<Journal Name>New Journal of Chemistry

Supporting Information

Triazine-polycarboxylate acids complexes: synthesis, crystal structure and photocatalytic activity

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Scheme, Figure and Table titles:

Table S1. Crystallographic data and the structure refinement of complex **3**

Complex	3
Formula	C32H36N10O8Zn
M ($g \cdot mol^{-1}$)	754.08
Crystal system	Triclinic
Space group	P-1
a (Å)	9.491(2)
b (Å)	13.025(3)
c (Å)	16.033(3)
α (°)	106.161(4)
β(°)	91.155(4)
γ(°)	109.772(3)
V(Å3)	1777.1(6)
Z	2
Dcalc(g.cm-3)	1.409
Crystal size (mm)	0.44×0.23×0.12
F(000)	784
M(Mo Kα) (mm-1)	0.755
θ (°)	2.30-22.80
Reflections collected	7357
Independent reflections(I>2σ)	4757(2724)
Parameters	469
Δ(ρ)(e Å-3)	0.346and-0.283
Goodness of fit (GOF) on F2	1.027
Ra	0.0632(0.1205)b
wRa2	0.1300(0.1570)b

*[a]$R=\Sigma \left| F_O-F_C \right| / \Sigma \left| F_O \right|$, $wR_2=\{\Sigma[w(F_O^2-F_C^2)^2]/\Sigma[w(F_O^2)^2]\}^{1/2}$; $[F_O>4\sigma(F_O)]$.

[b]Based on all data.

Table S2. Selected bond lengths (Å) and angles (°) for the complexes **1**, **2** and **4**

Complex **1**			
Zn-O(1)	1.940(2)	Zn-O(2)	1.954(3)
Zn-N(1)	2.052(2)	Zn-N(3)	2.215(3)
Zn-N(2)	2.229(2)		
O(1)-Zn-O(2)	99.60(11)	O(1)-Zn-N(1)	136.35(11)
O(2)-Zn-N(1)	124.05(11)	O(1)-Zn-N(3)	100.49(11)
O(2)-Zn-N(3)	101.53(12)	N(1)-Zn-N(3)	73.15(10)
O(1)-Zn-N(2)	96.95(11)	O(2)-Zn-N(2)	105.80(11)
N(1)-Zn-N(2)	72.82(10)	N(3)-Zn-N(2)	144.43(10)
Complex **2**			
Co-O(1)	1.986(5)	Co-N(1)	2.029(6)
Co-O(4)#1	2.015(5)	Co-N(2)	2.196(7)
Co-N(3)	2.125(7)		
N(1)-Co-N(3)	75.6(3)	O(4)#1-Co-N(3)	108.1(2)
O(1)-Co-N(1)	129.6(2)	O(1)-Co-N(2)	96.6(3)
O(1)-Co-O(4)#1	98.6(2)	N(1)-Co-N(2)	73.9(3)
N(1)-Co-O(4)#1	130.3(2)	O(4)#1-Co-N(2)	91.0(2)
O(1)-Co-N(3)	103.6(2)	N(3)-Co-N(2)	149.4(2)
Complex **4**			
Cu(1)-O(1)	1.940(2)	Cu(1)-O(1W)	1.971(3)
Cu(1)-N(2)	2.004(3)	Cu(1)-N(1)	2.024(2)
Cu(1)-O(2W)	2.306(2)		
O(1)-Cu(1)-O(1W)	89.81(9)	O(1)-Cu(1)-N(2)	96.34(10)
O(1W)-Cu(1)-N(2)	171.35(10)	O(1)-Cu(1)-N(1)	171.61(10)
O(1W)-Cu(1)-N(1)	93.44(10)	N(2)-Cu(1)-N(1)	79.66(10)
O(1)-Cu(1)-O(2W)	91.66(9)	O(1W)-Cu(1)-O(2W)	88.12(10)
N(2)-Cu(1)-O(2W)	97.74(10)	N(1)-Cu(1)-O(2W)	96.18(10)

Table S3. Hydrogen bonds (Å) and angles (°) of the complexes **1, 2** and **4***

D–H ··A	*d*(D–H)/ Å	d(H ··A)/ Å	d(D ··A)/ Å	∠D–H ··A/ °
Complex **1**				
O7–H7 ··O3	0.82	1.88	2.688(4)	168.1
O5–H5A ··O7$^{\#1}$	0.82	1.81	2.623(4)	173.5
O8–H8 ··O2$^{\#2}$	0.82	2.19	2.998(9)	168.2
C17–H17A ··O8$^{\#3}$	0.96	2.54	3.248(10)	131.1
Complex **2**				
O5–H5 ··O7$^{\#1}$	0.82	1.87	2.637(12)	154.5
C7–H7 ··O2$^{\#2}$	0.93	2.52	3.393(12)	157.2
Complex **4**				
O1W–H1WA ··O3	0.85	1.83	2.630(3)	155.1
O3W–H3WA ··O1W	0.85	2.14	2.980(4)	170.7
O4W–H4WB ··O8	0.85	2.01	2.701(3)	138.2
O3W–H3WB ··O5	0.85	1.94	2.640(3)	138.9
O6W–H6WB ··O4	0.85	2.07	2.897(4)	164.2
N6–H6 ··O6$^{\#1}$	0.86	1.99	2.841(3)	172.2
N8–H8 ··O5W$^{\#2}$	0.86	1.98	2.822(4)	165.4
O1W–H1WB ··O6W$^{\#3}$	0.85	1.79	2.628(4)	170.9
O2W–H2WA ··O6$^{\#4}$	0.85	2.34	2.936(4)	127.3
O2W–H2WA ··N9$^{\#4}$	0.85	2.27	3.112(3)	172.2
O2W–H2WB ··O4$^{\#5}$	0.85	1.96	2.805(3)	178.0
O5W–H5WA ··O5$^{\#5}$	0.85	2.07	2.887(4)	160.0
O5W-H5WB ··O3$^{\#5}$	0.85	2.05	2.815(3)	150.2

*Symmetry transformation used to generate equivalent atoms: complex **1**: #1: -1-x, -1/2+y, -3/2-z; #2：-x, -1-y, -1-z; #3: x, -1/2-y, -1/2+z; complex **2**: #1: 1+x, y, z; #2: 3/2-x, -1/2+y, 3/2-z; complex **4**: #1: 2-x, -y, 1-z; #2: 1+x, -1+y, z; #3: 1+x, y, z; #4: -1+x, 1+y, z; #5: 1-x, 1-y, 1-z.

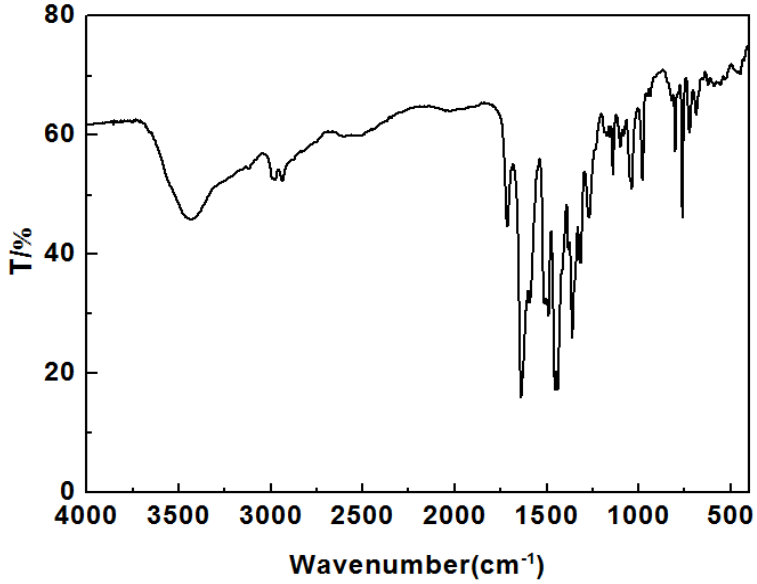

Fig. S1. IR absorption spectrum of complex **1**

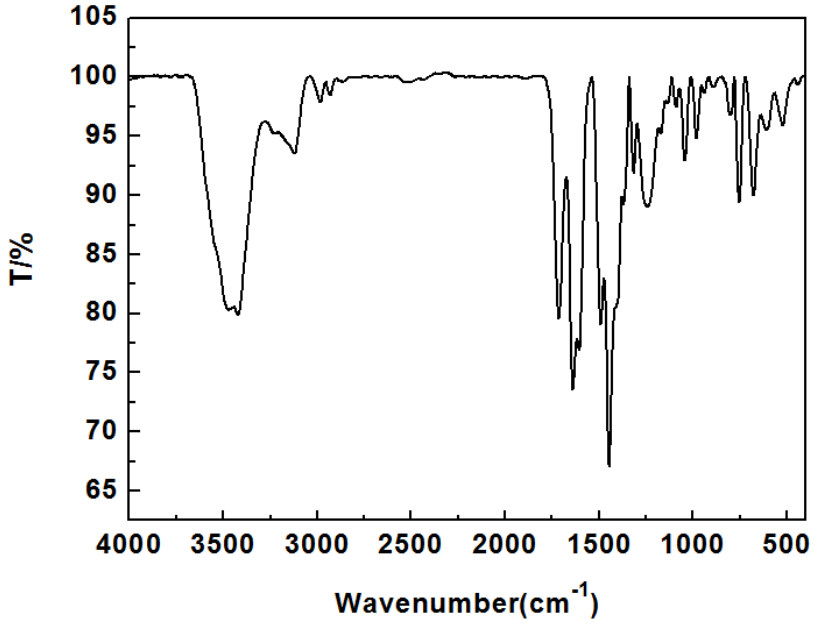

Fig. S2. IR absorption spectrum of complex **2**

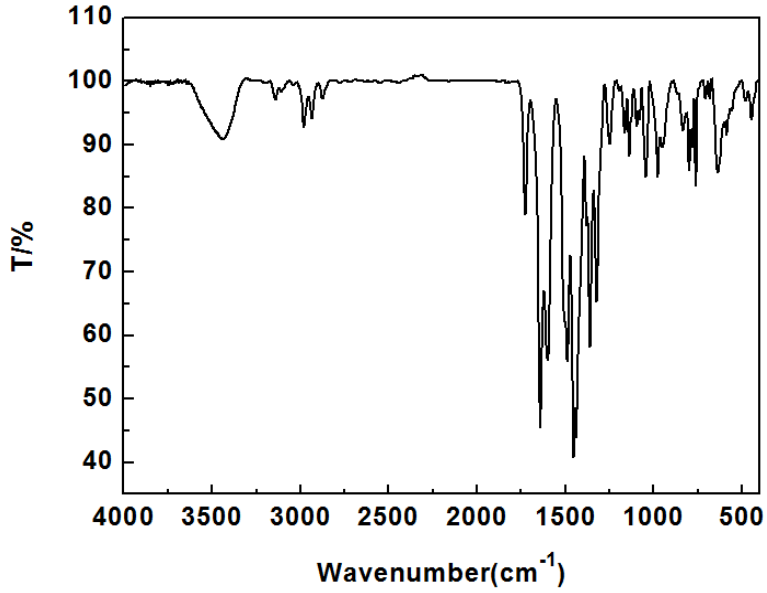

Fig. S3. IR absorption spectrum of complex **3**

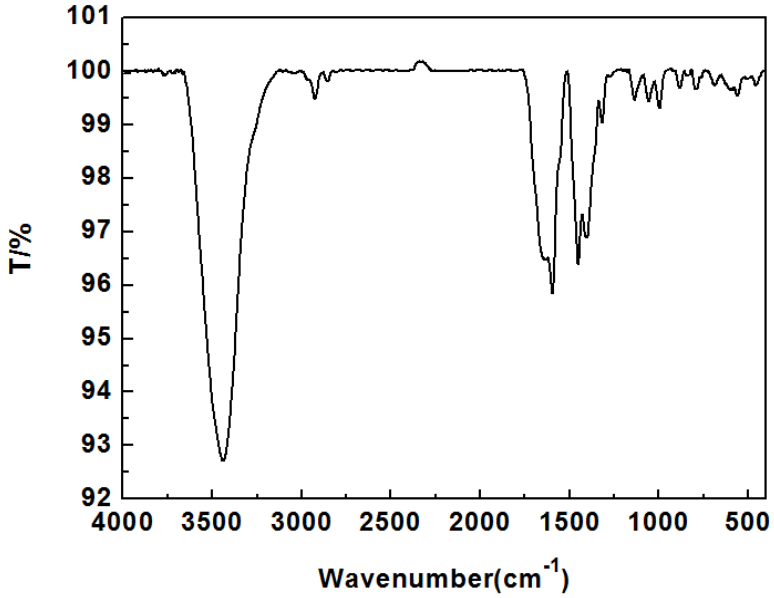

Fig. S4. IR absorption spectrum of complex **4**

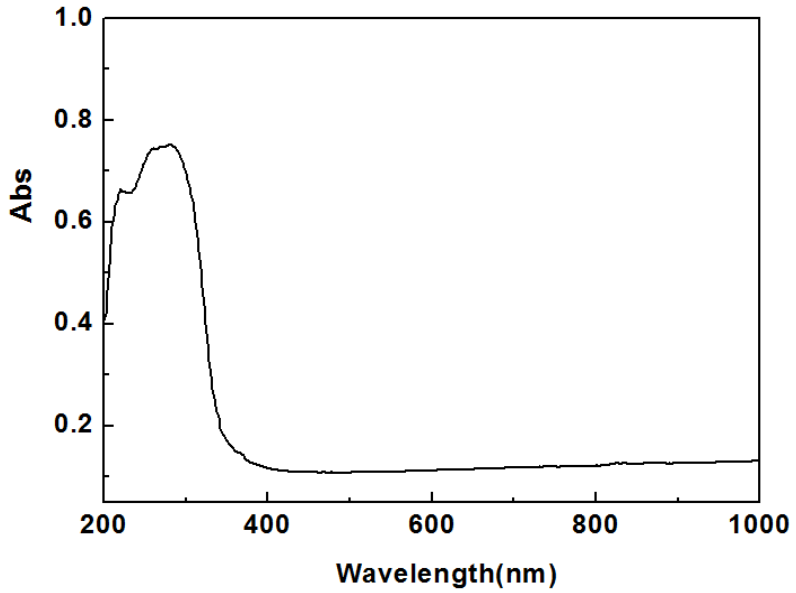

Fig. S5. UV-vis absorption spectrum of complex **1**

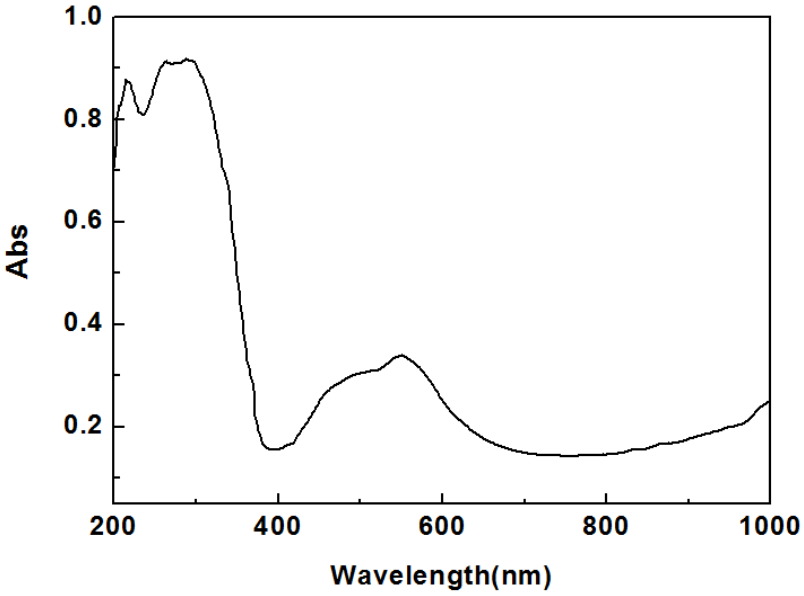

Fig. S6. UV-vis absorption spectrum of complex **2**

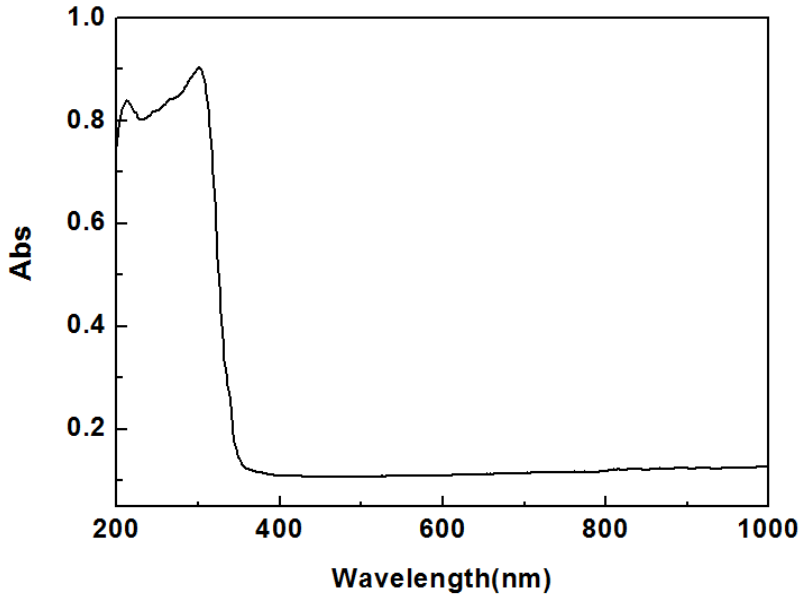

Fig. S7. UV-vis absorption spectrum of complex **3**

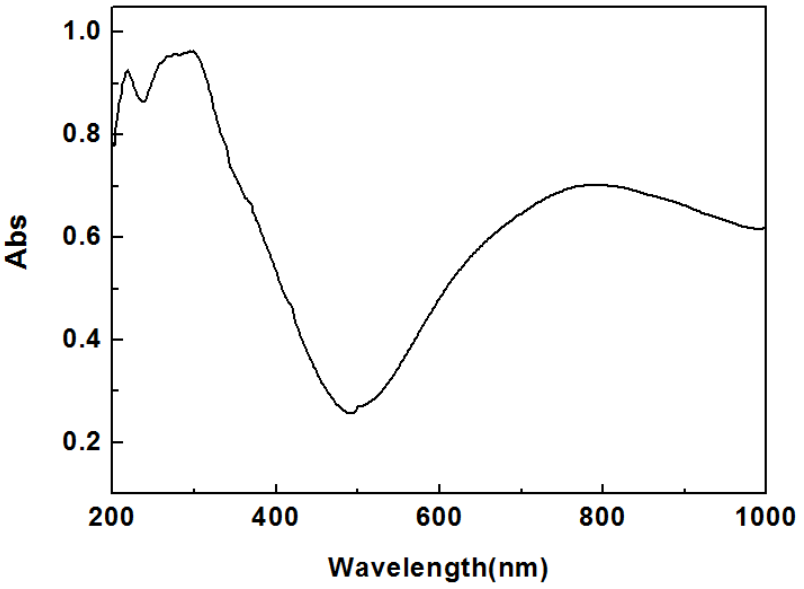

Fig. S8. UV-vis absorption spectrum of complex **4**

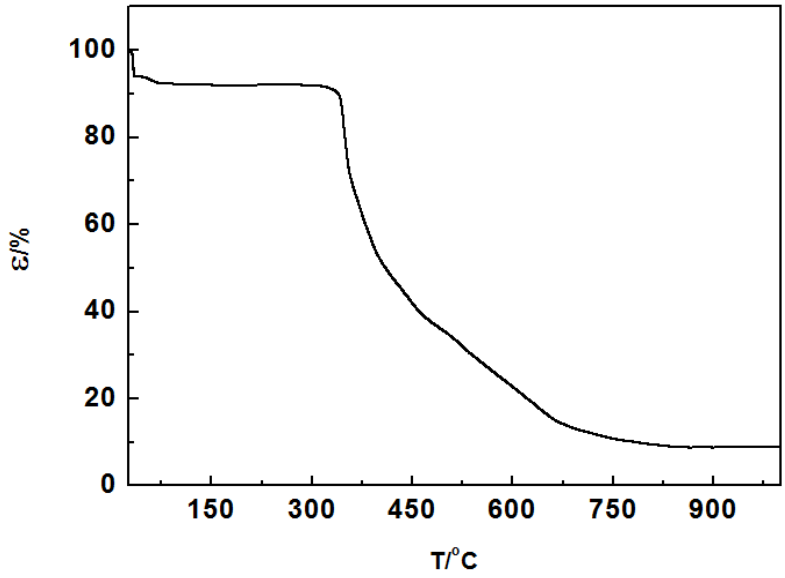

Fig. S9. TG curve of the complex **1**

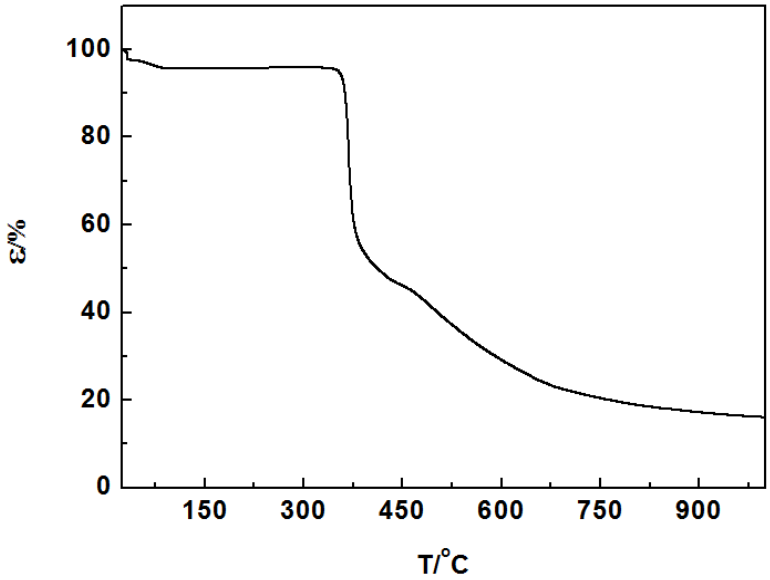

Fig. S10. TG curve of the complex **2**

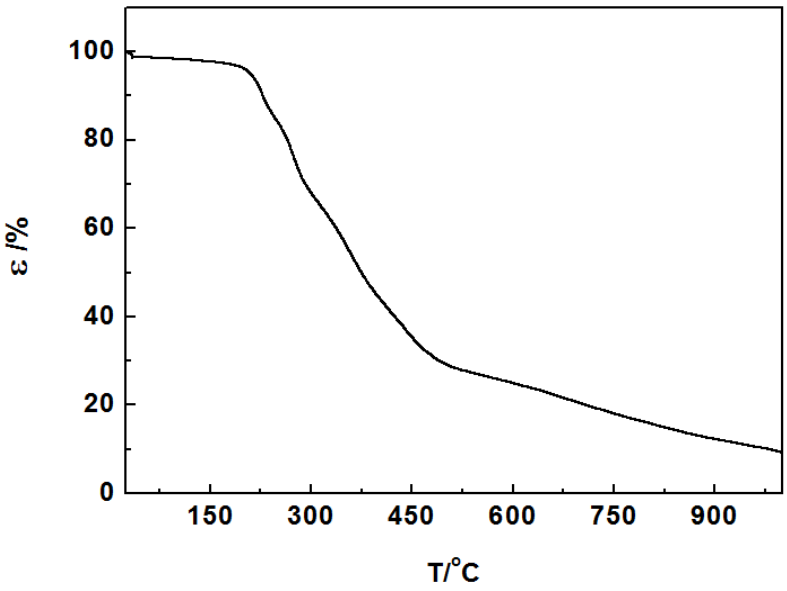

Fig. S11. TG curve of the complex **3**

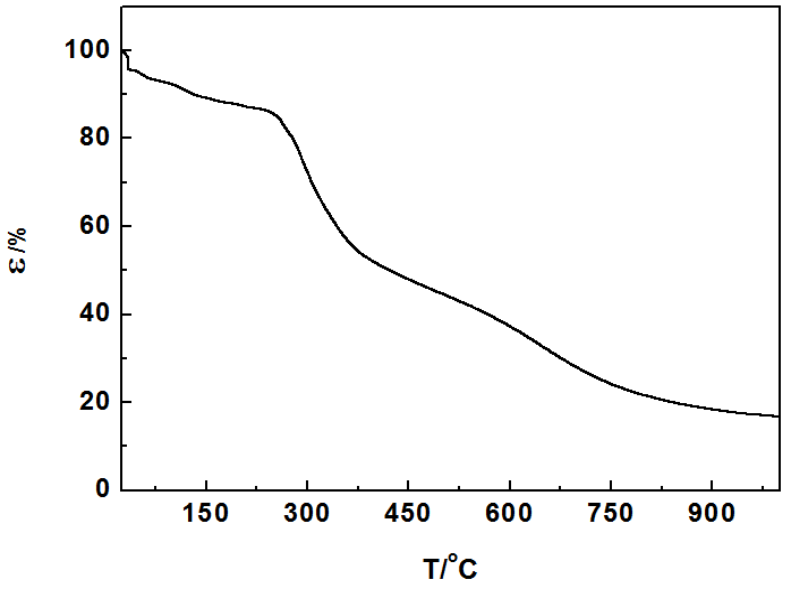

Fig. S12. TG curve of the complex **4**

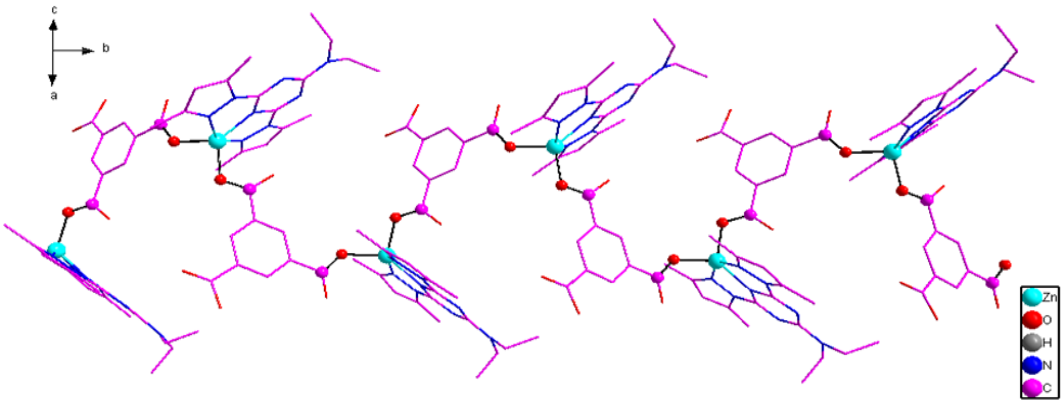

Fig. S13. The view of 1D chain of complex **1** (All H atoms are omitted for clarity)

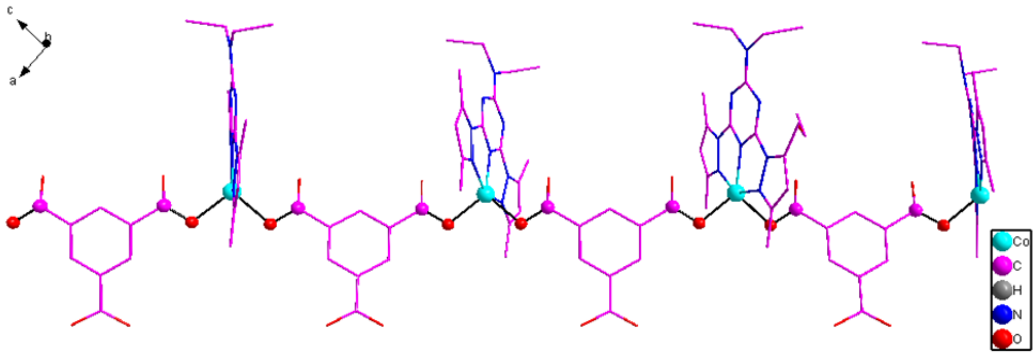

Fig. S14. The view of 1D chain in complex **2** (All H atoms are omitted for clarity)

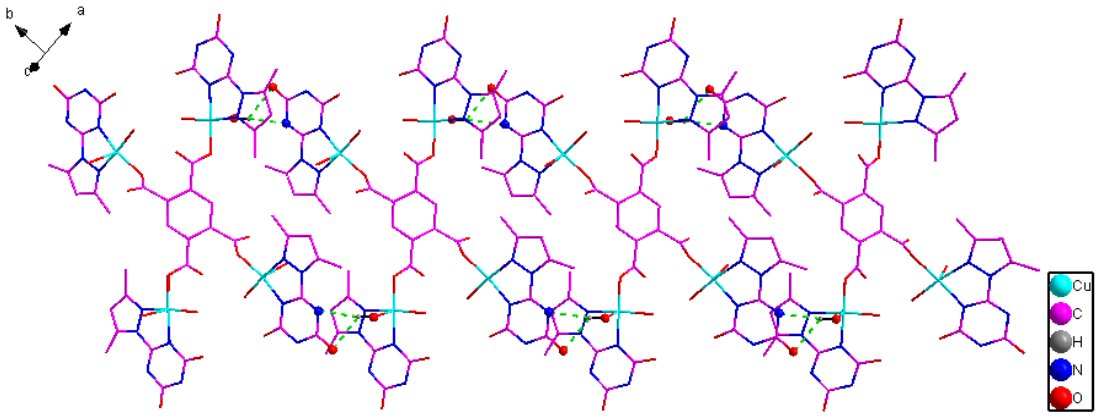

Fig. S15. The view of 1D chain via hydrogen bonds in complex **4** (All H atoms expert for the hydrogen bonds are omitted for clarity; Symmetry codes: #4: -1+x, 1+y, z)

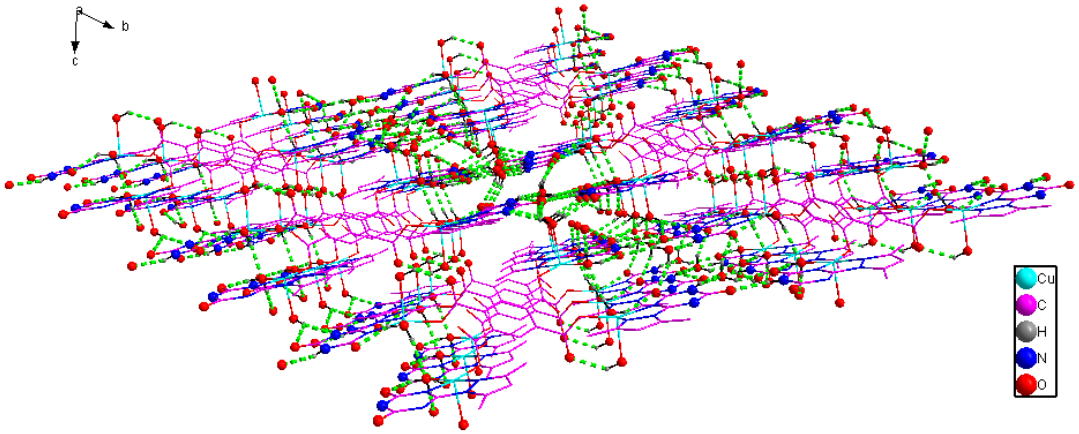

Fig. S16. The view of 3D network structure via hydrogen bonds in complex **4** (All H atoms expert for the hydrogen bonds are omitted for clarity; Symmetry codes: #1: 2-x, -y, 1-z; #2: 1+x, -1+y, z; #3: 1+x, y, z; #4: -1+x, 1+y, z; #5: 1-x, 1-y, 1-z.)