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BROAD LINE NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY OF P-NONYLPHENOLPOLYETHYLENEGLYCOL

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Abstract: The present work represents research into the broad line NMR spectrum of Arkopal dissolved in D_2O.

The phase structure and molecular mobility of different liquid crystal phases (including lyotropic systems as well) have been the object of much research Especially effective has been the use of broad line NMR spectroscopy method I1I. The line width and form of the absorption spectrum give information about the mobility of a mesogenic molecule as a whole, and also about the mobility of its constituent atomic groups I2I. For example, in a series of works I3I, I4I the influence of the length of the alkyl chain on the microscopic mobility and polymorphism of a detergent-water system is studied. With most types of surface active substances the hydrophilic heads give fewer possibilities of variation. An exception to this are some non-ionic detergents for example the p-alkyl phenolpolyethyleneglycols (Arkopals). For these substances the sizes of both the hydrophobic alkyl chains and the hydrophilic polar heads can be changed in wide ranges.

The present work represents research into the broad line NMR spectrum of p-nonylphenolpolyethyleneglycols with 9,6 mole ethyleneglycol (Arkopal 9,6) dissolved in D_2O, with respect to different weight concentrations of the detergent.

The proton absorption spectra of (Arkopal 9,6) dissolved in D_2O in weight concentrations from 10 % to 100 % were taken. We used a homemade NMR broad line spectrometer to record the spectra. The experiment was carried out at a temperature of about 25^oC.

According to Luzzati, lamellar and hexagonal liquid crystaline phases I5I are to be expected for the above-mentioned detergent.

In the lamellar phase, lateral molecular diffusion takes place in the plane of the layer; because of this the molecular axis does not turn in space, and a narrowing of the spectrum caused by the reorientation of the molecular axis absent. In the hexagonal phase, lateral diffusion has two components:
1) along the generant of the cylinder, along which the molecular axis also does not reorientate and
2) revolving around the axis of the cylinder, in which case the molecular axis must turn in space, due to which the spectrums narrow. Still more narrowing occurs in the intermediate optically isotropic phase (it has been observed by us), in which every lateral shift of the molecule changes the direction of its axis.

The absorption NMR spectra that were recorded are of a typical "super-Lorentzian" kind. We present each of the spectra as a sum of two Gaussian curves (with the help of a proper computer programme). As a result the following was obtained:

1) One of the components (we denote it with A) is the same for all the spectra; it has a width relatively narrow and is not dependent on the concentration. This is probably due to intramolecular thermal motion.

2) The second component, denoted by us with B ,is a considerably broader absorption curve with a width of several gauss and strongly depends on the concentration In our opinion it is connected with the mobility of the molecule as a whole.

Table 1 presents the half widths and the statistical weights of the two Gaussian curves as a function of the concentration of (Arkopal 9,6) . The concentration interval studied was divided into several subintervals: 1) from 0 % to C_1; 2) from C_1 to C_2 ; 3) around C_2; 4) from C_2 to C_3; 5) over C_3; where $C_1 \approx 40$ %, C_2 is in a narrow concentration interval around 50 %, C_3 70 %. The second and the fourth subintervals correspond to the hexagonal and lamellar phases respectively. The third subinterval corresponds to the liquid crystal intermediate optically isotropic phase . The first and fifth are probably isotropic micellar solutions with normal and reverse micelles.

From Table 1 it can be seen that component B is comparatively wide and has a high statistical weight at the hexagonal phase. This reflects the hindered mobility of the molecules and perhaps their dense packing.

In the narrow concentration interval around 50 % we observed an optically isotropic phase which we have provisionally called "cubic". This phase has a considerably smaller width of component B than in the neighbouring phases. In this case we assume that our "cubic" phase is not pure, but contains small domains with the characteristics of the other phases.

As was expected, component B has a maximum width in the lamellar phase, wider than at the hexagonal phase (Table 1). The statistical weight of B is highest in the lamellar phase as well - more than 50 %.

The first and fifth subintervals (the isotropic micellar solutions) will be the object of additional investigations. Here we will remark only that the existence of a broad line in these two intervals testifies to hindered molecular motion, which is probably caused by the formation of optically isotropic supermolecular structures with low mobility.

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concentration of detergent	H_B IgaussI	statistical weight K_B
10 %	2,3	51 %
20 %	2,5	50 %
30 %	2,4	53 %
35 %	2,5	53 %
40 %	2,6	64 %
45 %	2,6	60 %
50 %	2,1	49 %
55 %	2,9	53 %
65 %	2,9	56 %
70 %	1,8	50 %
80 %	2,7	50 %
90 %	2,9	53 %

TABLE 1