Electronic Supplementary Information

Magnetic Dimensionality and Crystal Structure of Two Copper(II) Coordination Polymers Containing Cu_6 and Cu_2 Building Units

Negar Rad-Yousefnia [a], Behrouz Shaabani *[,a], Maria Korabik*[,b], Marek Weselski [b], Mansoureh Zahedi [a], Ulli Englert [c], Rahman Bikas [d], Daria Szeliga [b], Marta Otreba [b], Tadeusz Lis [b]

[a] *Department of Inorganic Chemistry, Faculty of Chemistry, University of Tabriz, Tabriz, Iran*

**Email: shaabani.b@gmail.com (shaabani@tabrizu.ac.ir)*

[b] *Faculty of Chemistry, University of Wroclaw, F. Joliot-Curie 14, Wroclaw 50-383, Poland*

**Email: maria.korabik@chem.uni.wroc.pl*

[c] *Institute of Inorganic Chemistry, RWTH Aachen University, Landoltweg 1, 52074 Aachen, Germany*

[d] *Department of Chemistry, Faculty of Science, Imam Khomeini International University, 34148-96818, Qazvin, Iran*

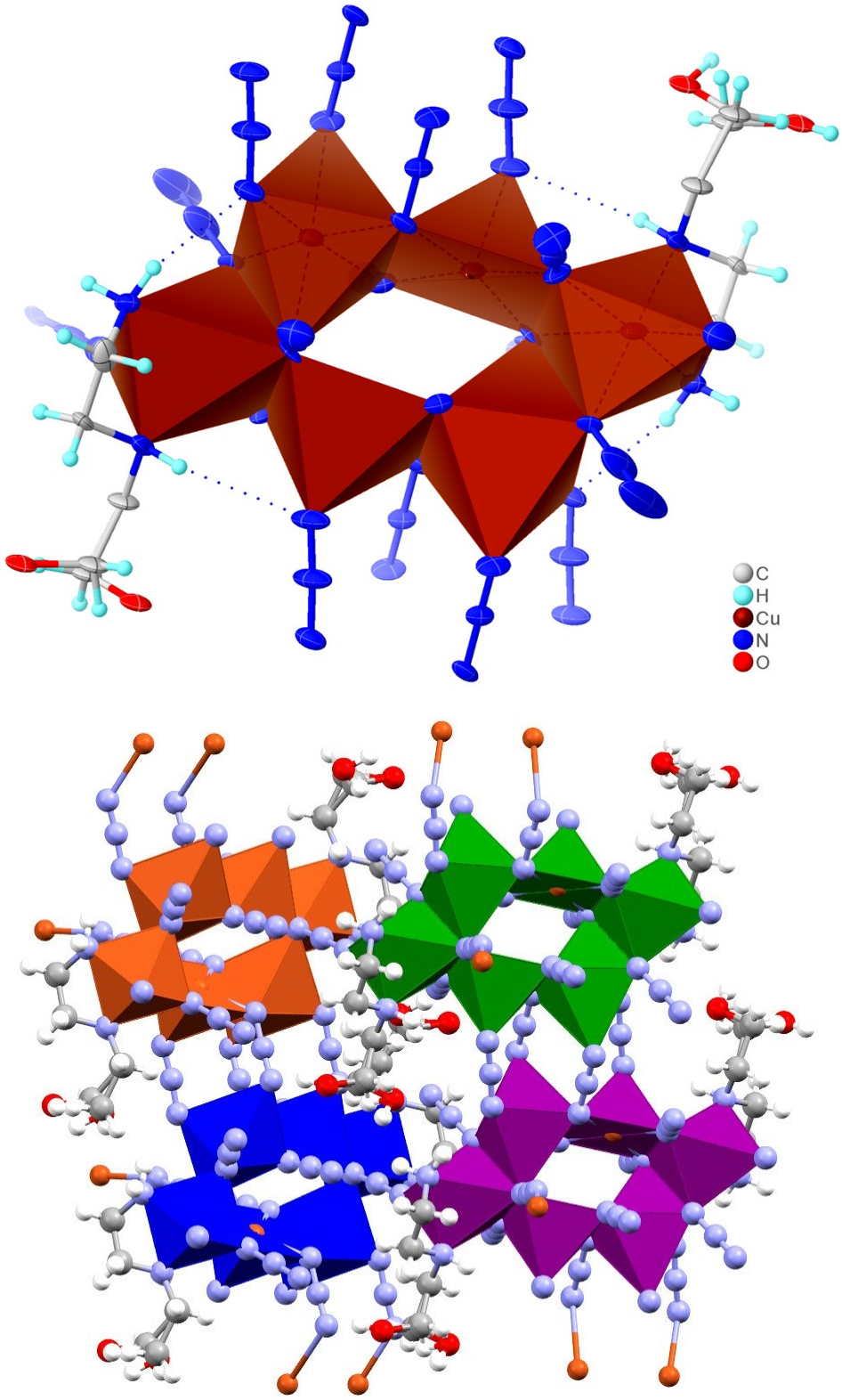

Fig S1: Coordination environment around the Cu(II) ions in hexanuclear units and the connection of hexanuclear units through azide bridges in the crystal structure of compound **1**.

The spin Hamiltonian of the hexanuclear copper-azido cluster with similar magnetic pathways to compound **1** and *J* parameter of interactions was written as[50, 56]:

$$\hat{H}_{hexa} = -2J(\hat{S}_1\hat{S}_2 + \hat{S}_2\hat{S}_3 + \hat{S}_3S_4 + \hat{S}_4\hat{S}_5 + \hat{S}_5\hat{S}_6 + \hat{S}_6\hat{S}_1)$$

Magnetic susceptibility for this model is given:

$$\chi_{hexa} = \frac{2Ng^2\beta^2}{kT}\frac{14 + 9\exp\left(-\frac{10J}{kT}\right) + 25\exp\left(-\frac{6J}{kT}\right)}{7 + 5\exp\left(-\frac{12J}{kT}\right) + 25\exp\left(-\frac{6J}{kT}\right)}$$

The molecular field term was used to describe intermolecular interactions (between hexanuclear units):

$$\chi_m = \frac{\chi_{hexa}}{1 - \chi_{hexa}\left(2zJ'/Ng^2\beta^2\right)}$$

The best fit gives parameters: g=1.83, J=3.56 cm-1, zJ'=0.53, R=2.2·10^{-3},

where $R = \sum_{i=1}^{n}\frac{(\chi_i^{\exp} - \chi_i^{calc})^2}{(\chi_i^{\exp})^2}$. Although the match of χ_m (T) is good, the parameters obtained are incorrect. The discrepancy between experimental and theoretical curve is also seen in $\chi_m T$ (T).

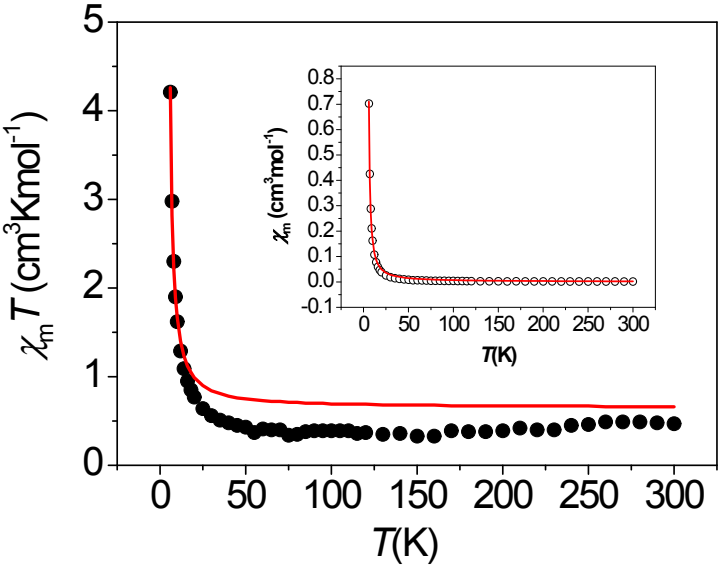

Fig S2: Temperature dependence of $\chi_m T$ product (magnetic susceptibility χ_m calculated per one Cu(II) ion). Inset represents $\chi_m(T)$ relation and the solid lines the best fitting of the data.

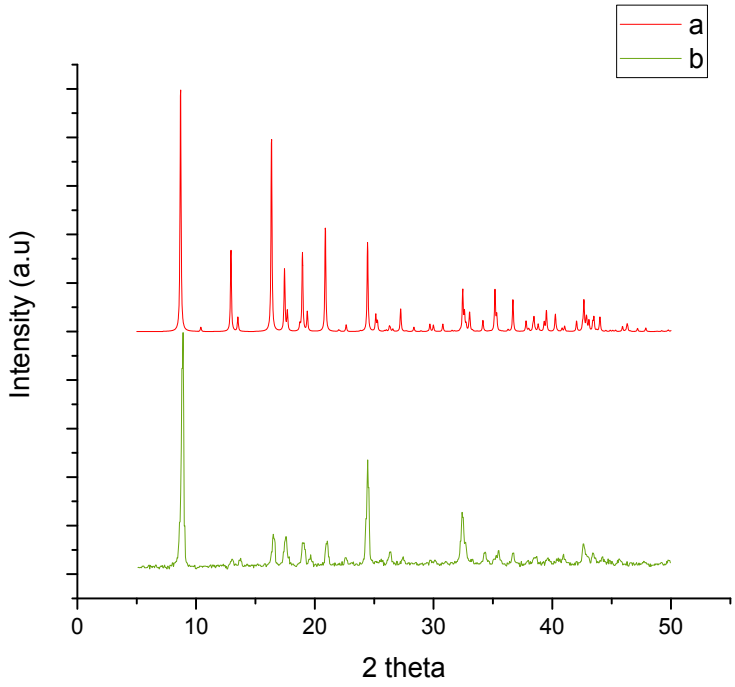

Fig. S3. XRD patterns of: simulated from the crystallographic data of compound **2** (a) and nanosheets of **2a** synthesized by using the ultrasonic method (b)

a b c

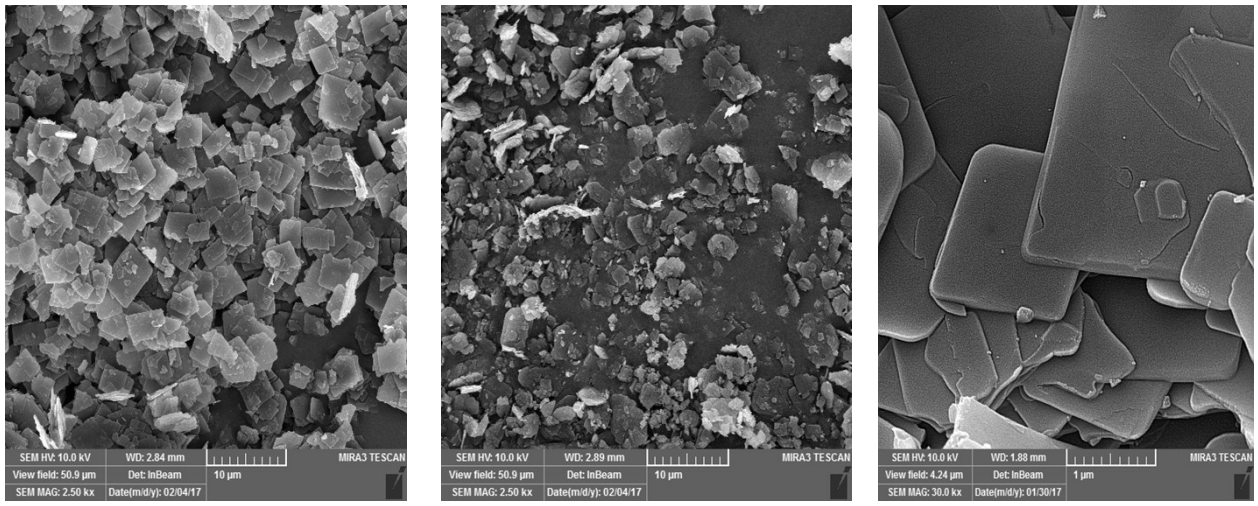

Fig. S4. a) SEM image of 2a prepared with $[Cu^{2+}]$=0.15 M, [HL]= 0.3 M, $[Fe^{2+}]$= 0.1 M and under a reaction time of 30 min; b) SEM image of 2b prepared with $[Cu^{2+}]$= 0.15 M, [HL]= 0.3 M, $[Fe^{2+}]$= 0.1 M and under a reaction time of 60 min; c) SEM image of 2c prepared with $[Cu^{2+}]$= 0.015 M, [HL]= 0.03 M, $[Fe^{2+}]$= 0.01 M and under a reaction time of 30 min.