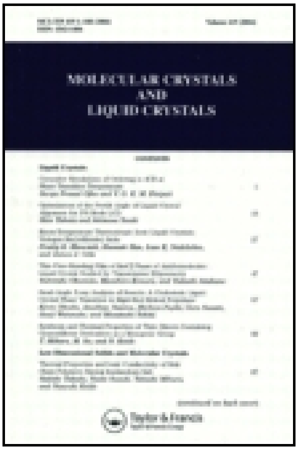

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Distribution of Hydrophobic Molecules and Solubilization in some Micellar Solution

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DISTRIBUTION OF HYDROPHOBIC MOLECULES AND SOLUBILIZATION IN SOME MICELLAR SOLUTION

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Abstract: The distribution of the hydrophobe molecules in the volume of some micellar solutions was checked by high resolution NMR spectra. The theoretical assuptions for the arrangement of the hydrocarbon chains in the micelle volume was confirmed.

The distribution of hydrophobic molecules in the volume of one micelle with various dopants and respectively with various properties was investigated experimentally. Usually one assumes that the hydrophilic heads of the amphiphilic molecules in the spherical micelles build up an outer spherical surface. The theory (1)(2) assumes that in the absence of a dopant in such a micelle the hydrophobic parts of the amphiphilic molecules have a maximum density at the micelle centre and much lower density at the periphery (hydrophobic - hydrophilic interface). The hydro phobic dopants dissolved in the micelle will then be settled mainly at the periphery.

In order to verify these assumptions high resolution NMR spectra of micellar solution of DBS /dodecylbenzene sulfonate/ with TEMPO and cyclohexane dopants (3) were recorded and investigated as well as TRITON X-100 and $CuSO_4$ dopants.

The TEMPO is a paramagnetic hydrophobic dopant. Its localization at various parts of the amphiphilic molecule is shown by the changing of the spectral lines of respective hydrogen atoms /according to Fox (5), Derzhanski (6), see too Abragam (7) / A small quantity of hydrophobic dopant, for example TEMPO, will be localized mainly at the peripheric micellar area. Its presence will influence on the broading and decreasing of the amplitude of the spectral line chiefly of the hydrogen atoms of the benzene ring. For example the ratio of the amplitude of the CH_3 group proton line and one of the benzene proton line is 1.94 in the absence of TEMPO and it increases up to 3.27 in the presence of TEMPO. The saturating amount of cyclohexane added equalizes the density in the micelle. The TEMPO is then distributed uniformly in all the micellar volume. Its influence over the CH_3 group spectra increases and comes closer to the influence of the benzene ring. The ratio of the amplitudes of the maximum lines of CH_3-A_{CH_3} and C_6H_4-$A_{C_6H_4}$ respectively can be a criterion for this influence. This ratio $A_{CH_3} / A_{C_6H_4} = B$ decreases as the hydrophobic dopant concentration increases (3).

Unlike the above said in TRITON micelles any radial gradient of the density will not be expected . As Ref.(4) showed these surfactant molecules are distributed in a more complicated way in spherical micelles. The surfactant molecules are at different distances from the centre of the micelle.That ensures amore uniformly filled volume with hydrophobic chains Besides,the hydrophobic and hyrophilic parts of this surfactant are less separated from each other. Thus one may conclude that the dissolved paramagnetic dopants, both hydrophobic and hydrophilic, influence equally all molecular parts of the surfactant.

The NMR spectra of 1% TRITON X-100 in D_2O were recorded.

i) without any paramagnetic dopant

ii)with a TEMPO dopant 1.25×10^{-6} weight concentration with respect to water

iii) with a $CuSO_4$ dopant

iv) with a TEMPO dopant and $CuSO_4$ dopant at the same concentration

Figures 1, 2, 3 and 4 represent cases i, ii, iii and iv respectively.

The ratio B obtains the following values corresponding to the four cases $B_i = 7.33$, $B_{ii} = 8.36$ $B_{iii} = 7.29$, $B_{iv} = 6.5$.

As we show above in the case of a micellar solution of the DBS the addition of paramagnetic dopants changes the value of B strongly $(\frac{3.27}{1.94} = 1.69)$.

Unlike this when one has the micelles of TRITON the value of B changes in very narrow intervals. That shows actually an equal influence of both paramagnetic dopants upon different parts of the

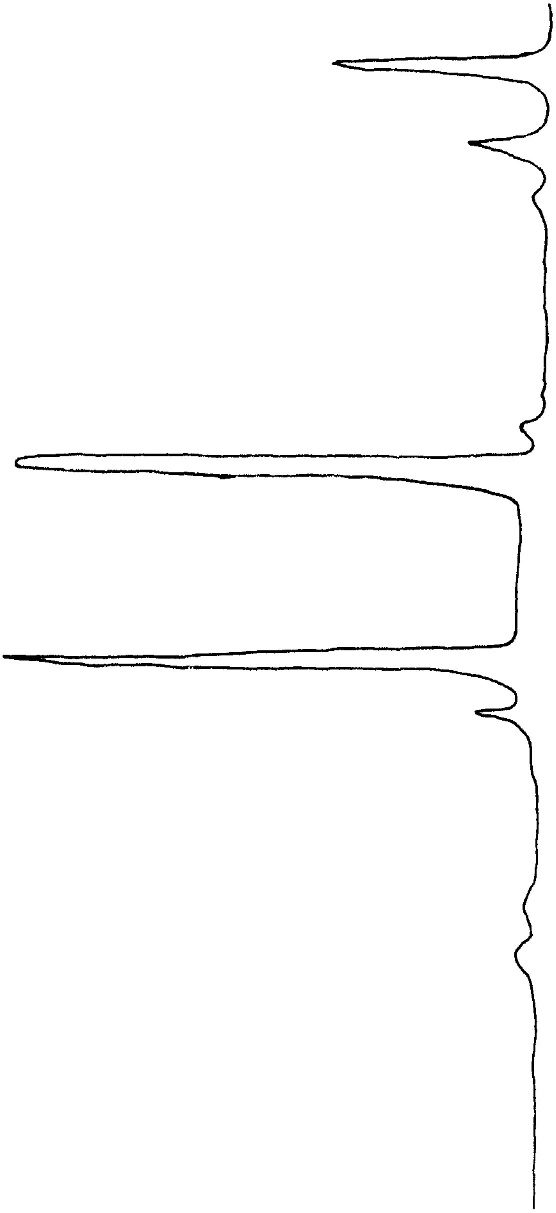

FIGURE 1

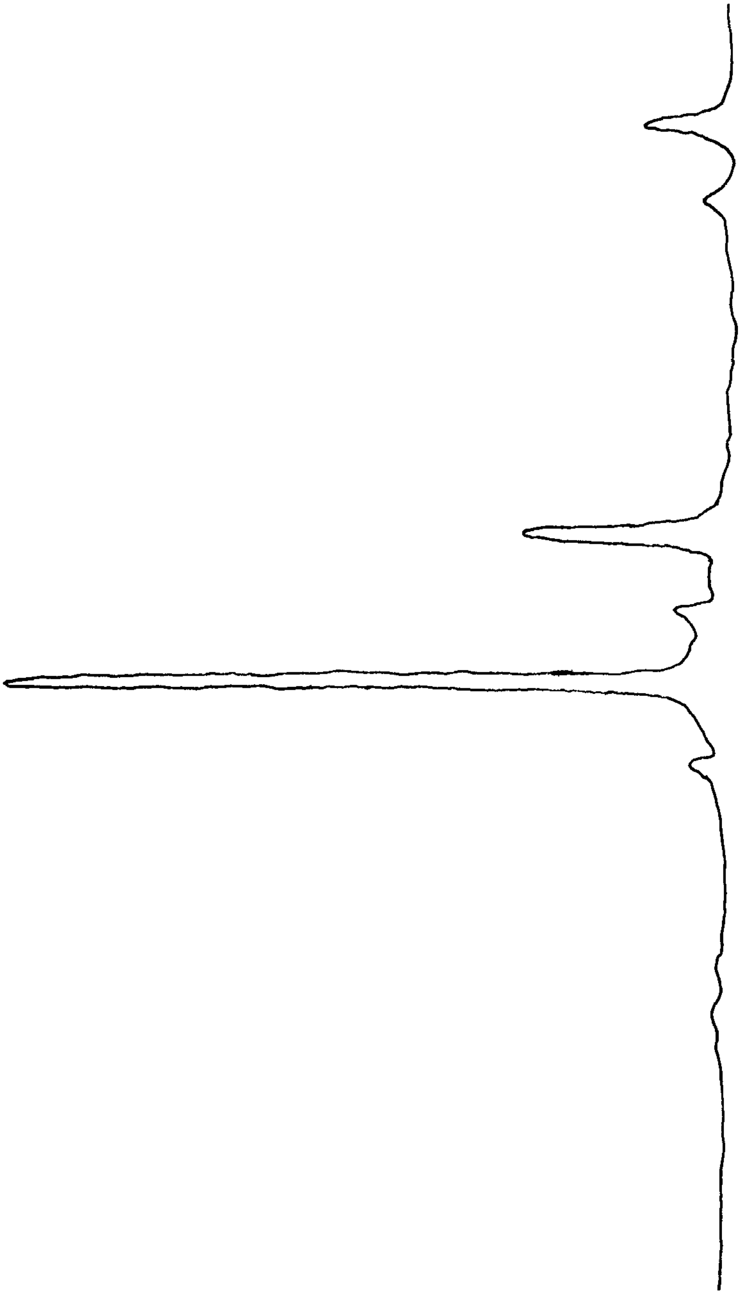

FIGURE 2

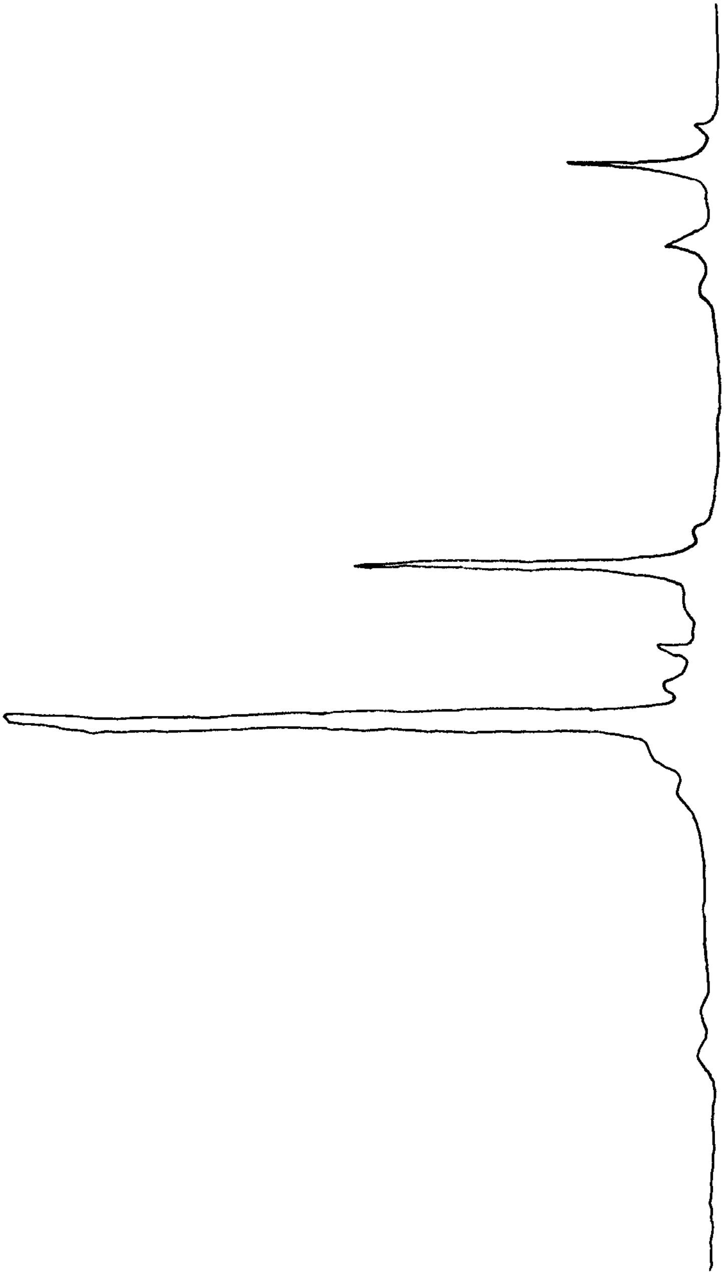

FIGURE 3

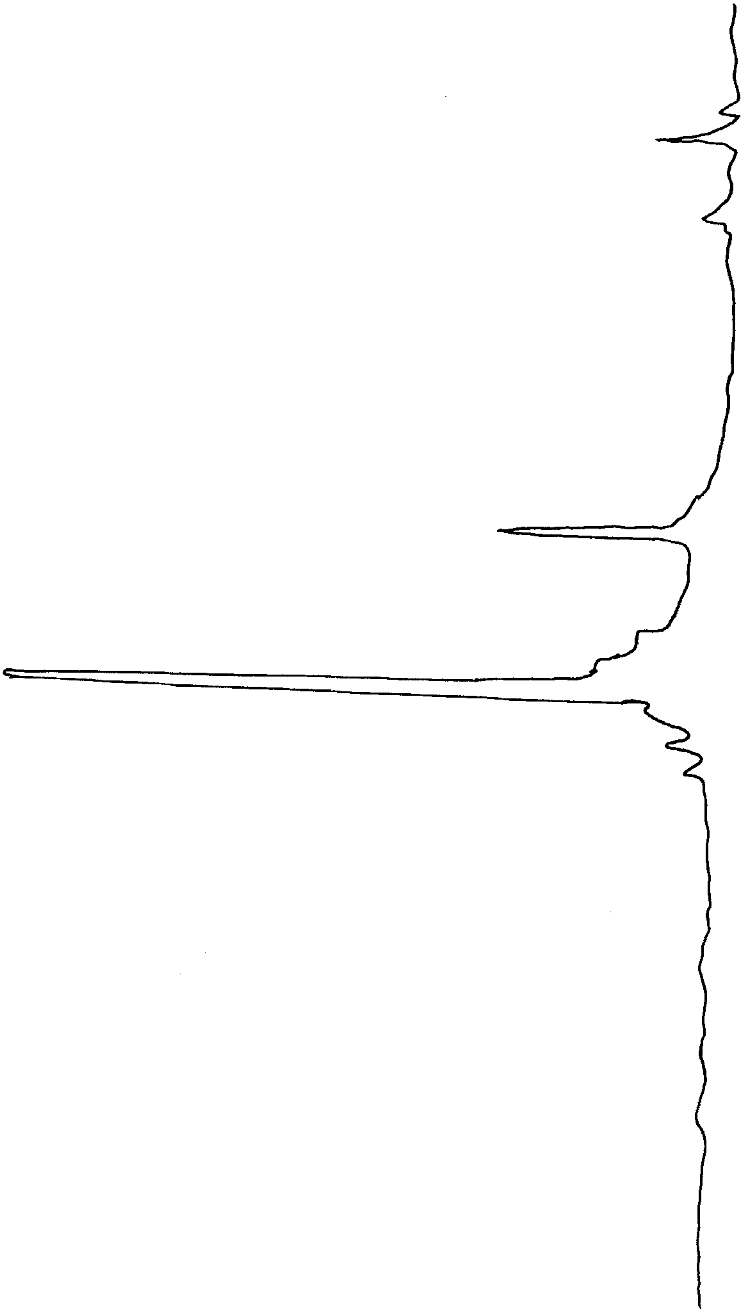

FIGURE 4

surfactant molecule.

Both paramagnetic dopants, in agreement with the above assumptions, broaden the spectral lines of the benzene ring and CH_3 groups in the same way.

References

(1) J.Charvolin and B.Mely, Mol.Cryst.Liq.Cryst.Lett. 41, 209, (1978)

(2) A.Derzhanski and I.Bivas, Phys.Lett.A 74A,372(1979)

(3) A.D erzhaski and A.Zheliaskova, Phys.Lett.A 72A 67, (1979)

(4) R.J.Robson and E.A. Dennis, J.Phys.Chem. 81, 1075 (1977)

(5) K.K.Fox, I.D.Robb and R.Smith, JCS Faraday Transactions I 3, 445, (1972)

(6) A.Derzhanski, A.Georgieva, K.Kotev and B.Atanasov, BBA, 214, 83, (1970)

(7) А.Абрагам, Ядерный магнетизм, Москва 1963