Electronic Supplementary Information (ESI) for

Two luminescent Cu(I) coordination polymers based on 1-(4-tetrazolephenyl)imidazole ligand for sensing of nitrobenzene

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Experimental section:

Single-Crystal Structure Determination. Suitable single crystals of **1-2** were carefully selected under an optical microscope and glued to thin glass fibers. Single-crystal X-ray diffraction analyses were performed on a computer-controlled X-ray diffractometer with graphite monochromated Mo Kα radiation ($\lambda_{Mo\text{-}K\alpha}$=0.71073 Å) at 293 K. Absorption corrections were made using the SADABS program.[1] The structures of **1-2** were solved using the direct method and refined by full-matrix least-squares methods on F^2 by using the SHELX-97 program package.[2]

Sensing experiments of nitrobenzene. The real-time sensing experiments of nitrobenzene were performed by using the sample of **1** as the starting material. The as-prepared sample of **1** was compacted onto a quartz plate to produce a thin film device, and then a drop of nitrobenzene was added. The resulting device was placed in a sealed quartz cuvette. After the emission measurement, the sealed quartz cuvette was opened to volatilize the nitrobenzene. This experimental setup is convenient for real-time monitoring the variation of emission intensity of **1** (Fig. S9). The sensing experiments of nitrobenzene for **2** were measured by the similar method.

Other Experimental details

All reagents and solvents were obtained from commercial sources. The IR spectra were recorded on a Perkin-Elmer SpectrumOne FT-IR spectrometer in the range 4000-400 cm^{-1}. Powder X-ray Diffraction (PXRD) were recorded using a Bruker D2 phaser with Cu-Kα source (λ = 154 Å) on glass surfaces of air dried samples (Figures S1-2).Thermogravimetric analyses (TGA) were performed on a Mettler Toledo TGA/SDTA 851e module. Samples were placed in open alumina pans in the temperature range 25-600 °C and were purged with a stream of dry N_2 flowing at 100 mL $min^{-1}$with heating rate 5 °C (Figure S3). The solid state fluorescence emission spectra of the samples were recorded of powdered samples in each case of equal weight (30 mg). Elemental anal calcd. For **1**（$C_{20}H_{14}Cu_2N_{12}$）, C, 43.67; H, 2.54; N, 30.57. Found: C, 43.51; H, 2.30; N, 30.34. IR (KBr, cm^{-1}): 3110 (w), 1617(m),1535 (s), 1483 (s), 1441 (s), 1306 (s), 1058 (s), 1229 (m), 1170 (w), 1094 (m), 954 (m), 1188 (w),845 (s),716 (w), 618 (w), (Figure. S7). Elemental anal calcd. For **2**（$C_{10}H_7Cu_2IN_6$）, C, 25.79; H, 1.50; N, 18.06. Found: C, 25.51; H, 1.17; N, 18.01.IR (KBr, cm^{-1}): 2934 (w), 1607 (s), 1545 (s), 1488 (s), 1441 (m), 1344 (m), 1297 (s), 1053 (m), 1229 (w), 1115 (w), 954 (w),850 (w), 845 (m), 785 (m), 654 (w) (Figure. S8).

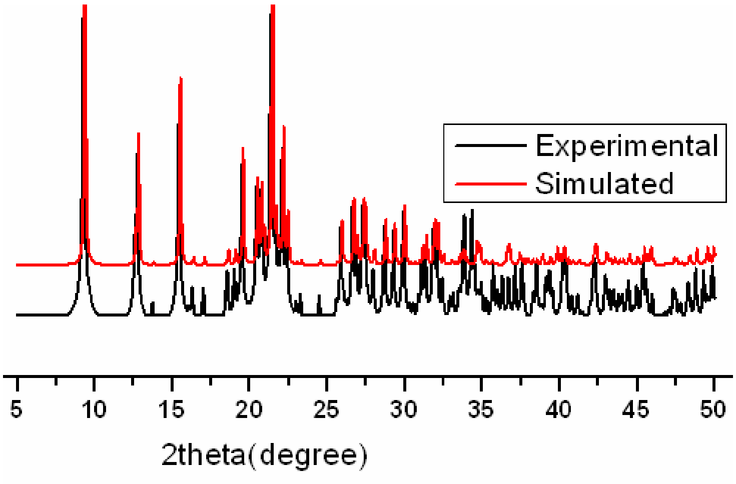

Figure S1. The PXRD patterns of **1.**

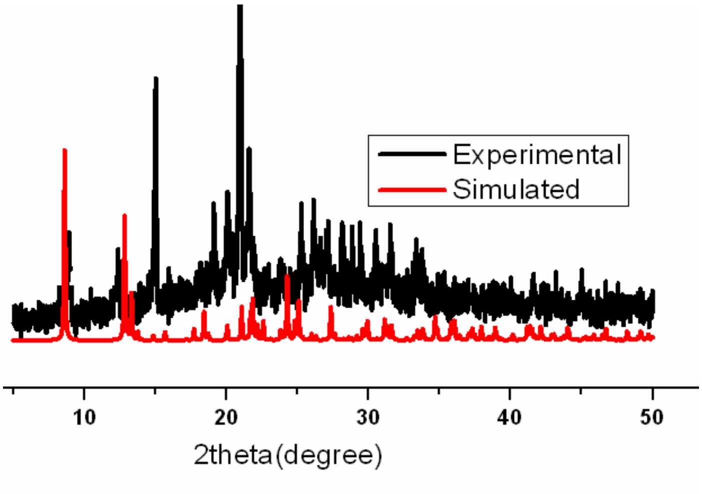

Figure S2. The PXRD patterns of **2.**

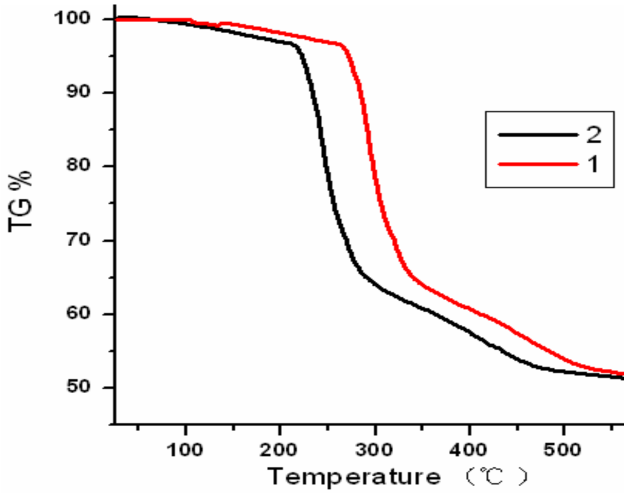

Figure S3. Thermogravimetric analyses of **1** and **2**. The thermogravimetric analysis for each compound reveals that there is no obvious weight loss before 150 °C, indicating the absence of solvent guests in the structure.

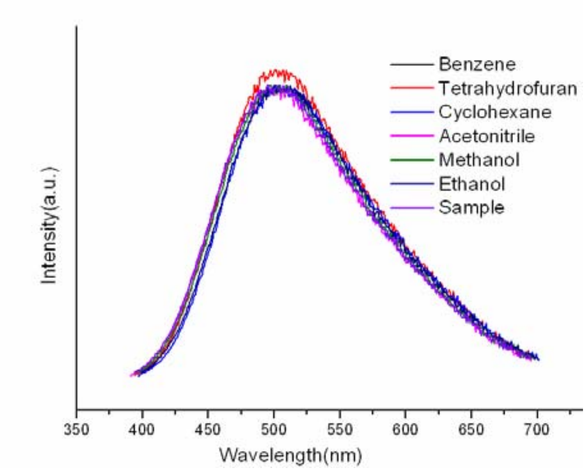

Figure S4. The solid-state emission spectra (λex = 360 nm) of **1** under different conditions. **1** was dispersed into these solvents, no obvious luminescent change was observed, suggesting that **1** can sense nitrobenzene.

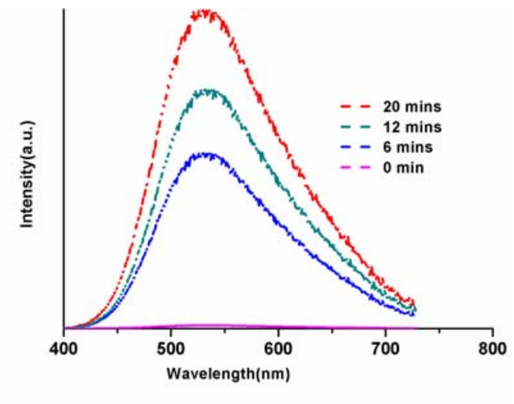

Figure S5. PL spectra of **2** quenching response to nitrobenzene solvent with time. The distinct fluorescence quenching response of **2** to nitrobenzene may due to the electrostatic interactions and the electron-deficient.

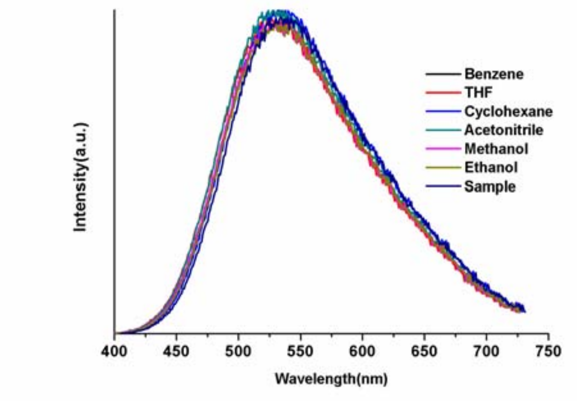

Figure S6. The solid-state emission spectra (λex = 360 nm) of **2** under different conditions. **2** was dispersed into above solvents, no obvious luminescent change was observed, suggesting that **2** can act as luminescent probe for sensing nitrobenzene.

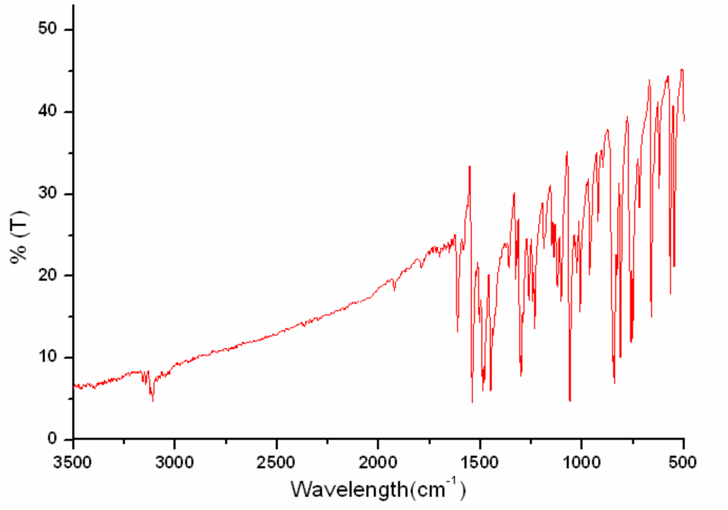

Figure S7. FT-IR (KBr) spectra of **1**.

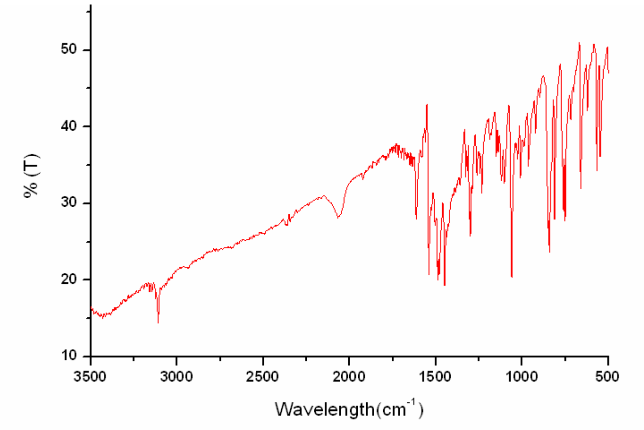

Figure S8. FT-IR (KBr) spectra of **2**.

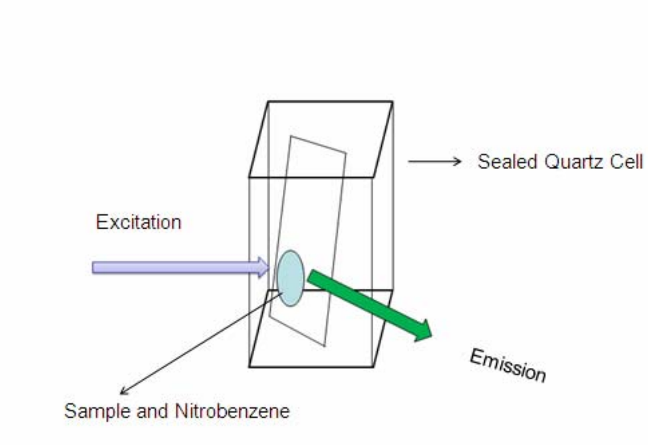

Figure S9.Experimental setup for the sensing of nitrobenzene.

Reference:

(1) Sheldrick, G. M. SADABS, Program for Area Detector Adsorption Correction, Institute for

Inorganic Chemistry, University of Göttingen: Göttingen, Germany, 1996.

(2) Sheldrick, G. M. SHELXL-97, Program for Solution of Crystal Structures, Institute for Inorganic Chemistry, University of Göttingen: Göttingen, Germany, 1997.