

# CHAPTER - XI

## *Inference / Conclusion*

Potential biological implications of various studies with apparently unique effect are discussed in this thesis. Systematic investigations provided valuable structural guidelines to design assembling supramolecular hosts with optimal composition for the effective encapsulation/ inclusion of imperative guests can lead to ideal delivery vehicles for the controlled delivery in the biological samples. Applications of sensitive new technologies, in particular, the spectroscopic techniques like  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR, 2D ROESY, UV, IR, Fluorescence, XRD, SEM, TEM have allowed detection of interaction in aqueous solution and also in some organic solvents.

*Chapter I – III* of the thesis comprises of the objective, novelty and applications of the research work, the imperative compounds i.e., electrolytes/solutes and solvents used and techniques of investigation. Moreover this also occupies the review of the works done allied with the dissertation.

A brief review of noteworthy means in the field of molecular as well as ionic interaction has been specified. The discussion includes ion-solvent/solute-solvent, ion-ion/solute-solute and solvent-solvent interactions in binary, ternary mixed solvent systems and of electrolytes in pure and non-aqueous solvent systems at diverse temperatures in terms of various derived parameters, estimated from the experimentally observed properties. Crucial assessment of diverse methods on relative merits and demerits on the basis of a range of assumption have been employed from time to time acquiring the single ion values (viscosity  $B$ -coefficient and limiting equivalent conductance) and their implications have been discussed. Molecular interactions are interpreted based on various derived parameters in the systems. Moreover the approximate quantum mechanical calculation and cell viability is also prepared in the present study. The experimental section is also discussed in details.

*Chapter IV* I have investigated geometry- optimized extended conformation obtained for amino acids (Tyrosine, Tryptophan) prevailing in Aqueous Vitamin C Solutions is studied in this part. Solute – solvent interactions are maximum in Tyrosine is observed. C-13 NMR spectroscopic data's along with Ab-initio are further reliable and supportive to learn the

Solute - Solvent interactions. Ascorbic acid (also known as Vitamin C) acts resembling a co-enzyme. This directs to the indispensable benefits of Tyrosine in attendance of Ascorbic acid in assorted catabolism reactions in human body. Ion-solvent interaction dominates above the ion-ion interactions in studied solution.

*Chapter V* Studies of transportation properties of diverse electrolytes in solvent media are of significance to obtain information on the behavior of ions in solution. Molecular interactions can be studied in solution phase by studying its thermodynamic, transport properties. These properties provide vital information about nature and strength of intermolecular forces operating among the components. The ion-ion interactions for LiCl, LiBr and LiI decreases with increase in temperature, which may be due to more solvation of ions. The temperature effect on B coefficient for LiCl, LiBr and LiI explains a positive sign of  $dB/dT$ , viewing thereby that LiCl, LiBr and LiI behaves a structure-breaker in (0.001, 0.003, 0.005) m aqueous ascorbic acid solution. This allows usage for a green battery with high capacity and high voltage in daily life. It also paves the approach for cheaper consumer electronics.

*Chapter VI* Physicochemical investigation of both inclusion and encapsulation complexes for  $\beta$ -CD and 18-Crown-6 with pyrrolidinium based ionic liquid are overviewed by me in the present work. In the first case ionic liquid combines with  $\alpha$ - and  $\beta$ -CD which has motivating variations in thermo chromic behavior of the dye molecules and would be desirable in the near future. On the other hand it was observed, 18-Crown-6 including hydrophobic ionic liquid has a vital role in electrochemistry. Such sort of inclusion complexes are used in recycling process.

*Chapter VII* Importance of this work lies behind the fact that if the co-solute ascorbic acid along with water is made to interact with oxalates the water along with Oxalates is removed from the body.

*Chapter VIII* this chapter deals precise measurements on geometry, spectroscopic, conductometric, ab initio methods. Aromatic nitriles have widespread applications in the production of dyes, pesticides and pharmaceuticals. They are used as intermediates in the synthesis of a assortment of pharmacologically active compounds which are used as sedatives, muscle relaxants, neuroleptics, etc. Benzonitriles are of immense interest in the ground of organic chemistry for the synthesis of pharmaceuticals, natural products,

herbicides, and agrochemicals. In the contemporary work substituted benzonitriles are being studied in order to find its novelty in many reactions in industries at high temperatures.

*Chapter IX* The present study adds a dimension in the field of contemporary science of controlled delivery of Tertiary-Leucine which is a derivatized amino acid by means of suitable host molecule as selected here as  $\alpha$ - and  $\beta$ -Cyclodextrin. Biological activity relates to non-toxic nature of the inclusion complexations.

*Chapter X* formation of supramolecular assemblies with Vitamins which would add to the controlled delivery in accordance with the pharmaceutical applications is studied here.

So, the whole thesis comprises of various assorted interactions with diverse imperative bio-active compounds in cooperation with the solution phase as well as in the inclusion phenomena.

*Further sketch of works would comprise of bio active molecules like Vitamins, Amino Acids along with their Derivatives etc which would regrow the importance of Supramolecular Chemistry along with Solution Chemistry in our day to day life to the hike.*

