

CHAPTER - X

CONCLUDING REMARKS

The aim of the works embodied in this thesis was to explore the assortment of interfaces of some Ionic Liquids by physicochemical approach. Here, I have studied the molecular as well as ionic interaction on ionic liquids in some solvent systems. 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.

The study reported in this thesis explains the procedures and results as well as the studies of the molecular interactions of ionic liquids in different solvent systems and somewhere ionic liquid as solvent media with other as solute. The overall goal was to look into the structure, property and interaction of ionic liquids in different solvent media. Therefore the systematic study of these properties has great importance in gaining a better knowledge about different interactions.

The volumetric, viscometric, interferometric, conductometric refractive index studies helped us to evaluate the extent of molecular interaction in a particular solution quantitatively whereas the spectroscopic measurements gave an insight into the type of molecular interaction occurring in any solution systems. Various types of interactions exist between the ions in solutions, and of these, ion-ion and ion-solvent interactions are of current interest in all branches of chemistry. These interactions help in better

understanding the nature of solute and solvent, that is, whether the solute modifies or distorts the structure of the solvent.

The study of density, viscosity, conductance and FT-IR of an ionic liquid (1-butyl-2,3-dimethyl imidazolium tetrafluoroborate) ([bmmim][BF₄]) in some assorted solvents like N,N-dimethylacetamide (DMA), Tetrahydrofuran (THF) and 2-methoxy ethanol or methyl cellosolve (MC), to investigate the solvation consequences analysed by different appropriate equations, reveal in Chapter IV. In conclusion it has been seen that the IL is more associated in MC than the other two solvents. It can also be seen that in the conductometric studies in THF the [bmmim][BF₄] mostly remains as triple-ions than ion-pairs but in MC and DMA the [bmmim][BF₄] remains as ion-pairs. There is more ion-solvent interaction in MC than DMA. The experimental values obtained from the volumetric, viscometric studies suggest that in solution there is more ion-solvent interaction than the ion-ion interaction and the extent of ion-solvent interaction of [bmmim][BF₄] in MC, DMA and THF, respectively.

Considering the special structure and properties of β -Cyclodextrin and N-butyl-4-methylpyridinium chloride ([C₄mpy]Cl), I have tried to investigate in Chapter V the complexation behavior between them using selected techniques as well as the stoichiometry of the inclusion complexes (ICs) formed by surface tension and conductance measurements. The results point out that β -CD and ([C₄mpy]Cl) finally form stable inclusion complexes (ICs) with a 1:1 stoichiometry. They both are promoting to each other due to hydrophilic and hydrophobic interactions among them. The experimental values

obtained from the volumetric, viscometric and refractometric studies also support the data and results observed from surface tension and conductance measurements.

To ascertain the nature of ion-association of ionic liquid (IL) tetrabutylphosphonium methanesulfonate [Bu₄PMS] in aqueous (H₂O) and non-aqueous polar protic/aprotic solvents, acetonitrile (CH₃CN), methanol (CH₃OH), nitromethane (CH₃NO₂), and formamide (HCONH₂) the different studies have been done which have been reported in Chapter VI. The solvation phenomenon is evident by the change of the variational intensity of characteristic bands in FTIR spectroscopy due to the presence of the [Bu₄PMS]. It concludes that the electrolyte (IL) exists as ion-pair in all the studied solutions. The tendency of the ion-pair depends on the size the charge distribution of the ions, and structural aspects (functional group of the solvents). The diffusion coefficient and the ionic mobility decrease from acetonitrile to formamide for both the [Bu₄P]⁺ and MS⁻ ions showing greater ion-solvent interaction in formamide than the other studied solvents. In all the solvents the electrolyte forms ion-dipole interactions as evident from the FTIR studies.

The volumetric, viscometric and acoustic behavior of solutes is very much useful in elucidating the various interactions occurring in solutions. Studies on the effect of concentration (molality), the apparent molar volumes of solutes have been extensively used to obtain information on solute-solute, solute-solvent, and solvent-solvent interactions. A systematic study on the density, viscosity, refractive index and ultrasonic speed of some amino acids in aqueous 1-butylpyridinium bromide ([BPy]Br)solutions at 298.15 K has been stated in Chapter VII to obtain the limiting apparent molar volumes (ϕ_V^0), experimental slopes (S_V^*) and viscosity *B*-coefficients, molar refraction (R_M) and limiting

apparent molar adiabatic compressibility (ϕ_k^0) in solution. The results point out that the association of the investigated amino acids, the L-Valine is greater than L-Alanine which is, in turn, greater than that Glycine. The refractive index and the molar refraction values suggest that the molecules of L-Valine are more tightly packed in the solution leading to higher solute-solvent interaction than L-Glycine and L-Alanine. The thorough study of amino acids in Ionic Liquid solution indicates that the solute-solvent interaction dominates over the solute-solute interaction. Moreover, this study demands a novelty of some amino acids prevailing in the aqueous solutions of 1-butylpyridinium bromide ([BPy]Br).

The nature of the formation of inclusion complexes of IL, 1-methyl-3-octylimidazolium chloride ([mocimm]Cl) insight into the β -cyclodextrin in $w_1=0.001, 0.003, 0.005$ mass fraction of aq. β -cyclodextrin media by conductance, surface tension and spectroscopic (UV-Vis and NMR) study have been revealed in Chapter VIII. The results point out that β -CD and IL finally form stable inclusion complexes (ICs) with a 1:1 stoichiometry. They both are promoting to each other due to hydrophilic and hydrophobic interactions among them. The experimental values obtained from the spectroscopic studies also confirm the data and results observed from surface tension and conductance measurements.

Density, viscosity, refractive index, conductance and FT-IR study of an ionic liquid, 1-butyl-pyridinium bromide ([bupy]Br) in assorted solvents (1,4 DO, THF and ACN) have been studied in Chapter IX to explore the solvation consequences analyzed by different appropriate equations. The results disclose that the salt is more associated in 1,4 DO than the other two solvents. It can also be found that in the conductometric study, the

[bupy][Br] in 1,4 DO and THF mostly remains as triple-ions than ion-pairs but in ACN the [bupy][Br] remains as ion-pairs. The experimental values obtained from the volumetric, viscometric and refractometric studies provide the same agreement as derived from conductometric study. Further, the extent of ion–solvent interaction of [bupy][Br] is enhanced by the following order:

1,4 DO>THF>ACN.

The overall consequential conclusion is caused due to the diverse permittivity of the solvents.

The broad studies of the different physicochemical, thermodynamic, transport and spectral properties of the ionic liquids in different solvents will be of sufficient in understanding the nature of the ion-solvent interactions and the role of solvents in different chemical processes. Here in this research work I have also tried to explore the formation of Host-Guest inclusion complexes between ionic liquids and cyclodextrins and the formed inclusion complexes have been confirmed by Conductance, Surface tension, UV-Visible and NMR spectroscopy. Such type of ionic liquids are very important in pharmaceutical industry, cosmetic and hygiene industries, food industries, paint industries and it also increases in speed of diagnostic test reaction. So, it may be concluded that our research work has adequate significance in the different branches of Sciences and demands a far reaching effect for the augmentation of the advanced research.