

## CHAPTER – A

### **A.1: Fundamental of the Research Work**

#### **A.1.1. Object and application of the research work:**

The study of physico-chemical techniques of solute-solvent<sup>1-3</sup> and solvent-solvent<sup>4-6</sup> systems are very useful because the physico-chemical properties play a pivotal role to explore the intermolecular interactions among mixed components especially to understand the such properties at microscopic and macroscopic levels. In order to understand the strength and nature of the interactions, transport properties of electrolytes, thermodynamic and acoustic studies involving binary and ternary systems of solvent and of one or more solutes in pure solvent and mixed solvent systems are very useful. The excess thermodynamic properties of the mixtures correspond to the difference between the actual property and the property if the system behaves ideally. Thus these properties provide important information about the nature and strength of intermolecular forces operating among mixed components.

The study of viscous synergy and antagonism is important, gives the mutual enhancement or decrement of the physico-chemical, biological or pharmaceutical activity between different components of a given mixture. Thus it helps to yield the desired physical structure and properties<sup>7</sup>. If the total viscosity of the system is equal to the sum of the viscosities of each component considered separately, the system<sup>8,9</sup> is said to lack interaction.

The applications and implications of the studies of reaction in non-aqueous and mixed solvents have been summarized by Meck<sup>10</sup>, Franks<sup>11</sup>, Popovych<sup>12</sup>, Bates<sup>13</sup>, Parker<sup>14</sup>, Criss and Salomon<sup>15</sup>, Marcus<sup>16</sup> and others<sup>17-19</sup>. The solute-solute and solute-solvent interactions have been subject of wide interest as apparent from Faraday Transactions of the chemical society<sup>20</sup>.

In solution chemistry the molecular interactions forms the basis of explaining quantitatively the influence of the solvent and the extent of interactions of ions in solvents. Estimates of ion-solvent interactions can be had thermodynamically and also from the measurement of partial molar volumes, viscosity *B*-coefficient and limiting ionic conductivity studies. Estimates of single-ion values enable us to refine our model of ion-

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solvent interactions. Acceptable values of ion-solvent interactions would enable the chemists to choose solvents that will enhance (i) the rates of chemical reactions, (ii) the solubility of minerals in leaching operations or (iii) reverse the direction of equilibrium reactions.

In spite of wide collections of data on the different electrolytic and non-electrolytic solutions in water, the structure of water and the different types of interactions that water undergoes with electrolytes are yet to be properly understood. However, the studies on properties of aqueous solutions have provided sufficient information on the thermodynamic properties of different electrolytes and non-electrolytes, the effects of variation in ionic structure, ionic mobility and common ions along with a host of other properties<sup>11,21</sup>.

In recent years, there has been increasing interest in the behavior of electrolytes or solutes in non-aqueous and mixed solvents with a view to investigate solute-solute and solute-solvent interactions under varied conditions. However, different sequence of solubility, difference in solvating power and possibilities of chemical or electrochemical reactions unfamiliar in aqueous chemistry have opened vistas for physical chemists and interest in these organic solvents transcends the traditional boundaries of inorganic, physical, organic, analytical and electrochemistry<sup>22</sup>.

Fundamental research on non-aqueous electrolyte solutions has catalyzed their wide technical applications in many fields. Non-aqueous electrolyte solutions are actually competing with other ionic conductors, especially at ambient and at low temperatures, due to their high flexibility based on the choice of numerous solvents, additives and electrolytes with widely varying properties. High-energy primary and secondary batteries, wet double-layer capacitors and super capacitors, electro-deposition and electroplating are some devices and processes for which the use of non-aqueous electrolyte solutions had brought the biggest successes<sup>23-25</sup>. Other fields where non-aqueous electrolyte solutions are broadly used include electrochromic displays and smart windows, photo-electrochemical cells, electro-machining, etching, polishing and electro-synthesis. In spite of wide technical applications, our understanding of these systems at a quantitative level is still not clear. The main reason for this is the absence of detailed information about the nature and strength of molecular interactions and their influence on structural and dynamic properties of non-aqueous electrolyte solutions.

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The influence of these solute-solvent interactions is sufficiently large to cause dramatic changes in chemical reactions involving ions. The changes in ionic solvation have important applications in diverse areas such as organic and inorganic synthesis, studies of reaction mechanisms, non-aqueous battery technology and extraction<sup>26,27,28</sup>.

As a result of extensive studies in aqueous, non-aqueous and mixed solvents, it has become evident that the majority of the solutes are significantly influenced by the solvents. Conversely, the nature of strongly structured solvents like water, is substantially modified by the presence of solutes<sup>29</sup>.

The knowledge of ion-solvent, solvent-solvent interactions in non-aqueous solutions<sup>18</sup> from practical and theoretical point of view is very important in many practical problems concerning energy transport, heat transport, mass transport and fluid flow. Besides finding applications in engineering branch, the study is important in understanding liquid theories.

The real understanding of the molecular interactions is a difficult task, as the aspect embraces a wide range of topics here we have analysed on a series of investigations based on the volumetric, viscometric, interferometric and conductometric behavior to study the chemical nature of the structure of solutes and solvents and their mutual and specific interactions in solution.

### A.1.2. Importance and scope of physico-chemical parameters:

The study of physico-chemical properties involves the interpretation of the excess properties to understand the nature of intermolecular interaction among the mixed solvents. The interactions between molecules can be established from a study of characteristic departure from ideal behavior of some physical properties such as density, volume, viscosity, compressibility etc<sup>30,31</sup>.

Density of solvent mixtures and related volumetric properties like excess molar volume are essential for theoretical as well as practical aspects. The sign and magnitude of excess molar volume imparts estimate of strength of unlike interactions in the binaries. The negative values of excess molar volume ( $V^E$ ) suggest specific interactions<sup>32,33</sup> between the mixing components in the mixtures while its positive values imply the dominance of dispersion forces<sup>32,33</sup> between them. The negative  $V^E$  values indicate the specific interactions such as intermolecular hydrogen bonding between the mixing components and also the interstitial

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accommodation of the mixing components because of the difference in molar volume. The negative  $V^E$  values may also be due to the difference in the dielectric constants of the liquid components of the binary mixture<sup>32</sup>.

Drug transport across biological cells and membranes is dependent on physico-chemical properties of drugs. But direct study of the physico-chemical properties in physiological media such as blood, intracellular fluids is difficult to accomplish. One of the well-organized approaches is the study of molecular interactions in fluids by thermodynamic methods as thermodynamic parameters are convenient for interpreting intermolecular interactions in solution phase. Also the study of thermodynamic properties of drug in a suitable medium can be correlated to its therapeutic effects<sup>26,27</sup> These facts therefore prompted us to undertake the study of binary or ternary solvent systems with 1,4-dioxane and 1,3-dioxolane or tetrahydrofuran as primary solvents with some polar, weakly polar and non-polar solvents as well as with some solutes. Furthermore, the excess properties derived from experimental density, viscosity and speeds of sound data and subsequent interpretation of the nature and strength of intermolecular interactions help in testing and development of various theories of solution.

Viscosity data provides valuable information about the nature and strength of forces operating within and between the unlike molecules. Recently the employment of computer simulation of molecular dynamics has led to significant improvement towards a successful molecular theory of transport properties in fluids and a proper understanding of molecular motions and interaction patterns in non-electrolytic solvent mixtures involving both hydrogen bonding and non-hydrogen bonding solvents<sup>34,35</sup>. The study of physico-chemical behaviors like dissociation or association from acoustic measurements and from the calculation of isentropic compressibility has gained much importance. Excess isentropic compressibility, intermolecular free length etc impart valuable information about the structure and molecular interactions in pure and mixed solvents. The acoustic measurements can also be used for the test of various solvent theories and statistical.

### A.1.3. Importance of solvents used:

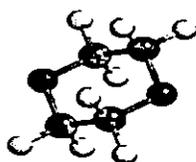
N,N-dimethylformamide, acetonitrile, acrylonitrile, dimethylsulfoxide, 2-butanone, some monoalkanols viz. methanol, ethanol, 1-propanol, 2-propanol, 1-propanol, 2-propanol,

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1-butanol, 2-butanol, 1-pentanol and isoamylalcohol, and some cyclic as well as acyclic ethers viz., 1,4-dioxane, 1,3-dioxolane, tetrahydrofuran, cyclohexylamine, cyclohexanone, butylacetate, butanone, butylamine, tert-butylamine, 2-butoxyethanol, some aromatic aldehydes viz. cinnamaldehyde, anisaldehyde and benzaldehyde along with water considered as a universal solvent have been chosen as main solvents in this research work. The study of these solvents, in general, is of great interest because of their wide use as solvents and solubilizing agents in many industries ranging from pharmaceutical to cosmetics.

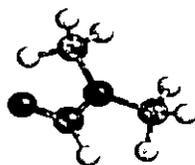
1,4-dioxane is very hygroscopic and miscible in all proportions with water. Its dielectric constant and dipole moment are 2.209 and 0.45D respectively at 25°C. However, its dipole moment rises with increase in temperature suggesting formation of boat form<sup>22</sup>.

1,4-dioxane is cyclic diether and they figure prominently in the high-energy battery technology<sup>38</sup>, in electrical conductance studies<sup>38</sup> and have also found application in organic synthesis as manifested from the physico-chemical studies in these media. 1,4-dioxane and 1,3-dioxolane differ in one methylene group and thus they differ in quadrupolar and dipolar order<sup>39</sup>.



1,4-dioxane

N,N-dimethylformamide is a non-associative aprotic protophilic solvent with a liquid range of -60°C to 153°C, low vapour pressure and good solubility for a wide range of substances. It is also used in the separation of saturated and unsaturated hydrocarbons and serves as solvents for vinyl resins, acid gases, polyacrylic fibres and catalyst in carbonylation reaction as well as in organic synthesis. It has also been used as the model of peptide linkage in studies aimed at understanding of protein denaturation studies<sup>40,41</sup>.

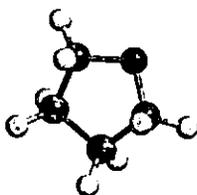


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### N,N-dimethylformamide

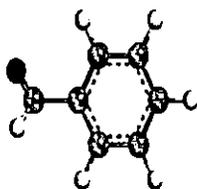
The increasing use of 1,3-dioxolane, 1,4-dioxane, tetrahydrofuran and their aqueous or binary liquid mixtures in many industrial processes have greatly stimulated the need for extensive information on their various properties. Viscosity and density of these liquid mixtures are used to understand molecular interactions between the components of the mixture to develop new theoretical models and also for engineering applications<sup>42,43</sup>.

Tetrahydrofuran and its mixtures are the very important solvents widely used in various industries. This is a good industrial solvent and figures prominently in the high-energy battery technologies and has sound its application in organic syntheses as manifested from the physico-chemical studies in this medium<sup>44</sup>



Tetrahydrifuran

Benzaldehyde is used- (i) for flavouring purposes, in perfumery; (ii) in the manufacture of dyes; and (iii) as a starting material for the synthesis of several other organic compounds, e.g., cinnamaldehyde, cinnamic acid, benzoyl chloride, etc<sup>45</sup>.



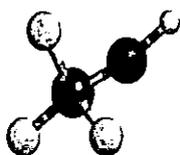
Benzaldehyde

Alcohols and their aqueous and non-aqueous mixtures are widely used in pharmaceutical industry as excipients in different formulations or as solvents. Alcohols have varied applications in chemical and cosmetic industries. These are useful in enology and as

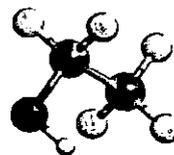
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an alternative energy source<sup>46</sup>. Knowledge of their physico-chemical characteristics helps to understand their behavior in a better way.

Methanol is used as solvent for paints and varnishes, antifreeze for automobile radiators, motor fuel, denaturant for ethanol, etc. It is obtainable commercially in adequate purity for most purposes, the principle impurity being up to 0.05% water usually be removed by distillation, or by use of molecular sieves and calcium hydride.



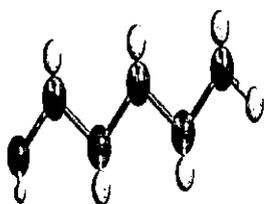
Methanol



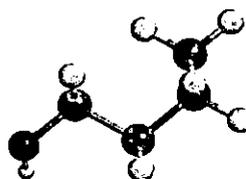
Ethanol

Ethanol has been used as a solvent in quantitative studies and 'Absolute' alcohol usually contains 0.01% water.

The Amylcohols are used fundamentally for the perfumes composition and the synthesis of fruit essences. They are also used as solvents for surfaces and lacquer baths, inks for paint and dyes for wool as well as in the chemical production of photographic and pharmaceutical substances . Furthermore, they are an intermediate in the production of amylacetate and other amyl esters.



Amyl alcohol



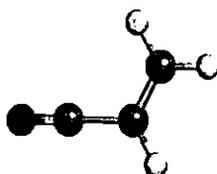
iso-amyl alcohol

The importance of iso-amyl alcohol in research field is implied for its usefulness in gas chromatography. It can isolate high quality RNA from even the hardest to isolate samples for immediate use in micro array application and it is also useful in most DNA applications<sup>47</sup>

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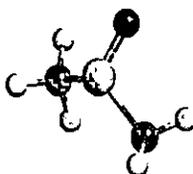
However, it is worth mentioning that 1,4-dioxane differs from alcohols in its behaviour towards water. Alcohols are usually structure makers whereas 1,4-dioxane acts as a net structure breaker<sup>48</sup>. Aqueous 1,4-dioxane mixtures have been found to be more basic than water and the basicity has been found to be maximum in the region 45-50 mass% of 1,4-dioxane<sup>49</sup>.

The study of mixtures of acrylonitrile in various solvents is of interest because of its wide use as an important industrial monomer for polyacrylonitrile as well as for investigating the effect of the simultaneous presence of the C=C double bond and the polar nitrile C≡N group on the molecular interactions. Further, the properties of liquid mixtures are also very important for polymer solubility, since some of the polymers which are insoluble in a single solvent can be dissolved in a solvent mixture. This behavior depends not only on the interactions between the polymer and each one of the liquids but also on the interactions between the liquids themselves. In fact, these interactions are decisive in determining the solubilization of the polymer and the coiling expansion of the polymer chains in solution<sup>50</sup>.



Acrylonitrile

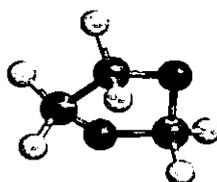
Dimethylsulphoxide is a powerful broad spectrum solvent for a wide variety of inorganic and organic reactants. Having low toxicity, it can be used in biology and medicine, especially for low-temperature preservation<sup>51</sup>.



Dimethylsulphoxide

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1,3-dioxolane is cyclic diether and it figure prominently in the high energy battery technology<sup>38</sup> and have also found application in organic synthesis as manifested from the physico-chemical studies in this media.



1,3-dioxolane

Water is the most widely used solvent in the chemical industries, since it is the most physiological and best tolerated recipient. However, in some cases, water cannot be used as a solvent because the active substance or solute is insoluble or slightly soluble in it. The non-aqueous solvents with common characteristics of being soluble or miscible in water are thus used. Such solvents can be used to prepare binary or ternary mixtures and they can serve different purposes such as increasing water solubility, modifying the viscosity, absorption of the dissolved substance.

The knowledge of the type and structure of the complex species in solution is essential for the optimal choice of solvents. Even though these solvents have drawn much focus in recent years as solvents for physico-chemical investigations, still a lot remains to be explored.

### A.1.4. Method of Investigations:

The phenomenon of ion-ion or solute-solute, ion-solvent or solute-solvent and solvent-solvent synergy, and antagonism, are intriguing. It is desirable to explore these interactions using different experimental techniques. We have, therefore, employed four important methods, viz. densitometry, viscometry, ultrasonic interferometry and conductometry in our research works.

Viscosity and density have been used to interpret the synergic and antagonic behavior in the solvent mixtures. The values of synergic and antagonic interaction indices determine the nature of the molecular package. Thermodynamic properties of solutions are not only

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useful for estimation of feasibility of chemical reactions in solution, but they also offer one of the better methods of investigating the theoretical aspects of solution structure.

Thermodynamic properties, like apparent molar volume, partial molar expansibility, etc. obtained from density measurements, are generally convenient parameters for interpreting ion-ion and ion-solvent interactions in solution.

The change in solvent viscosity by the addition of electrolytes is attributed to inter-ionic and ion-solvent effects. The *B*-coefficients gives a satisfactory interpretation of ion-solvent interactions such as the effects of solvation, preferential solvation and structure-breaking or structure-making capacity of the solutes.

The compressibility, a second derivative of Gibbs energy, is also a sensitive indicator of molecular interactions and provides useful information in such cases where partial molar volume data alone cannot provide an unequivocal interpretation of these interactions. Various acoustical parameters have been derived in carrying out the investigations.

The excess properties such as excess molar volume, viscosity deviations and deviation in isentropic compressibility along with the correlating equations explain molecular interactions in a more effective way.

The transport properties are studied using the conductance data, specially the conductance at infinite dilution. Conductance data obtained as a function of concentration are used to study the ion-association with the help of appropriate equations.

### A.1.5. Summary of the works done:

## Chapter-A

### Chapter A.1.

This chapter contains the object and applications of the research work, the reasons for choosing the main solvents and solutes and methods of investigation. This also includes a summary of the works relating to this thesis.

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### **Chapter A.2.**

This chapter contains the general introduction of the thesis and forms a background of the works embodied in the thesis. A brief review of notable works on the behavior of viscous synergy and antagonism, ion-ion or solute-solute, ion-solvent or solute-solvent and solvent-solvent interaction has been made. Also an attempt has been made to define these interactions. Various derived parameters dependent on density, viscosity, ultrasonic speed of sound and conductance along with their importance in solution chemistry has been discussed. Several semi-empirical models to estimate dynamic viscosity of binary liquid mixtures have been discussed. Ionic association and its dependence on ion-size parameters as well as relation between solution viscosity and limiting conductance of an ion has been discussed using Stokes' law and Walden rule. Critical evaluations of different methods employed frequently for obtaining the single ion values (viscosity  $B$ -coefficient and limiting equivalent conductance) and their implications have been discussed stressing the importance of the work associated with the thesis

### **Chapter A.3.**

This chapter contains the experimental section mainly involving the source and purification of the solvents and solutes used and the details of the experimental methods applied for measurement of the thermodynamic, transport and acoustic properties.

## **Chapter-B**

### **Chapter B.1.**

This chapter includes the study on interaction between solvent-solvent occurring in binary mixtures of acrylonitrile with some aromatic aldehydes by volumetric, viscometric and acoustic measurements. The excess molar volume ( $V^E$ ) and viscosity deviations ( $\Delta\eta$ ) have been derived from density ( $\rho$ ) and viscosity ( $\eta$ ) data of the binary mixtures of acrylonitrile with anisaldehyde, cinnamaldehyde, and benzaldehyde measured at 298.15, 308.15, and 318.15K. The data have been correlated with the Grunberg-Nissan equation. Moreover, deviations in isentropic compressibility ( $\Delta K_S$ ) have been calculated from ultrasonic speed

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measurements of these binary mixtures at 298.15, 308.15 and 318.15 K. The results have been discussed in terms of molecular interactions and structural effects.

### Chapter B.2.

In this chapter Densities and viscosities and ultrasonic speeds have been measured for the binary mixtures of cyclohexylamine and cyclohexanone with butyl acetate, butanone, butylamine, *tert*-butylamine and 2-butoxyethanol at 298.15 K over the entire composition range. From density and viscosity data, the values of excess molar volume ( $V^E$ ) and viscosity deviation ( $\Delta\eta$ ) and Gibbs excess energy of activation for viscous flow ( $G^{*E}$ ) have been determined.. Furthermore, deviation in isentropic compressibilities ( $\Delta K_S$ ) have been calculated from ultrasonic speed measurements of these binary mixtures at 298.15 K. These results have been fitted to Redlich–Kister polynomial equation to estimate the binary coefficients and standard errors between the experimental and the computed values. The density and viscosity data have been analyzed in terms of some semiempirical viscosity models and the results have been discussed in terms of molecular interactions and structural effects.

### Chapter B.3.

Study of densities, viscosities and speeds of sound have been measured for the ternary liquid mixtures of 1,4-dioxane + N,N-dimethylformamide + monoalkanols as a function of the composition at 298.15 K. From the experimental measurements excess molar volumes ( $V^E$ ), viscosity deviation ( $\Delta\eta$ ), Antagonic Index ( $I_A$ ) The speeds of sound of these ternary mixtures have been measured over the whole composition range at the same temperatures (298.15K) and also, the isentropic compressibilities ( $K_S$ ) and excess isentropic compressibilities ( $K_S^E$ ) have been evaluated from the experimental data. The variation of  $V^E$ ,  $\eta_{\max}$  and  $I_A$  with the number of carbon atoms are also shown. The results get a clear idea about the type and amount of molecular interactions between them and also given us an idea about antagonism. The lower monoalkanols are found to associate more with others molecules whereas self-association between the alcohol molecules was found to increase with increasing chain length because as the chain length of the alkane groups in the alkanols

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increases, their electron releasing ability increases, thereby decreasing the polarity of the –OH group. In case of isomers, steric effect becomes the deciding factor. Here due to large and complex size of the secondary alkanols compared to the primary ones, the 1,4-dioxane molecules cannot easily disrupt the molecular package formed between DMF and alcohols. Thus, the mutual attraction remains greater for the 2°-isomers. an example is shown here:

### Chapter-C

#### Chapter C.1.

In this chapter electrolytic conductivities of some alkali metal halides,  $\text{MX}$  ( $\text{M}^+ = \text{Li}^+, \text{Na}^+ \& \text{K}^+$ ;  $\text{X}^- = \text{Cl}^-, \text{Br}^- \& \text{I}^-$ ),  $\text{NaBPh}_4$  and  $\text{Bu}_4\text{NBr}$  have been investigated in 20, 40 and 60 mass% of dimethyl sulfoxide (DMSO) in DMSO + Acetonitrile mixtures at 298.15 K. The conductance data have been analyzed by the Fuoss conductance equation in terms of the limiting molar conductance ( $\Lambda_0$ ), the association constant ( $K_A$ ) and the association diameter ( $R$ ). The limiting ionic conductances have been estimated from the appropriate division of the limiting molar conductivity value of the “reference electrolyte”  $\text{Bu}_4\text{NBPh}_4$ . The cations are found to be substantially solvated in both solvent mixtures whereas the anions appear to have weak interactions with the solvent molecules. The results further indicate that the coulombic forces play a major role in the ion association processes.

#### Chapter C.2.

In this chapter electrical conductances of some tetraalkylammonium halides have been measured in THF + 1,4-DO mixtures with 10, 20, and 30 mass percent at 298.15 K. Minima in the conductometric curves ( $\Lambda$  versus  $\sqrt{c}$ ) were observed for electrolyte concentrations dependent upon both the electrolyte and the binary solvent mixture. The conductance data have been analyzed by the Fuoss-Kraus theory of triple ions. A numerical evaluation of ion-pair and triple-ion formation constants ( $K_p$  and  $K_T$ ) were made and the results have been discussed in terms of molecular scale model. The existence of triple-ions might be inferred in solutions due to coulombic interactions and covalent bonding forces between the ions ( $\text{R}_4\text{N}^+ \dots \text{X}^-$ ).

### Chapter-D

#### Chapter D.1.

This chapter includes the volumetric, viscometric, and ultrasonic studies of tetrabutylammonium bromide in aqueous binary mixtures of ascorbic acid (0.00, 10, 20 and 30 mass % ascorbic acid) at different temperatures (298.15, 308.15, and 318.15) K. The experimental values of  $\rho$  were used to calculate the values of the apparent molar volume ( $V_\phi$ ). The limiting apparent molar volume ( $V_\phi^0$ ) and the experimental slope ( $S_V^*$ ) have been interpreted in terms of ion-solvent and ion-ion interactions respectively. The structure making / breaking capacities of the (1:1) electrolytes have been inferred from the sign of  $\left(\frac{\partial^2 V_\phi^0}{\partial T^2}\right)_p$  and  $\frac{dB}{dT}$ . The  $V_\phi^0$  and viscosity  $B$ -coefficient values for TBAB indicate the presence of strong solute-solvent interactions, and these interactions are further strengthened at higher temperatures and higher concentrations of ascorbic acid in ternary solutions. This study also reveals that TBAB acts as a water-structure promoter due to hydrophobic hydration in the presence of ascorbic acid and ascorbic acid has a dehydration effect on the hydrated TBAB.

#### Chapter D.2.

This is chapter consists of Partial molar volumes of oxalic acid and its salts, viz. ammonium oxalate, sodium oxalate and potassium oxalate, have been determined in 5 %, 10 %, and 15 % by mass of 1,3-dioxolane + water mixtures at  $T = (298.15, 308.15, \text{ and } 318.15)$  K and  $p = 0.1$  MPa. Structure making/ breaking capacities of oxalic acid and its salts have been expressed from the sign of  $\left[\frac{\partial^2 V_\phi^0}{\partial T^2}\right]_p$ , i.e. the second derivative of partial molar volume with respect to temperature at constant pressure. The viscosity data have been evaluated using the Jones-Dole equation and the derived parameters,  $B$  and  $A$ , have also been interpreted in terms of solute-solvent and solute-solute interactions, respectively. The oxalic acid and its salts behave as structure breakers in binary aqueous mixtures of 1,3-dioxolane.

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### **Chapter D.3.**

Proteins are complex molecules and their behaviour in solutions is governed by a combination of many specific interactions. One approach that reduces the degree of complexity and requires less complex measurement techniques is to study the interactions in systems containing smaller biomolecules, such as amino acids and peptides. The small amino acid molecules incorporate some of the structural features found in proteins and have been used as model compounds for specific aspects of proteins in aqueous solutions. Some studies have revealed that the presence of an electrolyte drastically affects the behaviors of amino acids in solutions and this fact can be used for their separation and purification. Therefore, in this chapter an attempt has been made to unravel the various interactions prevailing in amino acid in aqueous catechol solutions at 298.15 K

### **Chapter E**

In this chapter the dissertation ends with some concluding remarks mentioning the methods, various equations, importance and application of the work

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