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A NOVEL CHEMOSENSOR ACTING AS A FLUORESCENT "OFF-ON" ZN²⁺ SENSOR: EXPERIMENTAL, LOGIC GATE BEHAVIOR AND TD-DFT CALCULATIONS

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There is a huge scope for the exploration of the role of zinc in biological systems. Therefore, it is highly desired to develop a sensitive method for its detection. Unlike other metal ions such as Mn²⁺, Fe²⁺, or Cu²⁺, the Zn²⁺ in biological systems cannot be detected by spectroscopic methods, thus the fluorescence stands out as a method of choice. The Hqpzc, N-(quinoline-8-yl)pyrazine-2-carboxamide, as a small fluorogenic molecule with a selective "Off-On" switching behavior for detection of Zn²⁺ and a colorimetric sensor for Cu²⁺, comprises of quinoline as the fluorophore and pyrazine-2-carboxamide as the chelating group. This chemosensor exhibits a remarkable fluorescence response with a detection limit of 1.11×10^{-6} M when investigated in acetonitrile and the fluorescence intensity enhances significantly upon addition of one equivalent of Zn²⁺. The selectivity of Hqpzc for Zn²⁺ is based on the chelation-enhanced fluorescence (CHEF) mechanism. The binding mode of the Hqpzc with Zn²⁺ was investigated through Job's plot experiment, the fluorescence and UV-vis titration, ESI-MS, and density functional theory calculations. These results revealed that the binding stoichiometric ratio between Hqpzc and Zn²⁺ in acetonitrile is 1:1. The limit of detection (LOD) for Cu²⁺ is 1.48×10^{-5} M in acetonitrile solvent and the association constant (K_a) for Hqpzc-Zn²⁺ and Hqpzc-Cu²⁺ complexes are 3.837×10^4 and

7.352×10^7 M⁻¹, respectively. Other interfering ions such as Na⁺, K⁺, Ca²⁺, Mg²⁺, Fe²⁺, Co²⁺, Ni²⁺, Cu²⁺, Cd²⁺, Hg²⁺, Mn²⁺, Cr³⁺ and Al³⁺, show either no or slight change in the fluorescence intensity of Hqpzc in the presence of Zn²⁺. Notably, in the presence of Zn²⁺, the Hqpzc fluorescence exhibits reversibility with SCN⁻, and the fluorescent signals of Hqpzc are utilized to construct an INHIBIT type logic gate at the molecular level. Theoretical calculations, carried out with TD-DFT method, support the experimental observations.

Biography

Marzieh Sohrabi is a PhD student in Inorganic Chemistry, Isfahan University of Technology, Isfahan, Iran. Bsc. Azad University of Shahr-e-Rey, Tehran, Iran, 2003; MSc. Azad University of Shahr-e-Rey, Tehran, Iran, 2008. Research interest: Synthesis and characterization of emissive ligands and their metal complexes with their application as sensors for detection of biologically important ions such as Co²⁺, Cu²⁺, Zn²⁺. Construction of molecular probes for application in live cell imaging. Construction of molecular logic gates from chemical light switches based on emission properties of small molecules. Synthesis and characterization of emissive organometallic complexes and their application in biology as anticancer drugs, and computational chemistry.

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