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Betti base and its modified phthalonitrile derivative for the turn on fluorimetric detection of Hg^{2+} and Cr^{3+} ions

G.S. Amitha[a], Vijisha K. Rajan[b], B. Amritha[a], K. Muraleedharan[b], Suni Vasudevan[a,*]

[a] Dept. of Chemistry, National Institute of Technology Calicut, Calicut, 673601, Kerala, India
[b] Dept. of Chemistry, University of Calicut, Calicut, 673635, Kerala, India

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ABSTRACT

The Betti Base Phenyl-(2-pyridinylamino)-methyl-2-naphthalenol (BB) derived by the multicomponent Mannich aminoalkylations reaction from 2-naphthol, 2-aminopyridine and benzaldehyde. The modified phthalonitrile 4-((1-(phenyl(pyridin-2-ylamino)methyl)naphthalen-2-yl)oxy)phthalonitrile BBPN was obtained by aromatic nucleophilic coupling reaction of 4-nitrophthalonitrile with BB. The compounds were successfully characterized by common spectroscopic and single crystal XRD techniques. The compounds BB and BBPN was exhibited a selective and sensitive fluorescence detection tendency towards mercuric Hg^{2+} and chromium Cr^{3+} ions respectively by the fluorescence turn on processes. Job's plot method is employed to obtain idea about the stoichiometric interaction of metal ions with fluorescent probes. Theoretical calculation was done by Density Functional Theory DFT-B3YLP in order to get atomistic insights into the coordination geometry of Hg^{2+} and Cr^{3+} with BB and BBPN respectively. The limit of detection (LOD) of Hg^{2+} with BB and Cr^{3+} with BBPN was estimated respectively as 9.7×10^{-7} mol/L and 7.03×10^{-6} mol/L. The fluorescence enhancement of both compounds were induced by the inhibition of Photoinduced Electron Transfer (PET) process in which electron transfer happens from amino group to the fluorophore naphthol unit. The PET process was blocked upon binding of the sensors BB and BBPN with Hg^{2+} and Cr^{3+} respectively.

1. Introduction

The rational design and development of simple organic molecule based chemo sensors for the selective and sensitive detection of metal ions have gained considerable attention in recent days [1,2]. Previously a number of analytical methods have been adopted for the accurate and precise detection of metal ions including inductively-coupled plasma mass spectrometry (ICPMS) [3], chromatography coupled with mass spectrometry [4], atomic absorption spectroscopy (AAS) [5], atomic emission spectroscopy (AES) [6], X-ray fluorescence spectroscopy (XRF) [7], electrochemical techniques [8] etc. Nevertheless these analytical methods provide quantitative results; most of them require sophisticated instrumentation, time consuming sample pretreatment methods and are not applicable for direct analysis. As a consequence, significant attention has been devoted to develop simple organic molecules with remarkable optical responses such as colorimetric or/and fluorimetric towards various analyte. Therefore, researchers are focusing to design and synthesize organic molecules having specific metal ion recognition property with signaling mechanism. The distinct advantages of fluorescence-based chemo sensors include high sensitivity, specificity, low cost, facile mode of operation, and ability to provide real-time monitoring [9,10].A large number of fluorescent chemosensors have been reported to date, pertaining to the signaling mechanisms of photoinduced electron transfer (PET) [11], intramolecular charge transfer (ICT) [12], excited-state intermolecular proton transfer (ESIPT) [13], metal-ligand charge transfer (MLCT) [14], excimer/exciplex formation [15,16], fluorescence resonance energy transfer (FRET) [17] etc. Among the all above mentioned detection mechanism, Photoinduced electron transfer (PET) has been widely applied in the design of fluorescence sensors for protons and metal ions [18]. A PET fluorescent probe usually consists of two structural units: the receptor unit and the fluorophore unit, the receptor unit is used for specifically recognizing the target ion, which usually contains N, O and S atoms as chelator for ions, and the fluorophore unit is used for translating the host-guest recognition into fluorescence signal, which often contain naphthalimide, pyrene, BODIPY xanthene units, such as fluorescein, rhodamine, coumarins [19–24] etc. to provide a wide emission with considerable photophysical quantum yield. Generally, PET takes place from a lone pair of the coordinating atoms such as N, O, S, and P in the receptor to the HOMO of the excited fluorophore [25]. The presence of

* Corresponding author.
E-mail address: suniv@nitc.ac.in (S. Vasudevan).

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Conflict of interest

The authors declare no conflict of interest.

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Appendix A. Supplementary data

Supplementary material related to this article can be found, in the online version, at doi:https://doi.org/10.1016/j.jphotochem.2019.111904.

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