Chapter XII

Concluding Remarks

The aim of the present work was to study the physicochemical properties and to collect new experimental data on properties such as densities, viscosities, conductivities and speeds of sound for various binary liquid systems and salt solutions over the entire range of compositions and at different temperatures. Furthermore, the study involved the evaluation of the apparent molar properties, excess functions, interaction parameters from the experimental data and interpretation of the intermolecular interactions and tesing various existing models of speed of sound. The study was undertaken covering a wide range of solvents and solutes of varying physical and chemical properties. The various solvents and solutes used in the investigation had been chosen mainly on the basis of their industrial applications.

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 found its application in organic syntheses as manifested from the physico-chemical studies in this medium. The alkoxyethanols (2-ethoxyethanol and 2-Methoxyethanol) occupies an important place in many industrial processes such as pharmaceutical and cosmetics industry. Alcohols have varied applications in chemical and cosmetic industries. These are useful in enology and as an alternative energy source. Dimethyl sulfoxide (DMSO) has a wide range of applicability as a solvent in chemical and biological processes. Some alkali metal halides and acetate salts show numerous interesting properties that are now being actively investigated in many laboratories.

A study of densities, viscosities, and ultrasonic speeds for the binary systems of acetonitrile with tetrahydrofuran, 1,3-dioxolane, and 1,4-dioxane at various temperatures over the entire composition range lead to the conclusion that, strong specific interaction is present between acetonitrile and ethers molecules. Dipole-induced dipole interactions are present between the unlike molecules along with the interstitial accommodation of non associated acetonitrile molecules in to the clusters of ether molecules.

The study of excess thermodynamic and transport properties for binary mixtures formed by 2-Ethoxy ethanol with eight monoalcohols suggest that with the increasing chain length, the alkanols tends to dilute the unlike interaction and finally for the higher alkanols this unlike interaction becomes unfavorable. The theoretical values of the sound speed were calculated by using the free length theory, collision factor theory, the Nomoto Equation, the Vandeal Vangael ideal mixing relation, the impedance dependence relation and compared with the experimentally measured sound speed. The results showed that, the Nomoto equation and the Collision factor theory predicts the experimental data extremely well, whereas the Fee length theory gives the maximum deviation for the experimental set of binary mixtures.

The measurement of viscosities and densities of binary liquid mixtures of Tetrahydrofuran with normal hydrocarbons (n-pentane, n-hexane, n-heptane) demonstrates that, the forces between the unlike pairs of molecules are far less than that between like pair of molecules. The effect of temperature increase is to disrupt the homo and hetero association of component molecules in the mixtures.

The examination of the ion-solvent and ion-ion interactions of Resorcinol in 2-Methoxyethanol and Tetrahydrofuran reveals that weak solute-solvent (Resorcinol-ME/THF) interactions are present here, and such interactions increases with rise of temperature whereas the solute-solute interaction in the above case is very strong but diminishes with rise of temperature due to the breaking of non covalent bonding between the solute molecules.

The comparative study of electrical conductance of some alkali chlorides in Methanol - Carbon tetrachloride and - 1,4-dioxane systems gives a clear distinction between the nature of ionic association and mobility of ions in these two systems. It is found that, for these electrolytes having the common anion, as the size of the cation increases, the solvation decreases. All the salts are highly associated in both the solvent mixtures. Also the combination of a solvent of higher permittivity with the one having low viscosity of has comparatively higher mobility resulting in higher conductivity values. The values of Walden product for the studied electrolytes pass through a maximum at a particular mole fraction and then decrease continuously for all the lower mole fractions.

Density, viscosity and compressibility data have been determined for amino acids in aqueous TBAB solutions and the results have been used to estimate the volume and compressibility of transfer, number of hydrated water molecules and the viscosity B-coefficient values. With the increase in concentration of aqueous TBAB in solution, the partial molar quantities also increase. The contribution of the (NH_3^+, COO^-) group to $V_{2,m}^0$ of the amino acids is larger compared to that of the (CH_2) group and increases with the increase of TBAB concentration in the solution. The number of water molecules hydrated to amino acids increases with the increase in hydrophobic content of the amino acids indicating the predominance of hydrophobic interactions between the amino acid and TBAB with increasing number Carbon atoms in the former. It s concluded that, for Glycine and L-alanine, with increasing concentration of co-solute TBAB, more positive $\Delta_{tr}V_{2,m}^0$ and $\Delta_{tr}K_{2,m}^0$ values result indicating an enhancement in the ion-ion interaction. The increased number of hydrophobic groups in these amino acids leads to stronger interaction between the hydrophobic groups of amino acids with hydrophobic groups of TBAB thereby leading to negative volumes of transfer.

We have investigated the molecular interactions of four acetate salts i.e. ammonium acetate, potassium acetate, sodium acetate and lithium acetate in different mass % of water methanol binary solvent mixtures at different temperatures. The study indicates the presence of strong solute-solvent interactions which weakens with rise in temperature, suggesting more electrostrictive solvation at higher temperature. For lithium acetate and sodium acetate in methanol solutions 'caging or packing effect' seems to be present whereas, ammonium acetate and potassium acetate behaves just like common salts in methanol solutions. Lithium acetate and sodium acetate are structure makers in methanol water mixture whereas ammonium acetate and potassium acetate are structure breakers in this mixed solvent system.

A study conducted on the excess thermodynamic and transport properties of binary mixtures of DMSO with butyl acetate, tert-butyl alcohol, n-butyl amine and 2-butanone indicates the presence of Specific interaction between DMSO and n- butyl amine, DMSO + butyl acetate, DMSO + 2-butanone solvent system but in DMSO + t-butyl alcohol solvent system dispersion forces are prevailing.

Most of the present day knowledge on non-aqueous solutions have come from studies on various thermodynamic properties, e.g., density, transport properties, e.g., viscosity, conductance as well as acoustic properties, e.g., ultrasonic speed.

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

Extensive studies of the different physico-chemical, biological or pharmaceutical activity between different components of a given mixture will be of sufficient help in understanding the nature of the different interactions prevailing in systems.