Electronic Supplementary Material (ESI) for CrystEngComm.


# Synthesis, X-ray Crystallography, Thermogravimetric Analysis and Spectroscopic Characterization of Isostructural One-dimensional Coordination Polymers Based on Diaza-macrocycles Bearing Pyridine Side Arms as Anion Sorbents

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Supporting Information:

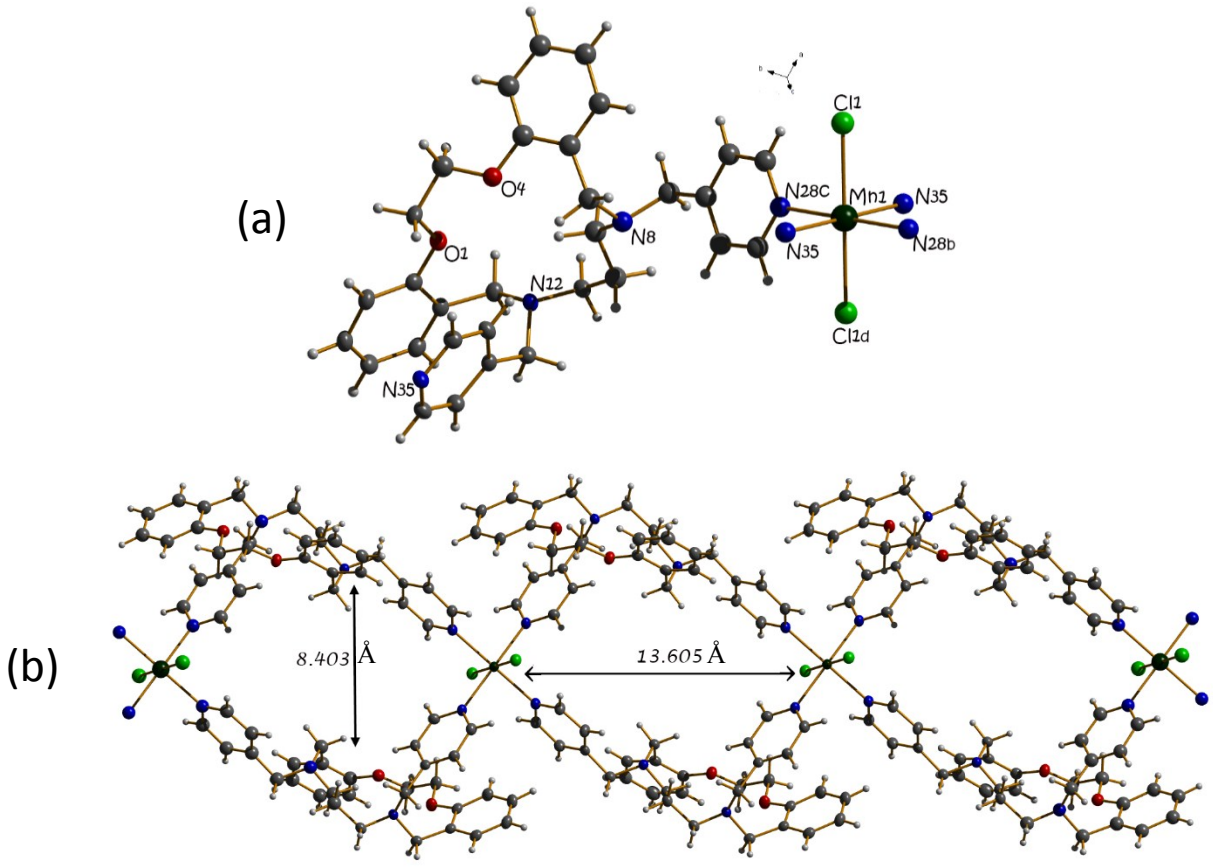



Fig. S1. The Coordination environment of Mn(II) ion in complex**1**(a), 1D infinite rod-shaped chain along *c* axis (b).

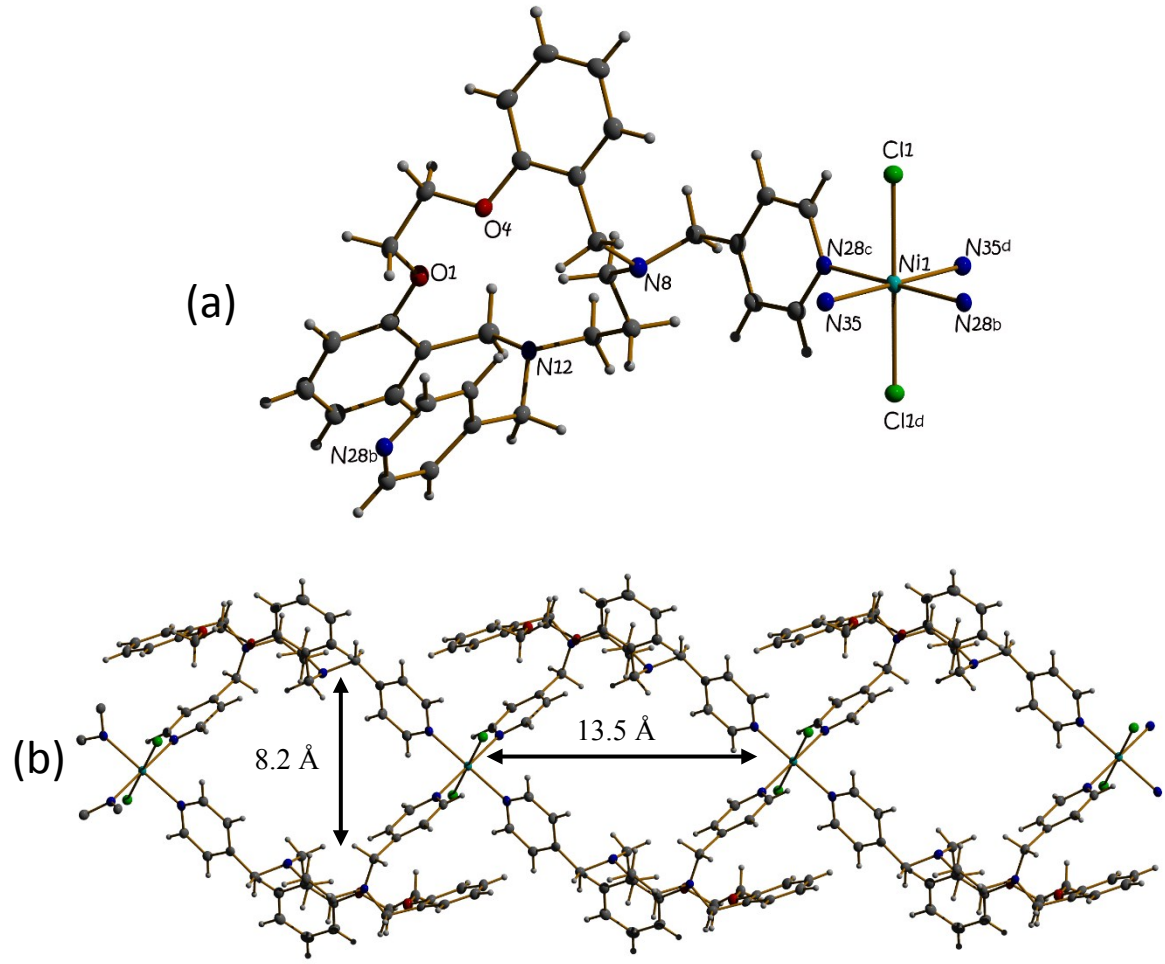

(a)
Cl1
O4
O1
N8
N28c
Ni1
N35d
N35
N28b
N12
Cl1d
N28b
(b)
8.2 Å
13.5 Å

Fig.S2. The Coordination environment of Ni(II) ion in complex **2**(a), 1D infinite rod-shaped chain along *c* axis (b).

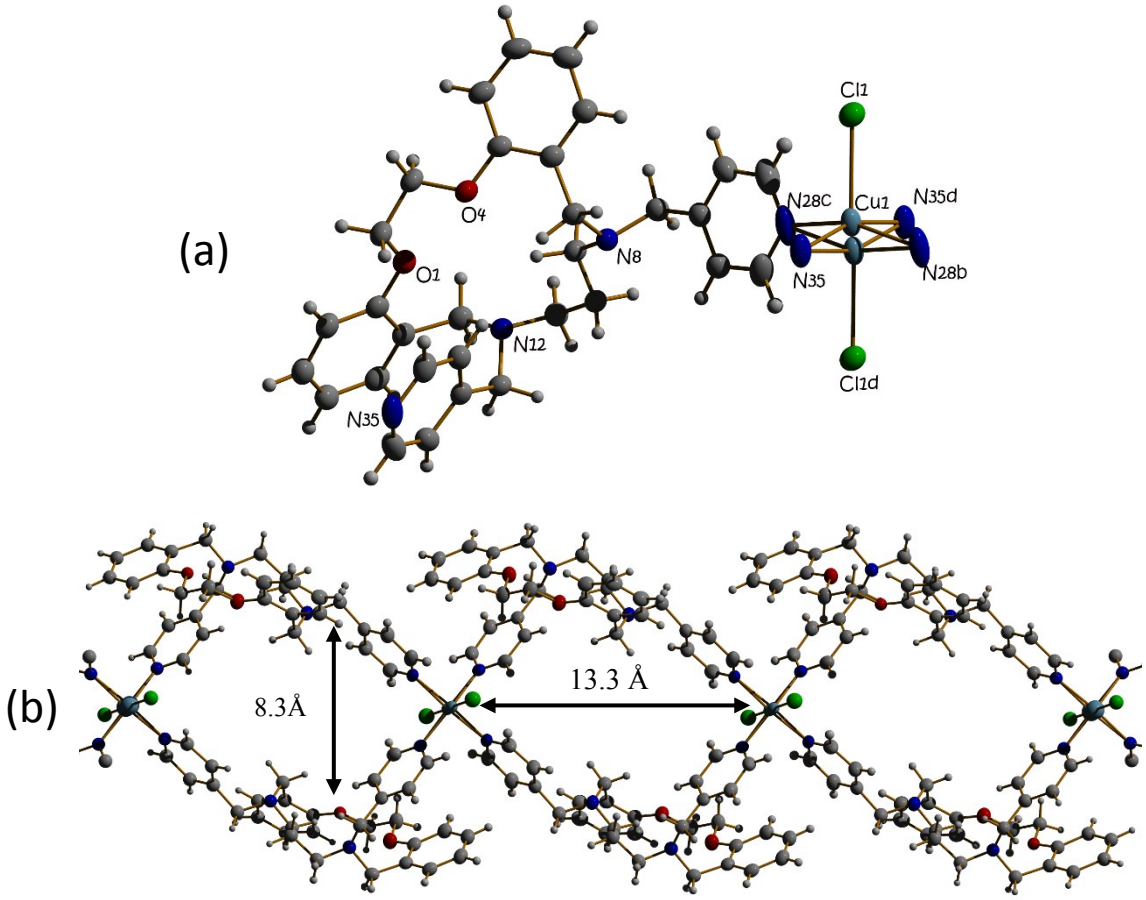



Fig.S3. The Coordination environment of Cu(II) ion in complex **3**(a), 1D infinite rod-shaped chain along *c* axis (b).

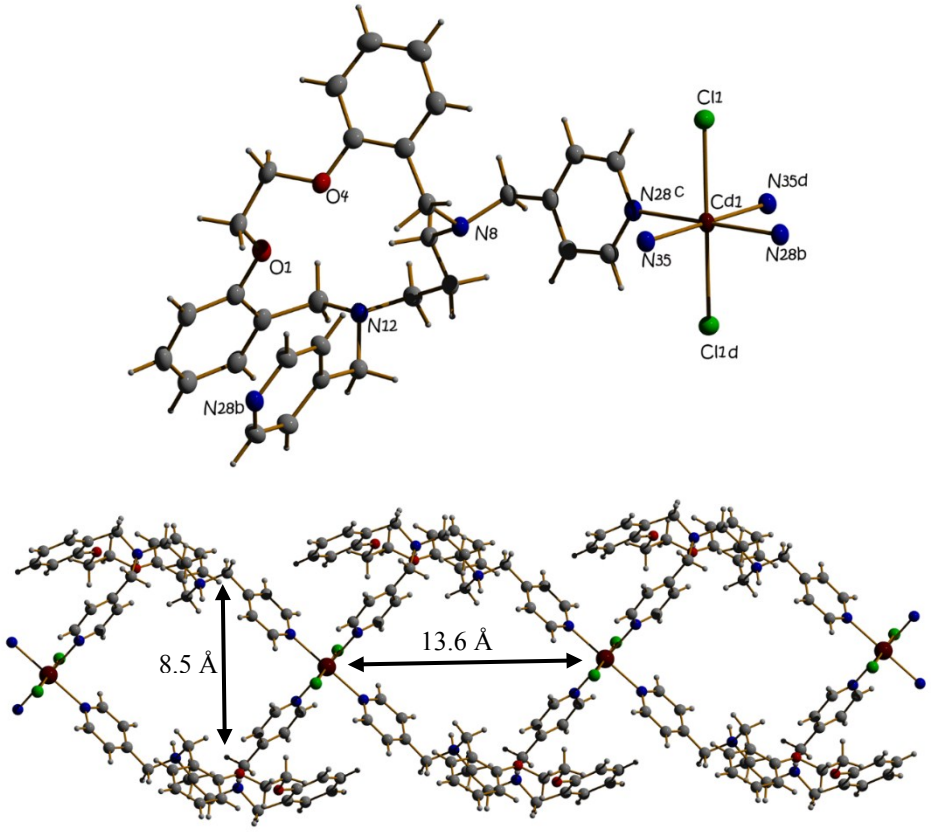



Fig.S4. The Coordination environment of Cd(II) ion in complex **4**(a), 1D infinite rod-shaped chain along *c* axis (b).

Table S1. Weak interaction data (°, Å) in **1**. Cg denotes the middle point of the six member.

| Analysis of Potential Hydrogen Bonds | | | | | | | |
|---|---|---|---|---|---|---|---|
| D | H | A | D−H | H···A | D···A | D−H···A | symmetry code |
| C(27) | H(27) | Cl(1) | 0.95 | 2.68 | 3.370(2) | 130 | -x,1-y,1-z |
| C(29) | H(29) | Cl(1) | 0.95 | 2.61 | 3.326(2) | 132 | x,y,-1+z |
| C(36) | H(36) | Cl(1) | 0.95 | 2.79 | 3.418(2) | 124 | - |
| C(9) | H(9A) | O(4) | 0.99 | 2.51 | 3.248(2) | 132 | - |
| Analysis of X−H···Cg(Pi-Ring) Interactions | | | | | | | |
| X−H(I) | | Cg(J) | H···Cg | X−H···Cg | X···Cg | X−H,Pi | |
| C(7) -H(7B) | | Cg(3) | 2.82 | 123 | 3.460(2) | 32 | 1-x,1-y,1-z |
| C(17) -H(17) | | Cg(1) | 2.91 | 139 | 3.677(3) | 57 | x,y,1+z |
| C(19) -H(19) | | Cg(3) | 2.85 | 149 | 3.696(3) | 58 | -1/2+x,1/2y,1/2+z |
| Analysis of Short Ring-Interactions with Cg-Cg Distances | | | | | | | |
| Cg(I) | | Cg(J) | | Cg-Cg Distance between ring Centroids | | | |
| Cg(4) | | Cg(2) | | 3.6558(12) | | | x,y,z |

Table S2. Weak interaction data (°, Å) in complex **2**.

| Analysis of Potential Hydrogen Bonds | | | | | | | |
|---|---|---|---|---|---|---|---|
| D | H | A | D−H | H···A | D···A | D−H···A | symmetry code |
| C(27) | H(27) | Cl(1) | 0.95 | 2.51 | 3.197(3) | 130 | -x,1-y,1-z |
| C(29) | H(29) | Cl(1) | 0.95 | 2.51 | 3.209(3) | 131 | x,y,-1+z |
| C(34) | H(34) | Cl(1) | 0.95 | 2.72 | 3.286(3) | 119 | x,1-y,2-z |
| C(36) | H(36) | Cl(1) | 0.95 | 2.67 | 3.253(3) | 120 | - |
| C9 | H9A | O4 | 0.99 | 2.52 | 3.264(3) | 132 | - |
| Analysis of X−H···Cg(Pi-Ring) Interactions | | | | | | | |
| X−H(I) | | Cg(J) | H···Cg | X−H···Cg | X···Cg | X−H,Pi | |
| C(7) -H(7B) | | Cg(3) | 2.73 | 122 | 3.359(3) | 33 | 1-x,1-y,1-z |
| C(17) -H(17) | | Cg(1) | 2.89 | 136 | 3.633(3) | 57 | x,y,1+z |
| C(19) -H(19) | | Cg(3) | 2.81 | 148 | 3.653(3) | 58 | - |

| | | | | | | | 1/2+x,1/2y,1/2+z |
|---|---|---|---|---|---|---|---|
| Analysis of Short Ring-Interactions with Cg-Cg Distances | | | | | | | |
| Cg(I) | | Cg(J) | | Cg-Cg Distance between ring Centroids | | | |
| Cg(4) | | Cg(2) | | 3.6502(16) | | | x,y,z |

Table S3. Weak interaction data (°, Å) in complex **3**.

| Analysis of Potential Hydrogen Bonds | | | | | | | |
|---|---|---|---|---|---|---|---|
| D | H | A | D−H | H···A | D···A | D−H···A | symmetry code |
| C(26) | H(26) | Cl(1) | 0.95 | 2.75 | 3.535(3) | 141 | 1+x,y,-1+z |
| C(27) | H(27) | Cl(1) | 0.95 | 2.55 | 3.365(3) | 143 | -x,1-y,1-z |
| C(29) | H(29) | Cl(1) | 0.95 | 2.48 | 3.307(3) | 146 | x,y,-1+z |
| C(34) | H(34) | Cl(1) | 0.95 | 2.72 | 3.427(3) | 132 | -x,1-y,2-z |
| C(36) | H(36) | Cl(1) | 0.95 | 2.69 | 3.421(3) | 134 | - |
| C(9) | H(9A) | O(4) | 0.99 | 2.53 | 3.271(3) | 131 | - |
| Analysis of X−H···Cg(Pi-Ring) Interactions | | | | | | | |
| X−H(I) | | X−H(I) | X−H(I) | X−H(I) | X−H(I) | X−H(I) | |
| C(7) -H(7B) | | Cg(11) | 2.70 | 121 | 3.323(3) | 34 | 1-x,1-y,1-z |
| C(17) -H(17) | | Cg(9) | 2.86 | 134 | 3.583(3) | 58 | x,y,1+z |
| C(19) -H(19) | | Cg(11) | 2.73 | 145 | 3.549(3) | 56 | - 1/2+x,1/2y,1/2+z |
| Analysis of Short Ring-Interactions with Cg-Cg Distances | | | | | | | |
| Cg(I) | | Cg(J) | | Cg-Cg Distance between ring Centroids | | | |
| Cg(12) | | Cg(10) | | 3.6423(15) | | | x,y,z |

Table S4. Weak interaction data (°, Å) in complex **4**.

| Analysis of Potential Hydrogen Bonds | | | | | | | |
|---|---|---|---|---|---|---|---|
| D | H | A | D−H | H···A | D···A | D−H···A | symmetry code |
| C(28) | H28 | Cl(2) | 0.93 | 2.67 | 3.3922(1) | 135 | |
| C(32) | H(32) | Cl(2) | 0.93 | 2.78 | 3.4688(1) | 132 | 2-x,1-y,2-z |
| C(25) | H(25B) | O(11) | 0.97 | 2.52 | 3.2460(1) | 132 | - |
| N(22) | H(22) | O(14) | 0.98 | 2.42 | 3.0359(1) | 120 | - |
| Analysis of X−H···Cg(Pi-Ring) Interactions | | | | | | | |
| X−H(I) | | X−H(I) | X−H(I) | X−H(I) | X−H(I) | X−H(I) | |
| C(4) -H(4A) | | Cg(3) | 2.88 | 124 | 3.5138(1) | 32 | 1-x,1-y,1-z |
| C(17) -H(17) | | Cg(9) | 2.95 | 140 | 3.7103(1) | 57 | x,y,-1+z |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(19) -H(19) | Cg(11) | 2.89 | 149 | 3.7251(1) | 59 | 1/2+x,1/2y,1/2+z |

| Analysis of Short Ring-Interactions with Cg-Cg Distances | | | |
|---|---|---|---|
| Cg(I) | Cg(J) | Cg-Cg Distance between ring Centroids | |
| Cg(2) | Cg(4) | 3.6710(1) | x,y,1+z |

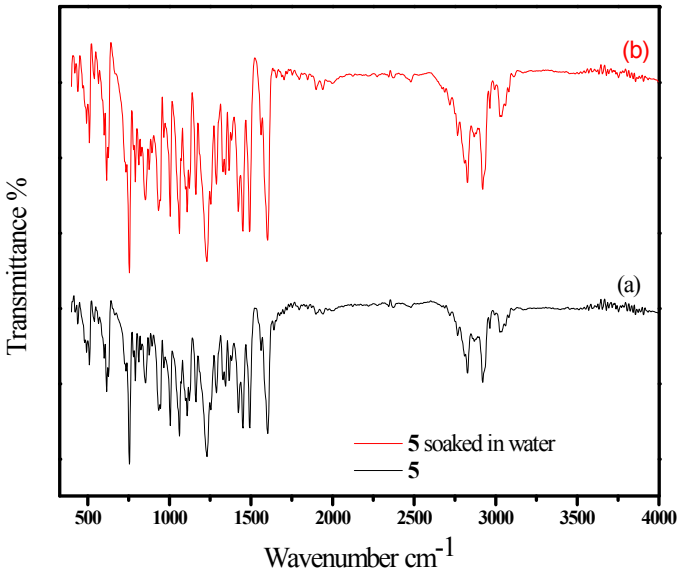
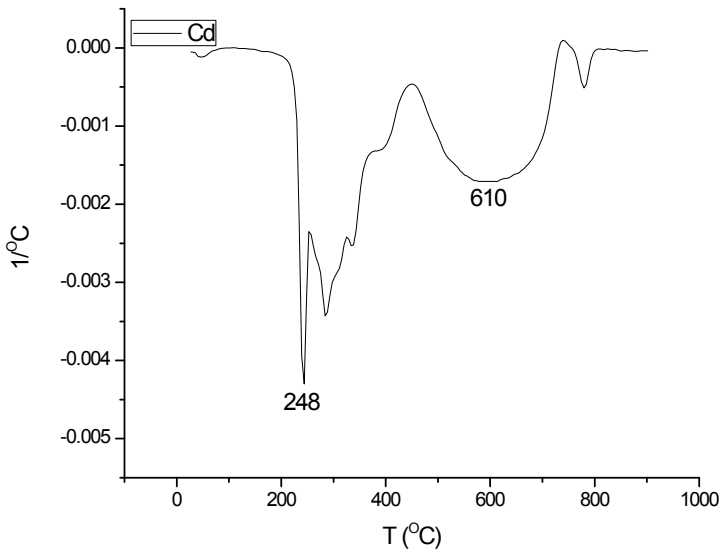
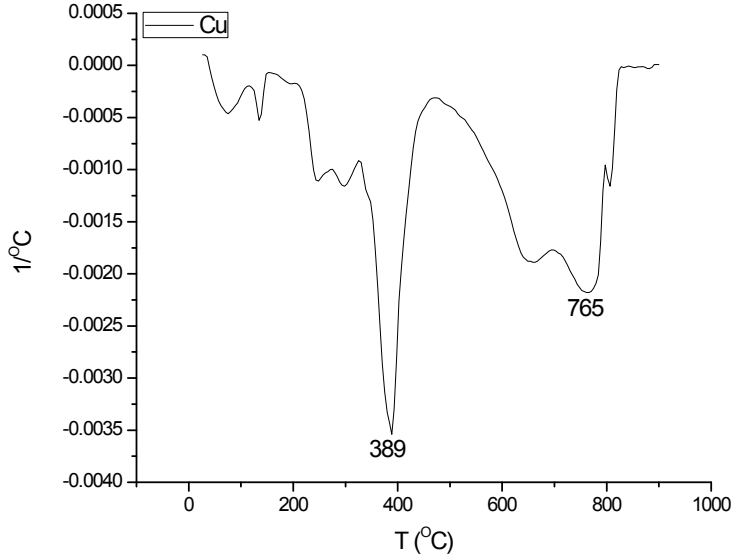
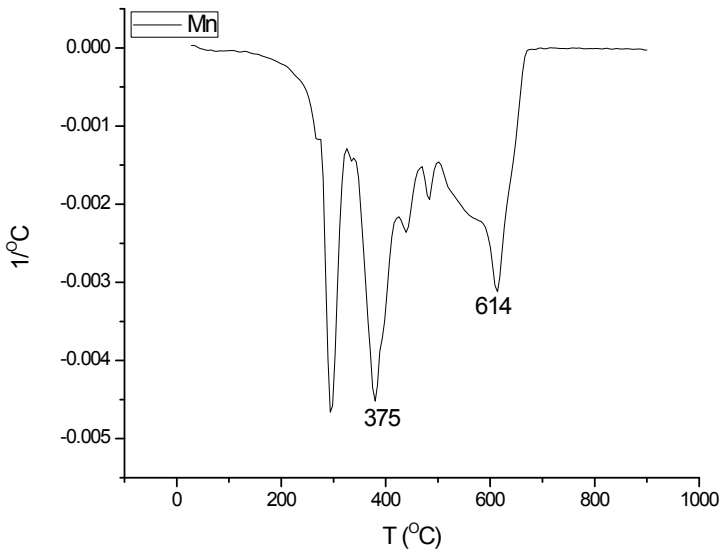
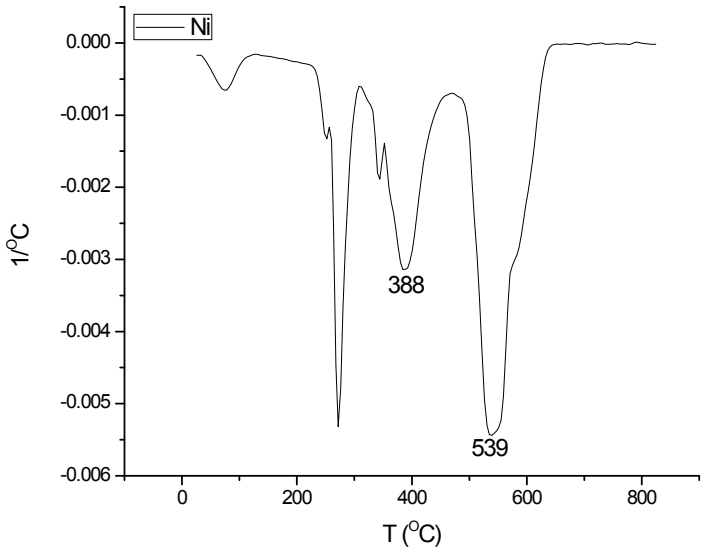



Fig. S5. FT-IR spectra: (a) as-synthesized **5**; (b) **5** soaked in water.


Cd
0.000
-0.001
-0.002
-0.003
-0.004
-0.005
1/°C
248
610
0
200
400
600
800
1000
T (°C)


Cu
0.0005
0.0000
-0.0005
-0.0010
-0.0015
-0.0020
-0.0025
-0.0030
-0.0035
-0.0040
1/°C
765
389
0
200
400
600
800
1000
T (°C)


Mn
0.000
-0.001
-0.002
-0.003
-0.004
-0.005
1/°C
614
375
0
200
400
600
800
1000
T (°C)


Ni
0.000
-0.001
-0.002
-0.003
-0.004
-0.005
-0.006
1/°C
388
539
0
200
400
600
800
T (°C)

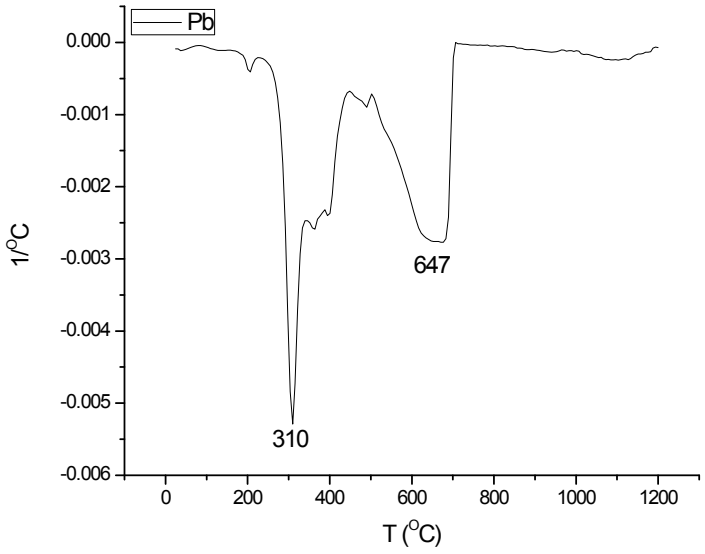



Figure S6. DTG curves of **1-5** coordination polymer.

Table S5. TG/DTG data and assignments of **1-5** coordination polymer.

| stages for Cd | $T_{max}$ of DTG | weight loss in TG (%) obs./calc. | | assignment |
|---|---|---|---|---|
| I | 284 | 45.50 | | ligand |
| II | 610 | 37.03 | 82.03/82.95 | ligand |

| Stages for Cu | $T_{max}$ of DTG | weight loss in TG (%) obs./calc. | | assignment |
|---|---|---|---|---|
| I | 75 | 2.4/3.05 | | $H_2O$ |
| II | 134 | 1.24/1.5 | | $H_2O$ |
| III | 389 | 32.6 | 80.32/84.16 | ligand |
| IV | 765 | 47.72 | | ligand |

| Stages for Mn | $T_{max}$ of DTG | weight loss in TG (%) obs./calc. | | assignment |
|---|---|---|---|---|
| I | 294 | 17.99/17.37 | | 3 DMSO |
| II | 375 | 40.24 | 75.82/73.45 | ligand |
| III | 614 | 35.58 | | ligand |

| Stages for Ni | $T_{max}$ of DTG | weight loss in TG (%) obs./calc. | assignment |
|---|---|---|---|
| I | 78 | 4.56/4.6 | 3 $H_2O$ |

| | | | | |
|---|---|---|---|---|
| II | 272 | 16.66/16.38 | | 3 DMF |
| III | 388 | 26.08 | 71.03/69.72 | ligand |
| IV | 539 | 44.95 | | ligand |

| Stages for Pb | $T_{max}$ of DTG | weight loss in TG (%) obs./calc. | | assignment |
|---|---|---|---|---|
| I | 206 | 2.59/2.76 | | DMF |
| II | 310 | 42.11 | 75.8/76.05 | ligand |
| III | 647 | 33.7 | | ligand |