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COLLOID CHEMISTRY AND ELECTROCHEMISTRY

Hexadecyltrimethylammonium Bromide Micellization in Glycine, Diglycine, and Triglycine Aqueous Solutions as a Function of Surfactant Concentration and Temperatures[1]

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Abstract—Micellization behavior of hexadecyltrimethylammonium bromide (HTAB) was investigated conductometrically in aqueous solutions containing 0.02 mol kg^{-1} glycine (Gly), diglycine (Gly–Gly), and triglycine (Gly–Gly–Gly) as a function of surfactant concentration at different temperatures. The critical micelle concentration (CMC) of HTAB exhibits a decreasing trend as the number of carbon atoms increases from Gly to Gly–Gly–Gly, favoring the micelle formation. The values of CMC and the degree of counterion dissociation of the micelles were utilized to evaluate the standard free energy for transferring the surfactant hydrophobic chain out of the solvent to the interior of the micelle, ΔG°_{HP}, free energy associated with the surface contributions, ΔG°_{S}, standard free energy, ΔG°_{m}, enthalpy, ΔH°_{m}, and entropy, ΔS°_{m} of micellization were also calculated. The results show that the micellization of HTAB in aqueous solutions as well as in aqueous Gly/Gly–Gly/Gly–Gly–Gly solutions is primarily governed by the entropy gain due to the transfer of the hydrophobic groups of the surfactant from the solvent to the interior part of the micelle. The CMC obtained by fluorometric method is in close agreement with those obtained conductometrically. Furthermore, decrease in the I_1/I_3 ratio of pyrene fluorescence intensity suggests the solubilization of the additives by the surfactant micelles and that this solubilization increases as the hydrophobicity increases from Gly to Gly–Gly–Gly.

Keywords: conductance, fluorescence, micellization, surfactant-amino acid/peptides interactions, micellization.

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INTRODUCTION

Surface-active molecules such as surfactants possess non-polar hydrophobic and polar hydrophilic groups in the same molecule and, thus, are amphiphilic in nature, form aggregates called micelles above a certain concentration range known as the critical micelle concentration (CMC) [1, 2]. It is well recognized that the self-aggregation of amphiphilic molecules and the resulting CMC is an important parameter in determination and optimization of various characteristic properties of micelles, used in many pharmaceutical, biotechnological, and chemical processes [3, 4]. The study of interaction between surfactant and protein molecules is of immense significance to understand various aspects of life processes [5]. However, due to the complex conformational and configurational three-dimensional structures of proteins, a direct study of surfactant-protein interaction is somewhat difficult. It is therefore useful and convenient to investigate the micellization behavior of surfactants in presence of model compounds (amino acids/peptides) [6, 7]. Amino acids are important biologically-active substances and are basic structural units of proteins. Moreover, amphiphilic molecules and amino acids are extensively present in biological systems.

However, amphiphiles are able to form aggregates only when they are dissolved in a suitable solvent. Thus, the aggregation behavior of a surfactant can be conveniently modified by using the solvents of varied nature. The usual way to vary the solvent properties is to add additives like electrolytes, which generally facilitate the formation of ionic micelles in aqueous solution, mainly by lowering the columbic free energy of the interface, resulting in decrease in CMC and an increase in micellar aggregation number [8]. On the other hand, polar and non-polar organic additives in aqueous solutions affect micellization in different ways—the former additive is solubilized in the palisade layer of the micelle while the latter one is solubilized in the micellar core [9]. Therefore, a systematic study of micellization behavior of surfactant in aqueous amino acids/peptides can provide valuable infor-

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