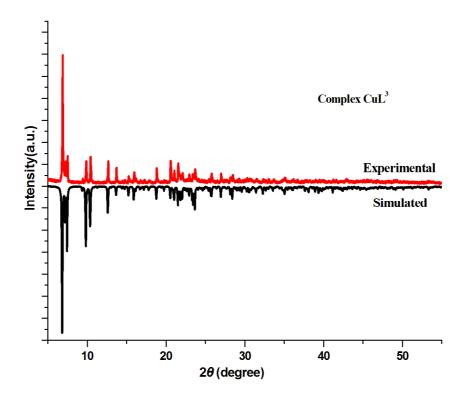


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Supporting information for article:

Synthesis, structure and photophysical properties of two tetranuclear copper(I) iodide complexes based on acetylpyridine and diphosphine mixed ligands

Bing-Jun Cao, Ran Li and Xi-He Huang



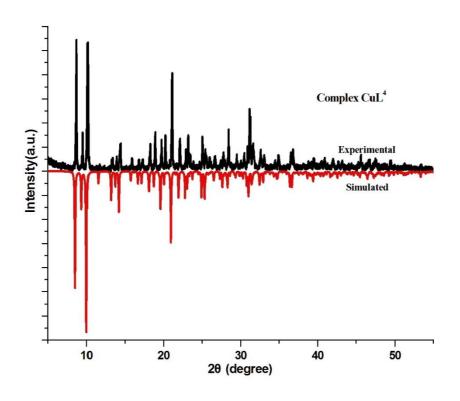


Figure S1. The experimental and simulated powder X-ray diffractions of CuL³ and CuL⁴

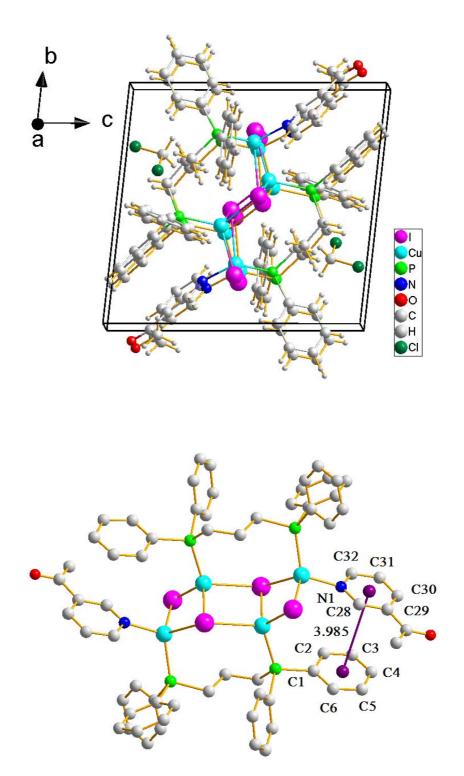


Figure S2. Packing diagrams of complex CuL^3 (up), and view of the intra-cluster $\pi \cdots \pi$ staking interactions (bottom). The purple ball represents the centroid of the phenyl or pyridine rings. The

distance between the centroid of the two rings (C1-C6), and N1/C28-C32) are 3.958(6) Å. The dihedral angle between the two rings is $8.5(5)^{\circ}$. H atoms are omitted for clarity.

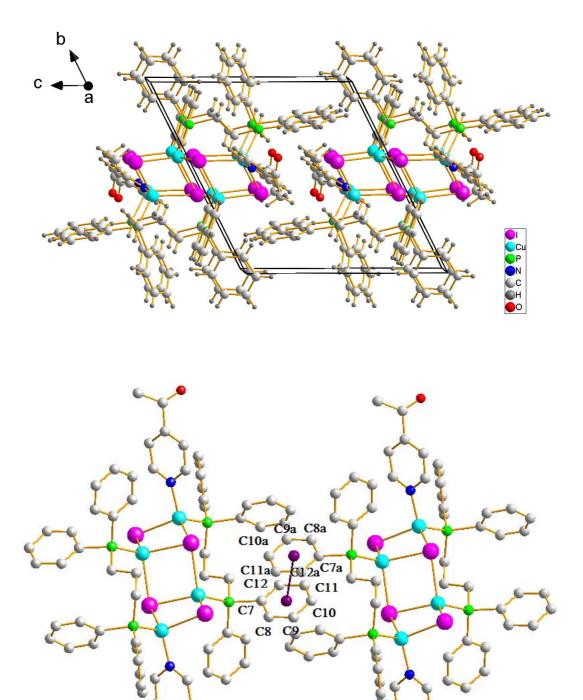
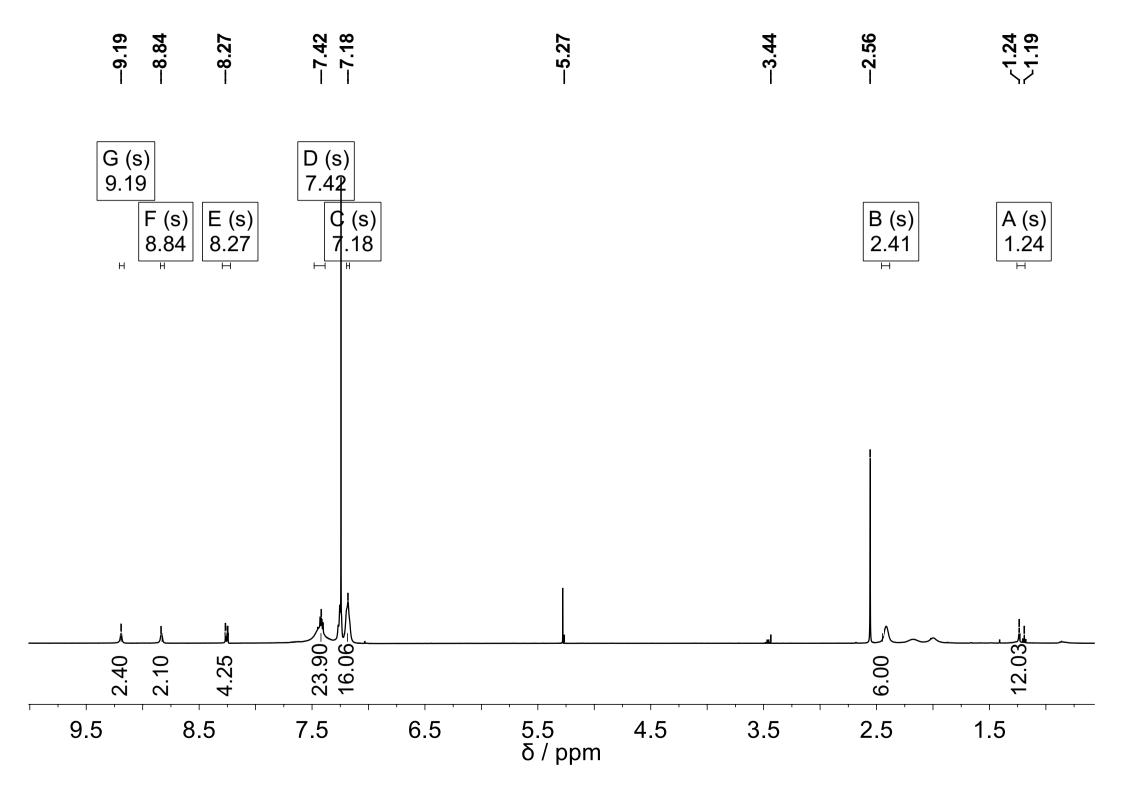
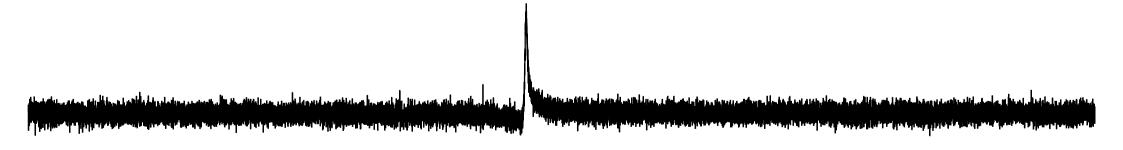
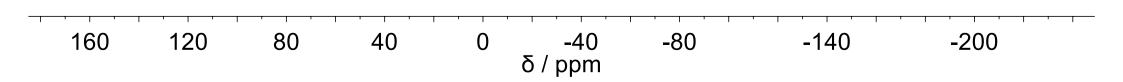


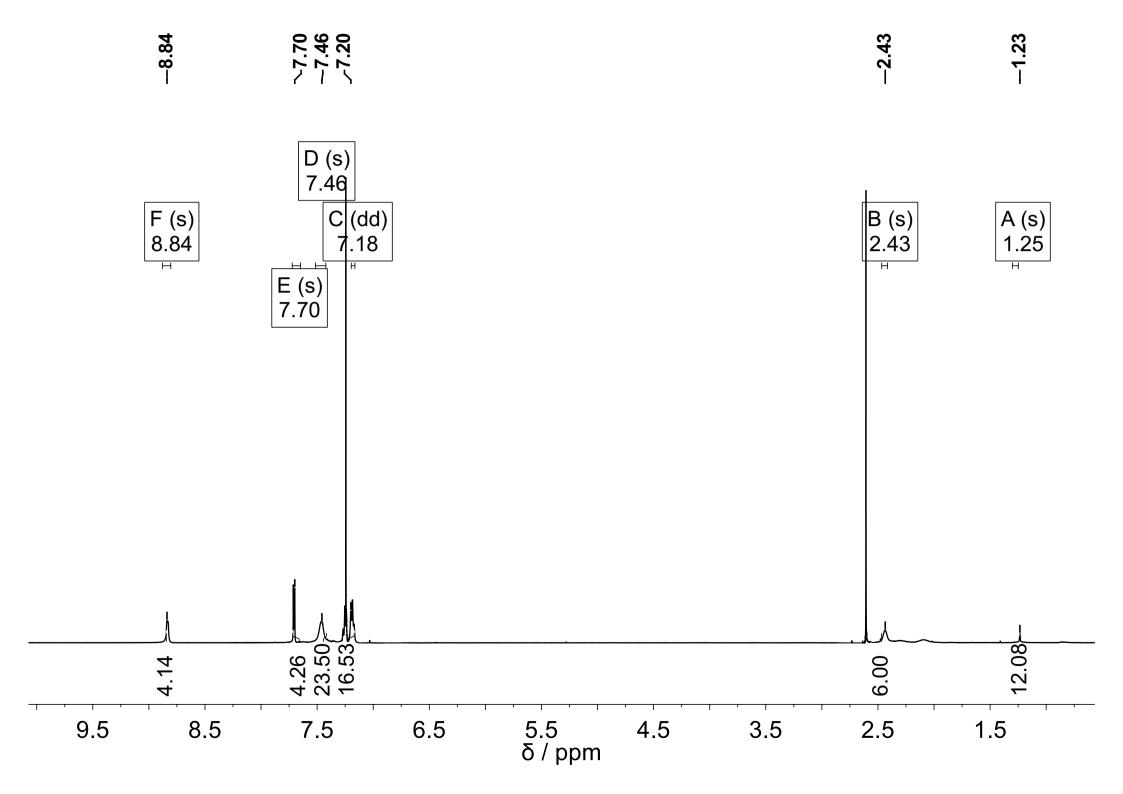
Figure S3. The packing diagrams of complex CuL^4 (up), and view of the inter-cluster $\pi \cdots \pi$ staking interactions (bottom). The purple ball represents the centroid of the phenyl rings. The benzene rings are parallel to each other. The distance between the centroid of the two rings is 3.816(9) Å [symmetry code: a) 2-x, -y, -z]. H atoms are omitted for clarity.



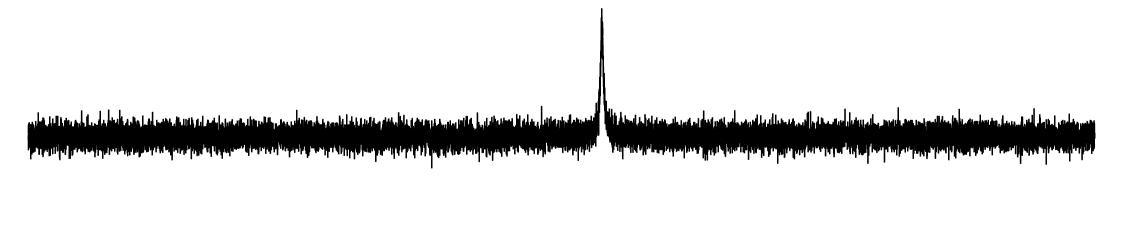












 $\begin{matrix} 0 \\ \delta \text{ / ppm} \end{matrix}$

-30

-90

50

110