

Electronic Supplementary Information (ESI)

Synthesis, Structures, and Magnetic Properties of Four Copper Compounds with 2,2'-Dinitrophenyl-4,4'-dicarboxylate

Ligands

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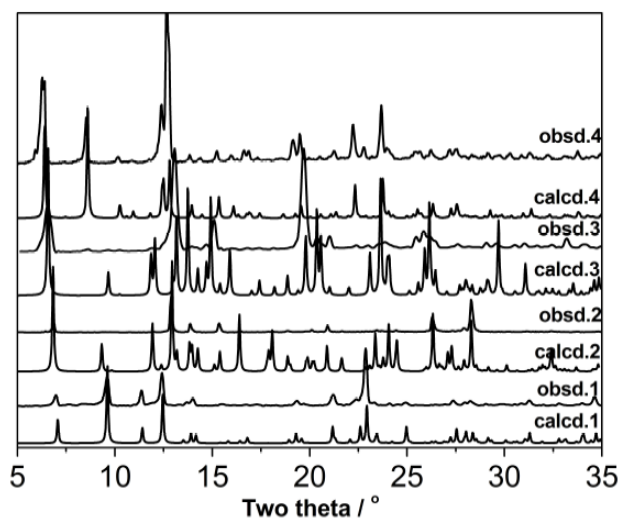


Fig. S1. PXRD patterns based on the X-ray single crystal diffractions and the observed sample for compound 1 – 4.

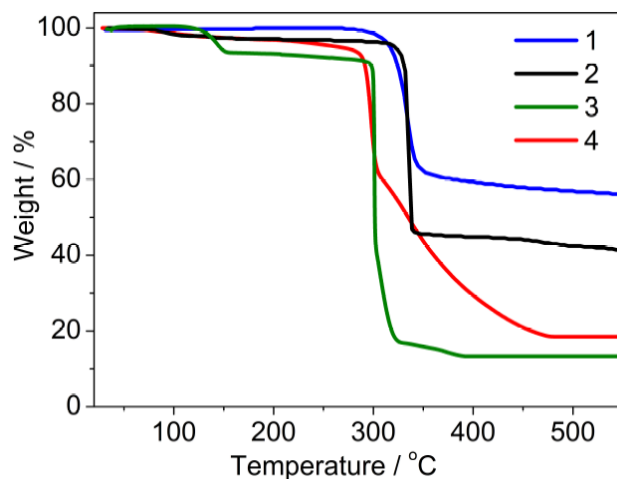


Fig. S2. The TGA plot of compound 1 - 4.

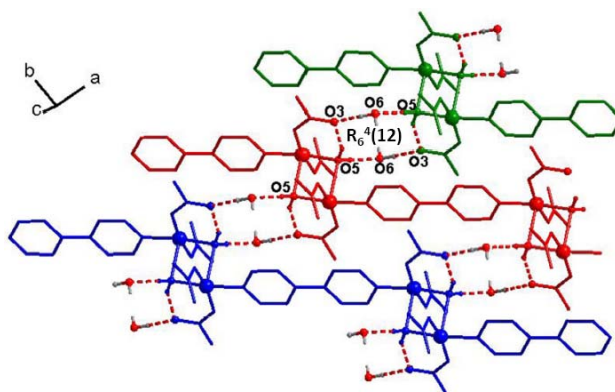


Fig. S3. View of the hydrogen bonding interactions between the guest H₂O molecules (O6) and bridging H₂O (O5), uncoordinated carboxylate oxygen atoms (O3).

Table S1. Selected bond lengths (Å) and angles (°) for compound 3.

| | | | |
|-----------------|----------|------------|----------|
| Cu1-O1 | 1.910(3) | Cu1-O4A | 1.956(3) |
| Cu1-O5 | 1.971(3) | Cu1-N1 | 1.992(3) |
| Cu1-O5B | 2.438(3) | | |
| O1-Cu1-O4A | 168.1(1) | O4A-Cu1-O5 | 90.3(1) |
| O1-Cu1-O5 | 86.1(1) | O4A-Cu1-N1 | 90.3(1) |
| O1-Cu1-N1 | 94.9(1) | O1-Cu1-O5B | 88.2(1) |
| O5-Cu1-N1 | 172.0(1) | O5-Cu1-O5B | 82.7(1) |
| O4A-Cu1-O5B | 102.5(1) | N1-Cu1-O5B | 89.4(1) |
| Cu1-O5-Cu1B | 97.3(1) | | |
| Hydrogen bonds: | | | |
| O5...O3A | 2.560(3) | O5-H...O3A | 146(3) |
| O5...O6C | 2.622(5) | O5-H...O6C | 165(2) |
| O6...O3D | 2.755(5) | O6-H...O3D | 166(3) |

Symmetry code: A x+1, y+1, z+1; B -x, -y, -z; C x, y, z; D -x, -y-1, -z-1.