QUANTUM TECHNOLOGIES, METAMATERIALS, AND THE FUTURE OF CB SENSING

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A Simple Benzothiazole-based Sensor For Cyanide Detection: Applications In Environmental Analysis And Bio-imaging

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Cyanide anion (CN-) is toxic to living organisms and the environment. Nevertheless, it is widely used in the production of pharmaceuticals, herbicides, metallurgy, and the mining of gold. Absorption of CN- through the lungs, gastrointestinal tract, and skin can affect the central nervous system, the respiratory enzymes, and cause hemoglobin poisoning. This can lead to vomiting, convulsions, loss of consciousness, and eventually death. Due to its historical use as a chemical warfare agent, there is also a potential risk of its use in terrorist activities. Thus, designing and synthesizing a robust, selective, and sensitive sensor for CN- is important to detect and quantify environmental and biological samples to ensure public health and safety. Consequently, extensive studies have been conducted to develop methods for its detection and quantification from pollutant sources. In recent years, numerous optical chemosensors for CNhave been developed. Herein, a simple benzothiazole-based (SU-1) CN- sensor has been designed and synthesized via a condensation reaction between 3-Ethyl-2-methylbenzothiazolelium iodide and 2-Hydroxy-1-naphthaldehyde. SU-1's structure was confirmed using 1H-NMR, 13C-NMR, HRMS, and single-crystal X-ray diffraction studies. Optical property examinations revealed that SU -1 displayed a colorimetric and fluorometric response in a DMSO/H2O matrix, changing color from red to colorless, visible to the naked eye, accompanied by a ~99 nm red shift in the absorption spectra upon CN- addition. This shift, due to the nucleophilic attack on the double bond of the benzothiazolium ring, disrupts π -conjugation, thereby blocking intramolecular charge transfer within SU-1. However, competitive anions (CH3COO-, N3-, HSO4-, S-2, ClO3-, NO2-, CO3-, F-, Cl-, Br-) showed negligible interference in the detection of CN-. The job's plot displayed a 1:1 binding stoichiometry ratio between SU-1 and CN- ions. The LOD was calculated to be 0.62 nM, which is far below the WHO's permissible CN- concentration in drinking water (1.9 µM). SU-1 demonstrated practical applications in analyzing environmental water samples and fluorescent imaging of intracellular CN- in live cell lines. Therefore, SU-1 can be a promising, sensitive, and selective chemosensor to monitor CN- in environmental and biological systems. Moreover, it introduces an alternative sensing approach as a chemical and biological defense technique by detecting and determining toxic chemical threats like CN- for effective hazard monitoring and enhancing protective measures for the environment, public health, and safety.

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