Electronic Supplementary Material (ESI) for CrystEngComm


# Structural variability of Co(II) and Ni(II) entangled metal-organic frameworks: effect of N-donor ligands and metal ions

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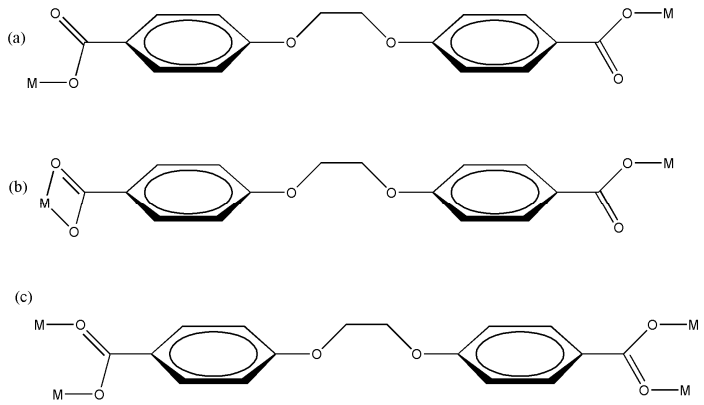


Chart 1 The kinds of coordinative modes of L1 ligand.

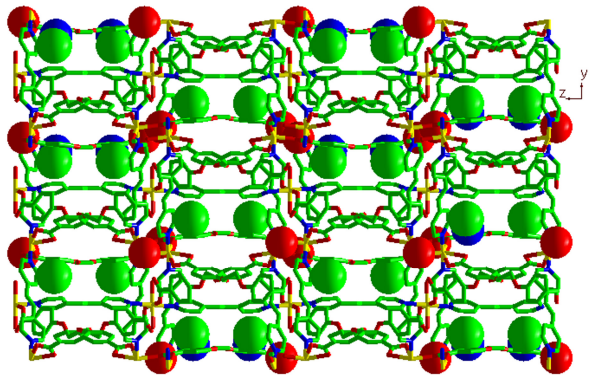

Fig. S1 The porous channels were occupied by guest solvents in **3**.

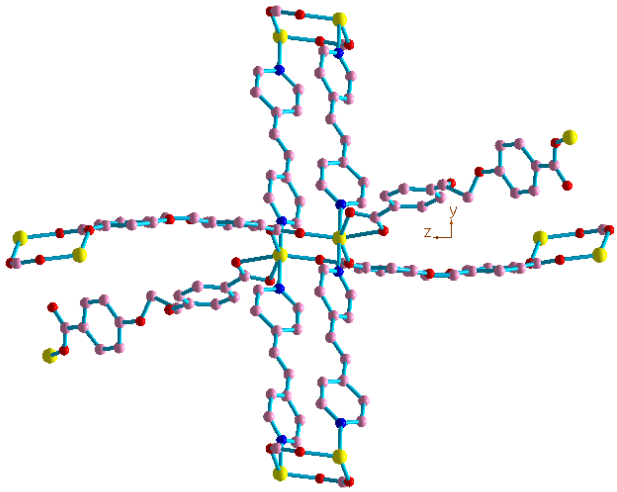


Fig. S2 The linkage cores for metal ions in **3**.

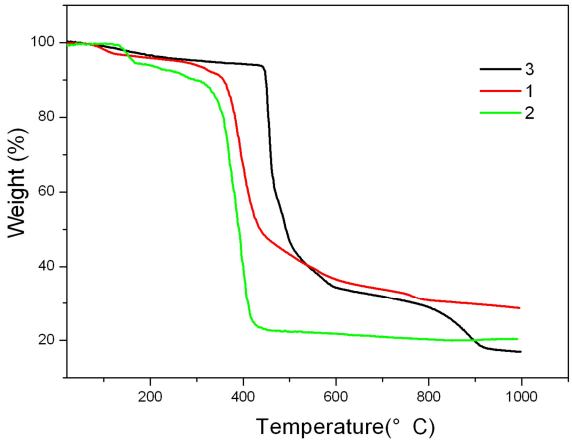


Fig. S3. TG curves of the complexes.

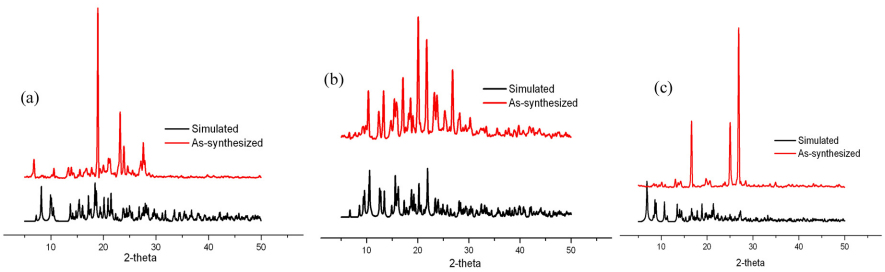


Fig. S4 Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination, the as-synthesized products in compound **1-3** (a-c).

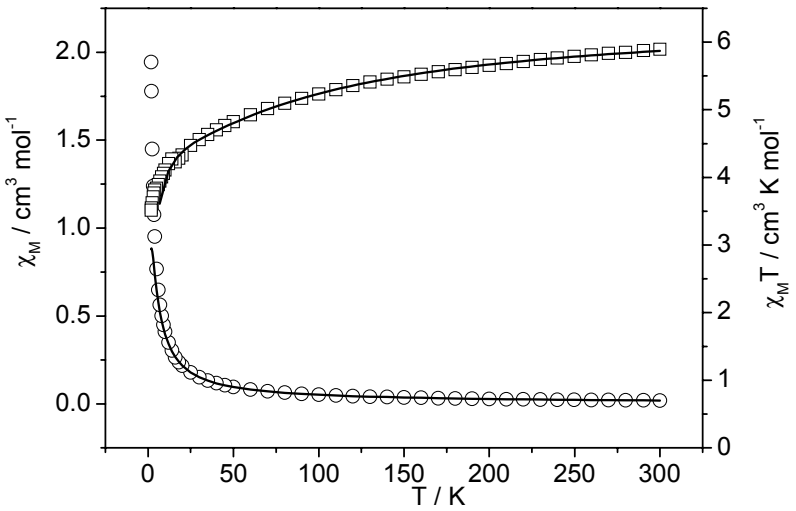


Fig. S5 Plots $\chi_M T$, $\chi_M$ and $\chi_M$ of versus T for **3**, solid lines represent fits to the data.

**Table S1. Selected bond distances (Å) and angles (°)**

Complex **1**

| | | | |
|---|---|---|---|
| Co1- O6 | 2.038(3)#1 . | Co1-O5 | 2.123(3)#1 |
| Co1- N2 | 2.123(3) #2 | Co1- N1 | 2.146(3) |
| Co1-O1W | 2.171(3) | Co1- O4 | 2.225(3) |
| O6- Co1- O5 | 171.41(11) | O6- Co1- N2 | 96.51(13) |
| O5 -Co1- N2 | 90.80(12) | O6- Co1- N1 | 84.50(12) |
| O5- Co1- N1 | 98.53(12) | N2- Co1- N1 | 101.27(12) |
| O6- Co1- O1W | 88.28(12) | O5- Co1- O1W | 87.47(12) |
| N1- Co1 -O1W | 168.84(13) | O6 -Co1- O4 | 111.52(12) |

Symmetry codes: #1: x-1, y+1, z; #2: x+1, y+1, z.

Complex **2**

| | | | |
|---|---|---|---|
| Ni1- N1 | 2.103(5) | Ni1- O5 | 2.069(4) |
| Ni1- O8 | 2.072(5) | Ni1- O1 | 2.074(4) |
| Ni1- O7 | 2.090(5) | Ni1- N2 | 2.093(5) |
| O5- Ni1- O1 | 176.28(16) | O8-Ni1- O1 | 89.01(17) |
| O5- Ni1- O7 | 94.06(16) | O5- Ni1- N2 | 92.65(16) |
| O8- Ni1- N2 | 174.0(2) | O7- Ni1- N1 | 176.03(17) |

Complex **3**

| | | | |
|---|---|---|---|
| Co1- O2#1 | 2.003(4) | Co1- O1 | 2.019(5) |
| Co1- N2 | 2.138(5) | Co1- O4 | 2.139(4) |
| Co1- N1 | 2.141(5) | Co1- O5 | 2.245(5) |
| Co2- O10#2 | 2.079(5) | Co2- N3 | 2.176(5) |
| Co2- O9 | 2.113(5) | Co2- O9#2 | 2.113(5) |

| | | | |
|---|---|---|---|
| O2- Co1-O4 | 152.15(18) | N2- Co1- N1 | 179.2(2) |
| O1- Co1-O5 | 149.60(18) | O10 -Co2-O10 | 180.000(1) |
| O9- Co2- O9#2 | 180.000(1) | N3- Co2- N3#2 | 180.000(1) |

Symmetry codes: #1: -x+2, -y+1, -z; #2: -x+1/2, -y+1/2, -z+1