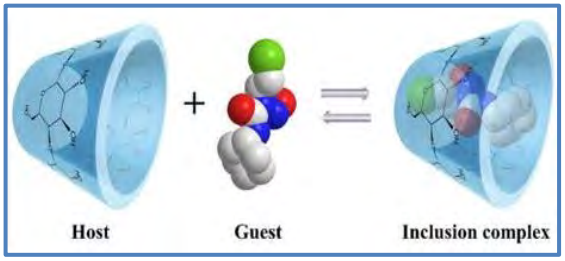
ABSTRACT

By the thesis title, I aim to demonstrate my profound understanding of the fields of amino acid-ionic liquid as well as vitamin-ionic liquid interaction in aqueous medium and supramolecular host-guest inclusion complexation. The supramolecular assembly has become increasingly important in drug release these days because of its exceptional bioavailability and unique capacity to change the solubility, stability, pharmacokinetics, and pharmacodynamics of the medication. They also show improved encapsulation, controlled release, and benign qualities.



The inclusion complexation of diverse bioactive compounds and their distinct photophysical properties in aqueous media are confirmed by the spectroscopic contribution. The development of supramolecular assembly can be qualitatively understood by the use of SEM analysis, powder XRD, ^{1}H-NMR, FTIR, and UV-visible analysis, all of which can satisfactorily express the inclusion phenomenon. Studying TGA and DSC can help to explain why such an arrangement is thermally stable. Confirming the data from the experimental research are studies of the supramolecular system using theoretical molecular modeling.

Significant information on a variety of thermodynamic properties of electrolytes and non-electrolytes, the impacts of variations in ionic structures, and the mobility of ions in addition to their common ions can be gained from the study of the physicochemical properties of solutions. Measurements of apparent molar volume (ϕ_v), limiting apparent molar volume (ϕ_v^0), molar refraction (R_M), limiting molar refraction (R_M^0), molar conductance (Λ), Surface tension (γ) and viscosity B coefficients obtained from various physicochemical methodologies are typically used to reveal the genesis of diverse interactions between amino acids, vitamins and ionic liquid in the aqueous phase.

This study has looked at the encapsulation of several biologically active compounds. There may be uses for these bioactive compounds in biological systems.

Pharmacological activity is frequently used to characterize the advantageous properties of bioactive compounds.

In host–guest chemistry, the application of macrocyclic hosts in molecular recognition, controlled release of a drug and sensing field has received considerable interest. The incorporation of guest molecules in the aqueous environment within the cavity of the host molecule such as α-cyclodextrin, provides new insight into molecular recognition (e.g. inclusion or complexation) through non-covalent interactions.

A general understanding of the development of an inclusion complex between the host and guest molecules can be obtained from supramolecular host-guest chemistry. The host's hydrophobic cavities can bind various guest compounds. The supramolecular assembly as a whole has been extensively researched recently in a variety of disciplines, including analytical chemistry and medication delivery. When combined with different guest molecules of the right size, cyclodextrin and its derivative appear to be the most promising host molecules for the formation of inclusion complexes.

Thus, the main goal of this thesis is to investigate the impact of supramolecular recognition and solution chemistry, which are unavoidably important due to their numerous applications in a variety of sectors, including the biological and pharmaceutical sciences.

SUMMARY OF THE WORKS

CHAPTER I

This chapter includes a full description of the research project, its scope, and its applications to modern science. It also explains the rationale for the selection of solvent systems, cyclodextrins, ionic liquids, and bioactive compounds. A summary of all the investigation techniques used in the research project is provided in this chapter.

CHAPTER II

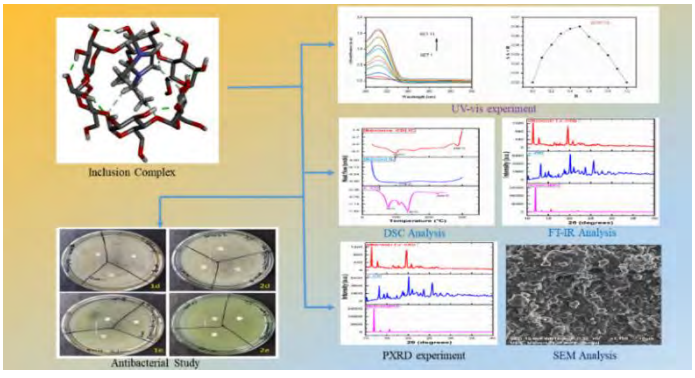
The earlier study on this topic, conducted by different scientists and researchers worldwide, is reviewed in this chapter. Additionally, a detailed explanation of the findings is provided in this chapter, which describes the forces that interact between the molecules. The theory underlying each of the investigation techniques—^{1}H-NMR, FTIR, UV-visible, Differential Scanning Calorimetry, Thermogravimetric analysis, Powder XRD, Scanning Electron Microscopy, Molecular Docking study, Antimicrobial study, Cytotoxicity study, Surface Tension, Conductivity, Density, Viscosity, and Refractive Index has been covered in detail here, along with the importance of their application to the research described in this thesis.

CHAPTER III

The experimental section is covered in this chapter. It discusses the names, compositions, characteristics, and uses of cyclodextrin, ionic liquids, solvents, and biologically active compounds that are employed in research projects. It also contains information about the instruments used in this research, their descriptions, and the specifics of the experimental procedures.

CHAPTER IV

This chapter consists of the formation of the new inclusion complex between the 1-butyl-2,3-dimethylimidazolium tetrafluoroborate [Bdmim]BF_4 ionic liquid (IL) and the host α-Cyclodextrin (α-CD) by a 1:1 ratio and newly formed inclusion complex was further explored by the ^{1}H-NMR, FT-IR, UV-vis spectroscopy, PXRD,



DSC, and SEM analysis. Molecular docking was also performed to investigate the encapsulation of the inclusion complex in which orientation and it have been seen that the IL [Bdmim]BF_4 enters into the α-CD cavity with a 1:1 ratio. It was further established with the help of Job's plot. The antibacterial activity of [Bdmim]BF_4 IL and its inclusion complex was also verified against some Gram-positive and Gram-negative bacterial strains.

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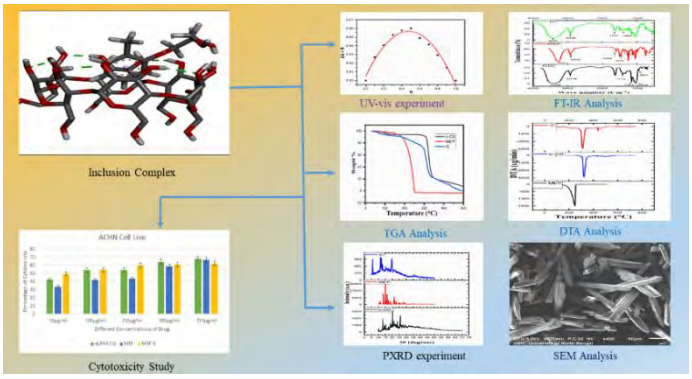
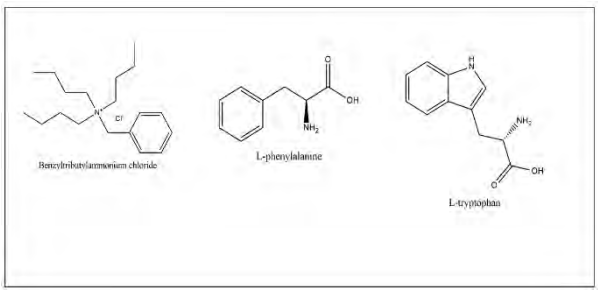
CHAPTER V

This chapter includes investigating the encapsulation of polyether compounds such as mephenesin (MEP) into the nano hydrophobic cage of α-cyclodextrin as a host molecule. The consequential inclusion system was characterized by UV–visible spectroscopy, ^1H NMR, PXRD, TGA, DTA, SEM, and FT-IR studies. Molecular docking was performed for the inclusion complex to discover the most proper orientation, and it was seen that the drug mephenesin fits into the cavity of α-cyclodextrin in a 1:1 ratio, which was also confirmed from the Job plot. Furthermore, a comparison was done based on cell viability between the drug and its inclusion complex ****Communicated*.**



CHAPTER VI

This chapter includes the solute–solvent interaction between ionic liquids (ILs) and amino acids (AA) in aqueous media plays a significant role in the optimization of several important biotechnological processes. L-Phenylalanine and L-Tryptophan (two solute molecules) interact with an ionic liquid (Benzyltributylammonium chloride) in an aqueous medium. Based on the different



parameters such as apparent molar volume, viscosity B-coefficient, molar refraction, molar conductance, surface tension at different temperatures and different concentrations from density, viscosity, refractive index, conductance, surface tension measurements have been used to explain the molecular level interactions. Using Masson equation, the experimental slopes and the limiting apparent molar volumes are obtained which explain the solute-solute and solute-solvent interactions. Hepler's technique and dB/dT values have been used to examine the structure-making and structure-breaking nature of the solutes in the solvents. Viscosity parameters, A and B obtained from Jones-Doles equation explained the solute-solute and solute-solvent interactions in the solution. Lorentz-Lorenz equation has used to calculate the molar refraction. The specific conductance and surface tension also explained the interaction properties. In our findings, we emphasized on the nature of solute–solvent interactions and the presence of structural effect on the solvent in solution to analyze the molecular-level interactions prevalent in the systems.

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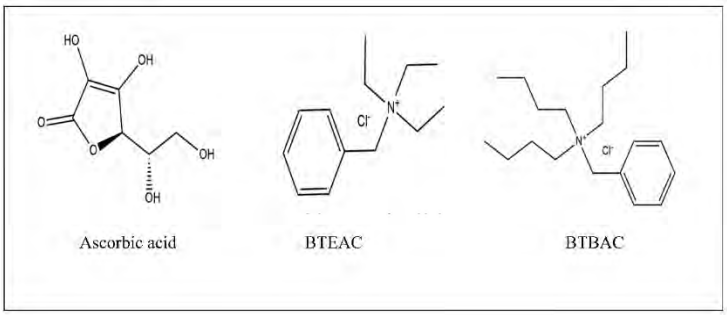
CHAPTER VII

In this chapter the densities, viscosities, conductances and surface tension of Vitamin C (Ascorbic acid) in Ionic Liquids viz: Benzyltributylammonium chloride (BTBAC) and Benzyltriethylammonium chloride (BTEAC) aqueous mixtures have been measured at 298.15K, 308.15K and 318.15 K. Apparent molar volumes (Φv), viscosity *B*-coefficients, molar conductances are obtained from these data supplemented with densities, viscosities and specific conductances, respectively. The limiting apparent molar volumes (Φv^0) and experimental slopes (Sv^*) derived from the Masson equation have been interpreted in terms of solute-solvent and solute-solute interactions, respectively. The viscosity data have been analyzed using the Jones-Dole equation, and the derived parameters *B* and *A* have also been interpreted in terms of solute-solvent and solute-solute interactions, respectively. The surface tension parameter has also been utilized to



support the investigation. The structure-making/breaking capacities of ascorbic acid in the studied ionic liquid systems have also been discussed.

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CHAPTER VIII

This chapter includes the concluding remarks about the research works done in this thesis.

CHAPTER IX

Bibliography and references of all the previous chapters has been included in this chapter.