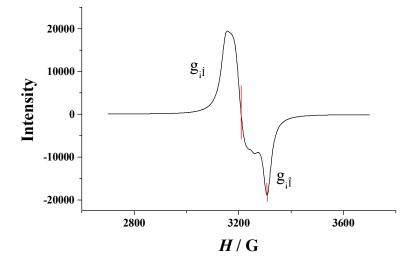
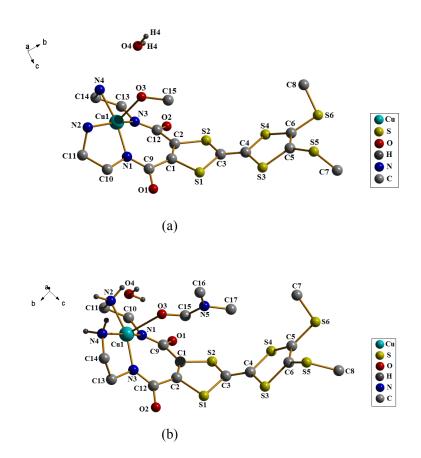
SI materials for Paper:

Cu(II) and Ni(II) dioxotetraamine complexes integrated with tetrathiafulvalene moiety, structures and solution chemistry

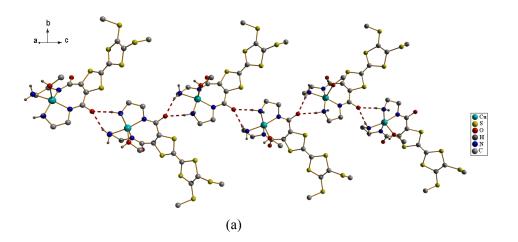
Zhe-Jun Lu, Jin-Po Wang, Qin-Yu Zhu*, Li-Bin Huo, Yu-Rong Qin, and Jie Dai*

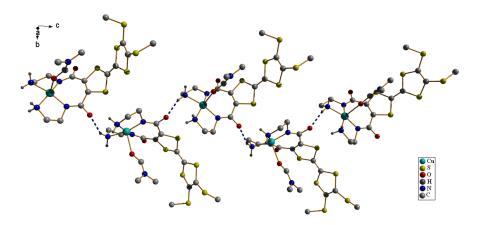


SI-Fig. 1. ESR spectra of 1 measured using powder sample at 110 K.

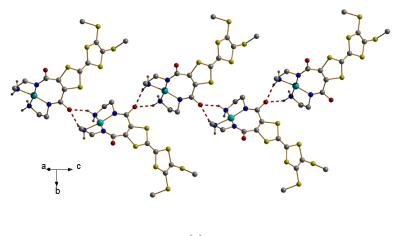


SI-Fig.2. Crystal structure of 2 and 3 with labeling schemes, hydrogen atoms are omitted for clarity except the hydrogen atoms of N–H and O–H. (a) $[CuL(CH_3OH)]\cdot 0.5H_2O$ (2), (b) $[CuL(DMF)]\cdot H_2O$ (3).



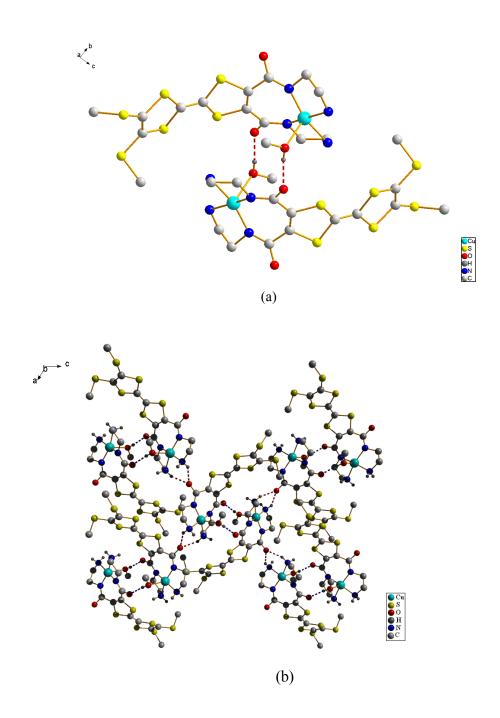


(b)

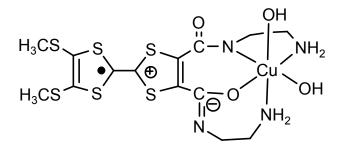


(c)

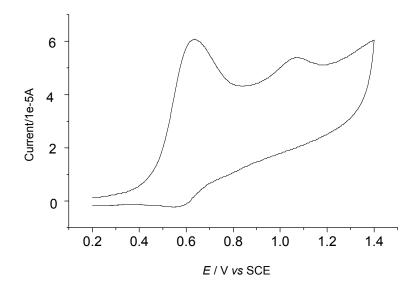
SI-Fig. 3. Similar to Figure 2, the band structure is also found in compounds 2-4 (2, a; 3, b; 4, c), that is the fundamental character of molecular arrangement for these type of compounds.



SI-Fig. 4. Cooperating with the N1–H1A····O2 and N2–H2B····O2 hydrogen bonds, hydrogen bonds that involve the imido oxygen atoms and the OH groups of methanol molecules (a) link the molecules of **1** into a 2-D aggregate (b).



SI-Fig. 5. Proposed structure of the TTF oxidized Cu(II) complex.



SI-Fig. 6. Irreversible CV curve of the free ligand.