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Title of thesis: "Thermodynamic and transport studies of amino acid – carbohydrate interactions in aqueous medium"

Abstract

The study of intermolecular interactions of amino acids in aqueous electrolyte/ carbohydrate solutions is very important as it provides an opportunity to have a better understanding of the behaviour of protein in such solutions. As most of the biological macromolecules are physiologically active in aqueous solutions, knowledge of water-protein interaction is necessary to understand the role of water solvated to soluble biomolecules in the living cells. The study of carbohydrate- protein interactions is very important for immunology, biosynthesis, pharmacology, and medicine. We intended to extend a detailed study of amino acid and carbohydrates (mono- and disachharides) in aqueous medium.

In aqueous protein solutions, the amino acid residues of a polypeptide chain interact with each other and with the surrounding water by these noncovalent forces. Therefore, the characterization of the thermodynamic properties of hydration can assist in the understanding of the conformational stability and the functional properties of proteins in solution. However, since proteins are particularly complex macromolecules, it is difficult to resolve the various interactions that participate in protein hydration. One of the useful approaches for interpreting the thermodynamic properties of protein solutions is the comparative study of various low molecular weight model compounds. Amino acids have been often used as the most convenient substances to estimate the individual contribution of monomeric units in proteins. The thermodynamic properties of protein-carbohydrate interactions in aqueous solutions assist in interpreting the solute-solvent interactions which help in understanding the conformational stability.

Thermodynamic and transport studies involving volumetric, viscometric, ultrasonic, surface tension and refractive index methods for the investigations of interactions of amino acids and carbohydrates in aqueous medium are very few. We have chosen thermodynamic methods for the present study, as these methods are important because changes in properties of the system caused by variations of temperature,

composition, and pressure can be studied without any reference to assumptions, models or hypothesis.

Ultrasonic speeds of sound, u , densities, ρ , viscosities, η , and refractive indices, n_D of amino acids and carbohydrates in aqueous medium have been measured at different temperatures. From these experimental data, apparent molar volumes, V_ϕ , apparent specific volumes, $V_{\phi,sp}$ as a function of the concentration of solutes, the standard partial molar volume, V_ϕ^0 , the experimental slope S_v , transfer volume from water to aqueous glycine solutions, $\Delta V_{\phi(w)}^0$, and partial molar expansibility of solute, E_ϕ^0 , $(\partial C_p^0/\partial P)_T$, $(\partial^2 V_\phi^0/\partial T^2)_p$, apparent molar isentropic compression, $K_{S,\phi}$, apparent molar isentropic compressions at infinite dilution, $K_{S,\phi}^0$, the experimental slope S_K , transfer compressibility, $\Delta_r K_{S,\phi}^0$, hydration numbers, n_H have been obtained. Falkenhagen coefficient A and Jones-Dole coefficient B , free energies of activation of viscous flow per mole of solvent, $\Delta\mu_1^{0\#}$, and solute, $\Delta\mu_2^{0\#}$, enthalpy, $\Delta H^{0\#}$, and entropy, $\Delta S^{0\#}$ of activation of viscous flow have been evaluated by using viscosity data. The molar refraction has been calculated by using measured refractive index data.

These parameters have been used to study the following possible interactions in the solution:

1. Hydrophilic - ionic interactions between ($-\text{OH}$, $-\text{C}=\text{O}$, $-\text{O}$) groups of carbohydrates and zwitterionic (NH_3^+ , COO^-) centres of amino acids.
2. Hydrophilic - hydrophobic interactions between ($-\text{OH}$, $-\text{C}=\text{O}$, $-\text{O}$) polar groups of the carbohydrate molecules and the nonpolar groups of amino acids.
3. Hydrophobic - Hydrophobic interactions between the nonpolar side groups of the carbohydrate and amino acids molecules.

Many investigators have shown that sugar and polyhydric alcohols increase the thermal stability of proteins or reduce the extent of their denaturation by other agents. Because of the complex behaviour of proteins in various solvents/cosolvents, it is convenient to study the model compounds (monomers of proteins), amino acids, peptides and their derivatives. The calculated derived parameters have been used to study the various possible interactions present in solutions.