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

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### Abstract

The selective chemosensing behaviour of imidazole bithiocarbohydrazone (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.

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