Novel Modified Asymmetrical Salan Ligands for Optical Detection of Cu^{2+}, Fe^{3+} Ions in Aqueous Media

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Abstract

Detecting metal ions in water is important in various fields, including agriculture, medicine, biology, and environmental protection. While many accurate methods exist for determining ion concentrations in aqueous media, most are expensive, time-consuming, and require laboratory conditions. Thus, industry seeks low-cost, portable, sufficiently accurate optical sensors for metal ions that can operate under real-world conditions. Schiff bases, imines, salens, and related organic ligands show promise for photochemical sensors of metal ions due to their room-temperature photoluminescence and chelation abilities, as well as their potential for high sensitivity and selectivity.

This work investigated the sensitivity and selectivity of novel asymmetrical salan-type ligands. The proposed ligands were essentially insoluble in alcohols and water. To address this issue, the ligands were protonated using trifluoroacetic acid (TFA).

The selectivity of the ligands was predicted using density functional theory (DFT) calculations. The chemical structures were confirmed using nuclear magnetic resonance (NMR), high-performance liquid chromatography-mass spectrometry (HPLC-MS), and Fourier-transform infrared spectroscopy (FTIR). The optical properties were investigated using photoluminescence (PL), diffuse reflectance, and transmittance spectroscopy.

Sensor testing was performed in a homemade system with a quartz cuvette equipped with a magnetic stirrer and integrated with a fiber optic system for time-resolved photoluminescence (PL) and transmittance (TM) measurements.

The proposed samples exhibited excellent selectivity and high sensitivity in the micro- and submicromolar ranges to Cu^{2+} and Fe^{3+} ions in alcohol and water media with varying pH levels. The interaction of ligand solutions with iron (III) resulted in a noticeable colorimetric reaction. The mechanisms of interaction are proposed.

It is well established that Cu^{2+} and Fe^{3+} ions are pivotal microelements that facilitate plant growth. Consequently, photochemical sensors based on asymmetrical salan ligands hold considerable potential for implementation in the agricultural sector, as well as environmental protection industry.

Acknowledgements

We acknowledge the project 'Novel optical nanocomposite sensors for analysis of micro and macro elements in corn plants', HE-MCSA-RISE-2022, Sens4Corn, grant number 101086364