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Sabeel M. Basheer, M. Muralisankar, T.V. Anjana, K.N. Aneesrahman, Anandaram Sreekanth

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Multi-ion Detection and Molecular Switching Behaviour of Reversible Dual Fluorescent Sensor

Sabeel M. Basheer, M. Muralisankar, T.V. Anjana, K.N. Aneesrahman and Anandaram Sreekanth*

Department of Chemistry, National Institute of Technology, Tiruchirappalli - 620 015, India.

*Corresponding Author: E-mail address: sreekanth@nitt.edu; Tel: +91 431 2503642

Abstract

The selective chemosensing behaviour of imidazole bisthiocarbohydrazone (IBTC) towards F^- and Cu^{2+} are studied via colorimetric, UV-Visible, fluorescence spectra studies, and binding constants were calculated. The ^1H NMR titration study strongly support that the deprotonation of IBTC followed by the hydrogen bond formation *via* N1–H1 and N2–H2 protons with fluoride ion. The fluorescence inactive IBTC-Cu complex became fluorescence active in the presence of perchlorate (ClO_4^-) ion. The selective detection of perchlorate ion was also explained. The F^- sensing mechanism of IBTC has been investigated by Density Functional Theory (DFT) and Time-Dependent Density Functional Theory (TDDFT) methods. The theoretical outcomes well reproduce the experimental results. And it concluded the N−H protons, nearby the imine group was first captured by the added F^- ion and then deprotonation happened followed by the formation of hydrogen bond. The IBTC found good reversibility character with the alternative addition of Ca^{2+} and F^-. The multi ion detection of IBTC was used to construct the NOR, OR and INHIBITION molecular logic gates.

Keywords: Chemosensor; TDDFT; Molecular logic gate; Molecular switches; Sensing mechanism.