

**“Zakopane” AMPERE NMR SCHOOL**  
virtual event

## **BOOK OF ABSTRACTS**

Edited by S. Jurga  
Adam Mickiewicz University in Poznań  
NanoBioMedical Centre

**21<sup>st</sup> June – 23<sup>rd</sup> July 2021**

# **“Zakopane” AMPERE NMR SCHOOL**

## **virtual event**

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**organized by**

**NanoBioMedical Centre  
and The Centre for European Integration  
Adam Mickiewicz University in Poznań, Poznań**



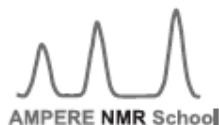
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# CONFORMATIONAL AND AGGREGATIONAL BEHAVIOR OF SOME SURFACTANTS IN AQUEOUS SOLUTIONS BY NMR OF $^1\text{H}$ AND $^{13}\text{C}$ NUCLEI

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Surfactants belong to actual chemical products, which are consumed in a large amount and find numerous applications in various areas. Amino-acid based surfactants attract an increasing interest, mainly because of their environmentally friendly properties. In comparison to conventional surfactants they are characterized in particular by a fast biodegradation and excellent antimicrobial and antifungal activities. Among them one of the most commonly used is sodium N-lauroyl sarcosinate (SLS).

To investigate the chemical and physical properties of surfactant solutions, a great number of experimental and theoretical methods have been used. Among them a special place can be assigned to nuclear magnetic resonance methods (used in the present study): NMR spectroscopy, NMR relaxometry, NMR diffusometry. Despite numerous studies of the properties of SLS in various systems, there are currently many questions that require clarification, in particular it concerns the value of the critical micelle concentration (CMC), conformational transitions in solutions and mixtures, local mobility of individual segments of amphiphilic molecules, etc. For example, as reported in the literature, the value of CMC for SLS lies in the range between 0.009 and 0.014 M, depending on the used method.

From the spectra it was possible to estimate the time scale of the internal reorientations of the COO-group at the room temperature: 3–5 ms. There is a relatively fast exchange of the SLS molecules between the monomer and micellar states: the exchange time is much less than 1 ms. Modern NMR spectrometers allow the measurements of relaxation rates for resolved spectral lines belonging to different molecular groups and, therefore, the investigation the local molecular mobility. For example, it was possible to obtain for the set of  $\text{CH}_2$  groups the correlation time of  $\tau_c \sim 10^{-10}$  s. The bigger values of spin-relaxation times for the  $\text{CH}_3$  groups indicate a higher mobility of these groups. Using the NMR method with a pulsed magnetic field gradient, the self-diffusion coefficients of surfactant molecules in the monomeric and micellar states were measured. The obtained data allowed us to refine the CMC values and develop a new method for estimating the decrease in the concentration of monomers with an increase in the total concentration of surfactants.

In practical applications the surfactant mixtures are often used because surfactants in mixtures exhibit new properties. In particular, mixtures of cationic and anionic surfactants are of interest for research. In the present study, in addition to SLS the dodecyltrimethylammonium bromide (DTAB) was chosen as the starting point. Data indicating the formation of mixed micelles in SLS+DTAB systems have been obtained. As a hypothesis, we suggest the electrostatic binding of molecules in the SLS+DTAB systems, which manifests itself in the broadening of the spectral lines for certain concentration regions. The spin-lattice relaxation times of  $^1\text{H}$  and  $^{13}\text{C}$  nuclei have been measured. Based on the relaxation of  $^{13}\text{C}$ , the reorientation times of the molecules are calculated. The bigger correlation times were observed for some molecular groups that correlate with the broadening of lines in the  $^1\text{H}$  spectrum for these groups.