

## **CHAPTER XIII**

### **Concluding Remarks**

The aim of the research works embodied in this thesis was to investigate to solution behavior of some food additives and drugs in different aqueous solvent media in terms of various thermodynamics properties.

The study of solution thermophysics of L-ascorbic acid in aqueous tetrabutylammonium hydrogen sulfate at 298.15, 308.15 and 318.15 K revealed that the standard partial molar volumes ( $\phi_V^0$ ) values for L-ascorbic acid are positive and increase when both the experimental temperatures and TBAHS content in the solvents increase. This trend in  $\phi_V^0$  values indicates the presence of strong solute-solvent interactions and such interactions further strengthen at elevated temperatures and with higher concentrations of TBAHS in the ternary solutions. The  $S_V^*$  values are smaller as compared to the  $\phi_V^0$  values for all the studied solutions and this fact indicates that the solute-solvent or ion-solvent interactions play a dominant role over the solute-solute or ion-ion interactions. The positive  $\Delta_t\phi_V^0$  values indicate that ion-hydrophilic and hydrophilic-hydrophilic group interactions predominate over ion-hydrophobic, hydrophobic-hydrophobic and hydrophilic-hydrophobic interactions.  $(\partial\phi_E^0/\partial T)_P$  and  $\Delta\mu_2^{0\neq}$  values support the fact L-ascorbic acid acts as a net structure promoter for the studied solutions. The viscosity  $B$ -coefficients also support the results obtained from  $\phi_V^0$  values  $S_n$  values indicated that L-ascorbic acid or its constituent ions remain solvated with primary solvation spheres in the aqueous solvent systems investigated.

The study of Volumetric and viscometric studies of thiamine hydrochloride in aqueous solutions of tetrabutylammonium hydrogen sulphate at  $T=(298.15-318.15)$  K revealed that the presence of strong solute-solvent interaction as their partial molar volumes are positive. The positive Hepler's constant  $(\partial\phi_E^0/\partial T)_P$  values suggest that thiamine hydrochloride is a structure maker in this solvent system. The values of Jone-Dole viscosity  $B$ -coefficient are also positive for all solvent systems. It is also indicative of structure promoting affinity of thiamine hydrochloride.  $S_n$  values

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indicated that the thiamine hydrochloride or its constituent ions remain solvated with primary solvation spheres in the aqueous solvent systems investigated and negative  $\Delta S_2^{0\neq}$  and  $\Delta H_2^{0\neq}$  values suggest that the transition state is associated with bond formation (between solute-solvent components) and decrease in order and the viscous process is exothermic in nature.

The study Solution thermodynamics of aqueous nicotinic acid solutions in presence of Tetrabutylammonium Hydrogen Sulphate indicated the presence of strong solute-solvent interactions and such interactions further strengthen at higher nicotinic acid concentrations but decrease at higher temperatures. These facts may be attributed to the predominance of ion-hydrophilic and hydrophilic-hydrophilic group interactions over ion-hydrophobic, hydrophobic-hydrophobic and hydrophilic-hydrophobic interactions. Also the trends in  $(\partial\phi_E^0/\partial T)_P$  and  $\Delta\mu_2^{0\neq}$  for TBAHS in the aqueous solutions of nicotinic acid suggest that TBAHS is a net structure promoter in the studied aqueous solutions and it has a dehydration effect on the hydrated nicotinic acid. Positive  $\Delta H_2^{0\neq}$  values suggest that the viscous process is endothermic in nature and positive  $\Delta S_2^{0\neq}$  values suggest that the slip plane is in ordered state.

The study of Volumetric and viscometric behaviour of pyridoxine hydrochloride in aqueous tetrabutylammonium hydrogen sulphate solutions at different temperatures indicated that solute-solvent interactions are predominant for pyridoxine hydrochloride in the presence of aqueous TBAHS solutions which get strengthened further with the increase of both temperature and TBAHS concentrations. The positive values of the Hepler constant  $(\partial\phi_E^0/\partial T)_P$  and  $\Delta\mu_2^{0\neq}$  suggest that the structure making behaviour of pyridoxine hydrochloride in the presence of aqueous TBAHS solutions.  $S_n$  values indicated that the pyridoxine hydrochloride remain solvated with primary solvation spheres in the aqueous solvent systems investigated. Positive  $\Delta\mu_2^{0\neq}$  values are also indicating that solute-solvent interactions in the ground state are stronger than in the transition state and the viscous flow is exothermic and enthalpy driven are confirmed by the negative values of  $\Delta H_2^{0\neq}$  and  $\Delta S_2^{0\neq}$ .

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The study of the Solution behavior of glycine and L-alanine in aqueous solutions of a tributyl methyl phosphonium based ionic liquid by volumetric and viscometric methods reveals that the  $\phi_V^0$  values for both glycine and L-alanine are positive and increase when both the experimental temperatures and  $[P_{4,4,4,1}][CH_3SO_4]$  content in the solvents increase. This trend in  $\phi_V^0$  values indicates the presence of strong solute-solvent interactions and such interactions further strengthen at elevated temperatures and with higher concentrations of  $[P_{4,4,4,1}][CH_3SO_4]$  in the ternary solutions. The  $S_V^*$  values are always smaller as compared to the  $\phi_V^0$  values for all the studied solutions. So the solutions are predominantly characterized by ion-solvent interactions rather than by ion-ion interactions. The standard partial molar volumes and viscosity  $B$ -coefficient are found greater in case of L-alanine than glycine. Therefore the ion-solvent interaction is greater in case of L-alanine than glycine.  $(\partial\phi_E^0/\partial T)_P$  values suggest that both glycine and L-alanine act as a net structure promoters for the studied IL solutions.  $S_n$  values indicated that the glycine and L-alanine or their constituent ions remain solvated with primary solvation spheres in the aqueous solvent systems investigated.

The study of solution properties and taste behavior of lactose monohydrate in aqueous L-ascorbic acid solutions at different temperatures: Volumetric and rheological approach reveals that solute-solvent interactions are predominant for lactose monohydrate in aqueous L-ascorbic acid solutions and such interactions get strengthened further with the increase of both temperature and L-ascorbic acid concentrations. The positive  $(\partial\phi_E^0/\partial T)_P$  values suggest that the structure making behavior of lactose monohydrate in the aqueous ascorbic acid solutions.  $S_n$  values indicated that the lactose monohydrate remain solvated with primary solvation spheres in the aqueous L-ascorbic acid solutions. The apparent specific volumes increase with the increasing concentration of L-ascorbic acid and therefore the sweetness decreases. Positive  $\Delta\mu_2^{0\neq}$  values indicate that solute-solvent interactions in the ground state are stronger than in the transition state and the viscous flow is entropy driven endothermic process as confirmed by the positive  $\Delta H_2^{0\neq}$  and  $\Delta S_2^{0\neq}$  values.

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The study of Effect of paracetamol in aqueous sodium malonate solutions with reference to volumetric, viscometric and refractometric measurements indicated that  $\phi_V^0$  values are positive and increase when both the experimental temperature and sodium malonate content in the solvents increase. This trend in  $\phi_V^0$  values indicates the presence of strong solute-solvent interactions and such interactions further strengthen at elevated temperatures and with higher concentrations of sodium malonate in the ternary solutions presence of strong solute-solvent interactions and such interactions further strengthen at higher sodium malonate concentrations in the ternaries. The viscosity  $B$ - coefficients for paracetamol in the studied solvent systems are positive and thus suggest the presence of strong solute-solvent interactions in the studies solutions. The apparent molar refractivity and UV-Vis spectroscopy have supported the conclusion obtained from both apparent molar volumes and viscosity  $B$ -coefficient. the trends in  $(d\phi_E^0/dT)_P$  and  $\Delta\mu_2^{0\neq}$  for paracetamol in the aqueous solutions of sodium malonate suggest that paracetamol is a net structure promoter in the studied aqueous solutions but the structure making tendency decreases with the increase in sodium malonate concentration in the ternary solutions.

The study of volumetric and transport properties of betaine hydrochloride drug in aqueous uracil solutions at  $T=(298.15-318.15)$  K indicated the presence of strong solute-solvent interactions and such interactions further strengthen at higher uracil concentrations in the ternaries. Also the trends in  $(d\phi_E^0/dT)_P$  and  $\Delta\mu_2^{0\neq}$  for betaine hydrochloride in the aqueous solutions of uracil suggest that betaine hydrochloride is a net structure promoter in the studied aqueous solutions but the structure making tendency increases with the increase in uracil concentration in the ternary solutions. The negative  $\Delta S_2^{0\neq}$  and  $\Delta H_2^{0\neq}$  values at all the experimental temperatures suggest that the transition state is associated with bond formation and increase in order and the overall viscous process is exothermic.

The study of Volumetric, acoustic and transport properties of metformin hydrochloride drug in aqueous D-glucose solutions at  $T=(298.15-318.15)$  K, the partial molar volumes ( $\phi_V^0$ ), viscosity  $B$ - coefficients and limiting apparent molar adiabatic compressibility ( $\phi_k^0$ ) for metformin hydrochloride in aqueous D-glucose

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solutions indicate the presence of strong solute-solvent interactions and such interactions further strengthen at higher D-glucose concentrations in the ternaries. Also the trends in  $(d\phi_E^0/dT)_P$  and  $\Delta\mu_2^{0\neq}$  for metformin hydrochloride in the aqueous solutions of D-glucose suggest that metformin hydrochloride is a net structure promoter in the studied aqueous solutions but the structure making tendency increases with the increase in D-glucose concentration in the ternary solutions. The negative  $\Delta S_2^{0\neq}$  and  $\Delta H_2^{0\neq}$  values at all the experimental temperatures suggest that the transition state is associated with bond formation and increase in order and the overall viscous process is exothermic.

Anyway, it is necessary to keep in mind that molecular interactions are very complex in nature and quite difficult to explore and interpret. Many forces may operate between the molecules in a solvent mixture and it is really difficult to separate and assign them all. Nevertheless, if careful experimental technique and methodology are used, important conclusions may be obtained regarding the nature of structure and order of the systems in solution phase. The knowledge of the type and structure of the complex species in solution is essential for the optimal choice of solvents for varied applications and proper understanding of the various interactions may constitute the basis of explaining quantitatively the influence of the solvents and ions in solution and thus pave the way for real understanding of different phenomena associated with solution chemistry and still a lot of systems comprising of food additives and drugs dissolved in different aqueous systems remains to be explored.