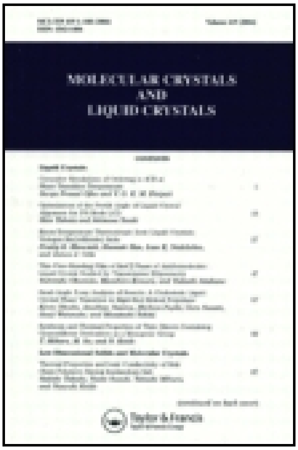

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A. Zheliaskova [a], S. Sagnowski [b] & A. Derzhanski [a]

[a] Institute of Solid State Physics, Liquid Crystal Department, 72 Lenin Blvd, 1784, Sofia, BULGARIA

[b] Institute of Nuclear Physics, Radzikowskiego 152, 31-342, Krakow, POLAND

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NMR OF THE TRITON X 114 - WATER MICELLAR SOLUTION

A.Zheliaskova[1], S.Sagnowski[2], A.Derzhanski[1]
[1]Institute of Solid State Physics, Liquid Crystal Department, 72 Lenin Blvd, 1784 Sofia, BULGARIA
[2]Institute of Nuclear Physics, Radzikowskiego 152
31-342 Krakow, POLAND

ABSTRACT Proton spin-lattice relaxation time T_1 has been measured as a function of temperature from 5°C to 50°C for the triton X 114 - water lyotropic binary system. Relaxation occurs to be nonexponential and is governed by two different processes: intramolecular movements and spherical micelle rotations.

INTRODUCTION

NMR investigations of liquid crystals have been extensively used to provide with the information about the mesophase structure, molecular arrangements,mobilities, and mechanism of binding of molecules. As a model compounds for complex biological molecules lyotropic liquid crystal systems are being used commonly.

Amphiphilic alkylphenylpolyethylene glycol (triton X 114) forms lamellar phase in water at certain concentrations[1,2]. Micelle aggregates are formed at low concentrations (10 - 20 weight percent) while the reversed micelle aggregates grow at high concentrations (20 - 90 weight percent) of the surfactant.

The purpose of this research is to study the spin-lattice relaxation mechanism in the lyotropic triton X 114 - water mixtures at low concentrations of the detergent.

MATERIALS AND METHODS

The investigated binary system composed of the Fluca's triton X114 detergent and perdeuterated water (99.98% of D_2O). Three samples of 10,15 and 20 weight percent of detergent were prepared.

T_1 measurements were performed at 8 MHz using Bruker SXP4-100 spectrometer. The technique of $(\pi-\tau-\pi/2)$ sequence was used.

Temperature of the sample was electronically controlled and did not vary by more than 0.1 K during an experiment. Over the temperature range studied (5°C - 50°C) the magnetization recovery was found to be nonexponential.

RESULTS AND DISCUSSION

In order to measure the spin-lattice relaxation T_1 for protons of the triton X 114 it was necessary to use deuterated water as a solvent.

The variation of T_1 as a function of tempereture suggests that the relaxation rate is a sum of two contributions governed by two different processes. We will call them a low temperature process (X) and a high temperature process (Y)[3]. Assuming that these mechanisms are of the Arrhenius type the least-squares fitting of the experimental data to the formula[4,5]

$$1/T_1 = \Sigma_i \; C_i\{\tau_i/(1 + \omega_o^2\tau_i^2) + 4\tau_i/(1 + 4\omega_o^2\tau_i^2)\}$$

$$i = X, Y$$

with

$$\tau_i = \tau_{oi}\exp(E_i/kT)$$

yields the values of C_i, τ_i and E_i for all investigated samples. Coupling constants C_X and C_Y along with the values of the correlation times τ_X and τ_Y calculated for the temperature T = 298 K are collected in Table 1.

TABLE 1.

c [%]	C_X $[s^{-2}]$	C_Y $[s^{-2}]$	τ_X [s]	τ_Y [s]
10	$3.5*10^9$	$1.3*10^8$	$0.7*10^{-9}$	$2.2*10^{-7}$
15	$3.3*10^9$	$0.8*10^8$	$0.9*10^{-9}$	$2.3*10^{-7}$
20	$3.1*10^9$	$1.1*10^8$	$0.9*10^{-9}$	$1.2*10^{-7}$

Similar investigation of the binary system triton X 114 - water were carried out at frequency 32 MHz for the concentration range 20 - 90 weight percent of the detergent[3]. The results showed also two relaxation processes which were attributed to the intramolecular movements in detergent molecule. One of them was shown to be connected with protons of the hydrophobic alkyl chains while the other one with protons of hydrophilic oxyethylene chains.

The low temperature process discovered in this study shows a similar behaviour as in the previous one[3] where the value of the correlation time was $\tau_X=1*10^{-9}$ s. This means that these processes have the same character: they are reflection of the intramolecular motions of protons in hydrophobic alkyl chains.

The correlation time for the second relaxation process (high temperature one) is $\tau_Y=2*10^{-7}$ s. This process we attribute to a slower motion. On the other hand τ_Y for three investigated samples shows a tendency to increase with the change in detergent concentration. This points to a formation of the spherical aggregates in this concentration range.

According to the Debye theory the correlation time for a spherical molecule of radius R can be expressed by the formula

$$\tau_r = 4\pi\eta R^3/3kT,$$

where η is the viscosity of the medium. From this formula the radius of micelle aggregate could be calculated. If we assume the viscosity of the solution to be approximately equal to the viscosity of pure water at the same tempereture (298 K) the calculated radius is R=60 Å. Robson at al.[6] investigated the amphiphilic triton X 100 with molecules similar to the ones studied in this research. He established the formation of spherical aggregates of radius R=47 A which is comparable with the value found from our experimental data. The difference between the two walues can be explained by the fact that in our calculations the increase of water viscosity due to solvation effect has not been taken into account.

The change of the high temperature correlation time τ_Y for the concentration increasing from 15 to 20 weight percent can be considered as an evidence of a change in micelle shape and increase of its size with the concentration.

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