Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

Conformation Induced Discrimination between Picric Acid and Nitro Derivatives/Anions with Cu-Pyrene Array: First Decision Making Photonic Device

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General Experimental Procedure

All reagents were purchased from Sigma-Aldrich and were used without further purification. The fluorescence spectra were recorded with a Cary Eclipse Fluorescence spectrophotometer, the excitation wavelength was fixed at 342 nm (λ_{ex} = 342 nm) in case of fluorescence measurements at 25°C in a 1 cm quartz cell with a slit width of 10 nm for both excitation and emission .UV-vis spectra were recorded on a Shimadzu UV-2450 spectrophotometer, with a quartz cuvette (path length, 1 cm). Scanning electron microscope (SEM) images were obtained with a field-emission scanning electron microscope (Hitachi S-4800).The synthesized complexes was dissolved in THF:HEPES (9.5:0.5) solution.

Tetrabutyl ammonium salts of F^-, Cl^-, Br^-,I^-, OH^-, HSO_3^-, CN^-, N_3^-, NO_3^- , CH_3COO^-, ClO_4^- , PO_4^{3-} and C_6H_5OH ,H_2O_2 , 4-nitrotoluene, 2,4-dinitrotoluene, 1,4-dinitrobenzene, picric acid were prepared in THF:HEPES (9.5:0.5) solution at 0.1M, 0.01M, 0.001M concentration and was used during the spectroscopic measurement.

Synthesisof complex 3

Asolution of pyrene-1-carboxaldehyde (0.50g, 2.17mmol) in ethanol:chloroform (1:1)was added drop wise to a solutionof diethylenetriamine(0.117 mL, 1.085mmol) in 20 ml of ethanol under reflux for 24 h. The formation of '**L**' was observed by monitoring of TLC and IR of the reaction mixture. For the *insitu*synthesis of copper complex,copper(II)chloride dihydrate ($CuCl_2{\cdot}2H_2O$) (0.6420 g, 3.77 mmol)in ethanol was added slowly to above solution. A dark green colored solid precipitated after 10 minutes of stirring. The precipitates were collected by the filtration. Yield: 88.7%;m.p. ≥ 300˚C; MS-*m/z* 742 (M^+) (**L**·2CuCl·H_2O).

Calculations for quantum yield

Fluorescence quantum yield was determined using optically matching solutions of pyrene (ϕ_R = 0.65 in ethanol) as standard at an excitation wavelength of 342 nm and quantum yield is calculated using the equation:

$$\phi_S = \phi_R \times A_R/A_S \times D_S/D_R \times (n_S/n_R)^2$$

ϕ_S and ϕ_R are the radiative quantum yields of sample and the reference respectively, A_S and A_R are the absorbance of the sample and the reference respectively, D_S andD_R the respective areas of emission for sample and reference,n_S and n_R are the refractive indices of the sample and reference solutions.

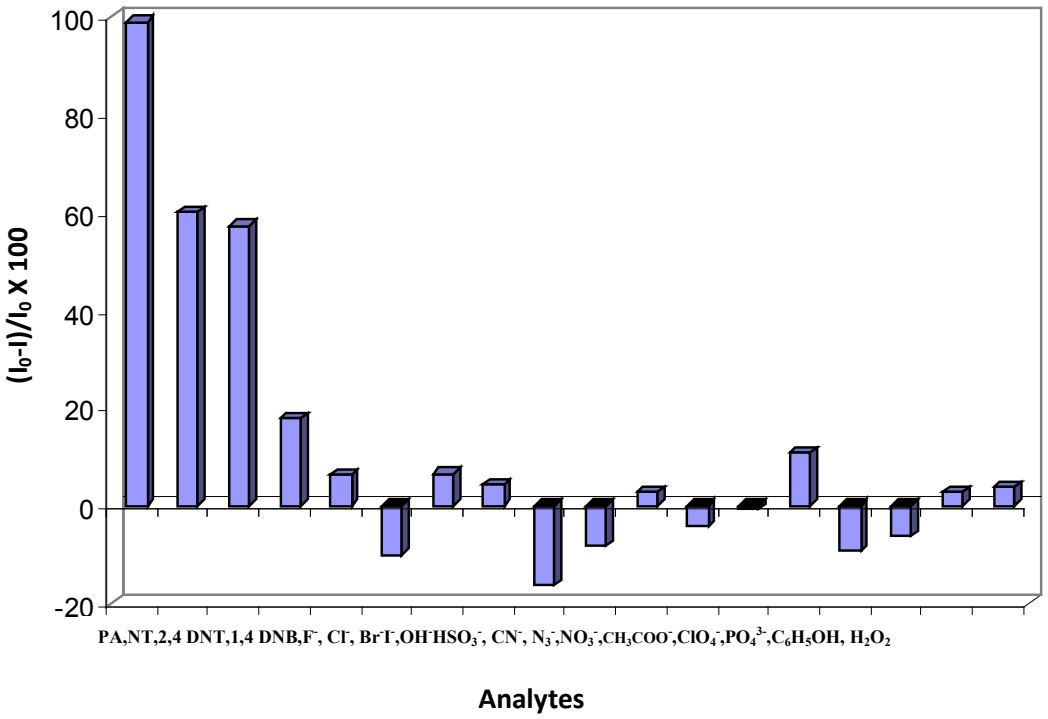


Figure S1. Fluorescence response of complex **3** (0.1 μM) in (THF:HEPES), 9.5:0.5 (*v/v*) among various anions and molecules.

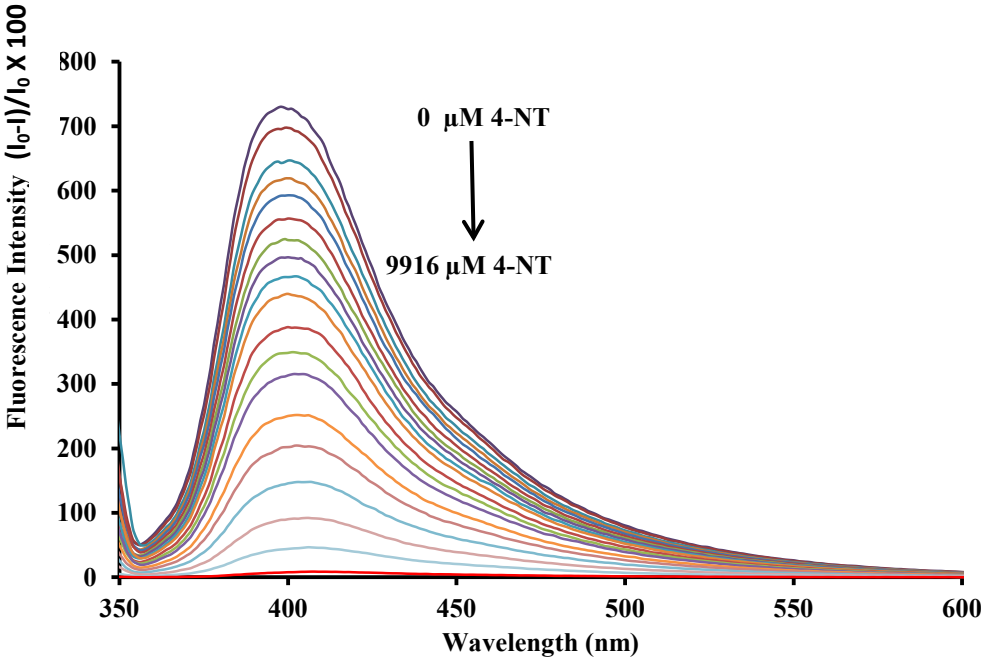


Figure S2. Change in emission spectrum of complex **3** (0.1µM) on addition of 4-nitrotoluene (9916µM) in (THF:HEPES), 9.5:0.5 (*v/v*).

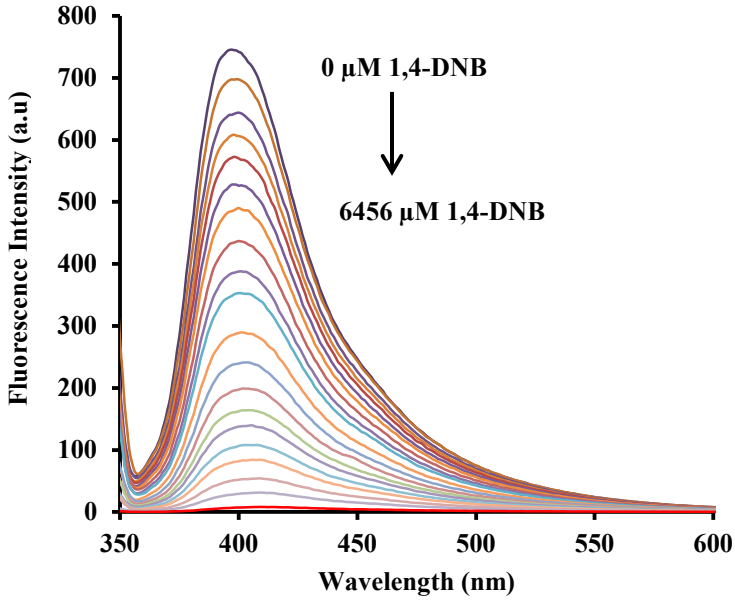


Figure S3. Change in emission spectrum of complex **3** (0.1µM) on addition of 1,4-dinitrobenzene (6456µM) in (THF:HEPES), 9.5:0.5 (*v/v*).

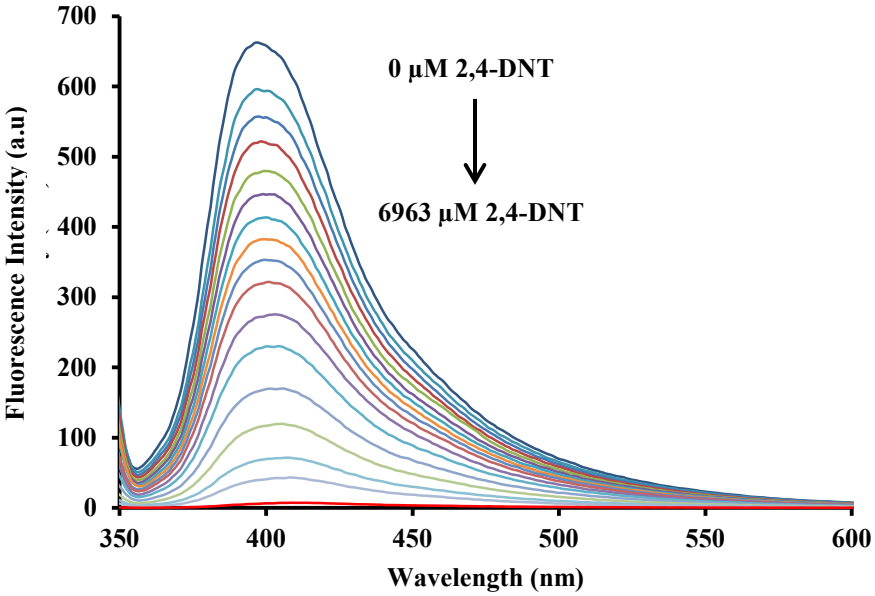


Figure S4. Change in emission spectrum ofcomplex **3** (0.1µM) on addition of2,4-dinitrotoluene (6963µM) in (THF:HEPES), 9.5:0.5 (*v/v*).

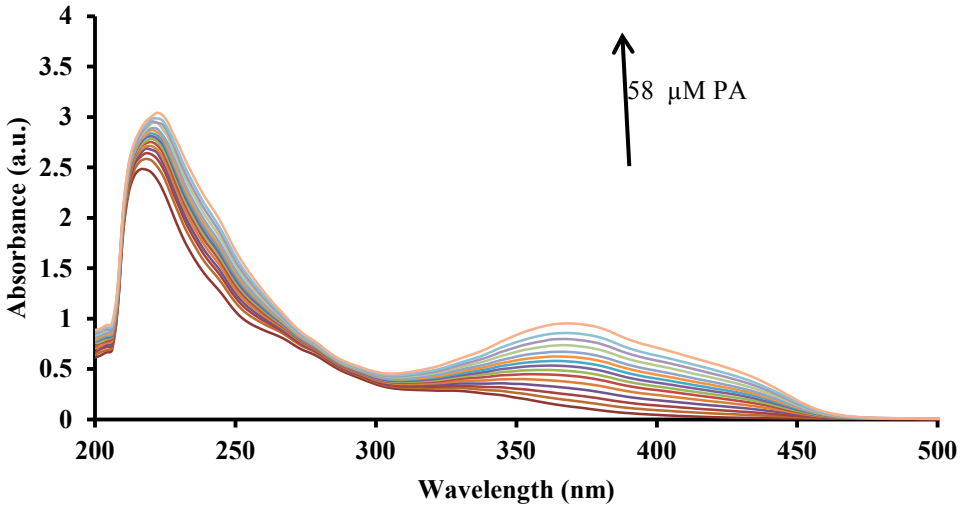


Figure S5. Change in absorption spectra of complex **3** (1µM) with the addition of 58 µM picric acid in a mixed aqueous medium of (THF:HEPES), 9.5:0.5 (*v/v*).

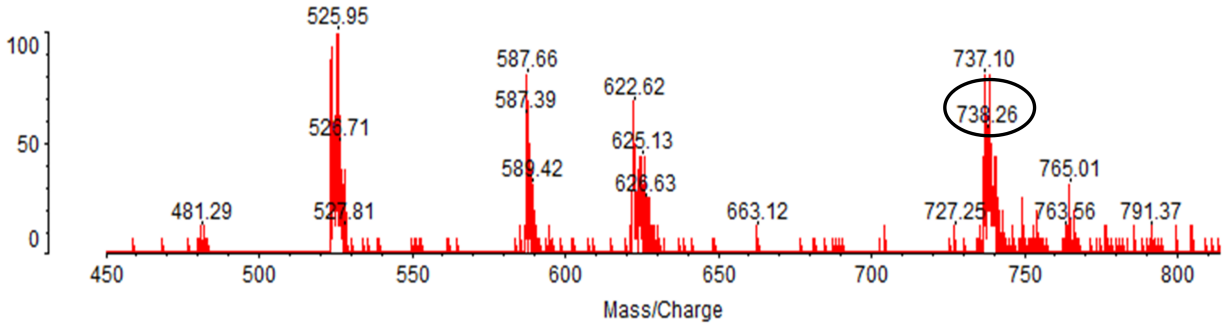
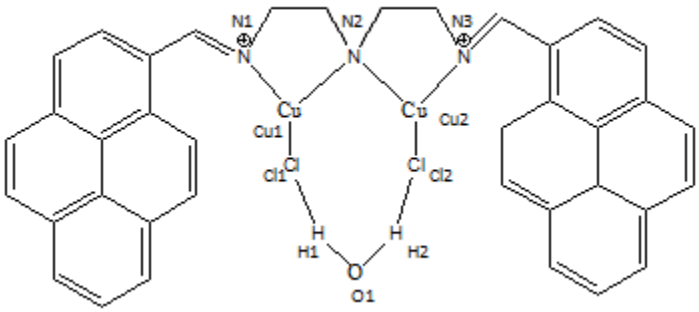


Figure S6.MALDI-TOF-MS spectrum of complex **3**



Hyperchem datafor complex **3.**The Hyperchem optimized structure for complex **3** is presented in Figure 3 in the main text.

Parameterscomplex **3**

N1-Cu1	1.867 A˚
N2-Cu1	1.978 A˚
N2-Cu2	1.978 A˚
N3-Cu2	1.865 A˚
Cu1-Cl1	2.219 A˚
Cu2-Cl2	2.219 A˚
H1-O1	0.971 A˚
H2-O1	0.971 A˚

NOTE: Using the HyperChem 10.0 professional; choose AMBER in Molecular Mechanics; run thegeometry optimization with Polak-Ribiere (conjugate gradient) algorithm.