

Supporting information belonging to the manuscript:

## Tripodal bis(imidazole)-based ligands and their chelation to copper(II)

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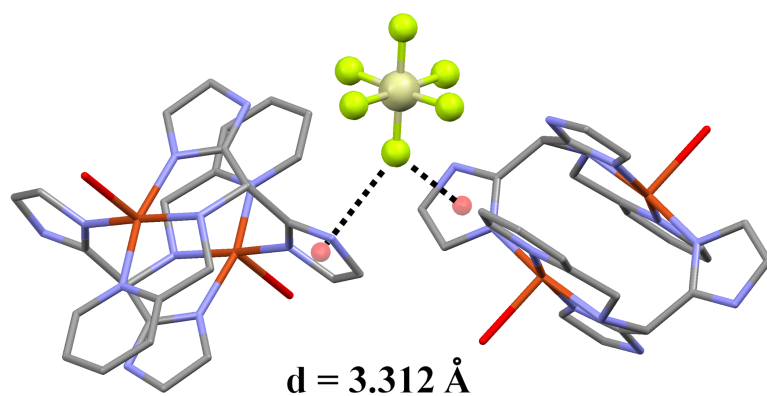
**Figure S2.** (a) crystal packing of compound **1** along ‘b’ in the unit cell. (b) the arrangement of the layered water clusters in **1**.

**Figure S3.** Hydrogen-bonding interactions between oxalate oxygens and the imidazole –NH, and the axially coordinated water molecules from the neighboring dinuclear [Cu<sub>2</sub>(L2)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]<sup>4+</sup> unit in **2**.

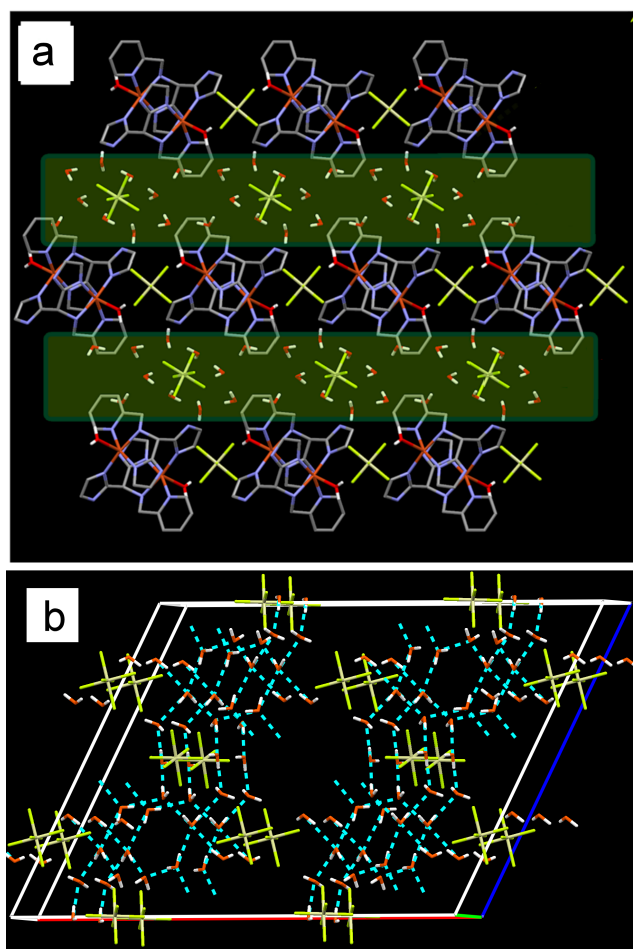
**Figure S4.** (a) 1D chain arrangement of compound **3**. (b) crystal packing of **3** along ‘a’. (c) showing the hydrophilic (H<sub>2</sub>O) channels along ‘c’, respectively.

**Figure S5.** Variable-temperature magnetic susceptibility measurements of compounds **1** (a), **2** (b) and **3** (c).

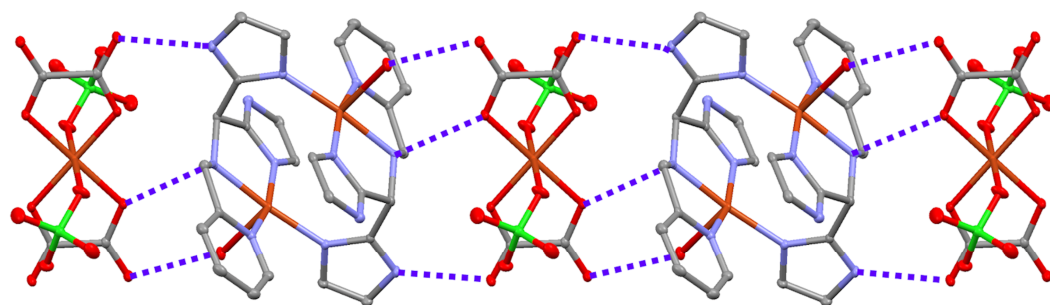
**Table S1** Selected bond angles (degree) for compounds **1-3**



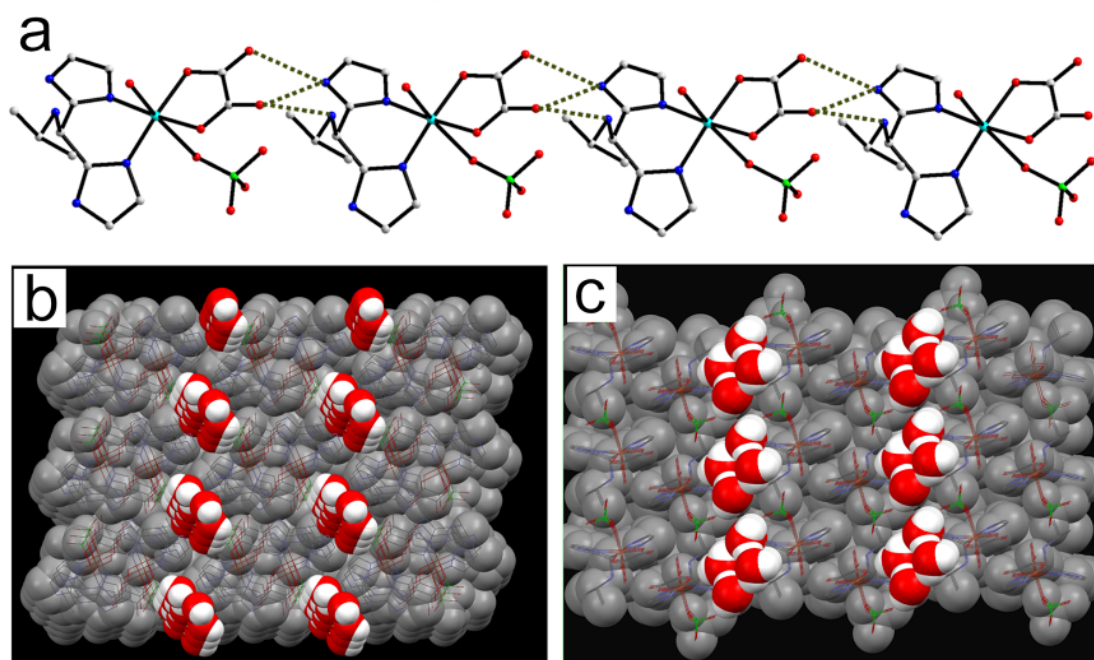
**Figure S1.** Representation of the  $\text{F}^-$ - $\pi$  interactions in **1**.



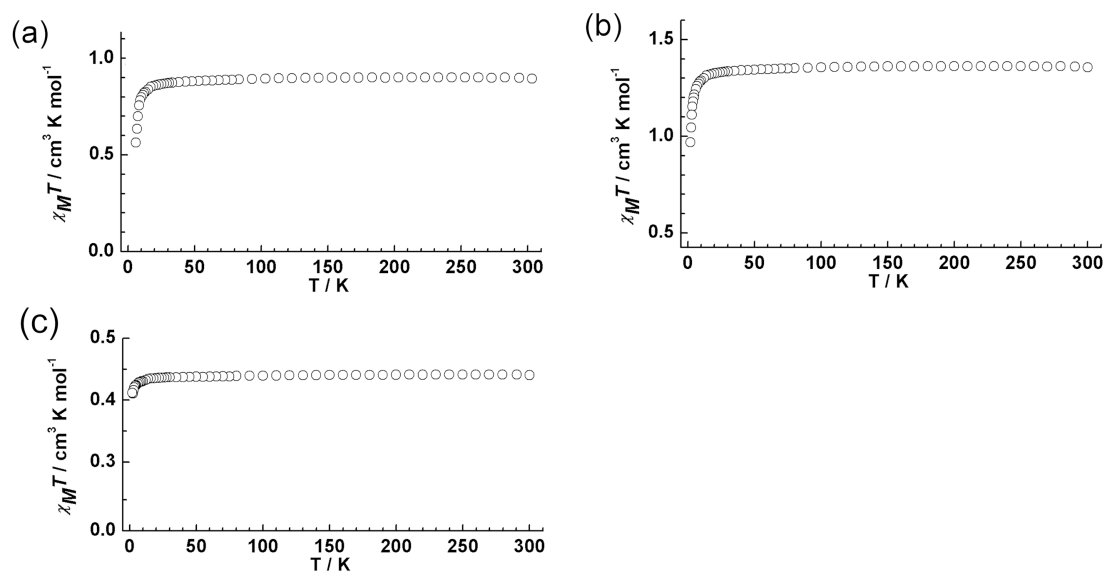
**Figure S2.** (a) crystal packing of compound **1** along 'b' in the unit cell. (b) the arrangement of the layered water clusters in **1**.



**Figure S3.** Hydrogen-bonding interactions between oxalate oxygens and the imidazole –NH, and the axially coordinated water molecules from the neighboring dinuclear  $[\text{Cu}_2(\text{L}2)_2(\text{H}_2\text{O})_2]^{4+}$  unit in **2**. (Water molecules and hydrogen atoms are omitted for clarity; hydrogen bonding interactions are indicated with dashed lines).



**Figure S4.** (a) 1D chain arrangement of compound **3**. (water molecules and hydrogen atoms are omitted for clarity; hydrogen-bonding interactions are indicated with dashed lines). (b) crystal packing of **3** along 'a'. (c) showing the hydrophilic ( $\text{H}_2\text{O}$ ) channels along 'c', respectively (grey: complex, red: water).



**Figure S5.** Variable-temperature magnetic susceptibility measurements of compounds **1** (a), **2** (b) and **3** (c).

**Table S1** Selected bond angles (degree) for compounds **1-3**

| <b>1</b> [Cu <sub>2</sub> (L1) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> ][SiF <sub>6</sub> ] <sub>2</sub> ·10H <sub>2</sub> O |            | <b>2</b> [Cu <sub>2</sub> (L1)(H <sub>2</sub> O) <sub>2</sub> ][Cu(C <sub>2</sub> O <sub>4</sub> ) <sub>2</sub> (ClO <sub>4</sub> ) <sub>2</sub> ].2H <sub>2</sub> O |           | <b>3</b> [Cu(ClO <sub>4</sub> )(C <sub>2</sub> O <sub>4</sub> )(HL2)H <sub>2</sub> O].2H <sub>2</sub> O |           |
|-----------------------------------------------------------------------------------------------------------------------------------|------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|---------------------------------------------------------------------------------------------------------|-----------|
| N21 Cu1 N31                                                                                                                       | 94.99(10)  | N5 Cu1 N1                                                                                                                                                            | 163.15(7) | O1 Cu1 O3                                                                                               | 84.68(5)  |
| N21 Cu1 N11                                                                                                                       | 162.59(11) | N5 Cu1 N3                                                                                                                                                            | 96.94(7)  | O1 Cu1 N3                                                                                               | 94.45(6)  |
| N31 Cu1 N11                                                                                                                       | 100.57(10) | N1 Cu1 N3                                                                                                                                                            | 98.07(7)  | O3 Cu1 N3                                                                                               | 174.41(6) |
| N21 Cu1 N18                                                                                                                       | 81.51(10)  | N5 Cu1 N2                                                                                                                                                            | 82.25(7)  | O1 Cu1 N1                                                                                               | 174.75(6) |
| N31 Cu1 N18                                                                                                                       | 171.75(10) | N1 Cu1 N2                                                                                                                                                            | 82.06(7)  | O3 Cu1 N1                                                                                               | 91.99(6)  |
| N11 Cu1 N18                                                                                                                       | 82.03(10)  | N3 Cu1 N2                                                                                                                                                            | 174.35(7) | N3 Cu1 N1                                                                                               | 89.25(6)  |
| N21 Cu1 O1                                                                                                                        | 98.42(10)  | N5 Cu1 O1                                                                                                                                                            | 90.86(7)  | O5 Cu1 N1                                                                                               | 90.30(6)  |
| N31 Cu1 O1                                                                                                                        | 97.04(10)  | N3 Cu1 O1                                                                                                                                                            | 94.03(6)  | O5 Cu1 N3                                                                                               | 89.72(6)  |
| N11 Cu1 O1                                                                                                                        | 87.46(10)  | N2 Cu1 O1                                                                                                                                                            | 91.58(7)  | O5 Cu1 O1                                                                                               | 86.01(6)  |
| N18 Cu1 O1                                                                                                                        | 90.88(10)  | N1 Cu1 O1                                                                                                                                                            | 95.68(7)  | O5 Cu1 O3                                                                                               | 95.74(6)  |
|                                                                                                                                   |            | O4 Cu2 O2                                                                                                                                                            | 95.09(6)  | O6 Cu1 N1                                                                                               | 103.53(6) |
|                                                                                                                                   |            | O4 Cu2 O4                                                                                                                                                            | 180.00(6) | O6 Cu1 N3                                                                                               | 89.25(6)  |
|                                                                                                                                   |            | O4 Cu2 O2                                                                                                                                                            | 84.91(6)  | O6 Cu1 O1                                                                                               | 80.26(6)  |
|                                                                                                                                   |            | O2 Cu2 O2                                                                                                                                                            | 180.00(6) | O6 Cu1 O3                                                                                               | 85.14(6)  |
|                                                                                                                                   |            | O6 Cu2 O2                                                                                                                                                            | 87.23(6)  |                                                                                                         |           |
|                                                                                                                                   |            | O6 Cu2 O4                                                                                                                                                            | 93.12(6)  |                                                                                                         |           |