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Critical Micelle Concentration and Self-aggregation of Hexadecyltrimethylammonium Bromide in Aqueous Glycine and Glycylglycine Solutions at Different Temperatures[1]

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Abstract—Conductivities, densities and ultrasonic speeds measurements of hexadecyltrimethylammonium bromide (HTAB) in aqueous solutions of glycine (Gly) and glycylglycine (Gly-Gly) have been made at various temperatures. The critical micelle concentration (CMC), the degree of ionization (β) of the micelles, standard free energy, enthalpy, and entropy of the micellization process (ΔG_m°, ΔH_m°, and ΔS_m°) for the present systems were estimated at different temperatures. The CMC values of HTAB in aqueous Gly and Gly-Gly were also evaluated by density and ultrasonic speed measurements. Apparent molar volumes, (V_ϕ), apparent molar volumes at infinite dilution, (V_ϕ°), apparent molar compressibilities, (K_ϕ), of HTAB in the pre- and post-micellar regions, and volume change on micellization (ΔV_ϕ^m) were also estimated. Large positive values of $T\Delta S_m^\circ$ and small negative values of ΔH_m° suggest that micellization process is driven primarily by entropy increase. The increase in ΔV_ϕ^m and K_ϕ with rise in temperature is indicative of less compact micellar structure of HTAB in presence of amino acid additives. These data suggest that amino acids are solubilised probably in the palisade layer of the micelle.

Keywords: hexadecyltrimethylammonium bromide (HTAB), critical micelle concentration (CMC), degree of ionization, apparent molar volumes and compressibilities, surfactant–amino acids interactions.

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INTRODUCTION

Surfactants are the surface–active agents, possessing the property of preferential adsorption onto the surfaces or interface of the phases and, thus, lower to a marked degree the surface or interfacial tension. They have unique structure, containing both non-polar hydrophobic groups (their tails) and polar hydrophilic groups (their heads) in the same molecule and, hence, are amphiphilic in nature. These amphiphiles are not only highly interesting from the physicochemical viewpoint but also are fundamental to life because of the fact that living things are made up of colloids comprising a wide variety of amphiphiles [1]. The surfactant molecules have tendency to aggregate into micelles in solution above a narrow concentration range called critical micelle concentration, CMC [1]. In recent years, surfactants due to their micellar properties are extensively studied in aqueous solutions in absence [2, 3] or in presence [4, 5] of additives due to their extensive employment in pharmaceutical [6, 7] and biotechnological [8, 9] processes. The vast majority of cationic surfactants are based on the N-atom carrying the cationic charge. They are widely used in industries and find numerous applications in our daily life [10].

Hexadecyltrimethylammonium bromide (HTAB) is used as an effective antiseptic agent against bacteria and fungi [10]. It has been widely used in the synthesis of gold nanoparticles [11] and is present in many household products [12]. Because of its industrial importance, we intend to study the thermodynamics of micellization of HTAB in presence of amino acids, glycine (Gly) and glycylglycine (Gly-Gly). These amino acids are considered to be structure-breakers in aqueous solutions [13] and also are of biological significance, being monomers of biopolymers, proteins. On the basis of their influence on the micellization process and their sites of solubilization, i.e., micellar core, micellar surface, or in the palisade layer, additives are classified as electrolytes and nonelectrolytes [4, 14] thereby, affect the thermodynamic properties differently. Literature survey indicates that study on the micellization behavior of hexadecyltrimethylammonium bromide in aqueous amino acids has been

[1] The article is published in the original.