INTERACTION BETWEEN TRITON X100 AND BRIJ 58 IN THEIR BINARY MIXED MICELLES

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Abstract
The micellization of the binary mixture of surfactants Triton X100 – Brij 58 in an aqueous solution was investigated using a spectrofluorimetric method with pyrene as a probe molecule. There are synergistic interactions between the micellar building units in the binary mixed micelles Triton X100 – Brij 58, which increase with increasing temperature. The analyzed binary mixed micelles possess molar excess entropy.

Introduction
Triton X100 is a commonly used surfactant, mainly as an additive in drug or vaccine formulation. Brij 58 is a dominantly used solubilizer and an emulsifier in the food, drug, and cosmetics industry. Their structures contain polyoxyethylene chains as hydrophilic parts of their molecules, significantly longer in Brij 58 than in Triton X100. The hydrophobic part in Triton X100 has an aromatic core and the hydrophobic part in Brij 58 has an aliphatic hydrocarbon chain. These traits lead to different behavior in terms of critical micellar concentration and affect the structure of their mixed micelle.

Experimental
Chemicals used for this study were taken from original manufacturer's packaging (Sigma Aldrich, Saint Louis, MO, USA). The critical micelle concentrations of pure surfactants and their binary mixtures in aqueous solutions were determined by the invasive spectrofluorimetric method, using pyrene as a probe molecule. Measurements were done with different molar ratios (α) of surfactants in their binary mixtures (α = 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9), in the temperature range of T = (273.15–323.15) K, with 5 K increments. All solutions of surfactants were prepared using pyrene-saturated water. First (I_1) and third (I_3) vibration band of pyrene emission spectrum, were recorded at 373 nm (I_1) and 384 nm (I_3). Obtained fluorescence measurement results (I_1/I_3 ratio) for different work solutions' concentrations were analyzed using software Origin Lab 9 (Northampton, MA, USA). The I_1/I_3 ratio vs. total concentration of surfactants plots were analyzed using a Boltzmann fitting, where the interception of two asymptotes was considered to be the critical micellar concentration of the examined surfactant mixture, at a given temperature. The calculations of thermodynamic parameters were done according to the Regular Solution Theory (RST) [1].

Results and discussion
In the monocomponent micelles of Brij 58, the globular and the elongated conformations of surfactant molecules are randomly distributed. The substitution of Brij 58 molecules, which hydrocarbon chains are in the globular conformations, with the molecules of Triton X100, reduces hydrophobic hydration [2,3]. This results in a synergistic interaction between different micellar building units in the examined binary mixed micelles. The mean value of the interaction parameter is negative, in the examined temperature interval T = (273.15–323.15) K. Synergistic interactions are usually the result of various factors (contributions). Enthalpic

contribution most likely originates from hydrogen bonds (in the hydrophilic shell of binary mixed micelles) between the terminal OH groups in the polyoxyethylene chains of Triton X100 molecules and the ether oxygens in the polyoxyethylene chains of Brij 58 molecules. Thermodynamic stabilization of the examined binary mixed micelles increases with increasing temperature. Namely, after replacing Brij 58 molecules that have globular conformations with Triton X100 molecules, the planar aromatic rings are incorporated into micelles, which increases hydrophobic interactions of Brij 58 hydrocarbon chains (with increasing temperature, the size - intensity - hydrophobic interactions also increase [4]). As the hydrophobic segment of Triton X100 is shorter than the hydrophobic segment of Brij 58, the hydrocarbon chains of Brij 58 have a favorable packaging effect, i.e., in the inner domain of the hydrophobic nucleus of the binary mixed micelle, the number of different conformational states of the Brij 58 hydrocarbon chains increases with increasing temperature.

Conclusion

For binary mixed micelles Triton X100 - Brij 58, the RST approximation of the zero value molar excess entropy cannot be taken. In the temperature interval T = (273.15–323.15) K, with increasing temperature, the thermodynamic stabilization of the binary mixed micelle Triton X100 - Brij 58 increases in an aqueous solution concerning the hypothetical ideal state (ideal binary mixed micelle).

References

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