

## CHAPTER X

### *Concluding Remarks*

In my thesis, I have tried to introduce some new type of inclusion complexes in host-guest chemistry which may help to employ in various field of science. The different kinds of physicochemical techniques have been performed to understand the different types of molecular as well as ionic interactions on ionic liquids in solution environments. I have studied interaction present in the inclusion complexes both in solution as well as in solid phase and to collect detailed information about the nature and strength of various interactions.

The surface tension, density and conductometric studies helped us to evaluate the extent of molecular interaction in a particular solution quantitatively whereas the UV-vis, fluorescence, FTIR and NMR spectroscopic measurements gave an insight into the types of molecular interactions occurring in any given systems. Scanning Electron Microscopy (SEM) gives information about the surface morphological structures of solid materials. ESI-MS study confirmed the stoichiometry ratio of a complexation process. The direct evidence for the complexation between host and guest molecule has been provided from the analysis of powder X-ray diffraction spectrum and the thermal stability of solid complexed materials have been demonstrated by TGA study.

In **chapter IV**, the interactions of DEPM with  $\beta$ -Cyd are investigated in liquid medium by UV-spectra in terms of Job plot and association constant (K). Both satisfy the formation of IC with 1:1 stoichiometry. Different pH environment shows that it has great influence on association constant (K). Determination of  $\Delta G$  value indicates that the process is thermodynamically controlled. The results come from  $^1\text{H}$ NMR, FT-IR, powder XRD and SEM studies suggest that the selected guest molecule DEPM

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monomer formed IC with nano hydrophobic core of  $\beta$ -Cyd effectively which will make possible DEPM to be solubilised in water successfully.

In **chapter V**, the obtained result of conductivity and the association constant ( $k_f$ ) for the complexation between 1-ethyl-1-methylpyrrolidinium hexafluorophosphate and 18C6 and DB18C6 can be explained in terms of the electrons donor ability of oxygen atoms to substrate. The thermodynamics parameters for this complexation process articulate that the overall complex formation path thermodynamically favorable. The five membered pyrrolidinium cationic head group is integrated into the macrocyclic polyether network via  $N^+ \cdots O^\delta-$  non-covalent ion-dipole, H-bonds and  $C-H \cdots \pi$  interactions (host-guest interactions) has been established by <sup>1</sup>HNMR. ESI-MS study confirmed the host-guest complexation process with 1:1 ratio. The FTIR spectroscopy study of the resulting solids between crown ethers and IL also gives distinct evidence about this host-guest complexation process.

In **chapter VI**, the solute-solvent interaction behavior of studied ionic liquid and amino acids in aqueous solution have been determined by conductance measurements at three different temperatures and spectroscopic studies. The ILs and amino acids systems in aqueous solution indicate the non-covalent interactions among them and causing an increase of hydrodynamic radii of ions and a decrease of their ionic mobility, hence we have got the result a decrease in molar conductance. It has been concluded from the association constant values of the selected ILs with AAs obtained by using Uv-vis and fluorescence measurements that among the two ILs, 1-butyl-3-methylimidazolium octylsulphate [BMIM][C<sub>8</sub>SO<sub>4</sub>] interact more firmly with L-tyrosine than L-phenylalanine and in each system both IL and AA have been promoted to each due to non-covalent such as strong hydrophobic- hydrophobic, weak  $\pi \cdots \pi$ , columbic force of attraction, H-bond

interactions etc. amongst themselves. The significant chemical shifts of ILs protons in presence of amino acids in  $^1\text{H}$ NMR studies also support the results obtained from other spectroscopic and conductance measurements.

In **chapter VII**, in this research, the interaction of NTHCL with  $\beta$ -CD and stability constant (K) of this complexation have been elucidating using UV-spectroscopy and fluorescence measurement. The job's method reveals that the NTHCL/  $\beta$ -CD forms 1:1 complex. Characterization by  $^1\text{H}$ NMR, ROSEY,  $^{13}\text{C}$ NMR, FTIR, PXRD have been performed and all of these techniques are utilised to support the complexation phenomenon.  $^1\text{H}$ NMR and ROSEY clearly suggest that the not only the aliphatic tail is involved but the tricyclic ring also participates in this process The resultant complex is found to be water soluble which can be used as regulatory releaser of the selected drug in human body and suitable for successive applications.

In **chapter VIII**, from the results of our experiments, it has been concluded that the UV-B protector sunscreen agent padimate O can form an inclusion complex with  $\alpha$ -CD and  $\beta$ -CD which can be used as regulatory releaser of this agent. The encapsulation of PMO molecule inside the hydrophobic core of cyclodextrins has been proved in aqueous medium by UV-Vis spectroscopy and in solid state by FTIR, Mass, XRD and TGA analysis. The stoichiometric behaviour with 1:1 ratio of the complexes has been confirmed through continuous variation job's method and ESI-MS experiments. The association constant values demonstrated PMO is somewhat in good agreement with  $\beta$ -cyd than  $\alpha$ -cyd and the thermodynamic parameters making the overall process thermodynamically favourable. FTIR spectroscopy, PXRD and TGA support the complexation phenomena and according to the results of PXRD and TGA techniques, it can be said that newly obtained PMO/  $\alpha$ -cyd and PMO/  $\beta$ -cyd complexes have different physicochemical properties compared to their free forms.

Thus it can be concluded that our work may be regarded as an alternation way to protect our skin from sun damage and beneficial to medicinal science.

In **chapter IX**, inclusion complexes between  $\beta$ -cyclodextrin and the selected amino acids are formed successfully in solution phase with 1:1 stoichiometry ratio which has been confirmed by surface tension,  $^1\text{H}$  NMR study. The amino acids- $\beta$ -CD interactions have been explained by density measurement. The group contributions to  $\phi_v^\circ$  facilitated to understand the proper interactions between the host and guest. The results come from PXRD suggest that the selected guest molecules monomer formed ICs with nano hydrophobic core of  $\beta$ -CD effectively. The aim of this work is to apply these three amino acids in complexed form by using  $\beta$ -CD in liquid medium in the field of controlled delivery systems.