Abstract

The studies on host-guest chemistry give a broad idea of intermolecular interactions where covalent bonds are not likely to form between the interacting species. Thus, most of this interaction has been performed by host-guest interaction. Among the host molecules, cyclodextrin seems to be the most promising to form inclusion complexes, especially with various guest molecules with suitable polarity and dimensions. In host-guest chemistry, an inclusion compound is a complex in which one chemical compound (the "host") forms a cavity in which molecules of a second "guest" compound are located. The definition of inclusion compounds is very broad, in molecular encapsulation; a guest molecule is actually trapped inside host molecule.

Solvation effect is an imperative branch of the physical chemistry, which deals the change in properties that arise when one substance dissolves in another substance. The investigation have been done for the solubility of substances and studied how it is affected in both the physical and chemical nature for the solute and solvent. There are three types of approach have been made to estimate the extent of solvation in physical chemistry. The first one involves the studies of transport properties as conductance, ionic mobility etc., of the electrolytes in aqueous and non-aqueous solvents and the derivation of various factors associated with ionic salvation; the second one is the thermodynamic approach by measuring the free energies, enthalpies and entropies of solvation of ions from which factors associated with solvation can be explain; and the third one is to use spectroscopic study where the spectral line shifts or the chemical shifts of the functional group of electrolytes or non-electrolytes in solvents has bee has been resolved qualitatively and quantitatively with their nature/mode of interactions.

Any compound which is very much important and essential to our environment systems is called the vital compound. In my work different kinds of Drugs, Amino acids and Ionic liquids are considered as vital compounds.

My Thesis is entitled as "**EXPLORATION OF INCLUSION COMPLEXES BETWEEN HOST AND GUEST MOLECULES AND SOLVATION EFFECT OF SOME VITAL MOLECULES IN VARIOUS ENVIRONMENTS**" and the summery of my research works are -

CHAPTER I

This chapter includes the objective, importance and applications of the research work, the reasons for choosing the host, guest molecules, vital molecules, solvents and methods of investigation. This also occupies the summery of the works done in this thesis.

CHAPTER II

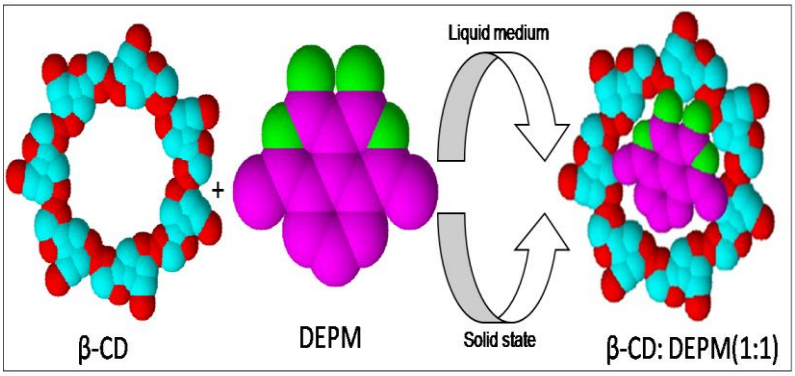
This chapter covers the general introduction of the thesis and forms a strong background of the works embodied in the thesis. A brief review of notable works in the field of host-guest chemistry and salvation effect has been given. Various derived parameters dependent on conductance, density, surface tension, UV-Vis spectroscopy, FTIR spectroscopy, fluorescence spectroscopy, NMR (1HNMR, 2D ROSEY, 13 CNMR, powder XRD, mass analysis, TGA and SEM analysis along with their importance in case of molecular interaction as well as ionic interaction (ion-solvent/solute-solvent and ion-ion/solute-solute interactions) in solution and in the field of inclusion chemistry have been discussed.

CHAPTER III

This chapter contains the experimental section which mainly involves the elementary information such as: structure, source, purification and application of the compounds and usefulness of the solvents used in the research work and the details of the instruments used for the study of the supramolecular host-guest chemistry and solution chemistry.

CHAPTER IV

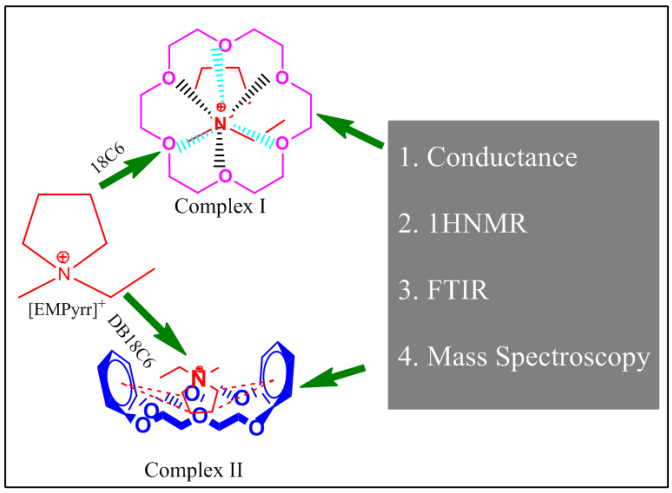
In this chapter, I have investigated the inclusion behavior of guest Diethyl phenylmalonate (DEPM) with beta cyclodexrin. The aim of this present work is to make soluble DEPM in aqueous medium through the formation inclusion complex into the hydrophobic hollow space of β-cyclodextrin (β-Cyd) which will provide a novel approach for designing drug delivery system in aqueous medium. The study of supramolecular complexation of DEPM with β-Cyd has been designed in both solution and solid state. In solution phase the evidences of the presence of non-covalent interactions in inclusion complex with 1:1 stoichiometry behaviour are obtained by investigating the UV-spectroscopy. The resultant solid of DEPM and β-Cyd is established by ^{1}H NMR, FTIR, powder XRD and SEM techniques. So, β-Cyd has the ability to encapsulate DEPM



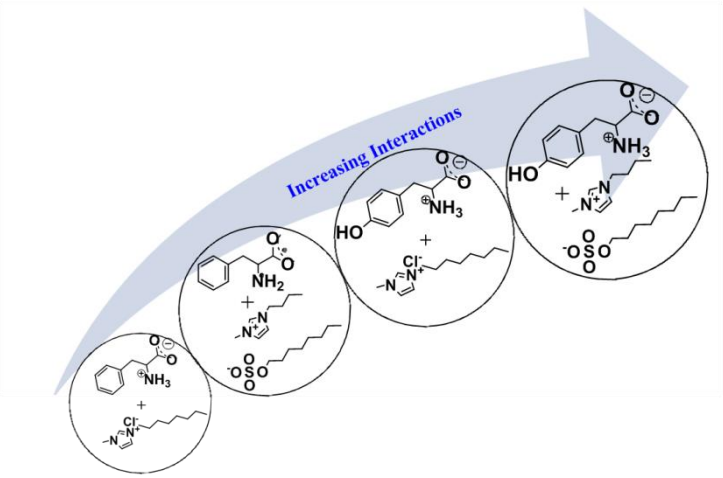
into their core without formation any covalent bonds and also increases the bioavailability of the water insoluble DEPM drug.

CHAPTER V

In this section complexation process of the selected macrocyclic crown compound viz. 18C6 and DB18C6 with 1-ethyl-1-methylpyrrolidinium hexafluorophosphate as a guest molecule have been intended in acetonitrile medium at by conductometry (three different temperatures), ^{1}HNMR and mass spectra. The formation constants of the complexes are evaluated in solution phase from the molar conductance-mole ratio values. The result shows that the stability of the resulting complexes with the same inward cationic moiety follows in the order 18C6:$[EMPyrr]^+$> DB18C6:$[EMPyrr]^+$ and based on the character of the crown ethers. The calculated thermodynamic parameters support this Complexation process. The host-guest complexations of the five-membered nitrogen containing cation with two different macrocyclic polyethers are supported by studying ^{1}HNMR. The electrospray mass spectrometry has been used to support the complexation process with proper stiochiometry ratio. The solid complex formation between the selected two crown ethers and the ionic liquid are established by FTIR study.



CHAPTER VI

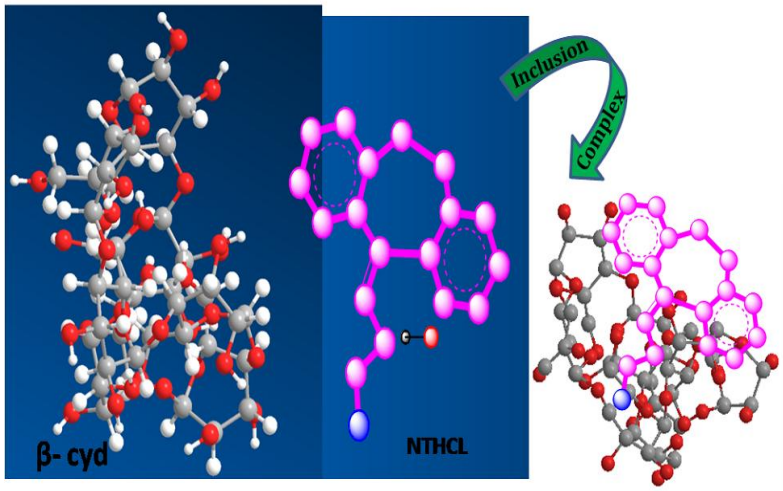


This chapter entails the Molecular interactions of two ionic liquids (ILS) 1-butyl-3-methylimidazolium octylsulphate [BMIM][C_8SO4] and 1-methyl-3-octylimidazolium chloride [MOIM]Cl with amino acids (AA) (AA= L-tyr, L-phe) in aqueous medium have been investigated by molar conductivities (Λ) at three different temperatures. Spectroscopic studies such as Uv-vis and fluorescence have been performed to investigate the association behavior order between the ILs and the selected amino acids and the spontaneity of this process. The 1HNMR spectroscopy has also been carried out to expose the change in electronic conditions of various protons of ILs in the presence of different amino acids. All the results that have been interpreted on the light of possible molecular interactions (non-covalent) operating in the ternary system and followed the interaction order of ([BMIM][C_8SO4] + L-tyr)> ([MOIM]Cl + L-tyr)> ([BMIM][C_8SO4] + L-phe)> ([MOIM]Cl + L-phe) in water.

CHAPTER VII

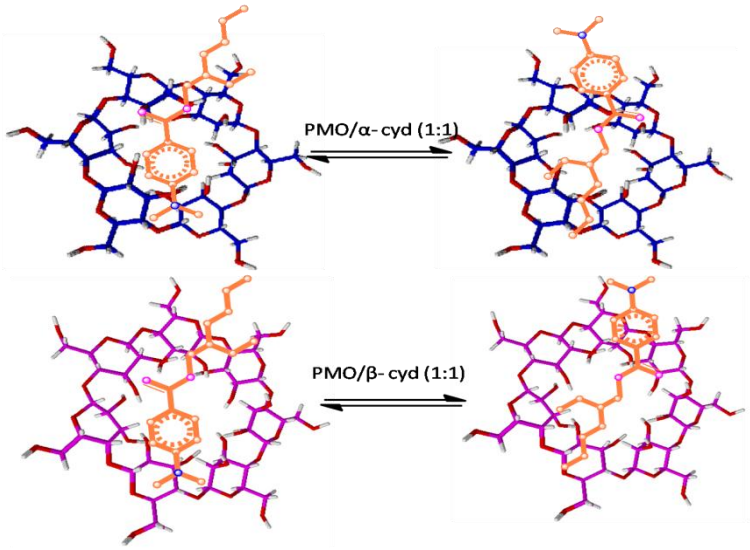
This chapter's study is related to characterise the formation, mechanism behaviour and importance of the complexation between nortriptyline hydrochloride (NTHCL), a class of tricyclic antidepressant (TCA) drug and also having neuroprotective effects, with β-cyclodextrin (β-Cyd) acts as an excellent drug-receptor. The continuous various method (Job plot), UV-spectroscopy, fluorescence measurements and powder XRD have been reported to confirm the inclusion complex with 1:1 stiochiometry with

the TCA aliphatic tail. A variant view of NTHCL/β-CD complex where the interaction of tricyclic ringring with β-Cyd cavity is presented in this work using 1HNMR, 13C NMR and FTIR spectroscopy. The most considerable evidence for inclusion of nortriptyline tricyclic ring and the protons located inside the β-Cyd cavity is the 2D NMR ROESY cross-peaks. Changes in chemical shifts in 1H NMR and behaviour of 2D ROESY cross peak suggest the inclusion complex formation.

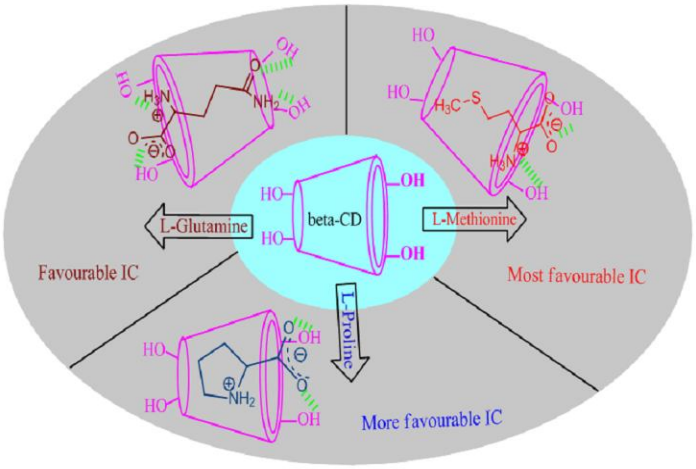


CHAPTER VIII

This chapter includes the exploration of the formation of inclusion complexes between water insoluble drug padimate O with α and β-cyclodextrin. The solubility of padimate O is enhanced by forming inclusion complex with these two cyclodextrins. The stoichiometry of the inclusion complex was determined with Job's plot method by UVVisible spectroscopy and found to be 1:1 stoichiometry. Mass spectra also support the inclusion process with 1:1 stoichiometry. The resultant solid of PMO/α-CD and PMO/β-CD has been established by FTIR and powder XRD techniques.



CHAPTER IX



This chapter includes the inclusion behaviour between β-cyclodextrin and amino acids (viz., L-Methionine, L-Proline and L-Glutamine) are established in aqueous medium. Such complexation of amino acids in aqueous medium without using any organic solvent provides great ideas in different industries. The complexes are characterized by ^{1}H NMR which proves the formation of inclusion complex. The interactions of β-CD with amino acids are analyzed by means of surface tension and density. Contributions of different groups of the guest molecules to the limiting apparent molar volume are determined. Additionally, the stoichiometry of the inclusion complexes is also determined to be 1:1 in all the three cases. The solid inclusion complex formations of β-CD with amino acids are confirmed by PXRD analysis.

CHAPTER X

This chapter contains the concluding remarks of the works related to the thesis.