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Title:	Cascade detection of fluoride and bisulphate ions by newly developed hydrazine functionalised Schiff bases
Authors:	Joshi, Mayank (/jspui/browse?type=author&value=Joshi%2C+Mayank) Choudhury, Angshuman Roy (/jspui/browse?type=author&value=Choudhury%2C+Angshuman+Roy)
Keywords:	Fluoride and bisulphate sensing Green-chemical synthesis Naked eye colour change Schiff base Spectrophotometry TD-DFT study X-ray structure
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Abstract:	Two hydrazine functionalized Schiff bases have been synthesized through the reaction between hydrazine and o-vanillin/salicylaldehyde compounds employing a green-chemical approach and characterized spectroscopically including XRD study. Crystal structure analysis reveals that both the chemosensors, N,N'-bis(o-vanilidine)hydrazine (P17) and N,N'-bis(salicylidene)hydrazine, (HARB) crystallize in monoclinic system with P21/n space group and exist in the locked forms through intramolecular H-bonding (~1.90 Å) between phenolic-OH and N atom of hydrazine. The chemosensors display excellent selectivity towards fluoride followed by bisulphate ions, over other potential competitor anions in acetonitrile. Binding stoichiometry of the individual chemosensor with F ⁻ is confirmed to be 1:1 and assessed with absorption study and ¹ H NMR analysis. Systematic DFT analysis reveals that the contribution of hydroxyl oxygen atoms to the HOMO increases sharply from the chemosensor to chemosensor-F ⁻ adduct (17% to 28%) leading to deprotonation of one hydroxyl group and consequently involvement in conjugation impeding the C=N isomerisation. Thus, the hydroxyl proton captured by F ⁻ restricts the C=N isomerisation as well as ICT character of both the chemosensors and confirms the cascade sensing mechanism for fluoride and bisulphate ions.
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