Chapter 6

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The studies involving the interactions of amino acid, nucleoside, nucleotides and essential metal ions may be helpful in understanding the molecular interactions of biomolecules in living systems. The excess or deficiencies of biomolecules in the body causes diseases. Metal ions also play a significant role in metabolic and physiological processes involving amino acids, nucleoside and nucleotides.

Various methods are available to study such interactions but the methods involving ultrasonic and thermodynamic studies are more convenient and precise for the said purpose. In the present study, an attempt has been made to discuss the systems containing tryptophan, glycine, adenosine and adenosine-diphosphate (ADP) in 0.05M, 0.01M and 0.005M zinc chloride and cobaltous chloride solutions, at 303.15K. A precalibrated bicapillary pyknometer was employed for the measurement of density, whereas ultrasonic velocity was measured with multifrequency ultrasonic interferometer. The viscosity was measured with precalibrated Ostwald type viscometer.

In the present study an attempt has been made to discuss the systems through experimentally and graphically calculated data. The following conclusions may be drawn.

1) The present work was undertaken with view to obtain information on biomolecular interactions operative in the presence of bio-essential metals like zinc and cobalt.
2) Literature information has shown that the presence of different metal cations will definitely affect the various parameters that define the interactions
3) The changes recorded in the measurable properties were the consequences of the interactions between water, biomolecule and transition metal chloride. The variations in the values of related parameters may be accounted to the non spherical 3d ion’s radii, effect of hydration energies, changes in coordination number, influence of
valence shell electronic configuration, steric effect, solvation involving inner coordination and outer hydrogen bonded sphere etc.

4) The experimentally calculated values of density and ultrasonic velocity were tried to fit into linear or polynomial equations respectively. Polynomial equation gives better fit than linear equation. Density data yields better fit than ultrasonic data.

5) For a fixed concentration of ZnCl₂ and CoCl₂ at experimental temperature, the values of density, ultrasonic velocity and relative viscosity increase with increase in the concentration of tryptophan, glycine, adenosine and adenosine diphosphate. Similarly the density, ultrasonic velocity and relative viscosities are found to increase with increase in the concentration of zinc chloride and cobaltous chloride. This clearly indicates that the concentration of amino acids, nucleoside, nucleotide molecules as well as the metal cations enhance the chances of interactions in the aqueous solutions.

6) The values of apparent molar volume (φᵥ) for all the biomolecules under study are positive. The limiting values of apparent molar volume (φᵥ₀) were calculated by linear plot of φᵥ versus molality (m). The (φᵥ₀) values of glycine and adenosine in aqueous solutions of ZnCl₂ and CoCl₂, are compared with (φᵥ₀) values of these in pure water. The values are found to be positive and higher in the presence of such metal cations. Many workers have investigated φᵥ₀ for amino acids in the presence of electrolytes such as NH₄Cl, LiCl, KCl, NaCl etc. and observed positive φᵥ₀ due to strong interactions of ions of electrolytes with the charge centers of amino acid. These ions have very little tendency to form complexes with amino acid. The situation is quite different in the presence of 3d transition metal cations like Zn²⁺ and Co²⁺. These ions have a strong tendency to coordinate with amino acids. Similar prediction may be stated in case of adenosine and ADP.

7) Compressibility data shows that the φᵥ values for glycine in the present study are much negative than in pure water. This will lead to the conclusion that in the presence of transition metal cations like Zn²⁺ and Co²⁺, the solutions becomes less compressible and this conclusion may be explained on the basis of formation of complex entity which occupies interstitial spaces of water structure imparting more stiffness to it. Similar interpretation may be valid for the systems containing tryptophan as well as
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adenosine. Whereas, comparatively adenosine diphosphate systems are found to be more compressible which may be due to the bigger size of ADP molecules, the intramolecular interactions between the various groups of ADP molecules and the formation of weak complex with metal cations.

8) The viscosity A and B coefficient are calculated by using Jones Dole equation. The values of Coefficients are negative (very small) for the systems containing glycine, adenosine and ADP while positive (small) for few cases in tryptophan system, thereby showing the presence of weak to very weak ion-ion interactions. On the other hand, the values of B-coefficients are positive and fairly large for the systems studied at different concentrations of all the biomolecules at 303.15K. This shows the presence of solute-solvent and ion-solvent interactions. The comparison shows that the values of B-coefficients (solute-solvent interactions) in various solutions of ZnCl₂ and COCl₂ are larger in magnitude than that reported for water. The higher ion-solvent interaction may be due to the complex entity formed between the biomolecule and metal ion. The B-values, for all systems in ZnCl₂ and CoCl₂ are nearly equal, this may be due to equal size or equal ionic radii of Zn²⁺ and Co²⁺ ion.

9) Hydration number values, for all the systems (with few exceptions), are higher in ZnCl₂ than that in CoCl₂. This may be due to electronic configuration and number of unpaired electrons in the d-sub shell. As the metal ion concentration decreases, the value of hydration number increases. This may indicate that the active centers on the biomolecules invites the water molecules more effectively, to cause solvation. This fact further support that the water molecules are more interactive towards the biomolecules in the body system and hence the water medium is considered to be the best medium for conducting all the metabolic activities in the living system.

10) The other parameters like isentropic compressibility specific acoustic impedance intermolecular free length, relative association, electrical conductance etc. are also found supportive towards the molecular interactions occurring in living systems.

11) It has been observed that the metal ions interact strongly with charged centers of the amino acids (in the form of zwitterions) resulting in decrease in electrostriction. But we feel that the fact cannot be explained only on the basis of electrostriction.
12) The literature survey and appropriate references in support of the work have been presented in this thesis and has been listed in the end of each chapter.

13) We conclude, that the ultrasonic and thermodynamic studies play an important role in understanding the interactions in solutions containing biomolecules. Polarities and molecular structure of various components in solutions influence the values of different acoustic and thermodynamic properties.

The interactions in such systems may be considered more than physical phenomena to occur in solutions. We have made an effort to apply it as a parameter for assessing the interaction between biomolecules and metal ions which may be useful to understand the molecular interactions in biological systems. Since actual mechanism for such interactions cannot be easily advanced, further work is required to throw light on interactions among biomolecules that play very important role in understanding the thermodynamics of many biological processes.