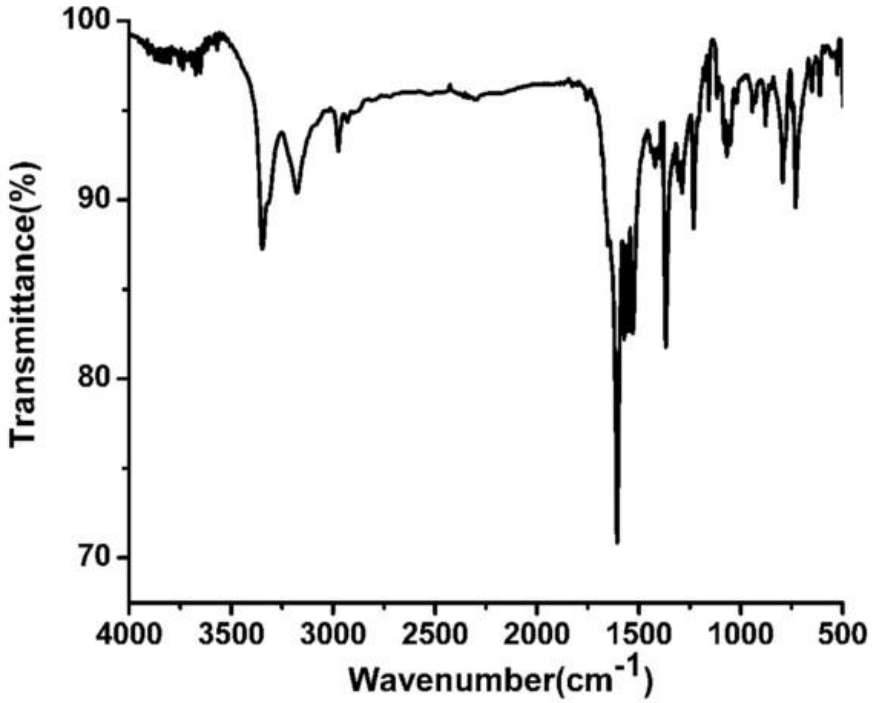

Fig. S8. IR spectra of compound **3**.

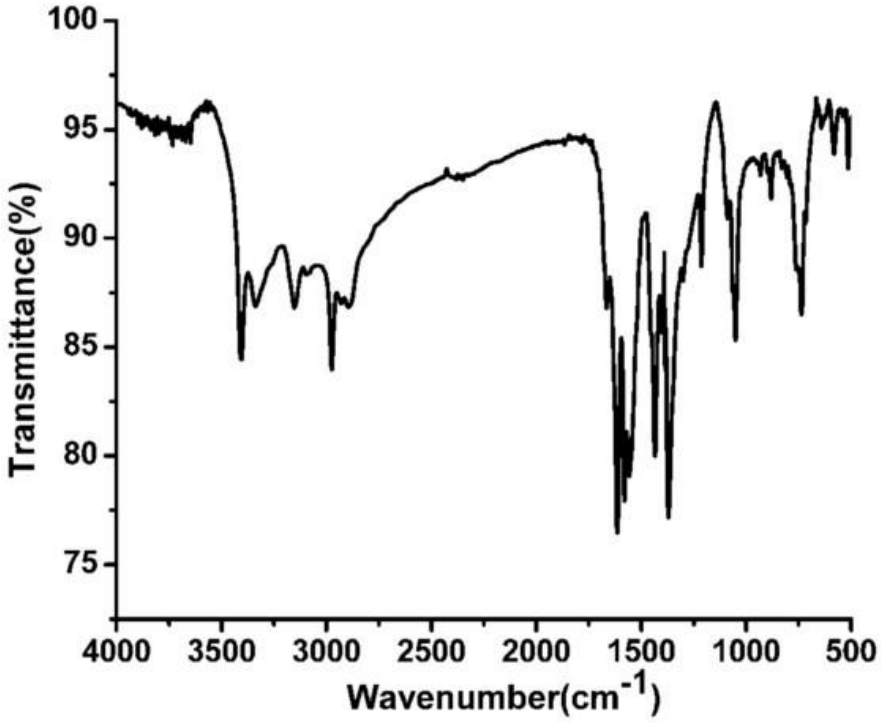

Fig. S9. IR spectra of compound **4**.

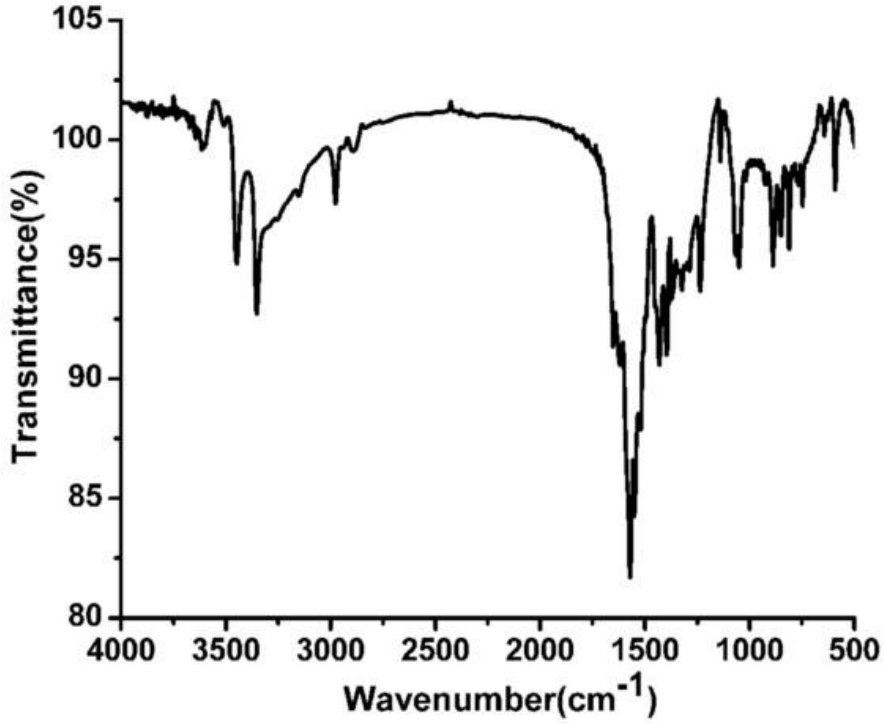

Fig. S10. IR spectra of compound **5**.