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Research Title: Synthesis and quantum chemical calculation of a highly sensitive and selective fluorescent chemosensor for detection of heavy metal ions

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ABSTRACT

Molecular structure and synthesis of fluorescent chemosensor based on dithieno pyrrole derivative as fluorophore, cyanoacetic, amide and amine moieties as ionophore were studied for detection of heavy metal ions. Electron contributions in the frontier molecular orbital and optical properties were conducted in the absence and the presence of metal ions. The fluorescence spectrum was measured the binding mode of metal/PY1A complex by various metal cations (such as Cd^{2+} , Fe^{2+} , Co^{2+} , Cu^{2+} , Hg^{2+} , Ni^{2+} , Pb^{2+} , Zn^{2+}) and metal concentrations. Comparison of the optical spectrum of complexes in the absence and the presence of buffer indicate that the absorption/emission intensity decreased when the buffer was added. The buffer concentrations (5%, 10%, 15% and 20% v/v) were examined. The results found that increase the proportion of the buffer affect to intensity by the decreased emission intensity with the appropriate concentration of this complexes is 10-15%

Keywords : Quantum chemical calculation, fluorescent chemosensor, pyrrole derivative