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Title: Salen Type Ligand as a Selective and Sensitive Nickel(II) ion Chemosensor: A Combined

Investigation with Experimental and Theoretical Modelling

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Abstract:

A novel tetradentate (N,O)-donor salen type Schiff base was designed, prepared and structurally characterized by different analytical techniques. This Schiff base ligand, (L = 2,2'-((1,2 phenylenebis(methanylylidene))bis(azanylylidene))diphenol) behaved as an effective chemosensor towards Ni(II) ion with specific selectivity. The Schiff base (L) displayed a remarkable ratiometric fluorescence enhancement upon binding with Ni(II) ion in acetonitrile (ACN) medium. The L-Ni(II) solution was distinguished indisputably with the naked eye colour change and the crystal was found to be red colour. L selectively detected Ni(II) ion in presence of  $other\ competitive\ cations\ like\ Mn(II),\ Fe(II),Co(II),\ Cu(II),\ Zn(II),\ Cd(II)\ and\ Hg(II)\ ions.\ This\ simple\ Simp$ but novel Schiff base might be used as a potential pH independent colorimetric and naked-eye chemosensor for Ni(II) ion. Most significantly, L exhibited geometry preferred selectivity towards Ni(II) ion and formed highly stable square planar Ni(II)-Schiff base complex. Single crystal X-ray diffraction study further authenticated that the nickel complex crystallized in orthorhombic system with P212121 space group in solid state. Density functional theory (DFT) calculations attested the experimental results very well. This sensing method could be applied in a wider concentration range and might be used as an alternative qualitative and quantitative test for the detection of Ni(II) ion in analytical chemistry.

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