SUMMARY OF ABSTRACT

The present study is primarily focused on the physico – chemical studies of biomolecules in aqueous electrolyte and aqueous non-electrolyte mixtures. The thesis is divided into eight chapters, the details of them is given below:

Chapter 1 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, and refractive index studies of the ternary aqueous liquid mixtures containing biomolecules. Thus, clearly emphasizes the need of the work.

Chapter 2 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 Ubbleohde viscometer, and refractive indices were measured using Abbe refractometer.

Chapter 3 In this chapter we present experimentally measured densities, ρ, viscosities, η and refractive indices, n_D of aqueous caffeine (0.05 M) and of solutions of amino acids, DL–alanine, D–phenylalanine and DL–threonine (0.01, 0.02, 0.03, 0.04 and 0.05 M) in aqueous caffeine at 298.15, 303.15, 308.15 and 313.15 K. From the experimental data of ρ, η and n, the apparent molar volume (ϕ_v), partial molar volume (ϕ_v^0) and slope (S_v^*), transfer volume [$\phi_v^0(tr)$], viscosity A and B coefficients, free energies of activation per mole of solvent ($\Delta\mu_1^{0\#}$) and per mole of solute ($\Delta\mu_2^{0\#}$), enthalpies (ΔH^*) and entropies (ΔS^*) of activation of viscous flow, and molar refraction (R_D) were calculated for all the amino acids in aqueous caffeine solution. The parameters were used to discuss the solute – solute and solute – solvent interactions in the aforementioned mixtures.

Chapter 4 In this chapter we report densities, ρ, viscosities, η and refractive indices, n_D of aqueous caffeine (0.5 M) and of solutions of amino acids; L-phenylalanine, L-tyrosine and L-histidine (0.01, 0.02, 0.03, 0.04 and 0.05 M) in aqueous-caffeine at 298.15, 303.15, 308.15 and 313.15 K. From the experimental values of ρ, η and n_D, various useful thermodynamic parameters evaluated for all the three amino acids in aqueous-caffeine solutions. These parameters are used to discuss the solute-solvent and solute-solute interactions in the aforementioned mixtures.

Chapter 5 In this chapter we extend our earlier study to the systematic study on amino acids, glycine, DL–alanine, L–serine and DL–valine in aqueous caffeine solution in the temperature range 278.15–313.15 K, which covers body temperature also. We report the densities, ρ, viscosities, η and refractive indices, n_D of glycine (Gly), DL–alanine (Ala), L–serine (Ser) and DL–valine (Val) each having concentrations 0.10, 0.20, 0.30, 0.40 and 0.50 M in 0.05 M aqueous caffeine solution at temperatures 278.15, 303.15, 308.15, 313.15 K. Using these experimental data, the various parameters computed are apparent molar volume, ϕ_v, limiting apparent molar volume, ϕ^0_v, relative viscosity, η_{rel}, Falkenhagen coefficient, A, Jones-Dole coefficient, B, hydration number, H_n, temperature derivative of B, $\delta B/\delta T$ and free energies of activation of viscous flow, $\Delta\mu^{0\#}_1$ and $\Delta\mu^{0\#}_2$ per mole of solvent and solute respectively. n_D values were used to calculate molar refractive index, R_D of the different solutes in aqueous caffeine solution. All these functions offer a convenient method to study the thermodynamic properties of amino acids (AAs) in various solvents, not easily obtained by other means.

Chapter 6 In this chapter we report the densities, ρ, viscosities, η and refractive indices, n_D of (0.01,0.02, 0.03, 0.04 and 0.05 M) DL-valine, L-isoleucine and L-proline in aqueous-DMSO (10 % DMSO v/v) at 298.15, 303.15, 308.15 and 313.15 K. The density data have been used to calculate apparent molar volume, ϕ_v and partial molar volume, ϕ_v^o. The viscosity data were analyzed by means of Jones-Dole equation. The activation parameters of viscous flow, namely, free energies of activation per mole of solvent, $\mu_1^{o\#}$ and per mole of solute, $\mu_2^{o\#}$, respectively, were obtained by using transition state theory. The refractive index data was used to calculate molar refraction, R_m, for all the three amino acids in aqueous-DMSO solvent mixtures. These thermodynamic parameters are used to discuss the solute-solvent/co solvent and solute-solute interactions in the aforementioned mixtures.

Chapter 7 In this chapter we report the densities, ρ, viscosities, η, and refractive indices, n_D of 0.1, 0.2, 0.3, 0.4 and 0.5M Gly, Ala, Ser, and Val in 0.2M aqueous D-glucose solution at 298.15, 303.15, 308.15, and 313.15 K. Various physical parameters like ϕ_v, ϕ^0_v, $\phi^0_v(tr)$, the viscosity A and B –coefficients, $\Delta\mu_1^{0\#}$ and $\Delta\mu_2^{0\#}$ respectively were calculated from the density and viscosity data. n_D values were used to compute molar refractivity, R_D of the ternary mixtures under study. All these parameters are discussed in terms of solute-solvent and solute-solute interactions occurring in the AA-glucose-water systems and the structure making/breaking tendency of the solutes in the given solvent.

In addition to this, group contributions have also been determined.

Chapter 8 In this chapter we report partial molar volumes, ϕ_v^0 at infinite dilution, partial molar volumes of transfer, ϕ_v^0(tr) and refractive indices, R_D of [0.02, 0.04, 0.06, 0.08 and 0.01M] amino acids in [0.005- 0.008 M] aqueous solutions of CTAB at different temperatures. Surfactants consist of two distinct parts-polar head group and apolar hydrophobic tail group. The self-aggregation of polar and hydrophobic groups leads to the formation of micelles above critical micelle concentration (CMC). While the hydrophobic interaction act as the vital driving forces for the formation of micellar aggregates and for binding of surfactant to protein, the electrostatic repulsion between polar head groups affects the size of micelle. The CMC of CTAB is reported as 8.2×10^{-4} mol dm^{-3}. Thus, the surfactant acts as micelles in these experiments.

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