Electronic Supplementary Material (ESI) for RSC Advances.


# Three Cobalt-Based Coordination Polymers with Tripodal Carboxylate and Imidazole-containing Ligands: Syntheses, Structures, Properties and DFT studies

**Long Tang*, Yu-Hao Fu, Huan-Huan Wang, Yi-Tong Wang, JiJiang Wang*, XiangYang Hou,**

## Supplementary Information

**Table S1** Selected bond lengths (Å) and angles (°) for compounds **1-3**

| Bond lengths and angles | Experiment | Bond lengths and angles | Experiment | Bond lengths and angles | Experiment |
|---|---|---|---|---|---|
| **1** | | **2** | | **3** | |
| Co(1)-O(6)#1 | 2.0104(18) | Co(1)-O(3)#1 | 2.0394(19) | Co(1)-O(1) | 1.973(2) |
| Co(1)-O(5)#2 | 2.0430(17) | Co(1)-O(4)#2 | 2.0639(18) | Co(1)-O(3)#1 | 2.009(2) |
| Co(1)-N(4) | 2.097(2) | Co(1)-N(1) | 2.128(2) | Co(1)-N(4) | 2.037(3) |
| Co(1)-N(7)#3 | 2.150(2) | Co(1)-N(4)#3 | 2.135(2) | Co(1)-N(7)#2 | 2.040(3) |
| Co(1)-O(1) | 2.1739(18) | Co(1)-O(1) | 2.1573(19) | | |
| Co(1)-O(2) | 2.2269(17) | Co(1)-O(2) | 2.2578(19) | | |
| O(6)#1-Co(1)-O(5)#2 | 115.23(7) | O(3)#1-Co(1)-O(4)#2 | 117.76(7) | O(1)-Co(1)-O(3)#1 | 119.27(11) |
| O(6)#1-Co(1)-N(4) | 93.07(9) | O(3)#1-Co(1)-N(1) | 87.48(9) | O(1)-Co(1)-N(4) | 110.06(10) |
| O(5)#2-Co(1)-N(4) | 91.25(8) | O(4)#2-Co(1)-N(1) | 87.23(8) | O(3)#1-Co(1)-N(4) | 106.71(11) |
| O(6)#1-Co(1)-N(7)#3 | 89.16(9) | O(3)#1-Co(1)-N(4)#3 | 91.51(9) | O(1)-Co(1)-N(7)#2 | 104.02(10) |
| O(5)#2-Co(1)-N(7)#3 | 87.29(8) | O(4)#2-Co(1)-N(4)#3 | 91.98(8) | O(3)#1-Co(1)-N(7)#2 | 92.61(11) |
| N(4)-Co(1)-N(7)#3 | 177.70(8) | N(1)-Co(1)-N(4)#3 | 178.24(8) | N(4)-Co(1)-N(7)#2 | 124.21(11) |
| O(6)#1-Co(1)-O(1) | 91.72(7) | O(3)#1-Co(1)-O(1) | 148.71(8) | | |
| O(5)#2-Co(1)-O(1) | 152.73(7) | O(4)#2-Co(1)-O(1) | 93.23(7) | | |
| N(4)-Co(1)-O(1) | 91.39(8) | N(1)-Co(1)-O(1) | 89.96(8) | | |
| N(7)#3-Co(1)-O(1) | 89.09(8) | N(4)#3-Co(1)-O(1) | 91.65(8) | | |
| O(6)#1-Co(1)-O(2) | 151.09(7) | O(3)#1-Co(1)-O(2) | 89.80(7) | | |
| O(5)#2-Co(1)-O(2) | 93.67(7) | O(4)#2-Co(1)-O(2) | 152.42(7) | | |
| N(4)-Co(1)-O(2) | 86.66(8) | N(1)-Co(1)-O(2) | 93.29(8) | | |
| N(7)#3-Co(1)-O(2) | 91.65(8) | N(4)#3-Co(1)-O(2) | 88.14(8) | | |
| O(1)-Co(1)-O(2) | 59.41(6) | O(1)-Co(1)-O(2) | 59.20(7) | | |

Symmetry transformations used to generate equivalent atoms: **1**: #1 -x+1, -y+1, -z+1, #2 x, y, z-1, #3 -x+1, -y+1, -z; **2**: #1 -x-1, -y+1, -z+2, #2 x, y+1, z-1, #3 x-1, y, z+1; **3**: #1 x+1, y, z+1, #2 x-1, y-1, z.

**Table S2** Hydrogen bond lengths (Å) and bond angles deg for **1** and **3**

| D-H···A | d(H···A)/Å | d(D···A)/Å | <DHA deg |
|---|---|---|---|
| **1** | | | |
| O3-H3A···O4#5 | 1.79 | 2.6478(18) | 176.95 |
| **3** | | | |
| O5-H5···O2#5 | 1.73 | 2.592(3) | 158.3 |

Symmetry code for **1**: #5 -*x* -2, -*y* + 2, -*z* + 1; for 3: #5 *x*-1, *y* - 1, *z*.

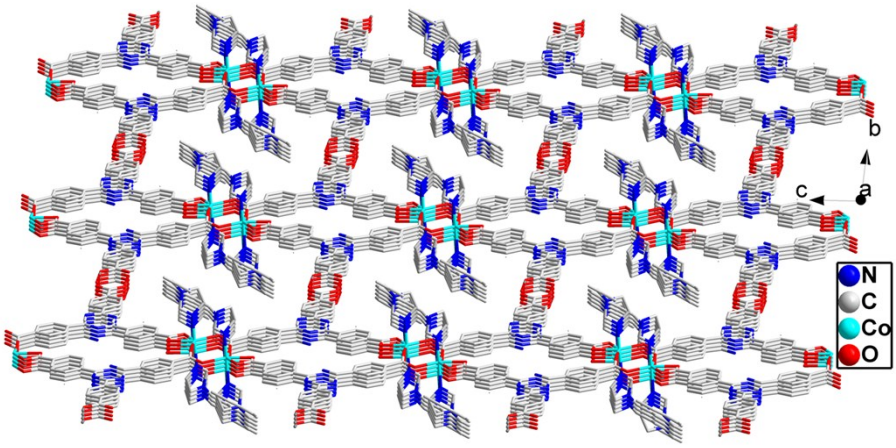


**Figure S1** The 3D supramolecular structure of **1**

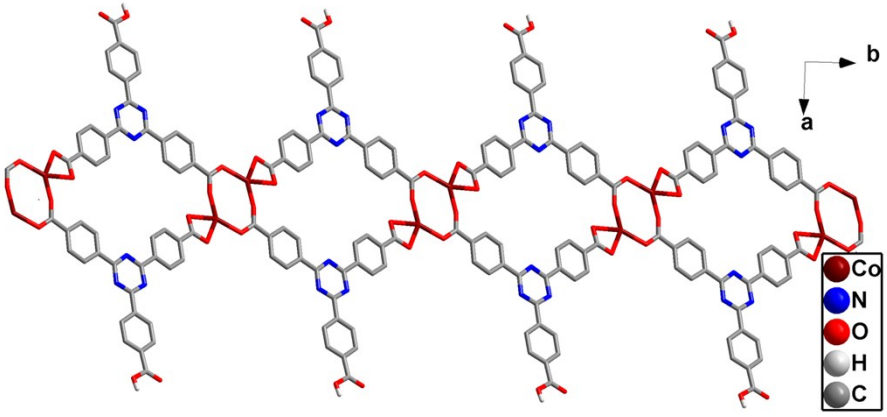


**Figure S2** The 1D double-strand chain of **2** view along [010] direction

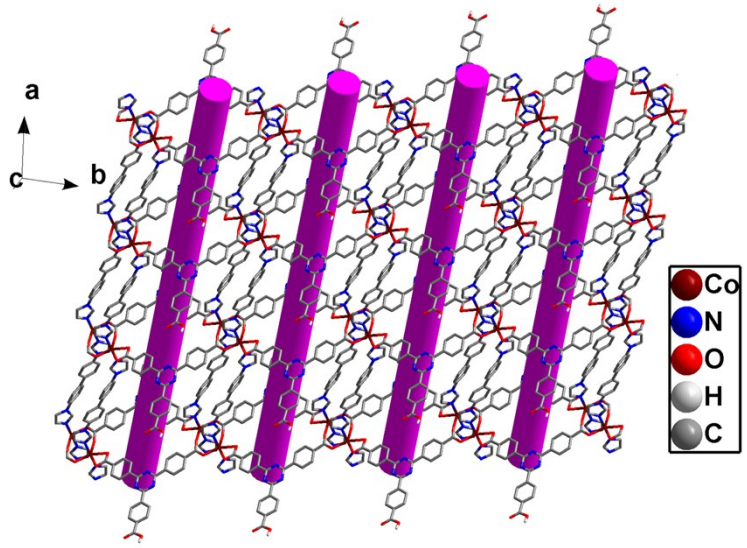


**Figure S3** The 2D layer structure of **2**

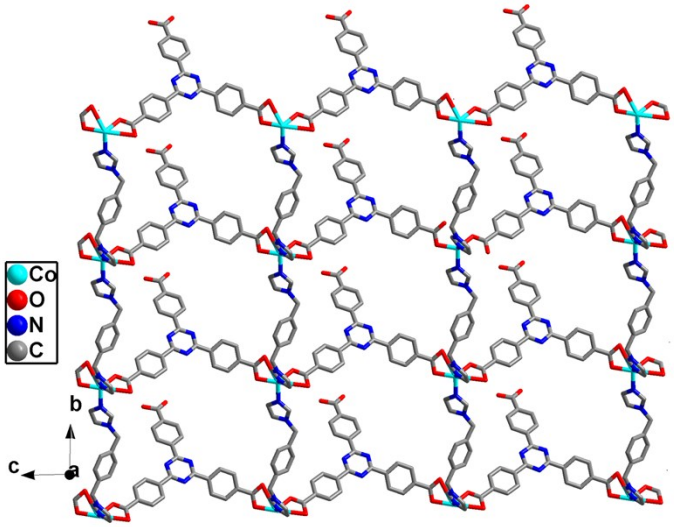


**Figure S4** The 2D layer structure of **3**

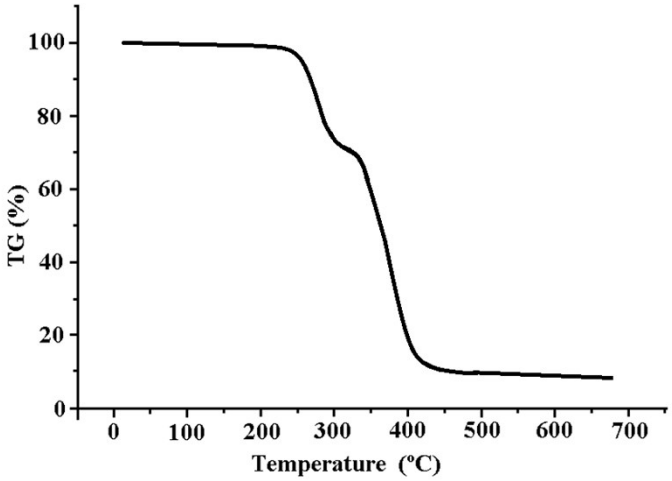


**Figure S5** TG curve of compound **1**

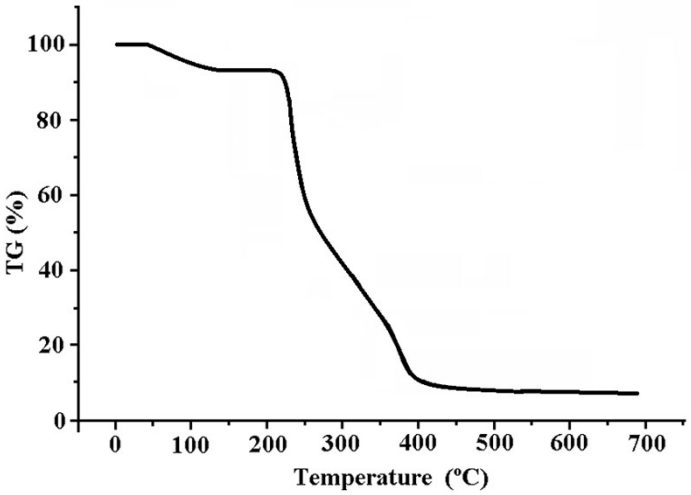


**Figure S6** TG curve of compound **2**

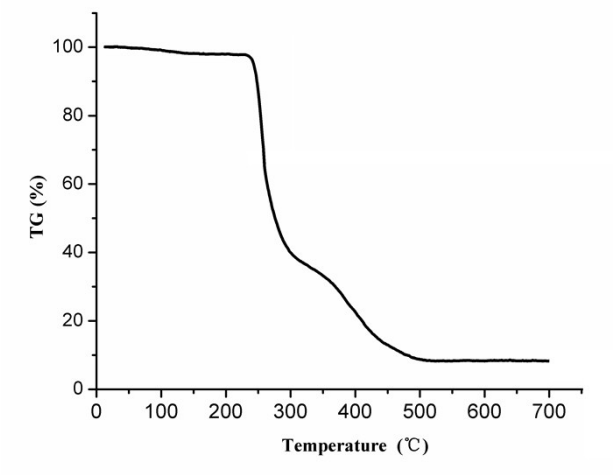


**Figure S7** TG curve of compound **3**