Chapter 1

Introduction

1.1. Chemistry of Host–Guest Interactions

In the realm of supramolecular chemistry, host-guest interactions characterize complexes formed by two or more molecules or ions united in distinct structural arrangements through forces other than full covalent bonds. This facet of chemistry revolves around molecular recognition and interactions facilitated by non-covalent bonding, which is crucial for maintaining the 3D structure of large molecules like proteins. Non-covalent interactions, categorized broadly into electrostatic or dispersive contributions, include ionic bonding, hydrogen bonds, van der Waals forces (Keesom force, dipole-dipole, Debye, dipole-induced dipole), and hydrophobic interactions. Key principles in supramolecular chemistry encompass molecular self-assembly, folding, recognition, host-guest chemistry, mechanically interlocked molecular architectures, and dynamic covalent chemistry. The understanding of non-covalent interactions is pivotal for unraveling biological processes relying on these forces. Biological systems often inspire supramolecular research, with the "host" being the larger molecule and the "guest" the smaller one, akin to enzyme and substrate in biological terms.

To design synthetic systems with specific functions, comprehending the thermodynamics of host-guest binding is crucial. Chemists focus on energy exchange in various binding interactions, employing techniques such as NMR spectroscopy, UV/visible spectroscopy, and isothermal titration calorimetry. Quantitative analysis of binding constants furnishes valuable thermodynamic information. The thermodynamic benefits of host-guest chemistry stem from the lower overall Gibbs free energy resulting from interactions between host and guest molecules. Exhaustive efforts are directed at measuring the energy and thermodynamic properties of these non-covalent interactions, seeking insights into their combinatorial effects on supramolecular structures. Thermodynamics serves as a vital tool for designing, controlling, and studying supramolecular chemistry, mirroring its importance in warm-blooded biological systems that operate within a narrow temperature range.

1.2. Host-Guest-based Optical Sensors

Host-guest chemistry has emerged as a promising avenue in the development of optical sensors, offering versatile and sensitive platforms for detecting various target analytes. These sensors rely on the specific interactions between a host molecule and a

guest molecule, resulting in measurable changes in optical properties. The host molecule acts as a receptor, selectively binding to the target analyte, leading to detectable signals such as changes in absorption, fluorescence, or refractive index.

One notable example of host-guest-based optical sensors involves the use of cyclodextrins as hosts. Cyclodextrins are cyclic oligosaccharides with a hydrophobic interior and a hydrophilic exterior, providing an ideal cavity for guest molecule encapsulation. Functionalizing cyclodextrins with appropriate recognition moieties enhances their selectivity, allowing for the creation of sensors with high sensitivity to specific analytes. In a study by Li et al. (2020), a host-guest-based optical sensor utilizing cucurbit [8] uril as the host molecule demonstrated remarkable sensitivity and selectivity towards paraquat, a toxic herbicide. The binding of paraquat with CB[1] induced a pronounced change in the sensor's fluorescence emission, enabling the detection of paraquat at low concentrations. Another significant advancement in host-guest-based optical sensors involves the incorporation of responsive polymers. In a work by Wang et al. (2019), a sensor based on a host-guest interaction between β-cyclodextrin and azobenzene-functionalized polymers exhibited reversible changes in UV-visible absorption upon exposure to specific ions[2]. Pictorial representations showing the various optical-based host-guest decorated systems are illustrated in **Figure 1.1**. The selectivity of the sensor was tailored by modifying the azobenzene groups, providing a versatile platform for ion detection. These examples highlight the potential of host-guest-based optical sensors in diverse applications, including environmental monitoring, biomedical diagnostics, and industrial processes. Continued research in this field holds promise for the development of highly selective and sensitive sensors for a wide range of analytes[3,4]

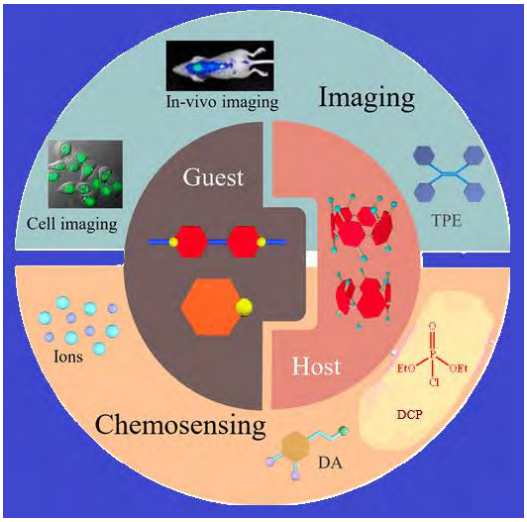

Figure-1.1: Pictorial representations showing the various optical-based host-guest decorated systems.

1.3. Colorimetric Chemosensor

Colorimetric chemosensors, rooted in host-guest interactions, have emerged as powerful tools in the field of chemical sensing. These platforms leverage the selective binding capabilities of host molecules with specific guest analytes, resulting in discernible color changes. The recent advancement in colorimetric chemosensors, emphasizes their applications in detecting various target molecules. The encompasses design strategies, sensing mechanisms, and potential real-world applications, highlighting the versatility and specificity offered by host-guest interactions in imparting selectivity to these sensing platforms. The integration of different host molecules, such as cyclodextrins, cucurbiturils, and calixarenes, with various guest analytes, showcases the broad scope and adaptability of colorimetric chemosensors. The importance of these sensors in fields like environmental monitoring, medical diagnostics, and food safety is also discussed. Additionally, insights are drawn from recent studies employing advanced analytical techniques and computational methods to enhance the understanding and optimization of these host-guest interactions. This review aims to provide a comprehensive overview of the current state-of-the-art in colorimetric chemosensors, laying the foundation for future developments in the field[5–7].

In the context of host-guest interactions within chemosensors, the D-π-A system typically involves the strategic incorporation of electron-donating and electron-withdrawing groups in specific positions. This configuration sets the stage for dynamic changes when a metal ion interacts with the sensor. Specifically, when a metal ion binds to the electron-donating group, the ability of this group to donate electrons diminishes, transforming the D-π-A system into an A-π-A system characterized by reduced conjugation. Consequently, this alteration induces a blue shift in the absorption band and enhances the likelihood of ligand-metal charge transfer (LMCT)[8–10].

Conversely, in scenarios where a metal ion binds to the electron-withdrawing group, it reinforces the D-π-A system, promoting the formation of metal-ligand charge transfer (MLCT). This modification results in the excited state being more stable than the ground state, manifesting as a red shift in the absorption spectra[11]. **Figure 1.2** Visual represents this phenomenon, highlighting the distinct shifts and charge transfer

processes associated with host-guest interactions in the context of the D-π-A system within chemosensors.

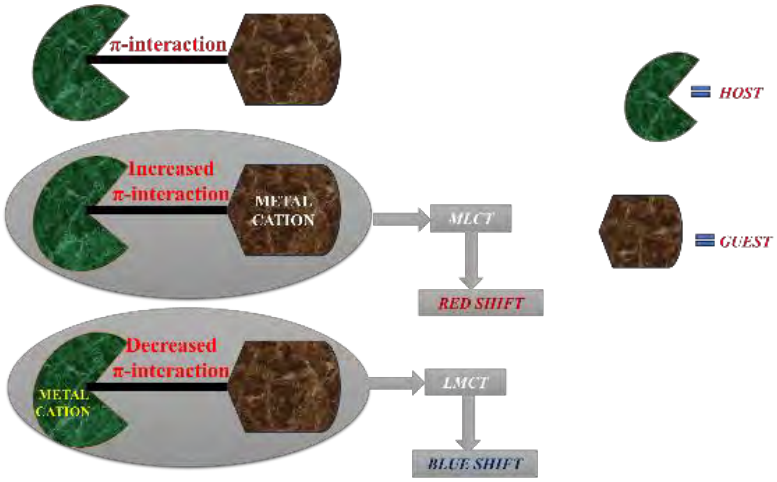

Figure-1.2: Pictorial presentation of the effect of binding of cation on the D-π-A system with spectral shifting in the absorption spectrum.

1.4. Fluorescent Chemosensor Based on Host-Guest Interactions

Fluorescent chemosensors act as adaptable guests within the host-guest system, displaying a remarkable capability to alter their fluorescence attributes when encountering distinct molecular recognition events or alterations in their ambient surroundings[12]. Their sensitivity lies in measuring variations in photophysical traits—fluorescence intensity, emission spectra, and lifetime decay—triggered by interactions with specific analytes like cations, anions, or neutral molecules, inducing fluorescent modulation. Within this intricate host-guest arrangement, the fluorescence method emerges as a powerful tool, offering high sensitivity, selectivity, cost-effectiveness, and adaptability for detecting analytes at incredibly low concentrations, often at sub-micromolar levels. Consequently, these fluorescent chemosensors play a pivotal role across diverse domains, including environmental monitoring, process control, food analysis, and bio-medicinal science[13–15]. Nevertheless, for these chemosensors to effectively function across varied applications, they must meet specific criteria [16]. Firstly, they must exhibit selective binding to the intended analyte amid the presence of other coexisting analytes—a crucial aspect within the host-guest relationship. Secondly, they should maintain intense fluorescence while being photostable, even in the presence of dissolved oxygen. Additionally, their emission wavelength must surpass 500 nm to minimize interference with the autofluorescence exhibited by certain biological samples. Ensuring minimal toxicity stands as another essential requirement. Lastly,

achieving adequate solubility within the desired medium is imperative. Various parameters like solvent characteristics, pH, and ionic strength significantly influence both binding efficiency and selectivity, as well as the photophysical characteristics of the fluorophore within this intricate host-guest network.

1.4.1. Signaling Pathways Associated with Chemosensors

The exploration of new sensing mechanisms within the realm of chemosensors has garnered significant attention, fueled by the quest to design innovative and efficient sensing technologies. This endeavor has given rise to a host-guest system where various conventional signaling mechanisms play a pivotal role. These mechanisms are intricately woven into the tapestry of chemosensor design, facilitating the dynamic interaction between recognition and signal reporting units.

Among the diverse array of established signaling mechanisms, several have emerged as key players in this host-guest system. Photoinduced electron transfer (PET), intramolecular charge transfer (ICT), metal-ligand charge transfer (MLCT), twisted intramolecular charge transfer (TICT), fluorescence resonance energy transfer (FRET), excimer/exciplex formation, aggregation-induced emission (AIE), C=N isomerization, and excited-state intramolecular proton transfer (ESIPT) are some of the noteworthy processes contributing to the rich tapestry of chemosensory responses. In essence, these mechanisms serve as the conduits through which the intricate dance between the host and guest takes place, allowing for the translation of molecular recognition events into discernible signals. Through the lens of the host-guest system, we delve into the nuanced interplay of these signaling mechanisms, each contributing to the fascinating landscape of chemosensor development. The various photophysical processes that are important and aligned with the present thesis work are discussed briefly in the next section.

1.4.2. Photoinduced Electron Transfer (PET)

In the realm of photoinduced electron transfer (PET), the interplay within a host-guest system becomes paramount. This phenomenon, triggered by the interaction of a photoactive substance with light radiation, orchestrates a fundamental electron transfer mechanism, often termed PET. Within this framework, a complex interplay of interactions unfolds within a fluorophore-spacer-receptor assembly.

Here, the fluorophore and receptor engage in a close embrace facilitated by the spacer, forming the crux of the PET mechanism (**Figure 1.3**). This intricate dance of

photon-driven transactions characterizes the essence of PET, which is pivotal in numerous fluorescent sensors designed for analyte recognition. These PET-based sensors manifest in two distinct classifications: turn-on and turn-off sensors. When devoid of an analyte, the PET sensor absorbs energy, prompting an electron shift from the highest occupied molecular orbital (HOMO) of the fluorophore to its lowest unoccupied molecular orbital (LUMO). Simultaneously, the HOMO of the free receptor, if at a higher energy level, facilitates PET, leading to a hindrance in emission transition or fluorescence quenching. However, when an analyte binds to the receptor, a shift occurs in the redox potential of the receptor, elevating its donor properties. Consequently, the relevant HOMO of the receptor lowers in comparison to the fluorophore's HOMO. This alteration prevents PET, subsequently enhancing the fluorescence of the chromophore. Sometimes, the receptor's role in the photophysical process is indirect. If the LUMO of the receptor-analyte complex bridges between the HOMO and LUMO of the fluorophore, a non-radiative pathway emerges via the LUMO of the analyte-bound receptor, causing fluorescence quenching.

In turn-on fluorescent sensors, PET engages the HOMO and LUMO levels of the fluorophore along with the HOMO level of the free receptor before analyte binding. Conversely, turn-off fluorescent sensors involve PET concerning the HOMO and LUMO levels of the fluorophore and the LUMO level of the analyte post-complex formation.

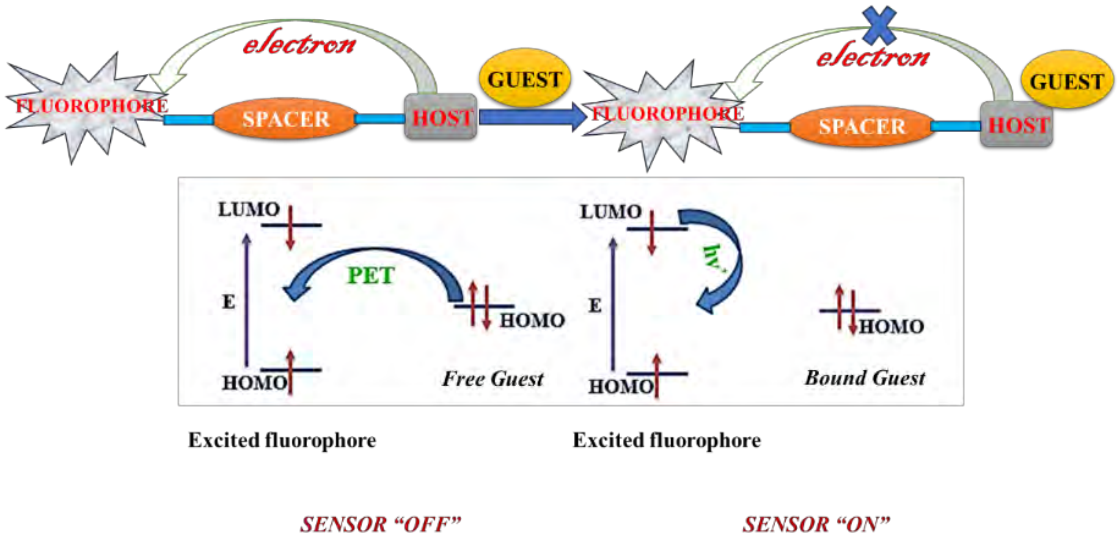

Figure 1.3: Schematic representation of the photoinduced electron transfer (PET) process.

1.4.3. Intramolecular Charge Transfer (ICT)/Photoinduced Charge Transfer (PCT)

As we delve into the diverse realms of host-guest systems, the interplay between electron-donating and electron-withdrawing groups assumes a central role in elucidating the intricacies of molecular dynamics. Within the tapestry of this multifaceted investigation, the orchestrated dance of electrons during intramolecular charge transfer becomes a key protagonist. In environments where electron-donating groups, such as -NH_2, -NMe_2, or -OCH_3, coexist with electron-withdrawing counterparts like >C=O or -CN, the intricate ballet of charge transfer unfolds. This dance, as evidenced by a wealth of spectroscopic contrivances, leads to the manifestation of distinct spectral signatures. The involvement of probing assorted host-guest interactions across various environments, each tailored to explore different target analytes. As these interactions manifest, the spectroscopic contrivances employed serve as discerning eyes, capturing the nuances of ICT. Through this lens, researchers can observe the shifts in dipole moments, alterations in Stoke shifts, and consequential changes in emission spectra, all of which contribute to a comprehensive understanding of the molecular landscape. In the context of different host-guest interactions, the impact of ICT on molecular properties takes center stage. Whether the host-guest system resides in solvents of varying polarities or interfaces with distinct target analytes, the intricate dance of electrons provides a nuanced spectroscopic fingerprint. A schematic illustration of ICT is shown in **Figure 1.4.**

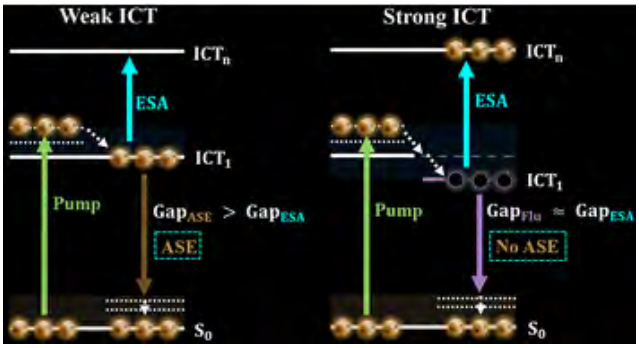

Figure 1.4: Schematic illustration of the ICT process.

1.4.4. Excited-State Intramolecular Proton Transfer (ESIPT)

In the exploration of diverse host-guest interactions prevailing in various environments, the study of excited-state intramolecular proton transfer (ESIPT) emerges as a compelling photophysical phenomenon. This phenomenon holds considerable utility across a spectrum of applications, including but not limited to fluorescent chemosensors, photochromic switching devices, and light-emitting materials[17–19]. The

crux of ESIPT lies in the migration of protons from a proton donor (-OH or -NH_2) to a proton acceptor (carbonyl oxygen or imine nitrogen) through an intramolecular hydrogen bond.

In the context of probing the host-guest interactions by diverse spectroscopic contrivances, the intricacies of ESIPT come to the forefront. Upon excitation, the chromophore undergoes structural and electronic changes as protons traverse from the acidic side to the basic side. As depicted in **Figure 1.5**, the chromophore initially adopts an enol form stabilized by an intramolecular hydrogen bond. Absorption transitions it to the singlet excited state of the enol form with no geometric alterations, followed by a rapid ESIPT process that stabilizes an intermolecular hydrogen bond by the keto form at the singlet excited state.

The fluorescence emission observed for ESIPT chromophores primarily originates from the keto tautomer, given its faster occurrence compared to the fluorescence process. Additionally, the deactivation of the keto form transpires through intersystem crossing (ISC) to the triplet excited state of the keto form. Noteworthy differences in geometry between the keto and enol forms, accentuated by an exocyclic double bond, facilitate a reduction in the energy gap between $S_0 \rightarrow S_1$ of the keto form, resulting in a substantial Stokes shift for ESIPT chromophores. This detailed exploration of ESIPT within diverse host-guest environments exemplifies the richness of molecular interactions elucidated through various spectroscopic methodologies.

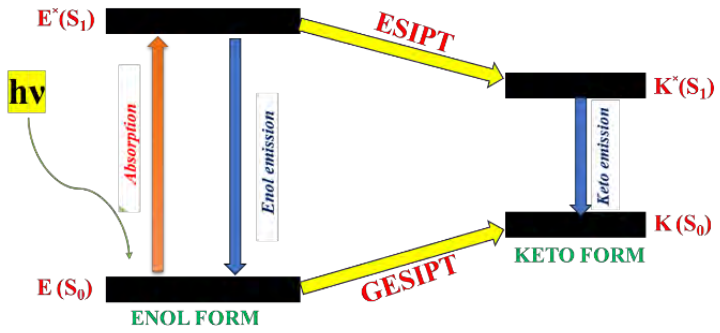

Figure 1.5: The photophysical cycle of the ESIPT process.

1.4.5. Aggregation-Induced Emission (AIE)

Exploring diverse host-guest Interactions across environments for analyte sensing through spectroscopic approaches: the intriguing realm of aggregation-induced emission (AIE) unfolds as a distinctive phenomenon within the landscape of host-guest interactions. Unlike conventional organic luminescent materials, which often encounter limitations in practical applications, particularly in organic light-emitting diodes and

luminescent sensing materials, AIE-based systems present a promising alternative with versatile applications in chemosensors and biosensors.

In the conventional scenario, most organic molecules showcase optimal photoemission efficiency in liquid states compared to their solid counterparts, owing to their inherent planar structural arrangement. However, their fluorescence efficiency takes a hit when aggregated, succumbing to the aggregation-caused quenching (ACQ) effect[20,21]. Innovative strategies come into play to overcome this limitation. Bulky substituents and branched chains are strategically incorporated into fluorophores[22,23], and the protection of chromophores is achieved through cyclic molecular wires utilizing supramolecular interactions.

Interestingly, an additional facet of AIE emerges, where certain organic molecules exhibit subdued emissive behavior in the liquid state due to unhindered intramolecular motions. However, when these molecules aggregate in the solid state, a transformative process known as "Aggregation-induced emission" (AIE) takes center stage, as depicted in **Figure 1.6**. Furthermore, an enhancement of this phenomenon, coined aggregation-induced emission enhancement (AIEE), manifests when luminophores exhibit even greater photoemission enhancement in the solid state than in the liquid state.

The versatility of AIE systems extends to their responsiveness to environmental stimuli, where analytes induce changes in the aggregation of AIE molecules through electrostatic, coordination, hydrophobic interactions, or the influence of polarity and viscosity. This unique attribute has paved the way for the development of a myriad of AIE-fluorescent sensors tailored for the detection of ionic species, gases, and biomolecules. Thus, the exploration of host-guest interactions within AIE frameworks not only offers insights into fundamental molecular behaviors but also holds tremendous potential for advancing the field of analyte sensing.

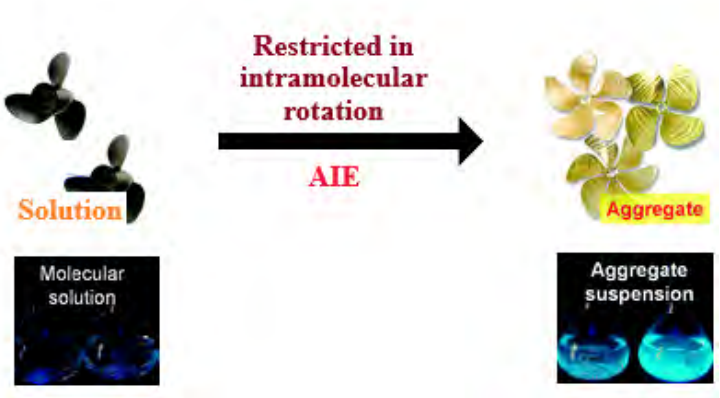

Figure-1.6: Pictorial representations of AIE phenomena.

1.5. Some Curious Sensing Mechanisms

1.5.1. Mechanisms of Action of Metal Ions Sensor

Delving into the intricate realm of host-guest interactions within diverse environments, our focus shifts towards unveiling the nuanced mechanisms underlying metal ions sensing—a crucial facet in analytical chemistry. In the multifaceted landscape of host-guest systems, the design and deployment of various spectroscopic contrivances emerge as powerful tools in elucidating these interactions, offering insights into the detection and quantification of target analytes.

Metal ions, with their distinct electronic configurations, pose unique challenges and opportunities in sensor development. Host molecules, equipped with tailored binding sites, serve as receptors capable of selectively recognizing and accommodating specific metal ions. The mechanism of action unfolds in a series of orchestrated steps within the host-guest framework.

In environments where metal ions abound, the host molecules act as selective chelators, forming stable complexes through coordination bonds. Spectroscopic techniques such as UV-visible absorption, fluorescence, and NMR spectroscopy become important instrumental techniques in tracking these interactions. The binding event induces alterations in the electronic and optical properties of the host molecule, leading to detectable changes in the spectroscopic signals.

For instance, in fluorescence-based sensors, the presence of a metal ion triggers a modulation in the emission intensity or wavelength. This phenomenon can be attributed to the disruption of the host molecule's electronic structure upon complexation. Similarly, UV-visible absorption spectra witness shifts and intensity changes reflective of the intricate interplay between the host and the guest displaying colorimetric changes.

NMR spectroscopy, with its ability to discern subtle changes in molecular conformation, provides an additional layer of understanding. Through chemical shift variations and alterations in peak patterns, the binding kinetics and structural rearrangements during host-guest interactions come into focus. The success of these spectroscopic contrivances lies in their collective ability to unravel the intricacies of host-guest interactions in diverse environments. By tailoring host molecules to exhibit high affinity and selectivity for specific metal ions and leveraging the sensitivity of spectroscopic techniques, we pave the way for the development of efficient and

responsive metal ion sensors. This exploration not only enriches our understanding of molecular recognition but also opens avenues for advancing analytical methodologies in environmental monitoring, medical diagnostics, and beyond.

1.5.2. Mechanisms of Action of Anion Chemosensors

In the captivating realm of diverse host-guest interactions, the mechanism underlying anion sensors unfolds with remarkable intrigue. Anion sensors, pivotal components in probing assorted environments for distinct target analytes, operate through a sophisticated mechanism reliant on specific spectroscopic contrivances.

Primarily designed receptors within the sensor possess an affinity for anions, exhibiting selectivity towards their unique properties. These receptors often entail electron-rich motifs, such as $-NH_2$, $-NMe_2$, or $-OCH_3$, juxtaposed with electron-withdrawing entities like >C=O or -CN. This strategic arrangement sets the stage for an intricate interplay—an intermolecular tango—wherein anions are drawn toward the electron-deficient sites.

Upon encountering an anion, the sensor undergoes a transformative interaction. Anions, commonly fluoride (F^-), chloride (Cl^-), bromide (Br^-), or iodide (I^-), cyanide (CN^-), and phosphate (PO_4^{3-}) engage in hydrogen bonding or electrostatic interactions with the receptor's functional groups. This binding event triggers a cascade of changes within the sensor's structure and electronic environment. Spectroscopic tools, ranging from UV-visible absorption to fluorescence emission, come into play at this juncture. The binding event between the anion and the receptor induces distinct alterations in the sensor's spectroscopic properties. For instance, a shift in absorption or emission wavelengths, changes in intensity, or alterations in fluorescence lifetime manifest as indicative signatures of the anion binding event. Thus, through a harmonious amalgamation of tailored receptors, anion recognition, and spectroscopic methodologies, these sensors stand as versatile tools, probing varied environments and elucidating the presence and behavior of diverse target analytes. Their mechanism of action not only explores host-guest interactions between chromo-fluorogenic hosts with anions but also unlocks a pathway toward understanding and navigating intricate molecular landscapes.

1.5.3. Mechanisms of Action of Chemical Warfare Agents (CWAs) Sensors

In the pursuit of comprehending diverse host-guest interactions within various environments, the exploration of spectroscopic contrivances holds immense promise,

particularly in the context of chemical warfare agents (CWAs) sensing mechanisms. This intricate interplay between hosts and guests extends its reach into the realm of safeguarding against potential threats, emphasizing the need for advanced sensor technologies designed to detect and identify target analytes associated with CWAs.

The mechanism of action underlying chemical warfare agents' sensors involves a strategic integration of host molecules specifically tailored to interact with these hazardous substances. These host molecules, acting as molecular recognition units, engage in selective and reversible binding with CWA analytes, thereby initiating a distinct host-guest interaction. This interaction forms the basis for the sensing process, as the binding event induces measurable changes in the spectroscopic properties of the sensor system. Various spectroscopic techniques, such as fluorescence spectroscopy, surface-enhanced Raman spectroscopy (SERS), and infrared spectroscopy, play pivotal roles in elucidating the nuances of these host-guest interactions. For instance, fluorescence spectroscopy capitalizes on the alteration in emission spectra resulting from the binding event, offering a real-time and highly sensitive detection method. Surface-enhanced Raman spectroscopy, on the other hand, exploits the enhancement of Raman signals upon analyte binding to provide detailed vibrational information, enhancing specificity in CWA identification. Infrared spectroscopy contributes by probing changes in molecular vibrations associated with host-guest interactions, further bolstering the sensor's capability to discern specific CWAs. The environmental adaptability of these spectroscopic contrivances is crucial, considering the diverse scenarios in which chemical threats may manifest. Whether in the field, industrial settings, or confined spaces, these sensors must exhibit robustness and versatility. The exploration of host-guest interactions exploring chromo-fluorogenic events within different environments not only refines sensor design but also amplifies their applicability across varied operational landscapes. In essence, delving into the host-guest interactions prevailing in environments rife with potential chemical threats unveils a sophisticated narrative of molecular recognition and sensing. By harnessing the power of diverse spectroscopic techniques, researchers can unravel the intricacies of these interactions, paving the way for advanced sensor technologies capable of safeguarding against the ominous presence of chemical warfare agents in our ever-evolving security landscape.

1.6. Literature Survey

1.6.1. International Status: The scientific communities around the world are actively affianced in designing and developing diverse colorimetric and fluorometric host molecules for detecting versatile target analytes influencing host-guest interaction. In this regard, Prof. Zheng-yin Yang and co-workers from Lanzhou University, Lanzhou, China have reported several OFF-ON-OFF chromo-fluorogenic host molecules for detecting the various target analytes. Among all his contributions, reports entitled "A simple fluorescent-colorimetric probe for selective switch-on detection of Al^{3+} in ethanol"[24] and "A chromone derivative as a colorimetric and "ON-OFF-ON" fluorescent probe for highly sensitive and selective detection of Cu^{2+} and S^{2-}," [25] are notable in these regards. The research group of Prof. Cheal Kim, Seoul National University of Science and Technology, Seoul, Korea has contributed to developing various chemosensors for selective and sensitive detection of several target analytes. Their work entitled "A novel fluorescent turn-on probe based on thiosemicarbazide-naphthalene for selectively detecting Zn^{2+},"[26] and "Fluoride detection with a colorimetric and fluorescent dual-mode chemosensor"[27] have skilled us how to develop chemosensor having selectivity and sensitivity towards detecting various target analytes in a single molecular platform by tailering the multiple functionalities. In this regard, several contributions in developing various fluoro-chromogenic chemosensors by Prof. Jong Seung Kim from Korea University, Seoul, Korea are noteworthy for the scientific communities who are interested in the thirsty area of chromo-fluorogenic chemosensors for detecting various target analytes [28–31]. Their testimony on fluoro and chromogenic chemo-dosimeters for heavy metal ion recognition in solution and biospecimens has highly inspired us to work in this field. Their findings on fluoride ion sensors based on calix luminophores modulating regioselectivity [32] have inspired us to work more in this field. Prof. Xiaoqiang Chen's group from China has also made significant contributions to the development of chromo-fluorogenic chemosensors to detect various target analytes[33].

1.6.2. National Status: The research and development on chemosensor and their application in the detection of several target analytes have attracted considerable attention from the Indian scientific community. Several research groups in India are actively engaged in investigating the selective recognition and quantification of various target analytes modulating versatile optoelectronic signaling. Among them, Prof. Anunay Samanta and co-workers (School of Chemistry, University of Hyderabad) have

made significant contributions to the design and development of various sensory materials. Their report on “pH-Regulated “Off–On” fluorescence signaling of d-block metal ions in aqueous media and realization of molecular IMP logic function [34] has taught us an understanding of the design and development of off-on metal ions chemosensors by modulating the various photophysical properties. Vinod Kumar and his group from Defence R & D Establishment, Gwalior, India, have contributed significantly to the development of various chromo-fluorogenic sensors for selective and sensitive detection of sulfur mustard simulants and nerve agents[35–39] which has highly motivated us to contribute more in this field. Recent work from Prof. Ghosh and his team from the Indian Association of Cultivation of Science (IACS), Kolkata, should also be notable while thrash outing the multitasking small molecules for various optoelectronic applications. Their findings on "Multitasking Behaviour of a Small Organic Compound: Solid State Bright White-Light Emission, Mechanochromism and Ratiometric Sensing of Al(III) and Pyrophosphate"[40] have encouraged us to work further in this field. Subsequently, Prof. Misra and his group from Vidyasagar University, Midnapore [41–43], and Prof. Das and coworkers from IIT Guwahati[44,45] have also made a significant effort to contribute to the sensing performance of Salen-type molecules. In this context, it is pertinent to mention here the recent contribution of Prof. M. Sarkar from the National Institute of Science Education and Research (NISER), Bhubaneswar,[46–48] towards decoding the various photophysical properties in the development of various chemosensors analytes to recognize and quantify different target selectively. All the findings and contributions pointed out above have equally motivated us to contribute further to designing and developing multitasking single, smart host molecules to detect various target analytes revealing the host-guest (analyte) interaction in their solid state and solution. However, the details elucidation of host-guest interactions’ mechanistic aspects in the sensory behavior of various chromo-fluorogenic host molecules and their real-world previling in different environments by diverse analytical contrivances are very are to date which is the main aim and objective of the present research work.

1.7. Conclusion

In summary, exploring diverse host-guest interactions in varied environments offers avenues to investigate different target analytes using various spectroscopic methods. These interactions, forming a crucial category with unique photophysical properties,

play a pivotal role in probing molecular intricacies. Comprising two or more components, these host-guest systems deviate from traditional electron-donor (EDA) frameworks, creating a dynamic interplay between the host and guest. These systems exhibit robust absorption within the visible and/or near-infrared spectrum, allowing tunability through strategic adjustments to the donor and acceptor components. Control over these factors opens avenues to design various chromo-fluorogenic hosts with the fine-tuning of unparalleled photophysical attributes, promising advancements in sensing devices.

In the present thesis, the main focus is on unraveling the intricate photophysical and sensorial intricacies of host-guest interactions with diverse chromo-fluorogenic host molecules with various target analytes. The research aims to delve into multifaceted interactions impacting absorption, emission spectra, and sensorial characteristics. The goals include synthesizing chromophoric systems, characterizing their electronic structures, exploring photophysical properties through sophisticated spectroscopy, and assessing sensorial attributes prevailing various host-guest interactions. This multidimensional approach contributes valuable insights to molecular design, applicable to developing sensory materials and devices, fostering progress in scientific and technological landscapes.

The references in the present thesis are organized in the following format:

Authors names, abbreviated journal name (in italics), year, volume number (bold) and page/article number, e.g.

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