

## **Iron-Based 1,10-Phenanthroline As ligands For Sensing Of Nitro Explosives**

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### **Abstract**

Here we report the sensing properties of the aqueous solution of Iron 1,10 phenanthroline(ferroin) 1 for simultaneous detection of nitroaromatic compounds by using UV-vis spectroscopy. We present the selective sensing of multi hazardous explosive compounds in water using a synthetic single probe. The probe is a bidentate ligand having phen ring as signaling and interacting moiety, respectively. The sensor showed different responses toward nitroaromatic compounds just by varying the concentration of detection. In water, the probe shows selective detection of PA. Due to the absence of the particular interaction of other nitroaromatics, the proposed probe is highly selective for PA detection with a low detection limit.

**Keywords:** UV-Visible, 1,10-Phenanthroline, Nitroaromatic, Explosive.

### **1. Introduction**

As powerful explosive compounds, TNT has elevated worldwide worries about public safety and can have severe effects on human health and the surroundings. For the safety of the native nation and the protection of the environment, the recognition of nitroaromatic explosives (NAEs) is of supreme importance. (Maiti et al., 2016) (Smith et al., 1999) NAEs are broadly used for the preparation of landmines, military operations, and criminal activities. These NAEs can spoil the environment by contamination of water resources as well as soil at

toxic levels, this can lead to hazardous effects on living organisms (Idros et al., 2017; Abubaker et al., 2018). Nitroaromatic compounds (NACs) are widely used as explosives (Acharyya & Mukherjee, 2014) (Sun et al., 2016)<sup>1</sup>. Surprisingly, picric acid (PA), being an important component of NACs family but also a solid irritant and allergen, (Bhalla et al., 2012) has been underestimated. PA is widely used in rocket fuels (Xu et al., 2011), glass, matches (Shanmugaraju & Mukherjee, 2015), leather industries, military explosives (Karthi et al., 2012). They are directly or indirectly released into the environment leading to the polluted soil, (Singh, 2007) water and ecosystems (Chakravarty et al., 2015) and causes numerous deadly diseases such as nausea (Zhu et al., 2013), skin irritation, abnormalities in liver and respiratory organs, etc.. Hence, sincere efforts need to be made for their rapid, sensitive, and selective detection. 1,10-phenanthroline behaves as an ideal candidate for recognition for cation/anion, amino acid, and DNA, RNA. (Alyapyshev et al., 2016) (Sie et al., 2018)

## **2. Materials and Instrumentations**

All the used chemicals and solvents are commercially available. Ferroin was purchased from Sigma-Aldrich. Chemicals were used without any further purification.

### **2.1. UV-Visible experiments-**

In a typical procedure, a dispersed aqueous solution of **1** (0.5 mM) was prepared. Further, a 3 mL aliquot of this aqueous solution was employed in a 1 cm quartz cuvette, and the absorbance response was recorded in the range of 200–800 nm. The Absorbance experiments were conducted after the periodical addition of freshly prepared nitroaromatics.

## **3. Results and Discussion**

### **3.1. Interaction of **1** with PA**

To examine the selectivity of **1**, the absorption spectra were recorded by the addition of analytes such as 3-NT (Nitrotoluen), 4-NT, 2,4-DNT (Dinitrotoluene), NB (Nitrobenzene), Cl-NB (Nitrochlorobenzene), and 2,4-DNB (Dinitrobenzen), but significant hypochromic shift was detected (Figure 1. (a)). In water, the UV-vis spectra showed red-shift upon addition of

PA(Picric Acid) and color change observed from pink to violet. The addition of other compounds did not show any changes in the UV-vis spectra of 1. Most nucleophilic position present in phen ring which attracts electron deficiency moiety. Such observations demonstrate that 1 senses more electronic-deficient analytes effortlessly. In conclusion, it was observed that 1 would be a selective sensor of nitroaromatics.(Rajak et al., 2019) PA is the most electronic deficient compound which showed a significant affinity towards probe 1.

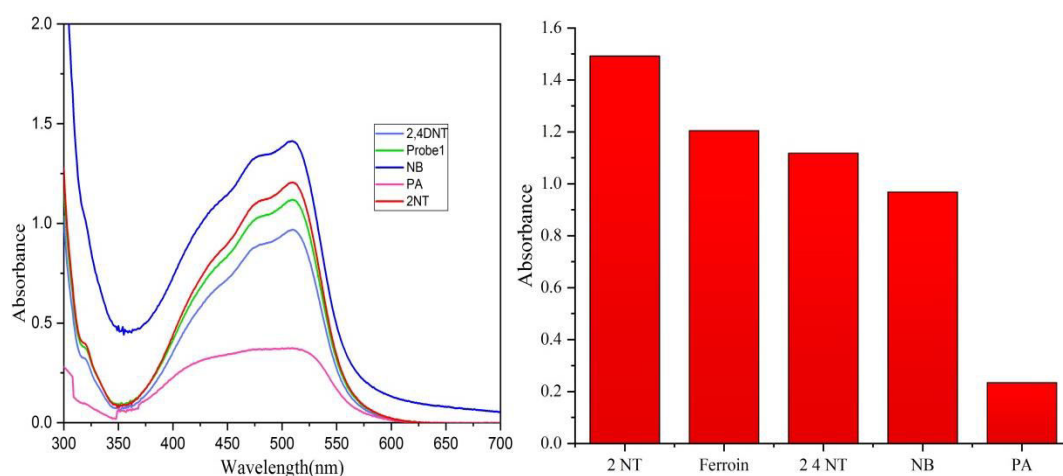


Fig. 1(a)UV-visible absorption spectra of probe 1 in the absence and presence of NACs in water (b) Plot of normalized absorbance of 1 (at 511 nm) upon addition of various NACs.

For the detection of PA present in an aqueous medium, a coordination complex formation method has been tried and resultant color changes have been noticed. Several concentrations (0–160  $\mu\text{M}$ ) of PA solutions were used for the purpose of complex formation. In each case (above 40  $\mu\text{M}$ ), we found a new peak at around 645 nm in addition to the peak of the probe 1. More interestingly, with the increase of concentration of PA solution, the absorbance of 511 nm peak decreased and that of 645 nm peak increased gradually (Fig. 2a). This phenomenon suggested that with the increase of the concentration of PA, complex formation enhanced with 1 might be through the H bonding.

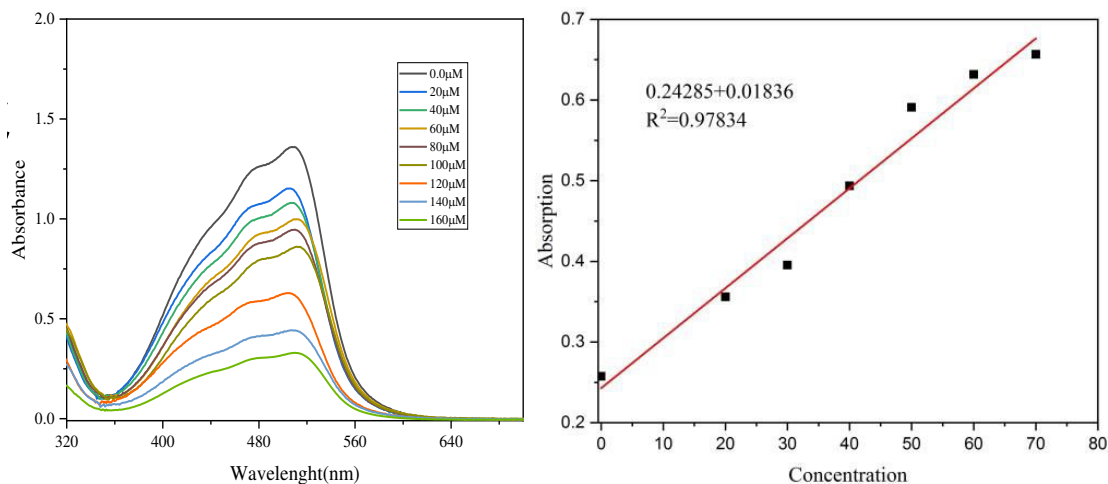


Fig.2-(a)UV–Vis spectra ofprobe 1 at varying concentrations of PA (b) Calibration curves between absorption ratios versus concentration of PA.

The change of the UV–Visible absorbance ratios (Ex645/511) was found to be linear with the concentration of PA. The calibration curve obtained from this ratio of the absorption coefficients of these two peaks (Ex645/511) versus concentration of PA enables one to estimate quantitatively the amount of PA present in water in  $\mu\text{M}$  levels (Fig. 2b). The formation of the complex is proved by the color change (detectable by the human eye) and the appearance of a peak at around 645 nm.(Frederix et al., 2003)

#### 4. Conclusion

Here, we have reported the utilization of commercial bidentate ligand Iron 1,10 phenanthroline as a sensor for the detection of hazardous explosive(PA) in water. The interaction between probe 1 and PA was proved by a color change from pink to violet. The probe is capable of showing the detection of all aromatic with the detection limit in the ppm range. In the probe showed a specific detection of PA with UV–Visible spectroscopy. Thus, using a single probe, PA can be selectively detected at the ppm level in the water. The probe should, therefore, be useful for many practical applications toward the detection of water pollution by these hazardous aromatic compounds. We believe that our conclusion will offer a substitute potential path to identify the nitroaromatic based organic compounds at traces level (ppm) and will motivate the researcher to understand the outcome from a theoretical basis.

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