crystals

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Supporting Information

Unprecedented Dinuclear Cu^{II} N,O-Donor Complex: Synthesis, Structural Characterization, Fluorescence Property and Hirshfeld Analysis

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1. Crystal Structure Determination of the Cu^{II} complex

Crystal data of Cu^{II} complex was collected at 273 (2) K (Mo-K alpha radiation (λ = 0.71073 Å)) by CCD area detector. The cell parameters of Cu^{II} complexes were determined by least square method. The LP calibration was used in SAINT program, while semi-empirical calibration was used in SADABS program. The structure was analyzed by direct method (SHELXS-2015) [1,2]. All non-hydrogen atoms were refined by full matrix least squares anisotropy. The positions of hydrogen atoms were calculated and fixed isotropically in the final refinement. The supplementary crystallographic data in this paper is included in the CCDC (1959387), which is available free of charge from the following website. www.ccdc.cam.ac.uk/conts/retrieving.html.

2. Infrared Spectra

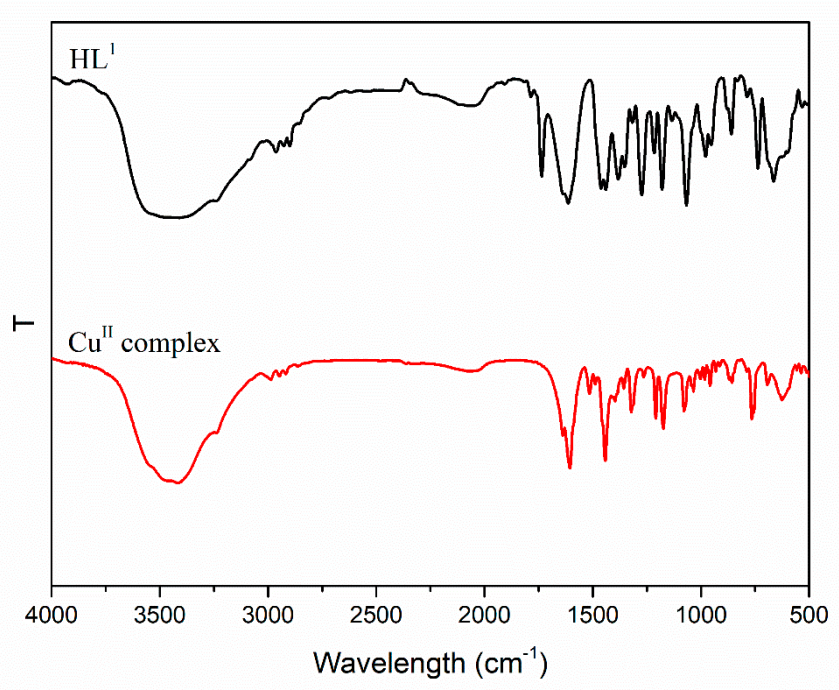

Figure S1. The infrared spectra of the ligand HL^1 and the Cu^{II} complex.

3. bonding constant

Benesi–Hildebrand (B-H) equation is widely used in all kinds of non key Systems for determining the bonding stoichiometry of ions and ligand.

$$\log (F - F_{min})/(F_{max} - F) = \log K + 2 \log [Cu^{2+}] \quad (1)$$

Where F_{min}, F_{max} and F are the emission intensities in the absence, presence of saturated Cu^{2+}, and addition of a given amount of Cu^{2+} concentration, respectively. $[Cu^{2+}]$ is the concentration of free Cu^{2+} [3].

References

1. G.M. Sheldrick, *SHELXS*-2016, Program for crystal structure solution, University of Göttingen, Göttingen Germany, **2015**
2. G.M. Sheldrick, *SHELXL*-2016, Program for crystal structure refinement, University of Göttingen, Göttingen Germany, **2015**
3. B. Valeur, M.N. Berberan-Santos, Molecular fluorescence: Principles and applications, DOI: 10.1002/9783527650002.