

CHAPTER- X

CONCLUDING REMARKS

The research work was designed to explore various interactions taking place in various systems inclusion of the various guest molecules inside the cyclodextrin molecules. It is well described that cyclodextrin molecules modify the physicochemical properties of the guest molecules after incorporation inside it. Therefore, various drug molecules as well as various ionic liquids having biological importance were studied whether they can be included inside the cavity of the host molecules. The aim of the works embodied in this thesis was to discover the interactions playing vital role in the solution phase and in the inclusion complexation. Here, the molecular interactions, ionic interactions in the solution phase, and the interactions taking place in the process of inclusion complexation of various ionic liquid molecules and drug molecules in liquid phase and solid phase were discussed. The molecular interactions occurring in the solution systems have been studied with the help of physicochemical, thermodynamic, transport and optical properties along with spectroscopic studies such as NMR, FT-IR, UV-Vis and Mass spectroscopic study.

The volumetric, viscometric, interferometric, conductometric refractive index studies helped us to estimate the extent of molecular interactions various solution systems quantitatively whereas the spectroscopic measurements gave an insight into the type of molecular interactions occurring in solution and solid phase. These interactions helped in better understanding the nature of solute and solvent in the solution phase and the inclusion complexation in both the solution and solid phase.

The thorough study represents the fact that the electrolyte lithium hexafluoroarsenate (LiAsF_6) remains mostly associated with the mixed solvent system in the binary mixture of EG and MeOH. This fact is supported by the study of conductivity of the salt LiAsF_6 in various mass fractions of EG in MeOH. The limiting apparent molar volume and viscosity B-coefficient values obtained for LiAsF_6 in the binary solution specifies the existence of strong ion-solvent interactions, which increase further with the increased mass fraction of EG in MeOH.

The thorough physicochemical and spectroscopic study that are discussed above lead to the conclusion that the ILs i.e., $[\text{BMIm}]\text{Cl}$ and $[\text{HMIm}]\text{Cl}$ associate to form host-

guest inclusion complexes with both the CDs. The proton NMR studies provides enough information which confirms the formation of ICs while Surface tension, Conductivity study and mass spectroscopic study supports the above mentioned phenomena and determine the 1:1 stoichiometry of the host-guest inclusion complexation. The Density and viscosity study again supports the phenomena of inclusion with a good agreement. Binding constants for the ICs have been determined with the help of the conductivity study by using a non-linear programme. Finally, the formation of the host-guest inclusion complexes has been found most feasible in case of the [BMIm]Cl- β -CD system than the other combinations. Based on the above information the plausible inclusion structures have been speculated. In the field of Nano-sensing, drug delivery and in many other fields these types of inclusion complexes have the extensive applications.

The work describes the inclusion phenomena between the IL [BMPy]PF₆ and α - and β -Cyclodextrin with the production of the aqueous soluble complexes. The Inclusion phenomena were confirmed by ¹H-NMR, FT-IR spectroscopy. Again the phenomena of inclusion and Stoichiometry of the complexes were confirmed by Job's plot obtained from UV-Vis spectroscopic study, Surface tension and conductance study. Binding constant calculated confirmed the good association between the host and guest and good feasibility of formation of the inclusion complexes. The process of inclusion is thermodynamically favourable, which is evident from the values of Gibb's free energy change and enthalpy values. The more feasible inclusion was obtained in case of the complexation with α -Cyclodextrin.

The study of encapsulation of TBPMS inside CDs in aqueous medium was found successful. A clear picture of inclusion was found in the solid form from the analysis of ¹H-NMR, 2D-ROESY, FT-IR and EI-MS study. The study of conductance, surface tension and UV-Visible spectroscopy in the aqueous solution confirmed the above phenomena of inclusion. The 1:1 stoichiometric ratio of host and guest in the inclusion complexes was confirmed by the conductance and surface tension study for both the cyclodextrins. This fact of stoichiometry was further supported by the EI-MS experiment of solid ICs. The binding constants of the ICs calculated and the thermodynamic parameters obtained by calculation confirmed the higher stability and the feasible formation of the ICs. Taking in account all the above observations a schematic representation of the inclusion was depicted. Now days, these types of ICs are of great interest in various industries as these are environmentally non-hazardous.

The entire study reveals the formation of host-guest inclusion complex of 1:1 stoichiometry. The $^1\text{H-NMR}$ and FT-IR studies confirm the formation of inclusion complexes between the drug molecule and CD molecule. The same conclusion is also supported by the experimental data derived from density and viscosity measurements. The single break point at the concentration near to 5mM of CD in each case obtained from the surface tension study indicates the formation of the inclusion complexes with 1:1 stoichiometry. From the UV-VIS spectroscopic data, binding constant calculated using Job's plot, clearly explains the formation of more effective inclusion complex with PTX than 2-PAM and the formation of IC with $\beta\text{-CD}$ is more feasible than $\alpha\text{-CD}$. Taking all the parameters and results in account the plausible mechanism of the inclusion has been depicted. The qualitative and quantitative idea of the formation of host-guest ICs of $\alpha\text{-CD}$ and $\beta\text{-CD}$ with PTX and 2-PAM reveal substantial applications in drug industries and medicinal sciences.

The viscosity, density and refractive index study of the solution of Li- Oxalate, Na-Oxalate, K-Oxalate in aqueous uric acid solvent of different concentration leads to the conclusion that solute solvent interaction is predominant over the solute-solute interaction and solute-solvent interaction is higher in case of K-Oxalate than sodium oxalate and which is greater than Li-Oxalate. One plausible reason is the size of the metal ion. The hydrated size of the K^+ is less compared to that of the Na^+ and which is less than Li^+ . Due to this size factor the K^+ comes more closer compared to that of the others. The same can be concluded for Na-Oxalate than the Li-Oxalate. This result indicates that potassium oxalate can more easily penetrate into the accumulated uric acid in the joints of the human body than that of sodium and lithium oxalates thereby releasing the accumulated uric acid rendering the recovery of gout pain due to stronger solute solvent interactions as discussed above. This is an excellent agreement with that as reported earlier.

All the above discussed drugs and ionic liquids are highly significant in pharmaceutical industries, food industries, cosmetic and hygiene industries, paint industries. Thus, this may be concluded that the full research work has satisfactory consequences in the diverse fields of sciences and technology which demands a far-reaching influence for the intensification of the progressive research.