

CHAPTER XI

Concluding Remarks

The close relationship between the molecular conformation and biological activity for certain biologically important compounds is very fascinating. Concentrations of the solute (biologically important compounds) and temperature can often be used to judge the inter and intra-molecular interactions during their conformational changes. Most of the physico-chemical processes occur in aqueous media, so changes in the solutions structure caused by various solute or cosolutes and temperature may help in proper understanding of the molecular interactions in the aqueous phase. Therefore the aim of the research works embodied in this thesis was to investigate the solution behavior of some biologically important compounds in different aqueous solvent media in terms of various transport and thermodynamics properties.

In Chapter IV the partial molar volumes (ϕ_V^0) and viscosity B -coefficients of nicotinic acid in the aqueous sodium malonate solutions were reported and found to be positive and both these properties increase as the experimental temperature and sodium malonate molalities in the aqueous solutions increase. These results unveil that the solute-solvent or ion-solvent interactions are strong and there is structural enhancement at larger sodium malonate molalities even at higher temperatures. Also such interactions spur the solute-solute or ion-ion interactions ($S_V^* < \phi_V^0$). Standard transfer volume ($\Delta_t \phi_V^0$) and $\Delta_t B$ values suggest that ion-hydrophilic and hydrophilic-hydrophilic group interactions spur the ion-hydrophobic, hydrophilic-hydrophobic and hydrophobic-hydrophobic interactions leading to volume expansion. The ϕ_E^0 and $(\partial \phi_E^0 / \partial T)_p$ values suggest that nicotinic acid to act as an overall structure maker in aqueous sodium malonate solutions. The absorption spectra for nicotinic acid in various aqueous sodium malonate solutions also well corroborate with the above results.

In Chapter V the partial molar volumes (ϕ_V^0) and viscosity B -coefficients of L-ascorbic acid in the aqueous sodium malonate solutions are reported and found to be positive and both these properties increase as the experimental temperature and

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sodium malonate molalities in the aqueous solutions increase. Therefore these results are suggestive of strong solute-solvent or ion-solvent interactions and the studied solutions are characterized by structural enhancement at larger sodium malonate molalities even at higher temperatures and the solute-solvent or ion-solvent interactions spur the solute-solute or ion-ion interactions ($S_v^* < \phi_v^0$). The positive standard transfer volume ($\Delta_t \phi_v^0$) and $\Delta_t B$ all the experimental temperatures suggest that ion-hydrophilic and hydrophilic-hydrophilic group interactions characterize the studied solutions, rather than the ion-hydrophobic, hydrophilic-hydrophobic and hydrophobic-hydrophobic interactions leading to volume expansion due to reduced electrostriction of water by L-ascorbic acid. Again the ϕ_E^0 and $(\partial \phi_E^0 / \partial T)_p$ values suggest that L-ascorbic acid acts as an overall structure maker in aqueous sodium malonate solutions. The absorption spectra for L-ascorbic acid in various aqueous sodium malonate solutions also support the above results.

In Chapter VI the partial molar volumes (ϕ_v^0) and viscosity B -coefficients of paracetamol in the aqueous uracil solutions are reported. Both the properties were found to be positive and they increase as the experimental temperature and uracil molalities in the aqueous solutions increase. Therefore it is evident that the solute-solvent interactions are strong and the solution structure is enhanced at larger uracil molalities at higher temperatures. Again for the studied aqueous solutions, S_v^* values are found to be negative but always lesser than the ϕ_v^0 values, thus solute-solvent interactions spur the solute-solute interactions. Standard transfer volume ($\Delta_t \phi_v^0$) and $\Delta_t B$ values are all positive and increase when the uracil in the ternary solutions increases at all the experimental temperatures. These results are also well reflected by ϕ_E^0 and $(\partial \phi_E^0 / \partial T)_p$ values and paracetamol acts as an overall structure maker in the aqueous uracil solutions. These results were also substantiated by the absorption spectra of paracetamol in various aqueous uracil solutions.

In Chapter VII the partial molar volumes (ϕ_v^0) and viscosity B -coefficients of sodium pyruvate in the aqueous glycine solutions are reported. These properties are functions of solute concentrations and experimental temperatures. The ϕ_v^0 and

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viscosity B -coefficients are positive and both these properties increase as the experimental temperature and glycine molalities in the aqueous solutions increase. These results, thus, unveil that solute-solvent or ion-solvent interactions are strong and these interactions are greater than the solute-solute or ion-ion interactions. Also the standard transfer volume ($\Delta_t\phi_V^0$) are suggestive of the dominance of ion-hydrophobic and hydrophobic-hydrophobic group interactions over the ion-hydrophilic, hydrophilic-hydrophilic and hydrophilic-hydrophobic interactions and sodium pyruvate acts as an overall structure maker in aqueous glycine solutions. These results are also well reflected by the $\Delta\mu_1^{0\neq}$ and $\Delta\mu_2^{0\neq}$ values.

In Chapter VIII the partial molar volumes (ϕ_V^0) and viscosity B -coefficients of sodium pyruvate in the aqueous L-alanine solutions are reported. Both these properties are positive and increase as the experimental temperature and L-alanine molalities in the aqueous solutions increase. These results are suggestive of strong solute-solvent or ion-solvent interactions with structural enhancement at larger L-alanine molalities even at higher temperatures. Also S_V^* values suggest that the solute-solute or ion-ion interactions are weaker for the studied solutions ($S_V^* < \phi_V^0$). Again, the standard transfer volumes ($\Delta_t\phi_V^0$) suggest that ion-hydrophobic and hydrophobic-hydrophobic group interactions mainly characterize the overall solution structure of the studied aqueous solutions and cause volume compression (negative $\Delta_t\phi_V^0$ values) and sodium pyruvate acts as an overall structure maker in aqueous L-alanine solutions.

In Chapter IX the partial molar volumes (ϕ_V^0) and viscosity B -coefficients of caffeine in the aqueous uracil solutions are reported and these properties are suggestive of strong solute-solvent interactions with structural enhancement at higher temperatures and these interactions are greater than the solute-solute interactions. Also standard transfer volume ($\Delta_t\phi_V^0$) are suggestive of polar-hydrophobic, hydrophilic-hydrophobic and hydrophobic-hydrophobic interactions leading to volume contraction probably due to increased electrostriction of water by caffeine and caffeine acts as an overall structure maker in the aqueous uracil solutions. The absorption spectra for caffeine in various aqueous uracil solutions also support the

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above results. Pyridine and purine bases aggregate in aqueous solutions by stacking interactions, so there exists multiple equilibria and possibility of several ionic and tautomeric forms for a simple molecular species; thereby making the study of their molecular interactions in solutions a tough task.

In Chapter X Various volumetric and viscometric properties for the aqueous solutions containing nicotinic acid and sodium gluconate were determined and discussed in terms of the solute-solvent and solute-solute interactions. It was found that the solute-solvent interactions are dominant for nicotinic acid in aqueous sodium gluconate solutions and such interactions strengthen further when both the experimental temperature and sodium gluconate molalities increase in the solutions studied and nicotinic acid acts as an overall structure maker in aqueous sodium gluconate solutions. S_n values suggested that the nicotinic acid exists as solvated with primary solvation sphere in aqueous sodium gluconate solutions. An inspection of the apparent specific volume of nicotinic acid in the aqueous solutions studied revealed that although initially nicotinic acid tastes sweet but gradually it tastes sweet-bitter to bitter with increasing sodium gluconate content.

Anyway, molecular interactions are very complex in nature and quite difficult to explore and interpret, explicitly those involving biologically important compounds. Many forces may operate amongst the molecules in a solvent and it is really difficult to separate or quantify and assign them all. Nevertheless, if careful experimental technique and methodology are used, important conclusions may be reached 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 their applications and proper understanding of the various interactions that 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 various biologically important compounds dissolved in different aqueous systems remains to be explored.