scrambling would have been observed (even in the absence of production of allyl cation). The heat of formation of protonated fluorocyclopropane is unknown, but it can be crudely estimated from the calculated heat of formation of fluorocyclopropane (-28 kcal/mol)[21] by taking the proton affinity of fluorocyclopropane to be the same as that of 1-fluoropropane. Estimating this latter value to be equal to the proton affinity of fluoroethane plus the difference in ionization potentials of fluoroethane and 1-fluoropropane,[15] we gauge the $\Delta H_f°$ for F-protonated fluorocyclopropane to be on the order of 160 kcal/mol. The fact that vibrationally excited **1** neither yields allyl cation nor scrambles isotopic label en route to **2** testifies to the kinetic inaccessibility of protonated fluorocyclopropane.

These results show the utility of fluoride abstraction for assigning ion structures. The use of ^{19}F NMR to determine the extent and position of deuterium label in neutral products opens new avenues for explorations of ion rearrangement pathways and reactivity in the gas phase.

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Registry No. 1, 14665-81-7; **2**, 50457-57-3; **3**, 61207-57-6; D_2, 7782-39-0; F^-, 16984-48-8; *t*-BuF, 353-61-7; *t*-Bu^+, 14804-25-2; $(CH_3)_2CF_2$, 420-45-1; $CH_2{=}CFCH_3$, 1184-60-7; $(CD_3)_2C(OH)CH_3$, 53853-65-9; MeMgI, 74-88-4; $(CD_3)_2CO$, 666-52-4; $(Et_2N)SF_3$, 38078-09-0.

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Electron Spin-Echo Modulation Studies of Doxylstearic Acid Spin Probes in Sodium and Tetramethylammonium Dodecyl Sulfate Micelles: Interaction of the Spin Probe with D_2O and with Deuterated Terminal Methyl Groups in the Surfactant Molecules

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Abstract: Electron spin-echo studies have been carried out for a series of *x*-doxylstearic acids (x = 5, 7, 10, 12, and 16) in frozen aqueous solutions of sodium dodecyl sulfate and tetramethylammonium dodecyl sulfate in D_2O and of sodium dodecyl sulfate and tetramethylammonium dodecyl sulfate deuterated in their terminal methyl groups. Modulation effects due to interactions of the nitroxide groups with water deuterium and terminal methyl group deuterium have been measured as a function of x. The results are discussed in terms of the distributions of water and of terminal methyl groups measured separately in these micelles. In addition information is deduced about the probable conformations of the spin probe and surfactant molecules in the micelles. There is a profound influence of the counterion on all these factors as shown by the great difference between the sodium dodecyl sulfate and tetramethylammonium dodecyl sulfate micelles.

In several recent papers we have shown how electron spin–echo modulation (ESEM) spectrometry can be utilized to obtain information about the structure of micellar systems.[1-5] Electron spin–echoes originating from the photogenerated *N,N,N',N'*-tetramethylbenzidine (TMB) cation radical and from *x*-doxylstearic acid spin probes in rapidly frozen micellar solutions show deuterium modulation for samples prepared in D_2O or with surfactants deuterated in their head group or counterions. We have demonstrated that micellar structure is retained in these rapidly frozen solutions by electron spin resonance observation of TMB^+ in the thawed solutions, since in bulk solution TMB^+ has only a lifetime of microseconds! We have found that micellar structural factors play an important role in the photoionization efficiency of TMB. Substitution of the tetramethylammonium cation for the sodium cation in dodecyl sulfate micelles brings about enhanced interaction between the TMB cation and water as measured by ESEM. This was accompanied by a marked increase in the photoionization efficiency of TMB. We have postulated that the surfaces of sodium dodecyl sulfate (SDS) and tetramethylammonium dodecyl sulfate (TMADS) micelles differ on the molecular level.[4] While SDS micelles have a relatively compact head group structure, the head group structure of TMADS micelles seems to be more disordered or rougher perhaps

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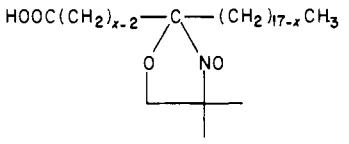
because the more hydrophobic counterions act as spacers between the head groups.[4,5]

In the present work we have studied the effect of such counterion substitution on the molecular organization in the hydrophobic core of the micelle. Using a series of *x*-doxylstearic acid spin probes with varying *x*, we have carried out studies of doxyl nitroxide interactions with deuterated terminal methyl groups on the surfactant molecules of TMADS and SDS in frozen micellar solutions. From the observed dependence of deuterium modulation depth on the *x*-doxyl group position, we have concluded that the average configuration of the surfactant molecules is different in TMADS as compared to SDS micelles.

The analysis was complemented by an investigation of the degree of water penetration into these two micellar systems since this is an area of some controversy.[6-8] By measuring deuterium interactions from D_2O as a function of *x* in a series of *x*-doxylstearic acid spin probes, we have been able to assess the distribution of deuterium nominally in the outer parts of the micellar structure.

Experimental Section

x-Doxystearic acid spin probes with the general structure



were purchased from Molecular Probes, Inc. (x = 5, 7, 10, and 12) and from Aldrich Chemical Co. (x = 16) and were used as received. D_2O was from Aldrich, SDS was from Eastman Kodak Co. or British Drug Houses or synthesized with equivalent results, and TMADS was prepared as described previously.[4]

Tetramethylammonium dodecyl-*12,12,12-d*$_3$ sulfate (TMADS-ω-d_3) and sodium dodecyl-*12,12,12-d*$_3$ sulfate (SDS-ω-d_3) were prepared as follows. Dodecanoic-*12,12,12-d*$_3$ acid (Prochem, B.O.C. Limited, L9317-9), 2.10 g, 0.0103 mol, was esterified by addition of freshly prepared diazomethane (from *N*-methyl-*N*-nitroso-*p*-toluenesulfonamide, Aldrich Diazald, by KOH in diethylene-glycol monoethyl ether) in dry diethyl ether until the yellow color of the diazomethane persisted. Gas chromatographic analysis (12 ft × $^1/_8$ in. 8% SP1000, 175 °C and 6 ft × $^1/_8$ in. 3% Dexil 300, 150 °C, Perkin-Elmer Sigma 3, flame ionization detection) showed this material to be free of impurities of shorter or longer chain length. Lithium aluminum tetrahydride (LAH, Aldrich, 95+%) reduction of the ester in dry diethyl ether (from LAH), using a 2-fold excess of hydride, 0.439 g, 0.013 mol, and reflux after the addition of the crude ester was complete, yielded the alcohol after hydrolysis with 1 N HCl, ether extraction, washing with saturated $NaHCO_3$ followed by brine and drying over anhydrous Na_2SO_4. The crude alcohol was concentrated and chromatographed on silica gel (Baker, flash chromatography grade) eluting with 1:2 ether in pentane. Gas chromatographic analysis (6 ft × $^1/_8$ in. 8% SP1000, 175 °C) of the fractions containing the alcohol showed no other alcohol or ester contamination at the detection limit (~ 0.01%). The entire yield of dodecanol-*12,12,12-d*$_3$ was sulfated with an equimolar quantity of freshly distilled chlorosulfonic acid (0.66 mL, 0.01 mol, bp 151-152 °C, laboratory atmospheric pressure, Fisher Purified Grade) by slow addition of the acid to a dry diethyl ether solution of the alcohol in an ice bath. After warming to room temperature and stirring for 1 h, the solution was poured onto 10 g of ice in a separatory funnel equipped with a Teflon stopcock to avoid grease. Butyl alcohol (25 mL, Fisher HPLC grade) was added and the aqueous layer extracted. The aqueous layer was further extracted twice with 10-mL portions of butyl alcohol, and the combined butyl alcohol extractions were washed 3 times with 10 mL of water to remove sulfuric acid. The success of these washes can be judged by the formation of slowly separating emulsions as the sulfuric acid is removed. The butyl alcohol layer was divided into two equal lots. The first was neutralized with 4.4 mL of 10% aqueous solution of tetramethylammonium hydroxide (Matheson, Coleman and Bell, TX381-9930, L8E26) to pH 7. The second was shaken with 10 mL of a saturated aqueous solution of Na_2CO_3 and the lower layer removed. The butyl alcohol from both solutions was then evaporated on a rotary evaporator at 50 °C until solids formed. A fresh 25 mL of dry butyl alcohol was added to each, the solids redissolved by heating to 50 °C, and the evaporation continued to remove water. The second evaporation was terminated at the first sign of cloudiness and the material hot filtered (50 °C) to remove inorganic salts. This concentration followed by hot filtration was repeated until no further solids insoluble in 20-30 mL of hot butyl alcohol could be obtained. When each final 20-mL butyl alcohol solution was cooled to 0 °C, white crystals of the surfactants were obtained. These were recrystallized twice from absolute ethyl alcohol to remove traces of butyl alcohol. After these were dried to constant weight under vacuum at room temperature, 1.10 g (64% theoretical) of tetramethylammonium dodecyl-*12,12,12-d*$_3$ sulfate was obtained. Anal. Calcd for TMAD-ω-d_3 (Galbraith Laboratories, Inc., Knoxville, TN): C, 56.10; H + D, 11.77; N, 4.09; 9.36% S. Found: C, 56.03; H + D, 11.76; N, 3.98; S 9.48. Similarly, the yield of sodium dodecyl-*12,12,12-d*$_3$ sulfate was 1.03 g (71% theoretical). Anal. Calcd for SDS-ω-d_3 (Galbraith): C, 49.46; H + D, 9.68; S, 11.00. Found: C, 49.40; H + D, 9.65; S, 11.25.

Samples of perprotiated sodium dodecyl sulfate (SDS) and perprotiated tetramethylammonium dodecyl sulfate (TMADS) were obtained as above from dodecanoic acid (Matheson, Coleman and Bell, lauric acid, CQ2984, L59).

The specificially deuterated surfactants were examined in D_2O by nuclear magnetic resonance spectroscopy. In both ^{13}C and ^1H spectra, the deuteration of only the terminal methyl group was confirmed. In addition, we have obtained fast atom bombardment mass spectra of these surfactants in glycerol. The m/e of the predominant $ROSO_3(M)_2^+$ ions confirmed the presence of only three deuteriums. This method also allowed an upper limit of 0.01% to be placed on the presence of similar surfactants of chain lengths other than 12 carbons and showed less than 1% dodecanol-d_3 based on addition of known amounts of the latter probable impurity.

Surfactant solutions of 0.1 M containing 0.4 mM *x*-doxylstearic acid were prepared in triply distilled, deoxygenated water. Details of the sample preparation have been published.[4,5,9] The two pulse ESEM spectra were recorded at 4.2 K from the $M_I = 0$ ^{14}N hyperfine transition on a home-built X-band spectrometer[10] using exciting pulse widths of 50 ns. Previous results have shown that the micellar structure is retained in frozen micellar solutions.[1]

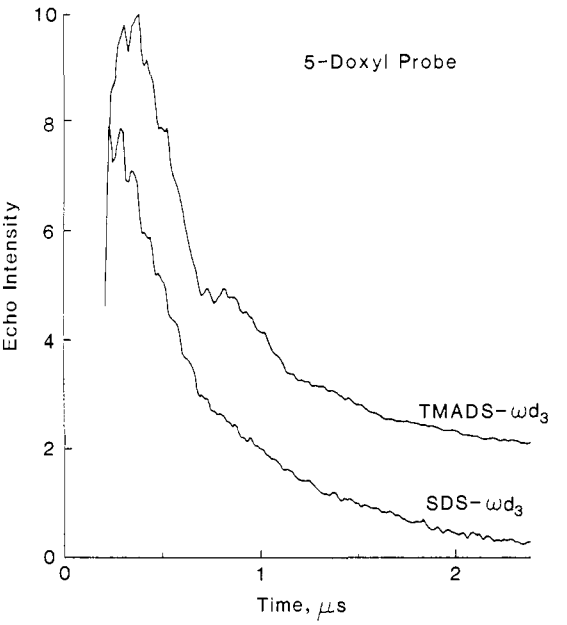


Figure 1. Two-pulse electron spin-echo spectra recorded at 4.2 K for 5-doxylstearic acid spin probe in SDS-ω-d_3 and TMADS-ω-d_3 micellar solutions.

Results

Two-pulse electron spin-echo envelopes were recorded from the $M_I = 0$ ^{14}N hyperfine transition (central line) of the nitroxide electron spin resonance spectrum. The results obtained for 5-doxylstearic acid in TMADS-ω-d_3 and SDS-ω-d_3 micellar solutions are shown in Figure 1. The echo decay curves exhibit modulations with periods of about 0.8 and 0.5 μs due to nitroxide interactions

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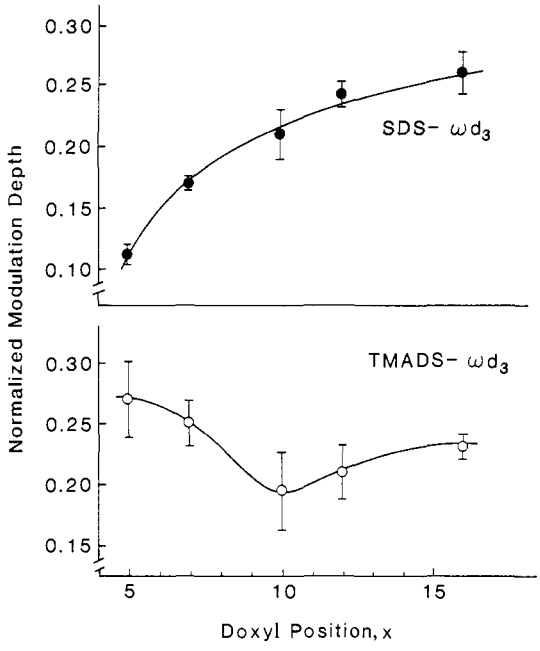

Figure 2. Dependence of deuterium ESE normalized modulation depth on the position of the doxyl group in x-doxylstearic acid spin probes in SDS-ω-d_3 and TMADS-ω-d_3 micellar solutions.

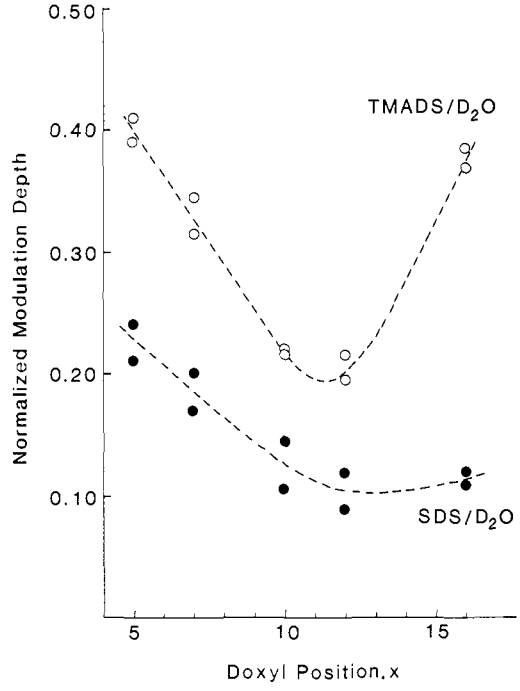

Figure 3. Dependence of deuterium ESE normalized modulation depth on the position of the doxyl group in x-doxylstearic acid spin probes in SDS/D_2O and TMADS/D_2O micellar solutions.

with protons and deuterons, respectively. Deuterium modulation for 5-doxylstearic acid is almost undetectable in SDS-ω-d_3 micelles, but it is clearly observed in TMADS-ω-d_3 micelles.

Similar ESEM patterns were obtained with the other x-doxylstearic acids in these two types of micelles. The normalized deuterium modulation depth was estimated by drawing a curve through the maxima and the minima of the modulation and measuring the fractional distance between these curves.[3-5] The normalized deuterium modulation depths are plotted vs. the doxyl group position, x, in Figure 2. The data represent duplicate and at least triplicate experiments for SDS-ω-d_3 and TMADS-ω-d_3 micelles, respectively, and the range of deviations is shown. In SDS-ω-d_3 micellar solution, the modulation depth increases smoothly with the increase of x. In TMADS-ω-d_3 micellar solution, however, the modulation depth decreases on going from $x = 5$ to $x = 10$ and then increases for higher values of x.

TMADS and SDS micellar solutions in D_2O were also studied with the x-doxylstearic acid spin probes for $x = 5$–16. Deuterium modulation was generally seen, and the normalized deuterium modulation depth for these micellar systems is plotted vs. x in Figure 3. The data represent at least duplicate experiments. Part of these data for $x = 5$, 7, and 10 was reported previously.[4]

Discussion

The choice of a 0.1 M surfactant concentration and the nature of the 0.4 mM x-doxylstearic acid spin probe Poisson distribution among the micelles have been discussed previously.[5] At 0.1 M surfactant concentration, the micelles are thought to be spherical or nearly so and to have aggregation numbers of 80 for TMADS and 75 for SDS which show that these micelles are very similar in size.[5,11]

The deuterium modulation depth depends on the number of interacting deuteriums and on their average distance from the spin probe. When an unpaired electron interacts with a spherically symmetrical distribution of 10 or fewer deuteriums, deuterium modulation is generally only detectable at interaction distances of less than 0.6 nm.[12] The intersection of a sphere of this radius with a micelle gives a maximum interaction volume for interacting deuteriums. When corrected for the volume of the doxyl group estimated from additive partial molar crystal volumes of atoms in combination[13] up to a distance of 0.6 nm from the nitroxide, a value of 0.67 nm^3 is obtained. We assume that the distributions of deuteriums from D_2O in the micellar–water interface or from deuterated terminal methyl groups on the surfactant are not significantly altered by changing the doxyl group position on the alkyl chain of the series of x-doxylstearic acid spin probes used. Thus the modulation as a function of x (Figures 2 and 3) is comparable in SDS and TMADS micelles and can be primarily interpreted in terms of the relative interaction distances for a fixed distribution of deuterium.

The maximum water interaction is probably obtained when the nitroxide occupies a position at the micelle radius. In a previous paper[5] we showed that the average interaction volume around a doxyl group was large enough for only one surfactant head group and counterion based on the surface density of head groups. Subtracting the head group and counterion volumes leaves 0.44 nm^3 in TMADS micelles and 0.56 nm^3 in SDS micelles for water and the hydrocarbon. We estimate that half of this volume is occupied by portions of the surfactant hydrocarbon chains, which leaves a volume for a maximum of seven water molecules in TMADS and nine water molecules in SDS to interact with the spin probe. Since the observed D_2O modulation is greater in TMADS compared to SDS, the implication is that the doxyl probes are distributed more deeply in SDS than in TMADS and/or that the Stern layer in TMADS is rougher than that of SDS, exposing more of the probe to the water. The average modulation should also reflect the hydration numbers of the head group and the counterion. Hydration numbers for these ions in aqueous and nonaqueous solvents[14] indicate a total hydration of seven and nine water molecules per surfactant molecule for TMADS and SDS, respectively, which is consistent with the estimate given above.

Estimation of the maximum number of interacting deuterated methyl groups is more difficult. The data for micelles with deuterium in the Stern layer[5] suggest that the spin probes are not radially arrayed on the average and hence may not often sample the core of the micelle where the simplest assumption would place most of the tail-end deuterium. The other extreme assumption of surfactant tail-end location places them evenly throughout the

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volume of the micelle. Below the Stern layer we assume the entire interaction volume, corrected for the doxyl group volume, to be filled with hydrocarbon. From the aggregation number and calculated micellar volume based on space filling models[15] and surfactant partial molar volumes,[16] we estimate 1.9 CD_3 groups or a total of 5.7 deuteriums interacting with the unpaired electron for both the SDS and TMADS micelles.

In agreement with other authors, we consider doxylstearic acid to have its carboxyl group in the Stern layer of the micelle,[9,17-22] leaving the doxyl group to seek its own location in the micelle in response to hydrophilic, hydrophobic, and steric forces.[5] In previous work we have shown that the average location of the nitroxide moiety in the doxyl group relative to a specifically deuterated part of a surfactant molecule in a micelle can be determined by ESEM. The most definitive results are for deuteration of the trimethylammonium head group in cationic micelles since in this case the location of the deuterium label with respect to the micellar structure is well-known.[5] In the present work we use a similar approach, but the location of the deuterium label is not as explicitly known. However, by looking at the entire complex of experiments, relatively unambiguous conclusions can be made about the conformations of the doxylstearic acid probes in the micellar structure and to a lesser extent about the surfactant conformations.

If the doxylstearic acid spin probe has a predominantly all-anti conformation, one expects that as x increases, the nitroxide group will be probing deeper toward the micelle core and farther from the micelle surface. This simple picture seems to be quite compatible with the results for SDS micelles. The results for the SDS/D_2O micelles in Figure 3 show that the normalized modulation depth decreases monotonically from $x = 5$ to $x = 12$ and then appears to level out between $x = 12$ and $x = 16$ for the series of x-doxylstearic acid spin probes studied. This is compatible with a model in which the bulk of the interacting D_2O is near the micellar surface region or Stern layer region, with the average interaction distance with the unpaired electron spin increasing as x increases. These results are also consistent with the results shown in Figure 2 for SDS-ω-d_3 micelles. If the surfactant molecules are predominantly in an all-anti conformation, the terminal methyl groups on the alkyl chains should be concentrated toward the center of the micelle and the the normalized deuterium modulation depth is expected to increase monotonically as x increases for the x-doxylstearic acid spin probes. This is exactly what is observed in Figure 2.

The overall qualitative picture seems clear. In SDS micelles the solvent water molecules are located predominantly in and near the Stern layer region or the outer portion of the micellar structure, while the terminal methyl groups on the surfactant alkyl chains are located predominantly in the inner or core region of the micellar structure. Considerations of the interaction distances involved[5] indicate that the 7-doxylstearic acid probe would need at least a single gauche conformation in the alkyl chain to have an interaction distance of less than 0.6 nm with Stern layer deuteriums. Thus, the probes and the surfactant molecules need not be constrained to be in an all-anti conformation to be consistent with the experimental results. Such statistical disorder of the surfactant and probe chain conformations is to be expected.

We now consider similar experiments on TMADS micelles in which the sodium counterion has been replaced by a tetramethylammonium counterion. We have previously shown that this counterion substitution has a profound influence on the micellar surface structure.[4] The interactions of the series of x-doxylstearic acid spin probes with D_2O in TMADS micelles are shown in Figure 3. There are two distinct differences from the analogous results in SDS micelles. Firstly, the modulation depth is significantly higher in the TMADS micelles. This indicates a greater concentration of water in the Stern layer or a different conformation of the spin probe in the TMADS micelles compared to the SDS micelles. Secondly, the deuterium modulation depth goes through a minimum for $x = 10$–12 and increases significantly for the $x = 16$ nitroxide spin probe. This is most easily understood if the nitroxide spin probe has a bend in its alkyl chain due to adjacent gauche conformations so as to allow both the carboxylate and the nitroxide groups to reside close to the Stern layer. A bent spin probe molecule suggests a different average conformation of the surfactant molecules in the TMADS micelle as compared to the SDS micelle.

While there is some uncertainty in the locus of the solvent water in micelles,[6-8] this is less true of the locus of micellar counterions. Thus, it is relevant to compare the results of the x-doxylstearic acid spin probes with deuterated water in TMADS micelles with the interactions of the same spin probes with deuterated counterions in TMADS micelles which have been studied previously.[5] The normalized modulation depth vs. doxyl position for TMADS-d_{12} micelles is shown in Figure 4. The parallelism between these results in Figure 4 and the TMADS/D_2O results

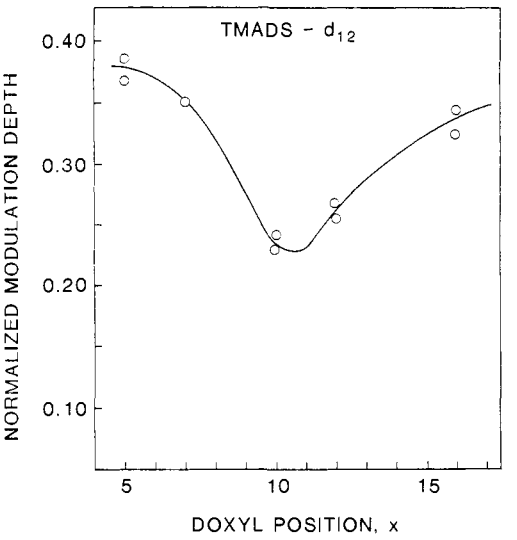

Figure 4. Dependence of deuterium ESE normalized modulation depth on the position of the doxyl group in x-doxylstearic acid spin probes in TMADS-d_{12} micellar solutions.

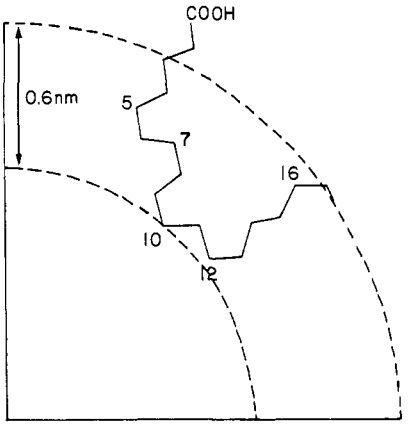

Figure 5. Schematic drawing of a cross section of a TMADS micelle showing a probable conformation of an x-doxylstearic acid molecule; the doxyl group is not shown. Only full cis or trans bond conformations are shown in this oversimplified two-dimensional representation.

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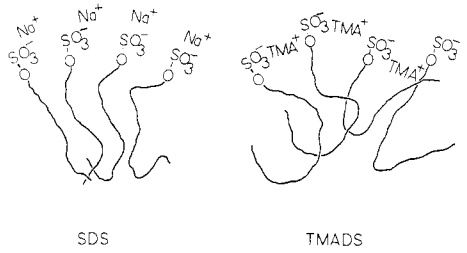

Figure 6. Schematic drawing of sections of SDS and TMADS micelles emphasing the structural differences in the head group arrangements and the alkyl chain conformations. TMA^+ refers to the tetramethylammonium cation.

in Figure 3 is striking. This seems to suggest that the locus of water in TMADS micelles is indeed predominantly in the Stern layer region and that at least the 12- and 16-doxylstearic acid spin probes are bent so that the alkyl end of the probe molecule samples the micellar surface or Stern layer of the micelle. Figure 5 shows a schematic representation of a possible conformation of a spin probe molecule in TMADS micelles with a bent alkyl chain which allows the 16 position to sample the micellar surface.

The TMADS-ω-d_3 micelle results in Figure 2 vs. the doxyl probe position show unexpected features. The normalized modulation depth decreases, instead of increases, with increasing x-doxyl position to about $x = 10$ and increases slightly for $x = 12$ and 16. This is only consistent with the primary locus of the methyl termini of the alkyl chains of the TMADS surfactant molecules near the micellar surface. However, the changes in the amplitudes of the normalized modulation depths vs. the x-doxyl position are relatively small, implying a reasonably uniform distribution of the surfactant alkyl chain ends throughout the TMADS micelle. Still, there is a greater probability for the chain ends to be located in the region that the 5-doxyl and 7-doxyl positions probe, consistent with the larger volume fraction of the outer part of the micelle. Even a random statistical distribution of chain ends implies a higher probability for the surfactant molecules in TMADS micelles to bend and to have their alkyl chain ends sample the micellar surface than is the case in SDS micelles.

Figure 6 shows a schematic drawing comparing sections of SDS and TMADS micelles based on our results and analysis. In SDS micelles the head groups are fairly compact and the alkyl tails are predominantly extended. In TMADS the head groups are spaced out by the tetramethylammonium counterions and also displaced vertically with respect to one another so as to increase the surface roughness and the thickness of the head group layer. In TMADS micelles the alkyl tails are more loosely packed than in SDS micelles, leading to significant chain bending.

Evidence from nuclear magnetic resonance and fluorescence quenching studies[23] and from the kinetics of chemical reactions in micelles[24] supports the contention that the hydrophobic tail of the surfactant molecules can sample the micellar surface. These conclusions have largely been reached on experiments involving SDS micelles. It would be very interesting to make similar measurements comparing SDS and TMADS micelles since our work indicates that such effects are much stronger for TMADS micelles.

Theoretical studies have also been carried out by several groups in which it has been concluded that the surfactant alkyl chains have considerable freedom of movement and that all segments including the alkyl tails have significant probabilities for sampling the surface of the micelle.[25-28] However, these theoretical analyses have not included any effect of changing the counterion, which we have found here to be of extreme importance in affecting the surfactant conformation in the micellar structure. Dill and Flory[26] have considered the effect of micelle surface curvature on the distribution of hydrocarbon chains in micelles by means of a statistical mechanical analysis. In micelles of reduced curvature, they found that the hydrophobic chains are packed with more order near the center than near the outside of the micelle and that the maximum in the distribution of terminal methyl groups is shifted toward the micellar center. This prediction could be used to explain the difference found between SDS and TMADS micelles if the SDS micelles had reduced average curvature compared to TMADS micelles. However, since SDS and TMADS micelles have similar aggregation numbers, their average surface curvatures should be similar. Alternatively we might equate the theoretical effect of reduced surface curvature with tighter molecular packing which may be considered characteristic of our SDS micelle results. In the TMADS micelles both our results and other results[29] indicate that the tetramethylammonium counterions act as head group spacers. This would reduce the surface density of head groups and alkyl chains, leading to looser molecular packing and more chain bending.

Conclusions

The structures of frozen SDS and TMADS micelles have been studied with x-doxylstearic acid spin probes and electron spin–echo modulation techniques. These two types of micelles present contrasting structural characteristics which reflect the importance of the surfactant counterions on the internal micellar structure. The SDS micelles appear to have a reasonably compact head group structure with a low degree of water penetration and relatively well-organized alkyl chains. The SDS terminal alkyl groups are concentrated near the center region of the micelle. In contrast, the TMADS micelles show a more open head group structure with significant water penetration into the Stern region and a locus of terminal alkyl groups that is broadly distributed throughout the micelle with some higher probability in the outer region of the micelle. This suggests that the TMADS molecules have more gauche and even bent conformations compared to the SDS surfactant molecules.

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Registry No. TMADS-ω-d_3, 94519-28-5; SDS-ω-d_3, 94519-29-6; SDS, 151-21-3; TMADS, 2536-43-8; $CD_3(CH_2)_{10}CO_2H$, 79050-22-9; $CD_3(CH_2)_{11}OH$, 94519-30-9; D_2O, 7789-20-0; 5-doxylstearic acid, 29545-48-0; 7-doxylstearic acid, 40951-82-4; 10-doxylstearic acid, 50613-98-4; 12-doxylstearic acid, 29545-47-9; 16-doxylstearic acid, 53034-38-1.

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