Supporting Information

Tuning the Framework Topologies of Co^{II}-doped Zn^{II}-Tetrazole-benzoate Coordination Polymers by Ligand Modifications: Structures and Spectral Studies

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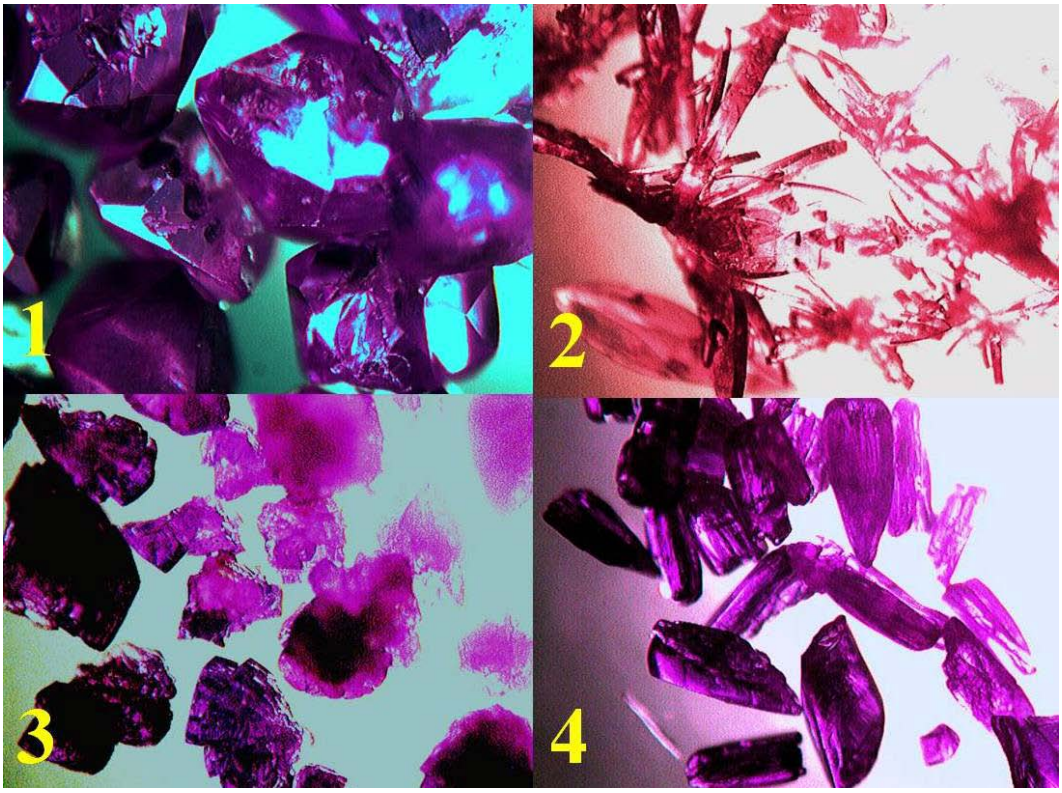
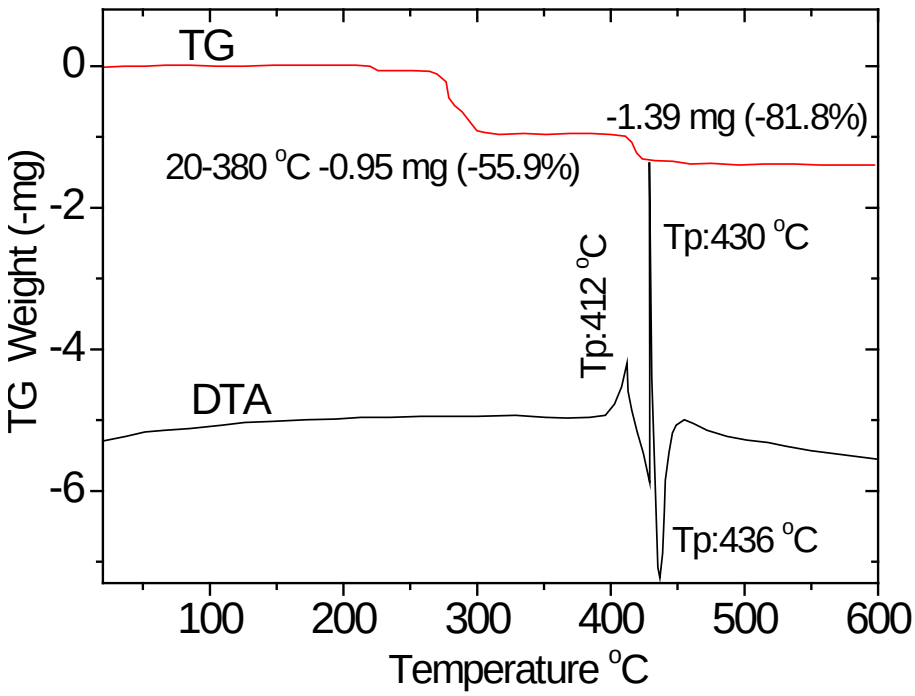
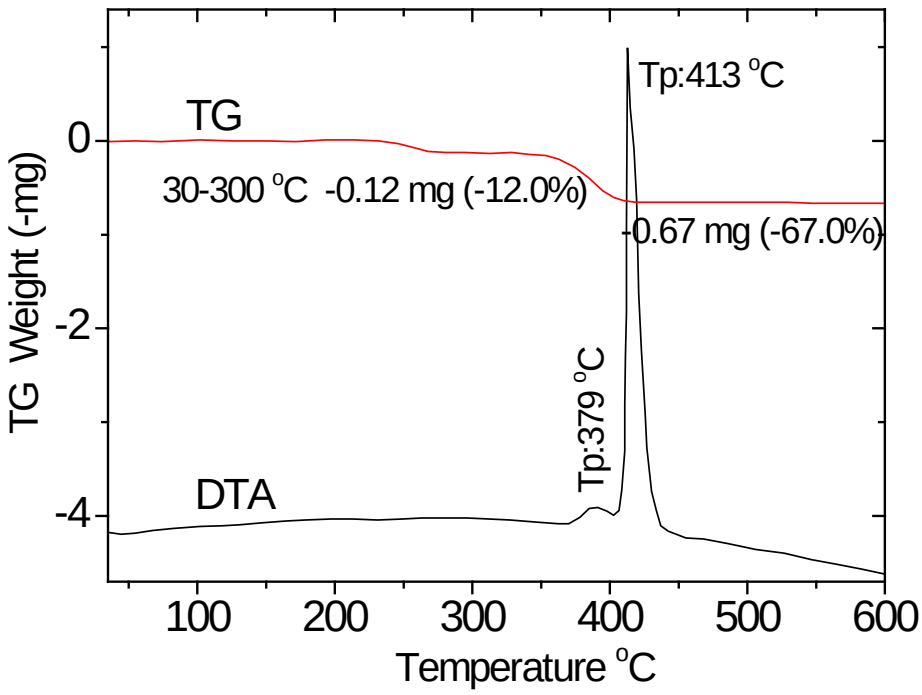


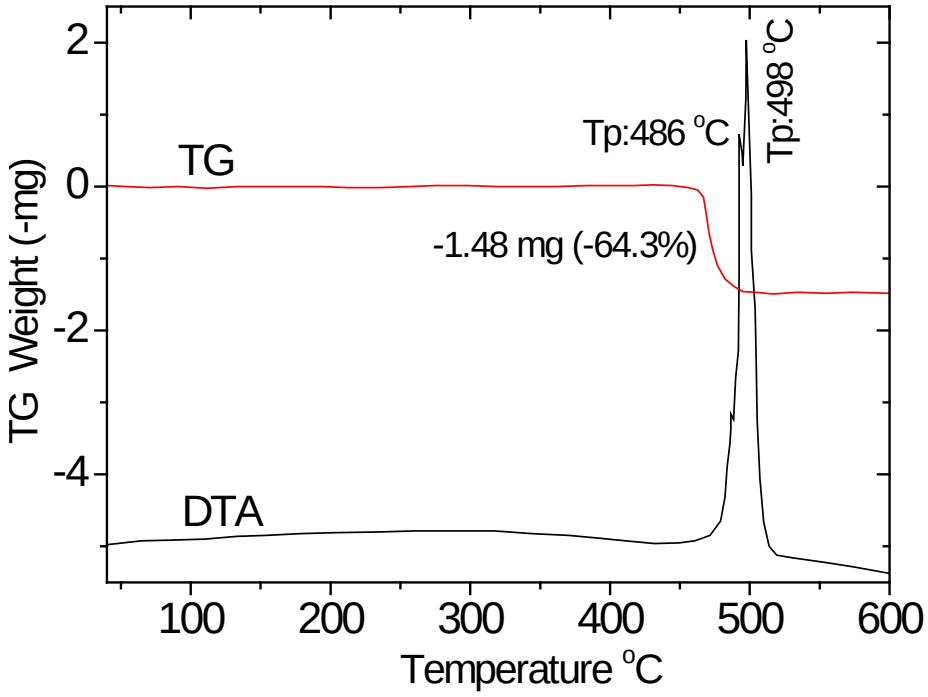
Figure S1. Photos of the crystals of **1-4** showing the existence of Co^{II} in the complexes.


TG
DTA
-1.39 mg (-81.8%)
20-380 °C -0.95 mg (-55.9%)
Tp:430 °C
Tp:412 °C
Tp:436 °C
TG Weight (-mg)
Temperature °C
0
-2
-4
-6
100
200
300
400
500
600

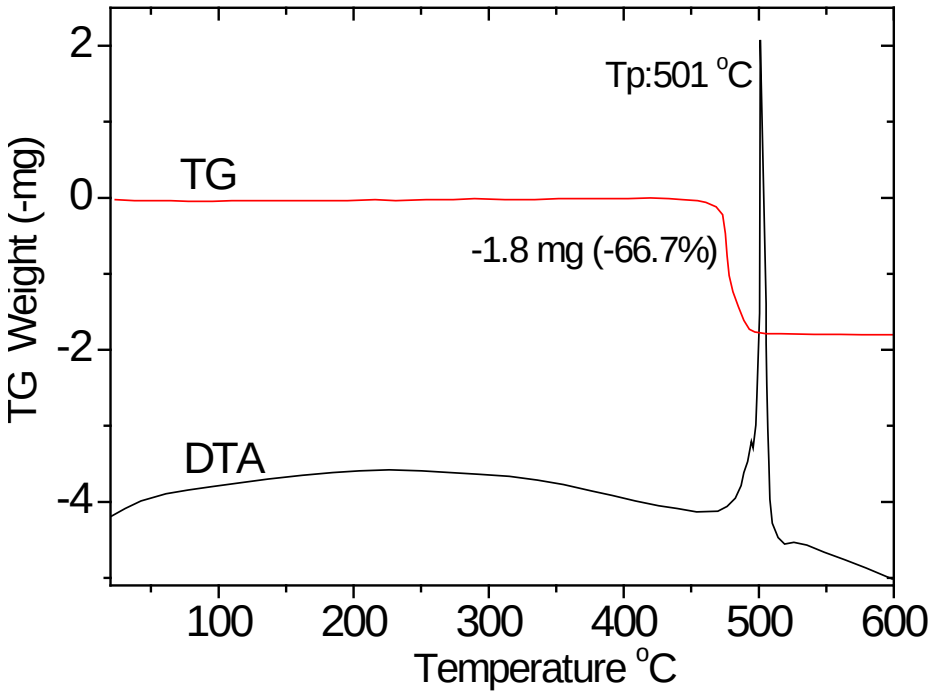
(a)


TG
DTA
Tp:413 °C
30-300 °C -0.12 mg (-12.0%)
-0.67 mg (-67.0%)
Tp:379 °C
TG Weight (-mg)
Temperature °C
0
-2
-4
100
200
300
400
500
600

(b)

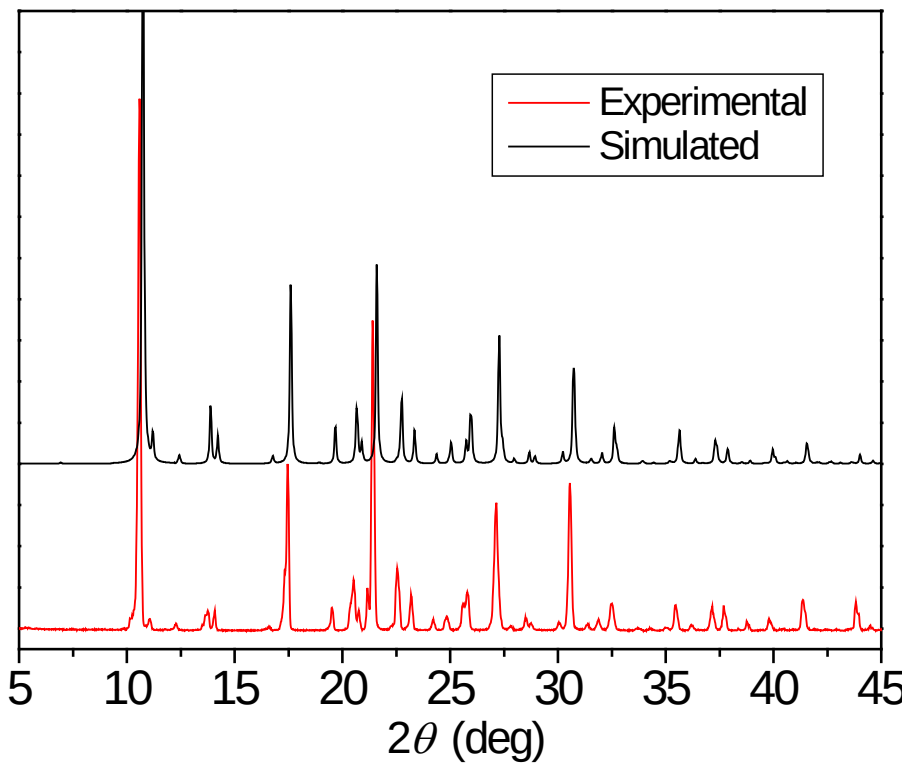


(c)

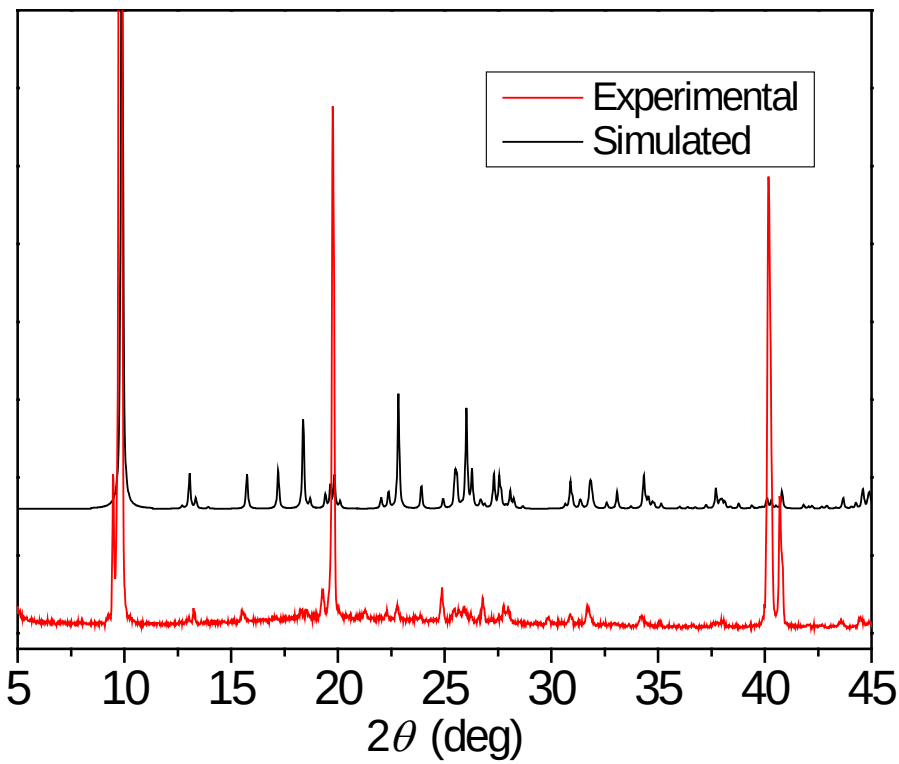


(d)

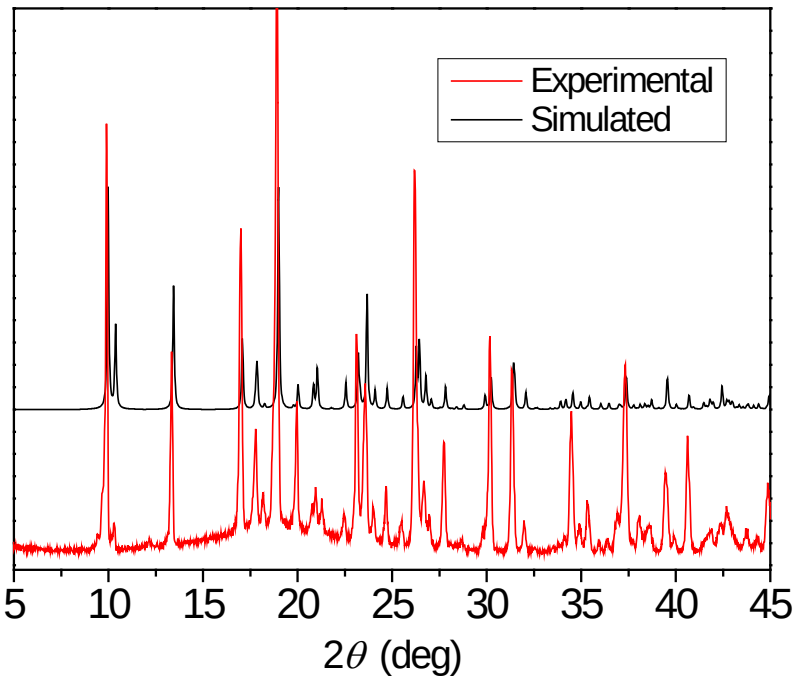
Figure S2. Thermogravimetric (TG-DTA) curves for: (a) **1**, (b) **2**, (c) **3**, and (d) **4**.


Experimental
Simulated
5
10
15
20
25
30
35
40
45
2θ (deg)

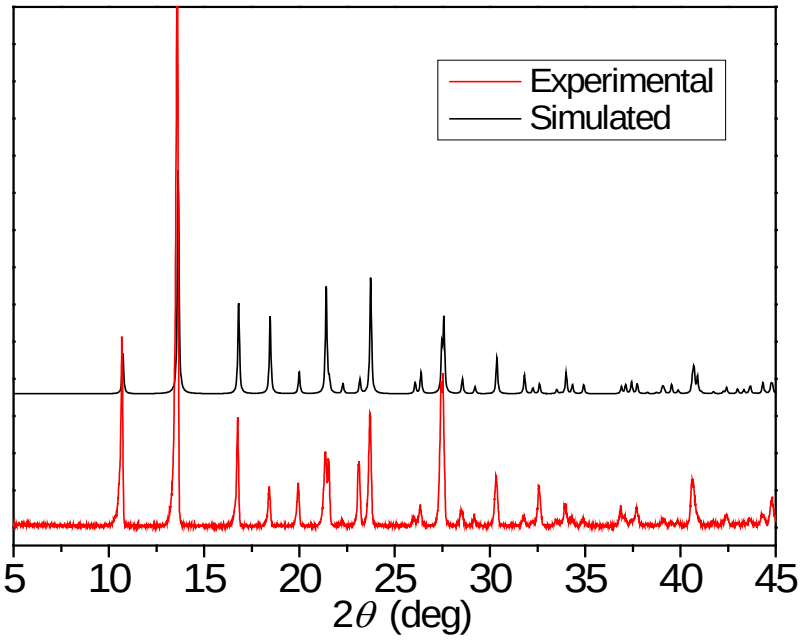
(a)


Experimental
Simulated
5
10
15
20
25
30
35
40
45
2θ (deg)

(b)



(c)



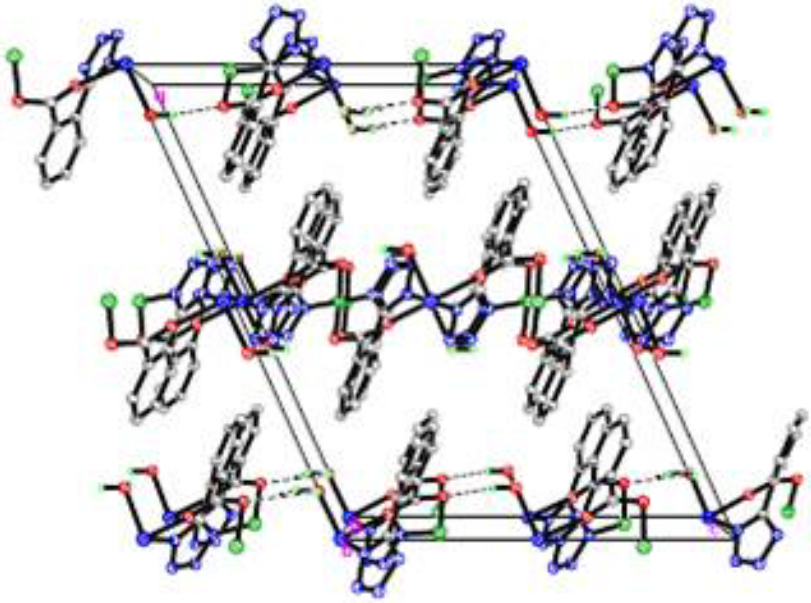
(d)

Figure S3. XRPD patterns of: (a) **1**, (b) **2**, (c) **3**, and (d) **4**.

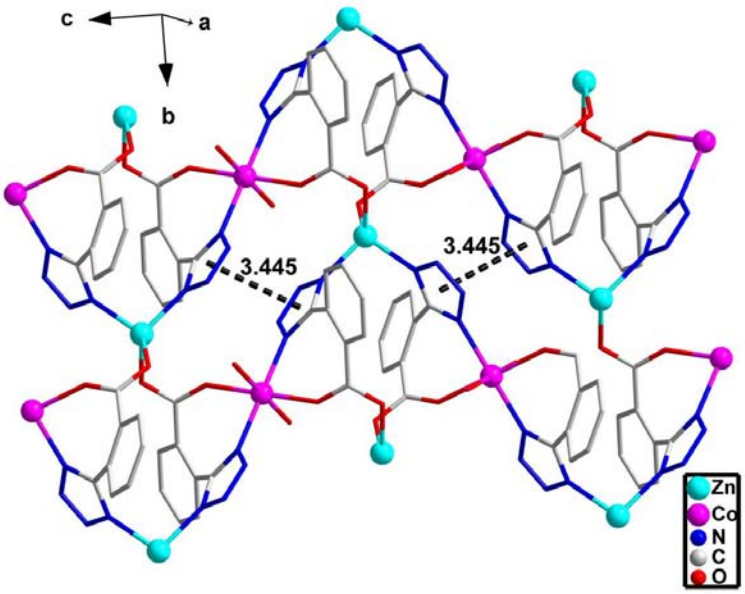
Table S1 Hydrogen-bond parameters in complex **2**.

D–H…A	D–H [Å]	H…A [Å]	D…A [Å]	< D–H…A[^{o}]
O(1W)-H(1A)...O(1F)	0.85(2)	2.012(18)	2.7999(19)	155(3)
O(1W)-H(1B)...N(3G)	0.846(11)	2.167(18)	2.956(12)	155(4)

Symmetry codes: F x,-y+1,z+1/2; G -x+1,-y+2,-z+1.



(a)



(b)

Figure S4. a) The packing pattern of **2**, intermolecular H-bonding shown as dashed line.

b) Intramolecular π···π stacking interactions (black dashed) in **2**, H atoms omitted for clarity.

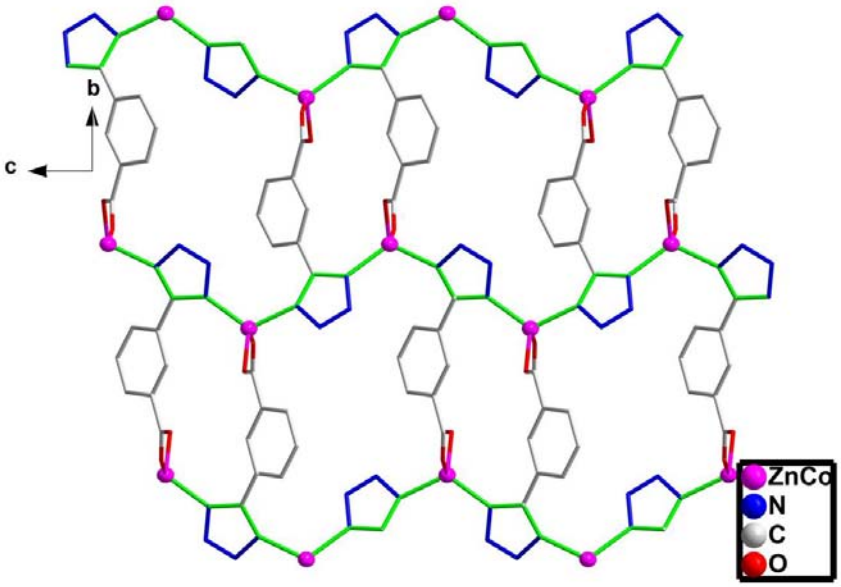
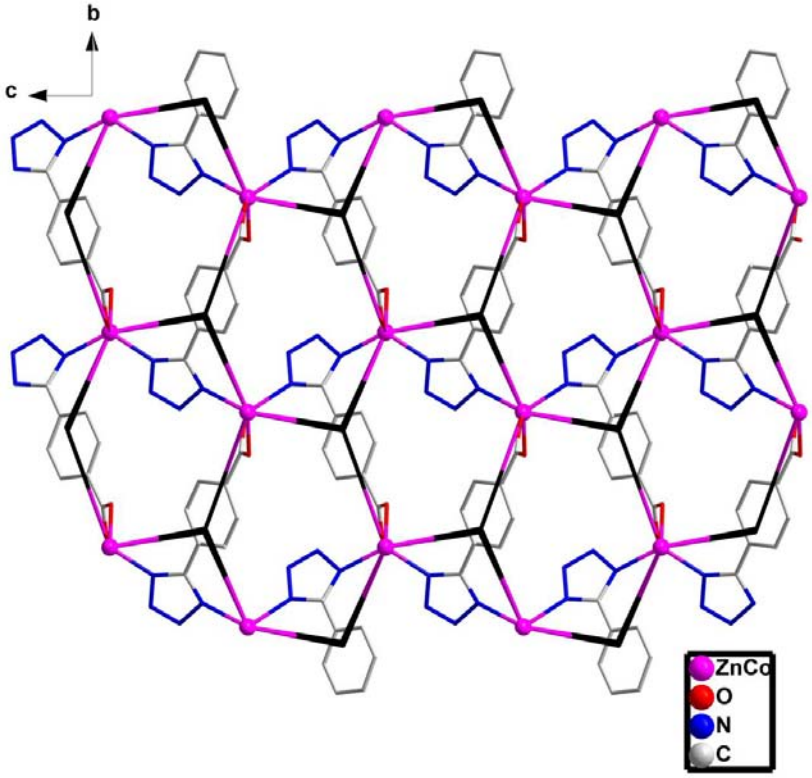
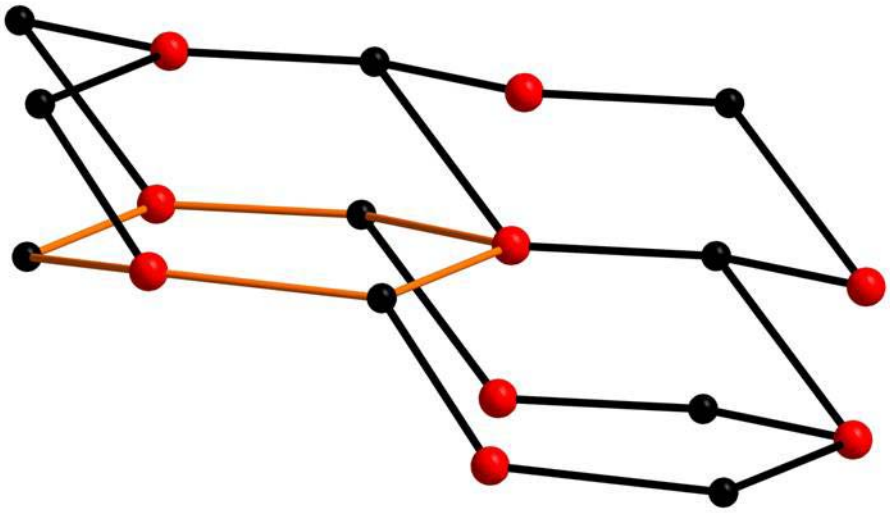


Figure S5. The 2D hexagonal sheet substructure in **3**, **z**igzag chain of M centers linked by bridging tetrazole ligands (green), H atoms are omitted for clarity.



(a)



(b)

Figure S6. a) The 2D hexagonal sheet substructure in **4**; b) highlighted shortest circuts of six-membered chair rings (black) and six membered twisted ring (brown) in different colors respectively in complex **4**.

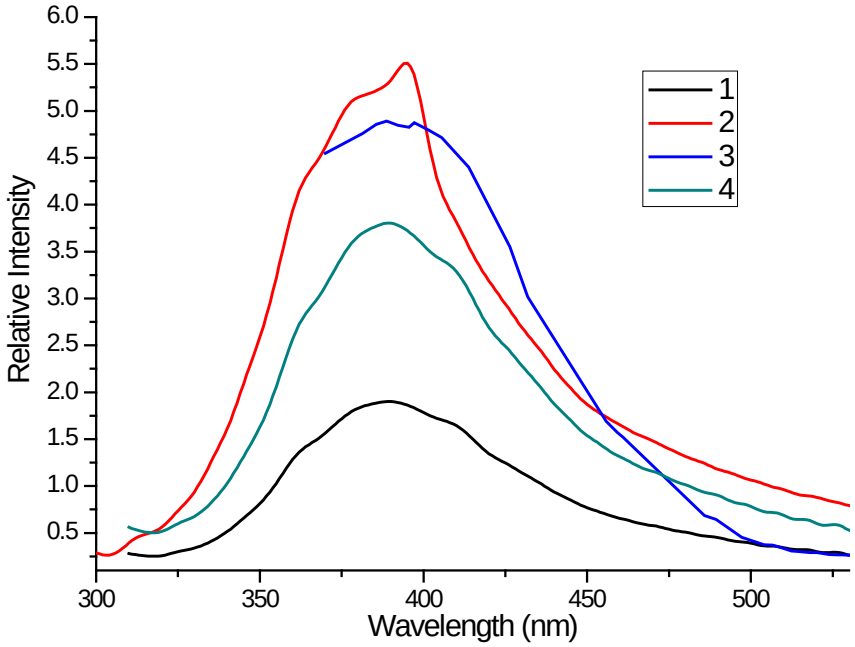
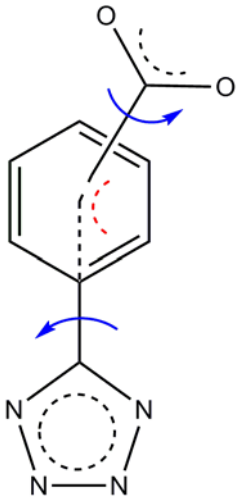


Figure S7. Emission spectra of complexes **1**-**4** in the solid state.



Scheme S1. The twisting mode of the carboxyl and tetrazoyl out of the plane of the aromatic ring.