



# Effect of caffeine on the micellization and related thermodynamic parameters of sodium dodecyl sulphate, hexadecyltrimethylammonium bromide and triton x-100: a physicochemical study

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### **ABSTRACT**

Effect of caffeine on the micellization of anionic surfactant (SDS), cationic surfactant (HTAB) and non-ionic surfactant (Tx-100) was investigated using the conductometric and tensiometric techniques. The thermodynamic parameters such as change in Gibbs-free energy,  $\Delta G_m^0$ , change in enthalpy of micellization,  $\Delta H_m^0$ , change in entropy of micellization,  $\Delta S_m^0$ , change in Gibbs-free energy of transfer,  $\Delta G_{m,trans}^0$ , surface excess concentration,  $\Gamma_{\rm max}$ , minimum area per surfactant molecule,  $A_{\rm min.}$ , surface pressure,  $\Pi_{cmc}$ , change in Gibbs-free energy of adsorption,  $\Delta G_{ads}^0$  and other related parameters were calculated to gain insights into the interactions of caffeine with different surfactants at different temperatures. The CMC in mole fraction units,  $\chi_{CMC}$ , values of SDS in caffeine are low, while that of HTAB are large in comparison with the values reported in water. The negative values of  $\Delta H_m^0$  and  $\Delta G_m^0$  and the positive values of  $\Delta S_m^0$  are indicative of SDS-caffeine and HTAB-caffeine interactions.

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# 1. Introduction

The use of surfactants with additive-based systems is of immense potential particularly as transdermal permeation enhancers [1,2], as solubilising agents [3], as in various industrial applications [4] etc. The application of surfactants with other organic additives is now being explored in the area of chemo and biosensors as well [5]. Surfactants are amphiphilic molecules and consist of polar head group and a large non-polar moiety known as tail and thus can interact with both polar and non-polar compounds. They have a property to self-assemble in aqueous solution forming micelles, where their properties are different from those of the monomer molecules [1–3]. To evaluate various thermodynamic parameters of interaction or the mixed micelle geometry or the salt effects, the conductivity [6–9], surface tension [8,10], spin probe method [11], fluorescence [7,12,13], UV-visible spectroscopy [9,14,15], dynamic light scattering [7,13,16] are commonly performed. However, any modification in the properties of an aqueous surfactant solution system depends not only on the nature of the surfactant molecules but also on the use of external additives, such as cosurfactants, cosolvents, electrolytes, polar organics, non-polar organics, etc [4–7,10–12,16–20].