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Physico-Chemical Studies of Glycine, L-Alanine, L-Phenylalanine and Glycylglycine in Aqueous Triton X-100 at Different Temperatures

The densities, ρ and viscosities, η of glycine (Gly), L-alanine (Ala), L-phenylalanine (Phe) and glycylglycine (Gly-Gly) in aqueous Triton X-100 (TX-100) solutions have been measured as a function of amino acid/peptide concentration at 298.15, 303.15, 308.15 and 313.15 K. The experimental data have been utilized to evaluate various thermodynamic parameters, viz., apparent molar volumes, V_a , partial molar volumes at infinite dilution, V_a^∞ , partial molar isobaric expansibilities, α_p^∞ , partial molar volumes of transfer, $\Delta_a V^\infty$ and A and B -coefficients of viscosity, respectively. The hydration numbers have also been calculated. The results have been discussed in terms of interactions taking place in the present systems. The structure-making/-breaking ability of the solute (amino acid/peptide) in the presence of surfactant, Triton X-100 has also been considered.

Key words: Amino acids, peptide, Triton X-100, partial molar volume, viscosity coefficients

Physikochemische Untersuchung von Glycin, L-Alanin, L-Phenylalanin und Glycylglycin in wässriger Triton-X-100-Lösung bei verschiedenen Temperaturen. Es wurden die Dichten ρ und die Viskositäten η von Glycin (Gly), L-Alanin (Ala), L-Phenylalanin (Phe) und Glycylglycin (Gly-Gly) in wässrigen Triton X-100- (TX-100)-Lösungen als Funktion der Aminosäure/Peptid-Konzentration bei 298.15, 303.15, 308.15 und 313.15 K gemessen. Mit den experimentellen Daten wurden verschiedene thermodynamische Parameter (das scheinbare Molvolumen (V_a), das partielle Molvolumen bei unendlicher Verdünnung (V_a^∞), die partiellen molaren isobaren Ausdehnungsvermögen (α_p^∞), die partiellen molaren Transfervolumina ($\Delta_a V^\infty$) und die A - und B -Viskositätskoeffizienten) berechnet. Die Hydrationszahlen wurden auch berechnet. Die Ergebnisse wurden diskutiert hinsichtlich der in den jeweiligen Systemen stattfindenden Wechselwirkungen. Die strukturgebende und -brechende Eigenschaft der Lösungen (Aminosäure/Peptid) in Gegenwart von Triton-X-100 wurde ebenfalls berücksichtigt.

1 Introduction

Ionic and non-ionic surfactants have a wide applicability from both biological and technological points of view [1–3]. Surfactants are widely employed in pharmaceuticals [4, 5]. The functional properties and molecular characteristics of proteins are affected in the presence of surfactants, so protein-surfactant interactions are considered to be significant. Various techniques have been employed to study the

protein-surfactant interactions, such as fluorescence [6], calorimetry [7, 8], conductivity [9] and FTIR [10, 11]. Though there are several studies on protein-surfactant interaction reported in the literature [12–17], investigations on amino acid/dipeptide-surfactant interactions are few [18, 19]. Since, proteins are complex biomolecules, interactions of their smaller sub-units such as amino acids and peptides with surfactants can provide a better insight into the protein-surfactant interactions.

Triton X-100 is a polydisperse preparation of *p*-(1,1,3,3-tetra methylbutyl) phenoxy poly (oxyethylene glycol) containing an average size of 9.5 oxyethylene units per molecule. Its use is qualitatively as well as quantitatively maximizing the yield of membrane-bound protein and globular proteins under non-denaturing conditions is well known. Triton X-100 together with hydrophobic dyes is also used for the separation of amphiphilic proteins. The critical micelle concentration, CMC, plays an important role in the description of physical behaviour of surfactant solutions [20]. The CMC of TX-100, as reported by Huang *et al.* [21], is $2.8 \times 10^{-3} \text{ mol} \cdot \text{dm}^{-3}$, therefore, almost all the surfactant molecules in the present study should be aggregated as micelles.

2 Experimental Procedure

The amino acids and the peptide used in the present study were Gly (Merck, mass fraction >0.99), Ala (Loba chemie, mass fraction >0.98), Phe (Thomas baker, mass fraction 0.99) and Gly-Gly (Acros Organics, mass fraction 0.99). All the amino acids and peptide were recrystallized from aqueous ethanol solutions and dried in vacuum over P_2O_5 at room temperature for about 72 h. Analytical reagent grade TX-100 (BDH Chem. Ltd., Poole, England, mass fraction 0.995) was kept over molecular sieves (0.4 nm Sigma Union Carbide type) to reduce the water content, if any. Doubly distilled and deionized water was used for preparation of the solutions. Aqueous TX-100 (0.05 m) was used as a solvent to prepare solutions of 0.05, 0.10, 0.15, 0.20 and 0.25 m Gly, Ala and Gly-Gly and 0.02, 0.05, 0.08 and 0.10 m Phe. All the solutions were prepared by weight on Precisa XB-220A, Swiss make electronic balance with a precision of $\pm 0.0001 \text{ g}$.

The density and viscosity measurements were carried out using a single stem pycnometer and an Ubbelohde viscometer [22], respectively, as described in our previous papers [23]. The measured density and viscosity were precise up to $\pm 0.01 \text{ kg m}^{-3}$ and $\pm 3 \times 10^{-5} \text{ N s m}^{-2}$, respectively. The viscos-