Supplementary Material

Fluorescent Cu(II) complex exhibiting dual functional fluorescent sensor for selective, sensitive detection of pollutants acetone and Cd(II)

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Crystal structure determination

Single crystals of Cu complex (**1**) were coated with a trace of Fomblin oil and quickly transferred to the goniometer head of a Bruker Quest diffractometer with a fixed chi angle, a sealed tube fine focus X-ray tube, single crystal curved graphite incident beam monochromator, a Photon100 CMOS area detector and an Oxford Cryosystems low-temperature device. Examination and data collection were performed with Mo Kα radiation (λ = 0.71073 Å) at 150 K. Data reduction and unit cell refinement for complex **1** was performed using SAINT-Plus.[1] Using *OLEX2*[2] the SHELXL-2014/7 [3,4] software was used to solve the structure of complex **1** by the direct method, the refinement procedurebeing done by full-matrix least-squares, based on F2 values against all reflections. H atoms attached to carbon and nitrogen atoms as well as hydroxyl hydrogens were positioned geometrically and constrained to ride on their parent atoms. C-H bond distances were constrained to 0.95 Å for aromatic and alkene C-H moieties. N-H bond distances were constrained to 0.88 Å for planar (sp^2 hybridized) N-H groups.

Topology analysis

The analysis was performed with the ToposPro program package and the TTD collection of periodic network topologies [5]. The RCSR three-letter codes [6] were used to designate the network topologies.

Fluorescence Titrations

The fluorescence spectra of Cu^{2+} complex (**1**) predissolved in CH_3CN at 298 K. All titrations were performed by the successive addition of acetone and Cd^{2+} in an incremental fashion. Each titration was repeated several times to get an accurate result. No shape change but only intensity decrease (in case of acetone) or increase (in case of Cd^{2+}) was observed in the emission spectra during the titration process. The fluorescence quenching or enhancement efficiency (%) was calculated with $(1 - I/I_0) \times 100$, where I_0 and I are the fluorescence intensities before and after the addition of acetone or Cd^{2+}, respectively.

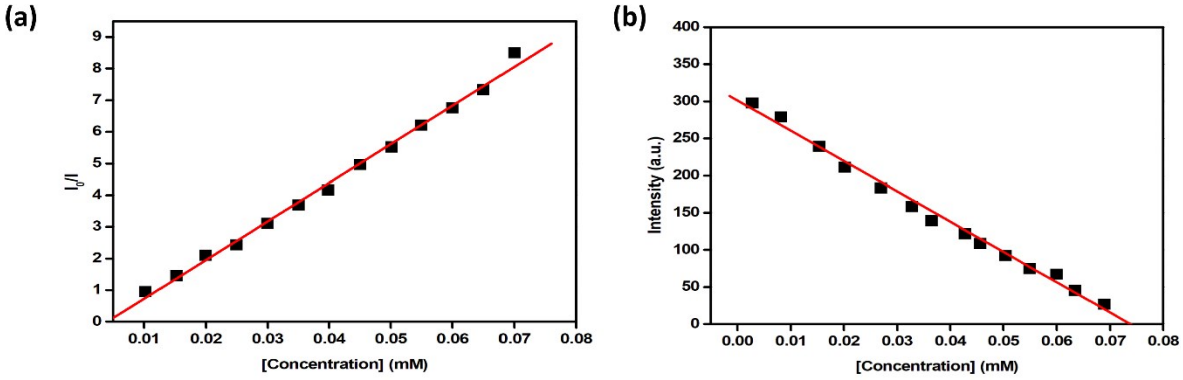

Fig S1- (a) Stern–Volmer plot for the fluorescence intensities of complex **1** upon addition of acetone (5.0×10^{-6} to 8.0×10^{-5} M), (b) The fitting curve of the luminescence intensity of complex **1** at different acetone concentrations (5.0×10^{-6} to 8.0×10^{-5} M).

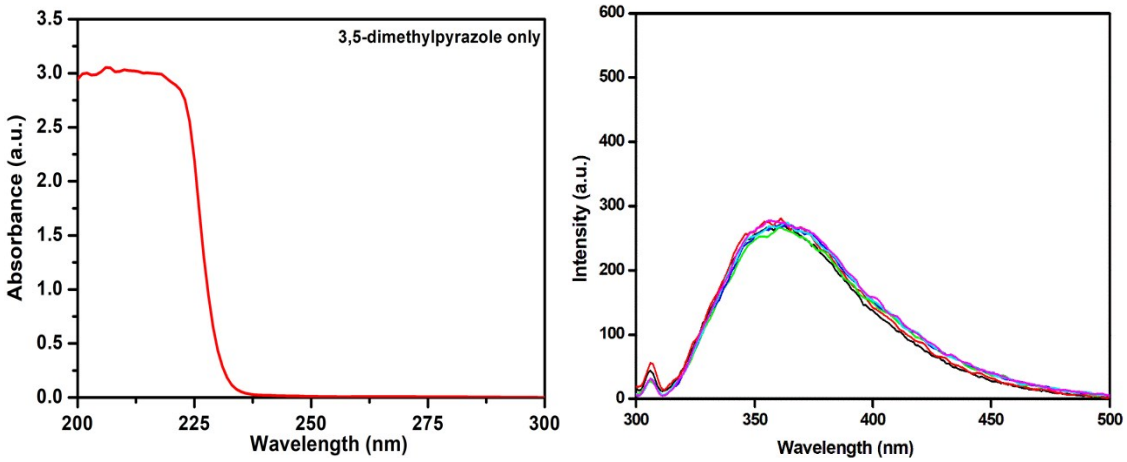

Fig. S2- (a) UV-vis spectrum of dmpy in acetonitrile, (b) Change in the fluorescence intensity of dmpy dissolved in acetonitrile (blank) upon titration with acetone.

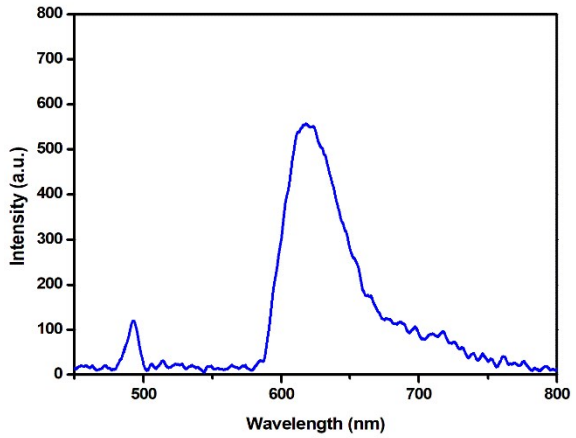

Fig. S3- Solid-state fluorescent spectra of complex **1** at room temperature (λex= 267 nm).

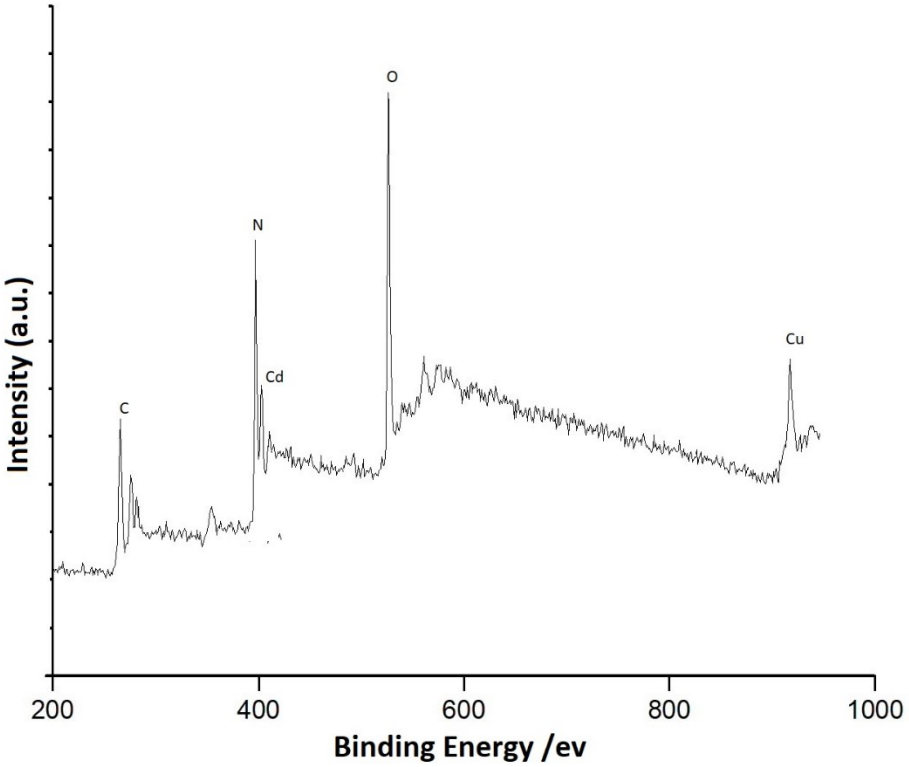

Fig. S4- The XPS of complex **1**/Cd^{2+} shows the typical peak of Cd^{2+} at 405.4 ev

References

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