Supporting Information In situ amination and side group effect of multifunctional heterocyclic thione ligand toward discrete and polymeric cluster constructions

Sheng Hu, * Fang-Yong Yu, Peng Zhang and Dian-Rong Lin

School of Chemical Engineering and Light Industry, Guangdong University of Technology,

Guangzhou, 510006, China. E-mail: husheng@gdut.edu.cn



Figure S1. The crystal packing of the adjacent hexanuclear copper molecules in compound 1.



Figure S2. The crystal packing of the adjacent (4,4) layers in compound 2.



Figure S3. The channel of 3 along the *c* axis features cross-shaped window.



Figure S4. TGA curve for an as-synthesized sample of 3 under a dinitrogen atmosphere.



Figure S5. Plots of *M* vs *H* for **3** at 1.8 K.



Figure S6. Simulated and experimental XRPD data of compound 1.



Figure S7. Simulated and experimental XRPD data of compound 2.



Figure S8. Simulated and experimental XRPD data of compound 3.



Figure S9. ¹H NMR spectra of the complex 1.





Figure S11. UV-Vis spectra of pure formic acid and the mother liquid collected after solvothermal synthesis of **1**.