

## Supplementary Material

# **Crystal Structures and Magnetism of Infinite Alternating Chains Arranged by Paddle-Wheel Dinuclear Copper and Mononuclear Copper Units**

*Huijun Li, Hongchang Yao, Erpeng Zhang, Yanyuan Jia, Hongwei  
Hou\*, and Yaoting Fan*

*Department of Chemistry, Zhengzhou UniVersity, Henan 450052, P. R. China*

E-mail: [huhongw@zzu.edu.cn](mailto:huhongw@zzu.edu.cn)

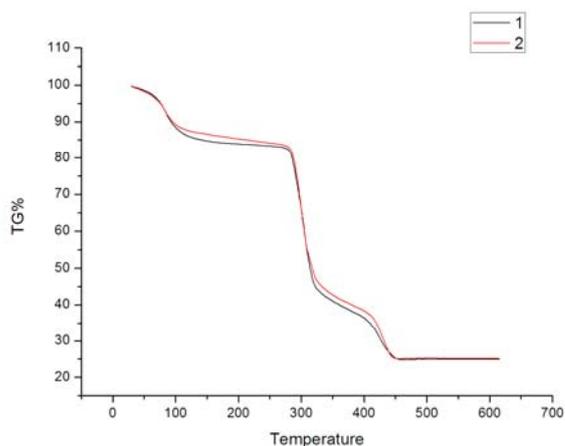


Fig. S1†. The TGA curves for **1** and **2**

**Thermal Analysis Studies.** To estimate the stability of the coordination architectures, thermogravimetric analyses (TGA) were carried out. The TGA curves for **1** and **2** are shown in Fig. S1†, TGA data of **1** shows that the first weight loss at 65.1 °C corresponding to the loss of a lattice water loss, and loses water in all by 280.4 °C. A plateau region is observed from 162.5 °C to 280.4 °C. The removal of the organic components occurs from 280.4-404.9 °C. The decomposed reactions end at 456 °C correspondence with the decomposition of CuO. For **2**, the TGA curve of **2** shows that the first step weight loss from 67.5 °C to 281 °C attributed to the gradual release of water molecules and coordinated water molecules. A plateau region is observed from 150.5 to 281 °C. And then, The second step weight loss from 281 to 409.5 °C corresponding to the decomposition of tci ligand, leading to the formation of CuO as the residue. Powder XRD patterns of the samples for **1** and **2** are in Fig. S2† characterized the phase purity.

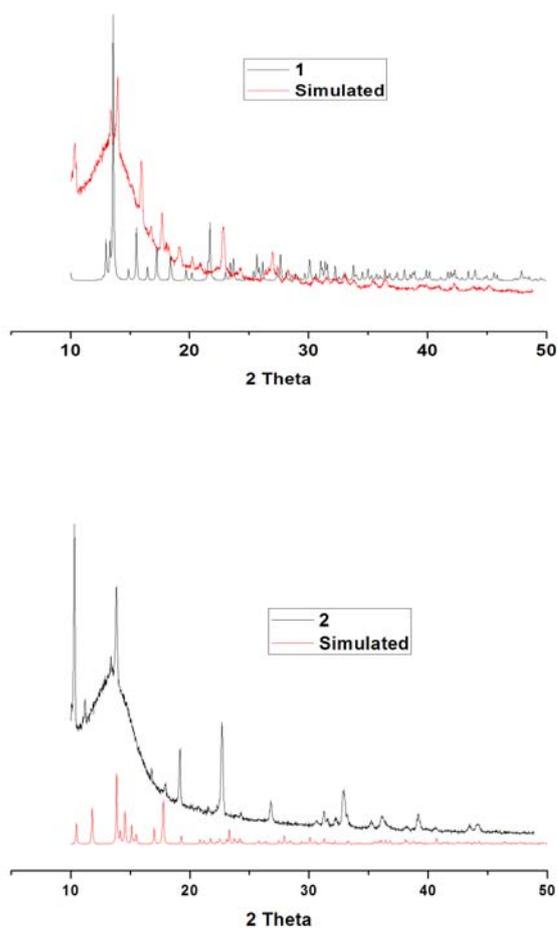


Fig. S2†. PXRD pattern of **1** (top) and **2** (bottom)

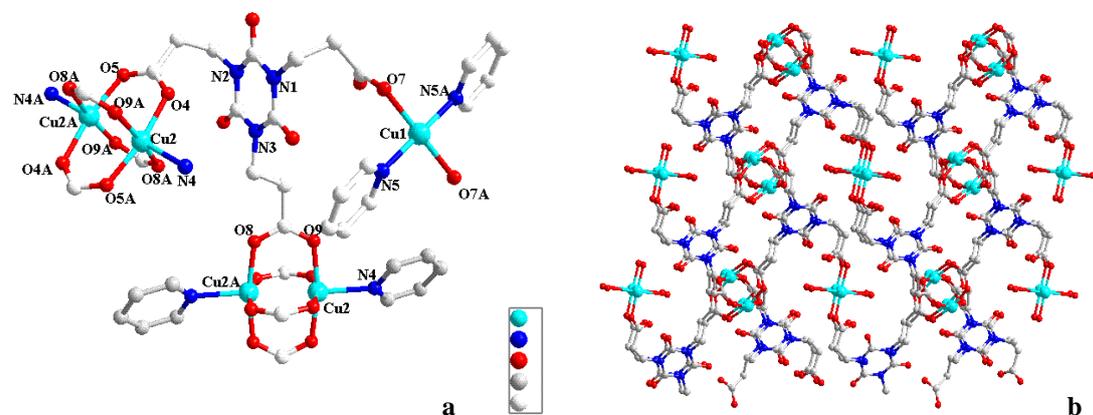


Fig. S3†. (a) The coordination environments of Cu(II) ions in **3** (b) the 3D framework of **3** based on isolated dinuclear cluster and mononuclear copper units.