CHAPTER-X

CONCLUDING REMARKS

The aim of the research work embodied in our thesis was to investigate the various interactions such as solute-solute, solute- solvent as well as molecular interaction associated with some ionic liquid and some biologically potent molecules(amino acids) prevailing in liquid environment. The different interactions involving ionic liquids and amino acids have been studied with the help of some physicochemical parameter, thermodynamic parameter, quantum mechanically computational study, transport phenomena, optical properties along with the help of spectroscopic investigations.

The volumetric, viscometric , conductometric, refractive index, surface tension measurement are very important properties is to used for the determination of ion-solvent interaction. Limiting apparent molar volume obtained from the density data and viscosity B – coefficients obtained from the viscosity measurements also gives the valuable information regarding the solute- solute and solute- solvent interactions.

In reality, the ion- solvent interactions is very complex in nature. There are strong electrical forces associated with the ions and ions with solvents , it is indeed not to separate them overall. However, if we noticed with carefully, valid conclusions can be obtained in many cases from apparent molar volume, viscosity, conductivity, NMR, UV-vis spectroscopy measurements relating to degree of freedom of structure and also order of the system.

In the chapter 1V deals with 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(298.15k,303.15k,308.15k) 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_8SO_4] 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}HNMR studies also support the results obtained from other spectroscopic and conductance measurements.

Density, viscosity, refractive index and conductance measurements in the chapter V has provided the valuable information about ion-dipole interaction and show that the solute-solvent interaction between BTAC ionic liquid and biologically potent molecules, L-Aspartic acid and L-Glutamic amino acid systems is higher than the solute-solute interaction. This is resulted by hydrophobic interactions which lead to volume contraction. The physico-chemical methodologies, describes the mode of interaction in solution. Calculation of limiting apparent molar volume, limiting molar refraction, viscosity B-coefficient and molar conductance makes it possible to identify the interaction as predominant solute–solvent interaction and indicate the predominance of solute-solvent interaction than the solute-solute interaction. The values of $(\delta\Phi_E^0/\delta T)_P$ and (dB/dT) have been calculated to provide the information that the solute–solvent interaction is structure-making. The extent of solvation is highest in L-Glutamic acid at 0.05m 313K and lowest in L-Aspartic acid at 0.01m 293K. The derived parameters obtained by analyzing various equations supplemented with experimental data sustain the same finale as discussed and explained above.

In the summary of this study obtained from chapter VI, it was found that there is a strong interaction between L-ascorbic and IL and it becomes stronger with rise in temperature. As molecules of L-ascorbic and IL have engaged each other, solute-co solute interaction is much greater than the solute-solute and solvent-solvent interactions in the ternary system.

In this chapter VII, aim of the present paper was to establish the nature of solute-solute and solute-solvent interactions in the solutions of TBMS + amino acid systems of several concentrations and temperatures (298.15K,303.15K,308.15K) for chemical and technological applications. The investigation of Physico-chemical parameters through density, viscosity, refractive index, surface tension and conductance study refers to the mode of interactions taking place in the amino acids; L-Arginine and L-Histidine in ionic liquid solutions of TBMS at different molalities (0.001,0.003,0.005) as well as different temperatures. In the present study, all the parameters were interpreted in terms of solute–solute and solute-solvent interactions occurring among the various components of the experimental solution mixtures. Analysis of apparent molar volume, limiting apparent molar volume, molar refraction, limiting molar refraction, viscosity B coefficient and surface tension signify the solute-solvent interaction is predominant over solute–solute interaction. The $(\delta\Phi_E^0/\delta T)_P$ and (dB/dT) values have been considered to illustrate the facts that, the solute-solvent interaction is significantly structure breaking which is further established by Hepler's constant values. From the study of the investigated solutions presence of strong solute-solvent interaction was observed and also

supposed to be more effective and predominant than the solute–solute interaction occurring in experimental systems. Amino acid L-Histidine fused with the imidazole ring undergoes a lower degree of interactions in the presence of ionic liquid (TBMS) as compared to L-Arginine. Surface tension indicated the starring role of the hydrophilic and hydrophobic character of solutes in molecular interactions with TBMS in aqueous solutions. Again, conductance data also recommends the mode of interactions going on between the solute and solvent thereby the presence of mobility in the solution phase. Ultimately, strong hydrophobic-hydrophobic interactions are playing an important role too. Furthermore, electrostatic and hydrophobic interactions are more predominant for the L-Arginine-TBMS system, associating the experimental outcomes. The experiment definitely would provide for a more inclusive understanding of such systems to a large extent.

From chapter VIII, Some physicochemical parameters density, viscosity, refractive index, conductance and surface tension measurements of aqueous solution of amino acid, L-Methionine in the ionic liquids, Benzyl tri-methyl ammonium chloride and Benzyl tri-ethyl ammonium chloride. The above results supported by some spectroscopic techniques FTIR, H^1NMR and UV-Vis spectroscopy and theoretically computational study provided the information that strong solute-solvent interactions dominate over the weak solute-solute interactions in the studied compounds. Further, L-Met in 0.005m BTEAC at 308.15K indicates highest solute-solvent interaction whereas, L-Met in 0.001m BTMAC at 298.15K shows the lowest. Again, mode of solute–solvent interaction is structure-breaking and the structure-breaking effect of L-Met is strongest in 0.001m aqueous BTMAC solution with highest packing or caging effect. The free energy of activation of viscous flow indicated greater solute–solvent interactions resulting in the formation of the transition state followed by breaking and altering the intermolecular forces prevailing in the solvent structure of the medium. Due to larger alkyl group, +I effect in BTEAC is greater than in BTMAC making the interaction more prominent in L-Met BTEAC solution, as there is presence of more lone pair availability of oxygen atom, making the interaction strong with the Ionic liquid.

From chapter IX, in the overview of this study, that there is a strong interaction between L-glutamine and BTBAC and it becomes stronger with rise in temperature and increase in mass fraction of BTBAC. All of these above physicochemical and spectroscopic along with computational works confirms the amino acids and IL (BTBAC) have engaged each other, solute-cosolute interaction is much greater than the solute-solute and solvent-solvent interactions in the ternary system.

It is very difficult to proper understanding the nature of ion-solvent interactions. However The wide range studies of the different physiochemical, thermodynamic, transport and

also spectral properties of the ionic liquid in different biologically potent molecules in liquid medium try to understanding the nature of ion- solvent interactions it is necessary to explained quantitatively the influence of the solvent and the extent of interactions associate with ions in solvents in solution chemistry.

In reality, the ion- solvent interactions is very complex in nature. There are strong electrical forces associated with the ions and ions with solvents it is indeed not to separate them overall. However, if we noticed with carefully, valid conclusions can be obtained in many cases from apparent molar volume, viscosity, conductivity, NMR, UV-vis spectroscopy measurements relating to degree of freedom of structure and also order of the system.

The ionic liquids and amino acid which used for my research work are very important in pharmaceutical industrial purpose, food industries, cosmetic and hygiene, paint industries, polymeric industry.

In the near future, we attempt to extend our research work with ionic liquids and amino acids; I hope that will certainly complement our present findings. In recent years, with the introduction of new synthetic technologies such as phase transfer catalysis, and catalysis, catalytic symmetric/asymmetric synthesis, the diversity of molecular interactions that can be studied has increased to the highest degree. I hope this thesis delivers a substantial launching point for the reader to begin their own investigation into the chemical natures of remarkable, however ionic liquids and natural amino acids. As more and more interesting and unusual ionic liquids and amino acid ionic liquids are discovered, the possibility for development of synthetic methods for these useful in different branch of science, academic, research area, industry and biologically important ionic liquids (ILS) and amino acids (AAS) grows up as well.