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Department: Chemistry
Title of the Thesis: Thermodynamic and Transport Studies of Some Organic Binary Liquid Mixtures and Mixtures of Amino Acids in Aqueous Surfactants / Carbohydrates

Abstract of the Ph.D. Thesis:

Thermodynamic is the basis of experimental science and therefore concerns with the macroscopic properties and the properties of systems containing many million of molecules. The problem of the microstructure and molecular dynamics in aqueous solutions has attracted much experimental and theoretical attention.

The thesis is divided into seven chapters and the details of them are given below:

Chapter I comprises the statement of the problem, importance of the work and an exhaustive and systematic review of the most recent literature on the volumetric, viscometric, ultrasonic, surface tension and conductometric studies of the binary non – aqueous and ternary aqueous liquid mixtures containing biomolecules.

Chapter II deals with the experimental details, i.e., standard methods of purification of the chemicals and details of the instruments and techniques used in the present study. For measurement of densities single stem capillary pycnometer has been used, viscosities were measured by using Cannon Ubbelohde viscometer, multifrequency ultrasonic interferometer has been employed, measurement of surface tensions have been carried out using a ring detachment tensiometer and for measurements of conductance conductivity meter has been used.

Chapter III In this chapter experimental data the densities (ρ), viscosities (η), and ultrasonic speeds (u), of pure cyclohexane, 1-butanol, 2- butanol, and those of their binary mixtures, with cyclohexane as common component, covering the whole composition range have been measured at 293.15, 298.15, 303.15, 308.15, 313.15, and 318.15 K. The variations of derived parameters mentioned above with composition offer a convenient method to study the nature and extent of interactions between the component molecules of the liquid mixtures, not easily obtained by other means.

Chapter IV This chapter presents conductivities, densities and ultrasonic speeds measurements of cationic surfactant, hexadecyltrimethylammonium bromide (HTAB) in aqueous solutions of glycine (Gly) and diglycine (Gly-Gly) amino acids have been made at various temperatures. The critical micelle concentration (cmc) and the degree of

ionization (β) of the micelles were determined from the conductivity data at different temperatures. Thermodynamic parameters such as standard free energy, enthalpy, and entropy of the micellization process (ΔG_m^o , ΔH_m^o , and ΔS_m^o) for the present systems were estimated by applying the charged pseudo-phase separation model. The volume change on micellization, ΔV_ϕ^m was also estimated.

Chapter V Surface properties of a cationic surfactant, hexadecyltrimethylammonium bromide (HTAB) in aqueous amino acids, glycine (Gly) and diglycine (Gly-Gly) were investigated at 298.15, 303.15, 308.15 and 313.15 K temperatures. The critical micelle concentrations (CMC) have been obtained and the surface properties calculated. The values of cmc and surface tension (γ_{cmc}) for the surfactant increase with an increase in temperature. The viscosity B – coefficients of Jones-Dole equation in pre- and post-micellar regions were analysed.

Chapter VI In the present chapter, we report the interaction between hexadecyltrimethylammonium bromide (HTAB) and aqueous serine and threonine amino acids has been studied by using conductivity, density and viscosity technique at 298.15 to 318.15 K. From the specific conductivities (κ) data, critical micelle concentration (CMC), degree of counter-ion dissociation (β), limiting molar conductivities at infinite dilution (Λ_m^o), equivalent conductivity of the solute at the cmc (Λ_{cmc}) and micellar aggregation number, (n) of HTAB have been computed. From the viscosity (η) data, intrinsic volume, $[\eta]$ have been evaluated.

Chapter VII In this section we report the volumetric and viscometric properties of amino acids glycine (Gly) and glycyglycine (Gly-Gly) have been obtained in aqueous beta cyclodextrin, (β -CD) solution at T = (298.15, 303.15, 308.15, 313.15 and 318.15) K by measuring the densities, ρ and viscosities, η , of ternary systems. From these experimental measurements, apparent molar volumes, V_ϕ , partial molar volume at infinite dilution, V_ϕ^o , experimental slope, S_V , isobaric expansibility, ϕ_E^o , and the partial molar volume of transfer at infinite dilution, $\Delta V_{\phi(tr)}^o$ were calculated by using density data. Falkenhagen's theoretical coefficient, A, Jones – Dole coefficient, B, free energies of activation of viscous flow per mole of solvent, $\Delta\mu_1^{o\#}$ and per mole of solute, $\Delta\mu_2^{o\#}$, enthalpy, $\Delta H^{o\#}$ and entropy, $\Delta S^{o\#}$ of activation of viscous flow have been evaluated by using viscosity data.