Supporting Information

A noel 3-D photoluminescent cuprous chloride polymer based on bifunctional imidazolate/tetrazolate bridges

Qiuling Tang, Jian Zhou,* Filipe A. Almeida Paz, Lianshe Fu,* Hong Xiao, Qi Zhou, and Ju Li

General Remarks. All analytical grade chemicals were obtained commercially and used without further purification. Elemental analyses (C, N and H) were performed using a PE2400 II elemental analyzer. IR spectra were obtained from a powdered sample pelletized with KBr on an ABB Bomen MB 102 series IR spectrophotometer in the range of 400–4000cm^{-1}. PXRD patterns were obtained using a Bruker D8 Advance XRD diffractometer with Cu Kα radiation (λ = 1.54056 Å). The photoluminescence spectra were recorded at room temperature with a modular double grating excitation spectrofluorimeter with a TRIAX 320 emission monochromator (Fluorolog-3, Horiba Scientific) coupled to an R928 Hamamatsu photomultiplier. The excitation source was a 450 W Xe arc lamp. The emission spectra were corrected for detection and optical spectral response of the spectrofluorimeter and the excitation spectra were corrected for the spectral distribution of the lamp intensity using a photodiode reference detector. Thermogravimetric analyses (TGA) were performed using a Mettler TGA/SDTA851 thermal analyzer under a N_2 atmosphere with a heating rate of 10 °C min^{-1} in the temperature region of 25–770 °C.

Crystal Structure Determination

Single-crystal X-ray diffraction data for **1** were recorded on a Rigaku Mercury CCD diffractometer using a ω-scan method with graphite monochromated Mo Kα radiation (λ = 0.71073 Å) at 173(2) K to a maximum 2θ value (50.20 °). Absorption corrections were applied using multi-scan technique. The structure of **1** was solved by Direct Methods (SHELXS-97) and refined by full-matrix least-squares techniques using the SHELXL-97 program. Non-hydrogen atoms were refined with anisotropic displacement parameters. The positions of H atoms attached to the C atoms were geometrically placed and H atoms were refined isotropically in a riding mode using the default SHELXTL parameters.

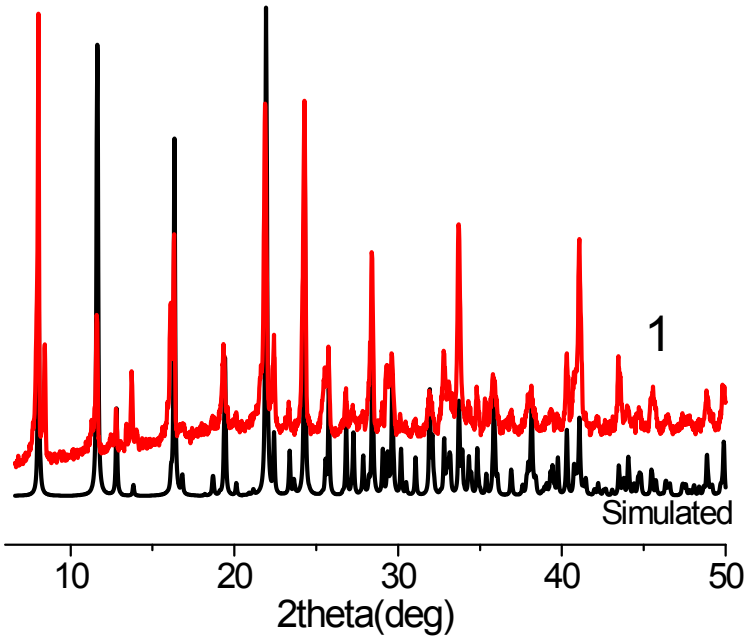

Fig. S1 Simulated and experimental powder XRD patterns of **1**.

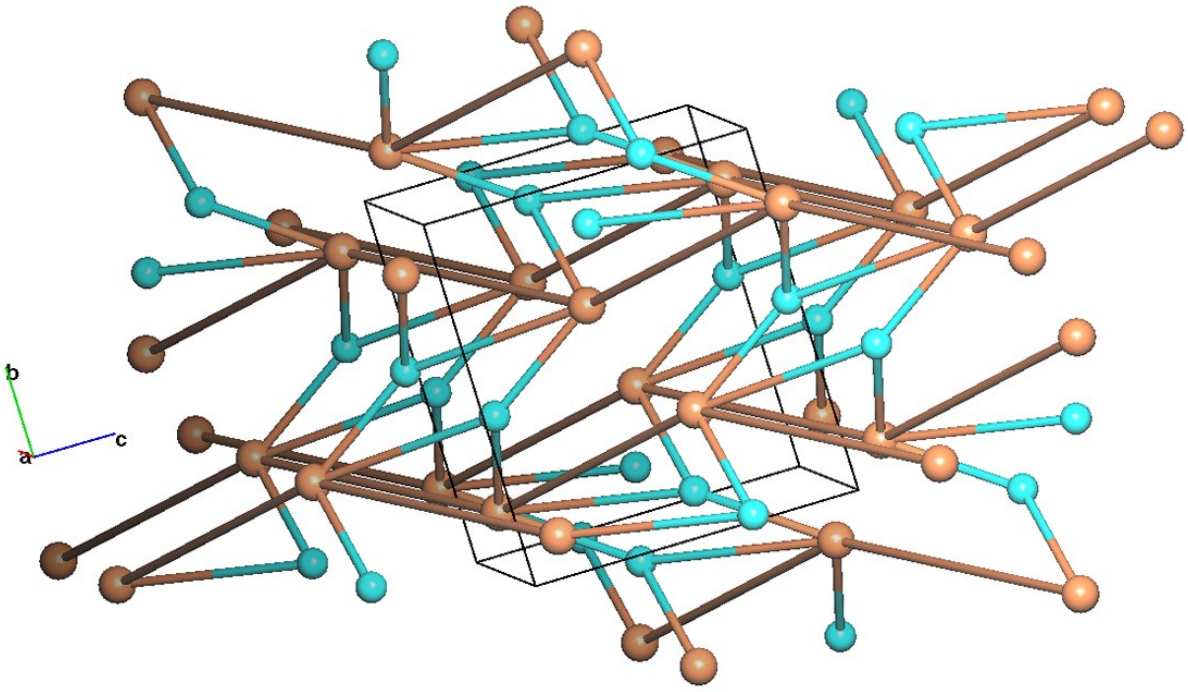

Fig. S2. Schematic representation of the topological representation of the bimodal **fsc**-3,5-Cmce-2(3,5)-connected network of $[Cu^{I}_{2}Cl(\mu_5\text{-L})]_n$in which the centres of gravity of the ligand and the Cu^{+} are taken as the nodes (in orange and blue, respectively).

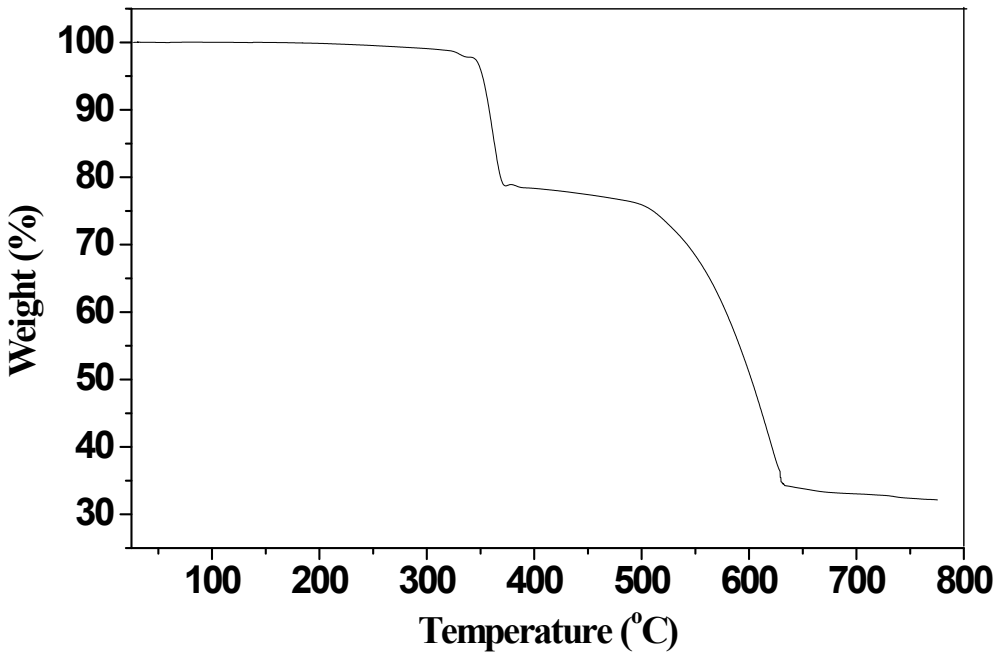

Fig. S3 Thermogravimetric analyses curves of **1**.

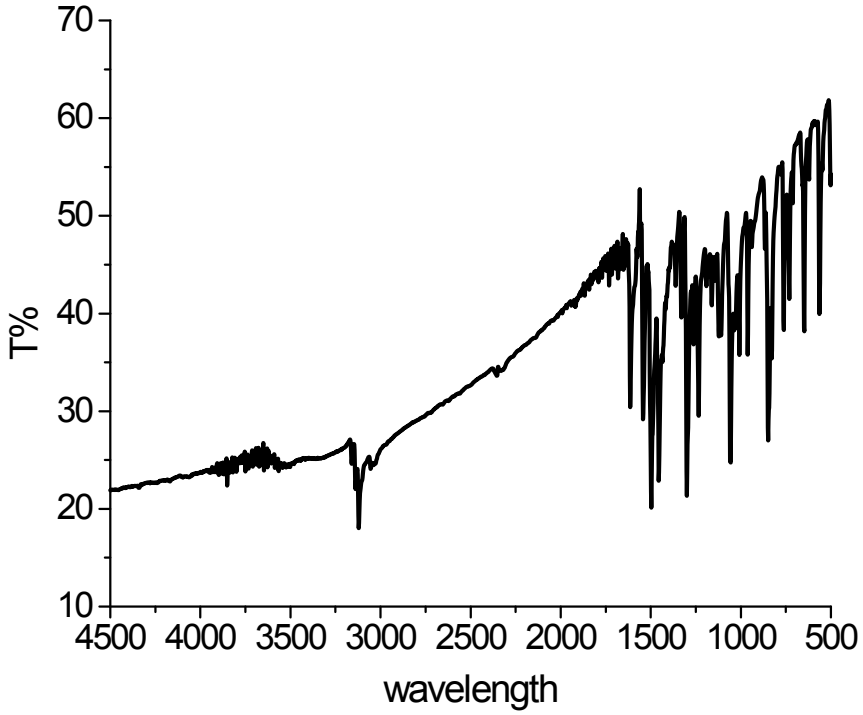

Figure S4 IR spectrum of **1**.