ABSTRACT

Fluoride ion detection in aqueous media is crucial for environmental monitoring, healthcare, and industrial applications. Regular monitoring of fluoride levels in drinking water is essential due to its dual impact on human health: insufficient intake harms dental health, while prolonged overexposure poses serious risks. The World Health Organization (WHO) has set a maximum permissible limit of 1.5 mg/L for fluoride in drinking water, necessitating treatment through fluoridation or de-fluoridation to maintain these levels.

Common techniques for fluoride quantification include Ion Selective Electrode (ISE), Ion Chromatography, ICP-MS (Inductively Coupled Plasma Mass Spectrometry), Atomic Absorption Spectroscopy (AAS), and Inductively Coupled Plasma Atomic Emission Spectroscopy (ICP-AES). However, these methods require advanced instrumentation and are not cost-effective for routine monitoring, especially in remote areas. ISE is economical but its accuracy is reduced by the presence of Al(III) ions. Optical methods (colorimetric and fluorometric) offer promising alternatives due to their ease of use and higher sensitivity. The SPADNS-Zirconium colorimetric method, though standard commercial method, is prone to interference from various ions, requiring sample pretreatment.

The thesis aims to develop methodologies for sensing fluoride ions in aqueous media using organic probe molecules with H-bonding recognition unit. Two hypotheses are explored: one based on Brönsted acid-base equilibrium and the other on Pearson’s hard-soft acid-base theory. The research validates that incorporating Ni(II) metal ion enhances the fluoride sensing affinity of organic chemosensors in aqueous medium and found the enhancement in colorimetric sensitivity up to 0.3 ppm with thiourea based tweezers. Additionally, it explores the use of common dyes like perylene tetracarboxylate and fluorescein as optical chemosensors. The potassium salt of these dyes, combined with Al^{3+} ion, serves as effective colorimetric and fluorometric sensors, achieving sensitivity up to 1 ppb in 100% water. These methods also mitigate interference from common ions. The effectiveness of the methodology was validated using both optical and electrochemical techniques on real-life samples.

Overall, the thesis advances practical and effective methodologies for fluoride ion detection in aqueous media, with potential applications in routine monitoring in fluoride-affected areas.