Multichromophoric open-cage silsesquioxanes as quantitative optical anion sensors

Motivation:

Developing sensors for trace-level detection of harmful environmental pollutants has been an important and intensively explored research area in recent years. Fluoride anion is still a valuable target for recognition and sensing because of its duplicitous nature. On the one hand, it is a valuable chemical for many industrial applications, organic synthesis, biological and medical processes, and the human diet, but on the other hand, it is considered a dangerous pollutant. Overexposure to F^- can be hazardous to the environment and humans. It causes, e.g. dental fluorosis, weakening of the bones, osteosarcoma and inhibition of neurotransmitter biosynthesis. Fluoride contamination of the environment and ground and surface waters is mainly generated by the leaching of fluoride-rich minerals and industry (that also generates organic waste liquors). The official limit in drinking water set by WHO (World Health Organization) is 1.5 mg L^{-1}. Due to this pollutant's negative impact, it must be monitored and removed. Therefore, it is crucial to design universal, stable, highly sensitive and selective fluoride anion sensors capable of qualitative and quantitative detection both in organic media and water environments. Based on literature reports, it still remains an immense challenge as a few divergent parameters should be compatible. Nevertheless, many contemporary methods suffer from disadvantages, including problematic sample preparation, the necessity of sophisticated equipment, and time-consuming operation. Furthermore, interference by ions containing oxygen, such as AcO^- and $H_2PO_4^-$, is a major problem for many known sensors.

The aim of the research:

This project addresses the problems posed and aims **to develop convenient, tailor-made quantitative optical fluoride anion sensor systems by designing and producing highly compatible, stable and resistant sensors, showing a quick response, selectivity, and accuracy, allowing quantification of the analyte and controlled reversible removal of an anion for application in organic solvents and aqueous media.** The project's premise is that the proposed silsesquioxanes are intended to facilitate more accessible encapsulation of ions in the cavity, and the response of the system tested by optical spectroscopy will be quantitatively dependent on the level of the analyte. The original strategy of this proposal concentrates not only on anion sensing and quantification but also considers many factors influencing, e.g. stability and enhancing selectivity and sensitivity of sensors by utilizing tailor-made host molecules with easier access to cavity and tunable linkers and chromophores, which is relevant for science, technology and development for sensing applications.

Expected impact of the research project:

The proposed research will allow for obtaining a library of host molecules with potentially interesting properties. An element of novelty in this project will be the use of incompletely condensed silsesquioxanes (IC-POSS) in the design of such sensors, which, due to their structure, will be able to more accessible and faster encapsulation of ions. These proposed chromophore-IC-POSS systems should lead to the discovery of extremely sensitive and selective quantitative optical fluoride anion sensors. Due to their unique structure and tailor-made substituents, it will be possible to apply them in organic media and aqueous solutions, which still remain a challenging area in the scientific world. Different topologies of proposed compounds may lead to the varied ability to anion recognition as a guest in silsesquioxane host cavity, which could revolutionize the field of fluoride ion detection. Furthermore, the proposed research also covers the aspect of greener and more sustainable chemistry regarding WHO environmental standards. Developing fast and more accessible sensors for harmful agents could have long-term effects. The proposed research could help on many fronts in the future to protect endangered species and natural areas, ensure safe drinking and bathing water, improve chemical waste management, and reduce the impact of harmful chemicals.