

CHAPTER-X

CONCLUDING REMARKS

In my research work, described in this thesis, I have tried to investigate the physicochemical properties of some ionic liquids and biologically active solutes in different aqueous and non-aqueous industrially important liquid systems respectively in terms of diverse interactions such as solute-solute or ion-ion, solute-solvent or ion-solvent and solvent-solvent. Thermodynamic, transport, optical and spectroscopic properties of solutions help to examine the molecular interactions. Systematic study made on these properties has great importance in gaining a better knowledge of these interactions. This study will find importance in Pharmaceutical, cosmetics, chemical industries.

The volumetric, viscometric, conductometric, refractive index and surface tension studies helped us to evaluate the extent of molecular interaction in a particular solutions quantitatively whereas the spectroscopic studies gave an insight into the type of molecular occurring in a given systems.

In Chapter IV, after a wide study on volumetric, viscometric and refractometric investigations of three simple amino acids in aq.18C6 reveals that the overall molecular interaction of amino acids with co solutes follows the order : glycine < L-alanine < L-isoleucine. Therefore, this behavior suggests that although ion-ion or hydrophilic-hydrophilic group interactions are predominant for glycine and L-alanine, ion-hydrophobic or hydrophobic-hydrophobic group interactions are predominant for L-isoleucine in aq.18C6 solutions. The size and number of carbon atoms of the alkyl groups of the amino acids also play an important role in determining the solvation consequences on the selected solvent systems.

In Chapter V, the extensive study based on surface tension and conductance data it was supported that an inclusion complex between studied IL and α -CD was formed. In NMR study, the changes in the chemical shift corresponding to H⁵ and H³ protons of host and guest establish the formation of IL- α -CD inclusion complex in aqueous solution. The Job plot of the UV-Vis spectrum proves also the inclusion complex formation in aqueous solution. The results point out that α -CD and IL finally form steady inclusion complex (IC) with a 1:1 stoichiometry. They both are

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promoting to each other owing to hydrophobic and hydrophilic interactions among them.

In Chapter VI, after a thorough investigation of interaction of Citric acid with Uric acid reveals that there is a strong interaction between citric acid and uric acid and it becomes stronger with rise in temperature. As molecules of uric acid are engaged with the citric acid's molecules, the accumulation among the uric acid molecules becomes less effective. Therefore, the process of crystallization and deposition of uric acid gets hampered in presence of citric acid. The above fact suggests that the relief of painful effect of gout can be achieved by consumption of more citrus fruits and by making warmth the affected area.

In Chapter VII, reveals the conductivity data communicates the complex formation of crown ethers with IL molecule, which are consistent with the surface tension measurements and ^1H NMR spectra. The studied complexes are mainly stabilised by hydrogen bonds and ion-dipole interactions play only a secondary role. Larger formation constant value for complex with 15-C-5 compared to that with 18-C-8 determined by conductivity study indicates that imidazolium cation form stable complex with 15-C-5 compared to 18-C-8 in aqueous solution. The 1:1 complexation of the imidazolium based IL by different crown ethers is driven by favourable stabilised interactions. This study also helps to get important information about the other host-guest systems having crown ethers. This complexation study of imidazolium ion provide further information on the nature of the complexation between positively charged organic guests and macrocyclic polyethers. This study is also significant for the understanding of the vital role of imidazolium cation in the design and construction of supramolecular host-guest materials.

In Chapter VIII, quantifies experimentally the ion-solvent interactions, solvation behaviour and solution structure of the three amino acids as a function of concentration in aq. $[\text{bmpyrr}]\text{PF}_6$. It is no doubt that the ion-solvent interaction is dominant over the interaction of ion or solute itself. The work also provided the qualitative and quantitative statement that the ion-solvent interaction or ion-solvation behaviour are higher for L-Histidine than L-Proline, which is in turn greater than L-Serine; and these ion-solvation is strengthen with increasing mass

fraction of [bmpyrr]PF₆ in aqueous media. The parameters resolved by the chemical analysis of different equations improved with experimental data sustain the same culmination discussed and explained in this study demanding the uniqueness of the work.

In Chapter IX, disclose the extensive study of IL, [BTMA]Cl in 1-Hexanol, 1-Heptanol and 1-Octanol leads to the conclude that, the IL is more associated in 1-Octanol than the other two solvents. It can also be found that in the conductometric studies in 1-Heptanol and 1-Octanol the [BTMA]Cl mostly remains as triple-ions than ion-pairs but in 1-Hexanol the [BTMA]Cl remains as ion-pairs. There is more ion-solvent interaction in 1-Octanol than 1-Heptanol than 1-Hexanol. The experimental values obtained from the volumetric, viscometric and refractometric studies also suggest that in solution the ion-solvent interaction is more than the ion-ion interaction due to the greater covalent interaction (van der Waals' interaction) between the hydrocarbon part of [BTMA]Cl and the hydrocarbon chain of 1-Alkanols. As the length of the alkyl-chain decreases the extent of van der Waals' force of attraction decreases hence the extent of ion-solvent interaction of [BTMA]Cl is enhanced by the following order:



The proper understanding of the solute-solute and solute-solvent interactions may form the basis of explaining quantitatively the influence of solvents and the ions in solution and thus pave the way for real understanding of different phenomena associated with solution chemistry.

Excess and bulk properties are fundamentally important in understanding the intermolecular interactions between dissimilar molecules and in developing the thermodynamic models. Furthermore, thermodynamic properties of solvent mixtures, containing substances capable of undergoing specific interactions, exhibit significant deviation from ideality arising not only from difference in molecular size and shape but also due to structural changes. It has been found that the addition of compound could either break or make the structure of solvent. Because a solvent's viscosity depends on the intermolecular forces, the structural aspects of the solvent

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can be inferred from the viscosity of solutions at different temperatures and concentrations.

Mixed solvents enable the variation of properties such as dielectric constant or viscosity, and therefore the solute-solute and solute-solvent interactions can be better studied. A number of conductometric and related studies of different electrolytes in nonaqueous solvents have been made for their optimal use in high-energy batteries and for understanding organic reaction mechanisms.

Spectroscopic techniques such as NMR, UV-Visible are very useful to quantify the host-guest chemistry. Nuclear magnetic resonance (NMR) is one of the most powerful spectroscopic techniques in analytical chemistry. It is an important tool for studies of host-guest complexes, for elucidating the structure of various complexes existing in the form of aggregates, ion pair or encapsulated system. By measuring chemical shifts (most commonly, proton) of different nuclei (host and guest) the binding activity between host and guest has been recognized. UV-Visible spectroscopy also helpful to understand the formation of inclusion complex, stoichiometry and association constant (using Benesi-Hildebrand method). There are various applications of Host-guest chemistry such as host-guest systems have been used to remove hazardous substances from the environment.

However, it is necessary to remember that the molecular interactions are very complex in nature. There are various forces existing in the molecule and it is not really possible to separate them all. Nevertheless, if careful judgement is considered, valid conclusions can be drawn in many cases relating to the degree of structure and order of the system.

To conclude it may be stated that diverse interactions studies of ionic liquid and biologically active solutes will be of immense helpful in understanding the nature of various interactions prevailing in varied solution environments.