УДК 544.77.022.532+538.955+004.942

NITROXYL SPIN PROBE IN IONIC MICELLES: A MOLECULAR DYNAMICS STUDY

V.S. Farafonov [a], A.V. Lebed [b]

V.N. Karazin Kharkiv National University, School of Chemistry, 4 Svobody sqr., 61022 Kharkiv, Ukraine

a) ✉ *farafonov@karazin.ua*   ⓘD *https://orcid.org/0000-0003-0785-9582*
b) ✉ *alebed@karazin.ua*   ⓘD *https://orcid.org/0000-0001-5175-816X*

The compounds containing nitroxyl radical (NO˙) are actively used as spin probes to examine colloid systems, including lipid membranes and micelles. Their electron paramagnetic resonance spectrum provides information about the composition of the medium, in particular, the content of water there. Yet, the proper treatment of the measurement results demands understanding the microscopic characteristics of the molecular probe. In the present paper, we extend our previous studies on the microscopic state of acid-base and solvatochromic probes in surfactant micelles to the field of spin probes. We report the results of molecular dynamics simulation of a common spin probe, methyl-5-doxylstearate, in micelles of anionic (sodium *n*-dodecyl sulfate, SDS) and cationic (*n*-dodecyltrimethylammonium bromide, DTAB) surfactants. The localization of the molecule within the micelles, its shape, composition of the local environment, hydration were quantified and compared with the available relevant experimental data. No significant dissimilarity was found in the characteristics of the probe molecule in both kinds of micelles. However, the characteristics of the O˙ atom carrying the unpaired electron are pronouncedly different, namely, in DTAB micelles it is less hydrated and forms less hydrogen bonds with water. Similar situation was observed for the COO group. The main reason was found to be the interactions with cationic surfactant headgroups, which screen the O˙ atom and COO group from water. These findings allowed revisit the point of view that the surface layer of DTAB micelles as a whole is less hydrated in comparison to that of the SDS ones.

Keywords: methyl-5-doxylstearate, sodium dodecyl sulfate, dodecyltrimethylammonium bromide, localization, conformation, hydration, hydrogen bond.

Introduction

The structure of micelles of ionic surfactants and their surface layers is an area of active research by modern experimental methods. While some information may be obtained directly, estimating many important properties demands using molecular probes. In the latter case, a compound called molecular probe is added to the micellar solution, and the change of its properties (with respect to its pure water solution) is experimentally registered. The properties include fluorescence spectrum (for fluorescence probes), apparent acidity constant (for acid-base probes), UV/vis absorption spectrum (for solvatochromic probes) and electron paramagnetic resonance spectrum (for spin probes). This change may be then related to such micelle properties as microviscosity, electrostatic potential, polarity, hydration, respectively [1–6]. However, to establish this relation, the knowledge of the state of the molecular probe in the micelle is necessary. It is usually obtained by means of nuclear magnetic resonance spectroscopy; yet, the method provides only rather general insight to the probe localization [7,8]. More detailed localization information is inaccessible for it.

Recently, the computational methods have been involved to the research, as well. Among them, the molecular dynamics (MD) simulations method became particularly popular because of its ability to capture both structural and dynamic properties of these objects. It allows direct observation of the microscopic details of the system, which are unachievable for most experimental means. Hence, the MD method was actively applied firstly to individual micelles [9,10], and then to micelles with solubilized molecular probes, including the fluorescent [11], acid-base [12], and solvatochromic [13,14] ones. Yet, for the group of spin probes such studies still are rather scarce [15–17], albeit they are numerous for lipid bilayers [18,19] and proteins [20,21].

In this work, we extend our studies on the microscopic state of solvatochromic and acid-base probes in micellar solutions to the field of spin probes. Their particular feature is the ability to estimate the water fraction (*i.e.* hydration) in the medium. The principle is based on an established linear correlation between i) the measured hyperfine splitting in electron paramagnetic resonance (EPR) spectrum of the probe and ii) the concentration of O–H dipoles in medium [22]. For solutions of surfactants,

which are not hydrogen bond donors, the latter equals to concentration of water. The result of measurement is usually presented as the ratio H between water concentrations in the medium and in pure water.

Among the variety of probes, we choose a rather popular representative methyl-5-doxylstearate (MDS, Fig 1). Its spin label is the nitroxyl radical NO$^{\cdot}$ containing the O atom with unpaired electron. The presence of the long hydrocarbon chain assures incorporation of the probe to the examined lipid bilayer or micelle. Particularly, it was previously employed to assess the water content in the surface layer of sodium *n*-dodecyl sulfate (SDS) and *n*-dodecyltrimethylammonium bromide (DTAB) micelles, Fig. 1: the former ones were found to have larger H and, thus, be hydrated stronger [5,6]. MDS has been already simulated in zwitterionic micelles of *N*-dodecyl-*N,N*-dimethyl-3-ammonio-1-propanesulfonate [17]. In this work we examine the microscopic localization and hydration of MDS molecule in SDS and DTAB micelles by means of MD simulation.

Figure 1. Structure formulas of the spin probe and surfactants considered in this work.

Simulation methodology

The simulations were carried out at standard conditions, maintained by means of Berendsen thermostat and barostat. The 3D periodic boundary conditions were imposed, time step equaled 2 fs. Electrostatic interactions were computed with the PME method, while van der Waals interactions were cutoff at 1 nm. GROMACS 5.0 software was employed.

The initial configurations were micelles of 60 monomers with an MDS molecule placed inside. This number corresponds to the aggregation numbers of these surfactants [23]. Three different initial configurations were prepared for each system. Simulations were run for 40 ns, the first 10 ns of the resulting trajectories were treated as equilibration and not used in calculations. The multistage procedure of preparation of initial configurations is described in detail in our previous papers [13]. Three 11 ns simulations in pure water were also performed, the first 1 ns was omitted in calculations as equilibration.

The potential models for compounds were derived in the framework of the OPLS-AA force field. SDS and DTAB models previously developed by us were taken [10,14]; water was described with the SPC model. The model for MDS was built following the accepted in OPLS-AA protocol. The atom types were assigned manually from the set available in the OPLS-AA. The atoms of ester group and the most of hydrocarbon radical were attributed with the respective built-in charges in the force field. Oppositely, the atomic charges in the doxyl moiety were computed *ab initio* because they are not present in OPLS-AA. At the first stage, the quantum-chemical computation of the electrostatic potential around the doxyl moiety including four adjacent CH_2 groups was performed (the parameters were: Hartree-Fock level of theory, 6-31G(d) basis set, vacuum medium). At the second stage, the potential was fitted with a set of point charges placed on atoms. To facilitate the process, the RED Server was employed: it automatically performs both steps for a specified molecule, providing the final point charges [24]. The produced potential model is shown in Appendix, Fig. A1.

Results and discussion

The first point of the study is understanding the location of the probe molecule. As a quantitative measure we used the distribution function of the distance (DFD) $p(r)$ defined as a time-averaged probability p to observe the chosen distance equal to r during MD. The DFD's were computed between the

micelle center of mass (COM) and indicative atoms of the probe molecule: the O˙ atom and the C atom of carboxyl group (C_{COO}). The DFD's between micelle COM and S or N atoms of the surfactant headgroups were also plotted to outline the location of the micelle surface. The graphs are shown in Fig. 2.

The positioning of the indicative atoms differs rather little: the peaks of C_{COO} and O˙ atoms are shifted by +0.15 nm upon going from DTAB micelles to the SDS ones. In both cases, C_{COO} is ~0.15 nm advanced towards water. To provide visual understanding, the typical configurations of MDS in micelles are shown in Appendix, Fig. A2.
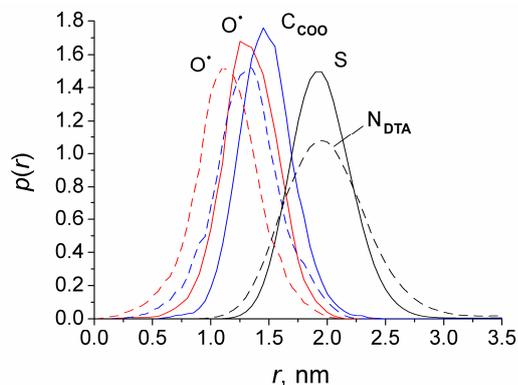
Figure 2. Distribution functions of distances micelle COM – O˙ (red), micelle COM – C in COO group (blue), micelle COM – surfactant S or N (black). Solid curves are for SDS micelles, dashed curves are for the DTAB ones.

The doxyl moiety is attached to a long hydrocarbon chain (17 C atoms). It is known that such chains tend to adopt a bent conformation because the straight conformation is statistically rather improbable. Further, the chain is longer than that in surfactant molecules (12 C atoms). It is interesting now to inspect the average curvature of the MDS molecule. We described it in terms of DFD between the C_{COO} atom and the C atom in the terminal CH_3 group, Fig. 3A. Small values indicate strong bend of the molecule and *vice versa*. According to the used potential model, the maximum value (that corresponds to the *anti* conformation of all C–C bonds) equals 2.0 nm. The calculated distribution functions are shown in Fig. 3B.

The distance mostly lies within 1.4–1.8 nm range, its preferable value is 1.6 nm indicating rather limited bend. No significant difference is present between the two surfactant solutions.

A

B
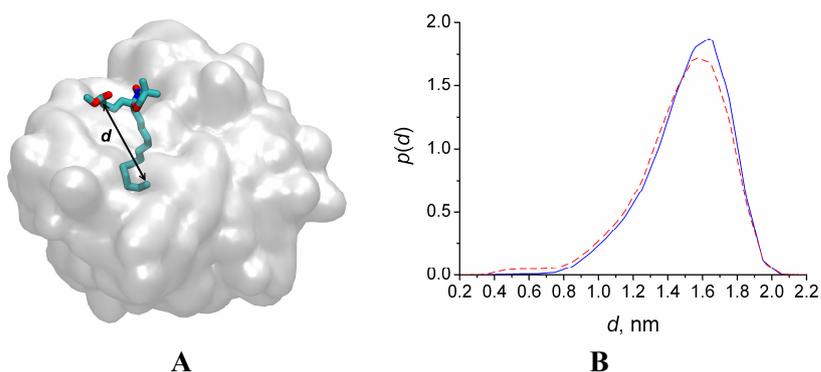
Figure 3. A: Definition of the distance d that characterizes the bend of MDS molecule (the gray surface represents the micelle hydrocarbon core); **B:** Distribution functions of d in SDS (blue solid curve) and DTAB (red dashed curve) micelles.

The investigated molecule is used to probe the water content in micelles. Therefore, the central point of our study is the inspection of composition of the solution located in the immediate vicinity of the MDS molecule, which is its microenvironment. We chose to inspect not only the microenvironment of the whole molecule, but also that of the COO moiety and the O˙ atom carrying the unpaired electron. The previously developed approach was used: for each time moment, the solution atoms

located within the 0.4 nm vicinity of any atom of the examined moiety were found and distributed into 3 groups depending on their kind (micelle hydrocarbon core, surfactant headgroups, and water). The time-averaged number of atoms in each group characterizes the medium the moiety is situated in. For convenience we converted these numbers to molar fractions. The latter are depicted in Fig. 4A.
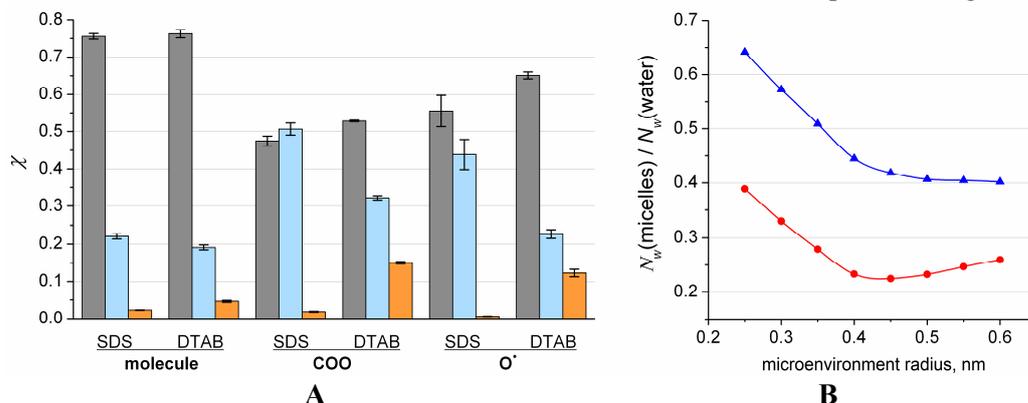
Figure 4. A: Microenvironment composition of the whole molecule and COO, O˙ moieties in micelles. The bars in triples correspond to (left to right): the micelle core atoms (gray), the water atoms (blue), the headgroup atoms (orange). **B:** The amount of water in the microenvironment of the O˙ atom in SDS (blue triangles) and DTAB (red circles) micelles relative to the pure water solution, calculated at different values of microenvironment radius.

The local environment of the whole molecule almost does not change upon going from one surfactant to another, the water content in it reaches ~20%. This is reasonable because the molecule contains only few atoms, which are expected to interact differently with cationic and anionic surfactants: the COO group and the two O atoms in doxyl moiety, all carrying high fractional charge ($|\delta| \sim 0.35$–0.5). For the COO group the difference becomes more pronounced: the water fraction in DTAB micelles is 19% lower than in SDS ones, mostly due to the increased fraction of headgroups (by 13%). The COO group in total is negatively charged, hence, it repels anionic headgroups and attracts the cationic ones. This effect was previously observed by us for acid-base and solvatochromic probes [12–14], where hydroxyl and carboxyl groups in neutral and, even more, anionic protolytic forms were strongly screened by cationic headgroups and, thus, had limited amount of water molecules around. The remaining 6% of the difference correspond to the increased fraction of hydrocarbon, which consequently is attributed to the slightly deeper immersion into micelles (Fig. 2A).

The situation for the O˙ atom is rather similar to that of the COO group. Because it is of a particular interest, we performed a more detailed analysis of its hydration. Firstly, we repeated counting water atoms around O˙ at the values of microenvironment radius other than 0.4 nm (namely, 0.25–0.6 nm). The results, N_w(micelle), were then related to the ones in pure water solution, N_w(water), Fig. 4B. Secondly, we determined the average number of O˙–water hydrogen bonds, n_{hb}. It equals 1.07±0.01 for pure water solution, 0.74±0.03 for the SDS one, and 0.46±0.03 for the DTAB one. This data proves much more aqueous environment of O˙ in the anionic surfactant than in the cationic one. This is caused firstly by the screening with the cationic headgroups (their fraction reaches 12% in DTAB) and secondly by the larger fraction of hydrocarbon around due to somewhat deeper localization in DTAB micelles (Fig. 2A).

Now we can consider the results of experimental measurements of SDS and DTAB solutions made using MDS in the light of the presented information about the microscopic state of this molecular probe. Specifically, in the works of Lebedeva *et al.* [5,6] the EPR spectrum of MDS was found to correspond to the molar concentration of water in the medium (relative to pure water) *H* equal to 0.68 and 0.44 in SDS and DTAB micelles, respectively. These values were then attributed to the whole surface layer of these micelles.

Matching these results with the data in Fig. 4B and n_{hb} values shows that they agree well with the values n_{hb}(micelle) / n_{hb}(water), which equal 0.69 for SDS and 0.43 for DTAB. Good match is also observed with the ratios N_w(micelle) / N_w(water) values of O˙ at microenvironment radius 0.25 nm: 0.64 for SDS and 0.39 for DTAB. These observations shed light on the microscopic reason of the O˙ EPR signal charge in micellar solutions. The effect of hydrogen bonding was assumed [22], but it was

not quantitatively shown in terms of the number of such bonds made by the probe with water. Further, the fact of almost quantitative agreement proves the adequacy of used model in the context of discussed problem.

On the other hand, attributing the measured H values to the entire surface layer appears to be unjustified. The localization of the molecule is similar in both micelles, its shape is similar, too (Fig. 2, 3). Given these conditions, its microenvironment should be much more hydrated in SDS micelles, if their surface layer actually contains more water. However, no considerable difference is observed (Fig. 4A). This allows suppose the overall similarity of water fractions in the surface layers of SDS and DTAB micelles, with the variations present in the local vicinity of the spin label only.

Conclusions

MD simulations of a spin probe methyl-5-doxylstearate in micelles of ionic surfactants sodium n-dodecyl sulfate and n-dodecyltrimethylammonuim bromide were performed. The localization of the molecule was examined and the hydration of the molecule and its moieties was calculated by counting water atoms in their microenvironments and counting hydrogen bonds made with water molecules. The molecule was found to be slightly deeper immersed into micelles of DTAB compared to SDS. The curvature and hydration of the molecule is also similar in both micelles. At the same time, the O˙ atom in nitroxyle radical is much better hydrated in SDS micelles than in the DTAB ones. This is caused mostly by its screening from water by cationic headgroups of DTAB and slightly deeper localization in the micelles. Therefore, it is concluded that the experimentally measured hydration values likely correspond not to the complete surface layer, but to the local environment of the spin label only. Importantly, the hydration values of the O˙ atom calculated in such a way quantitatively agree with the experiment. This proves the adequacy and usefulness of the approach and the model used for investigating local environments of molecular probes in micellar solutions.
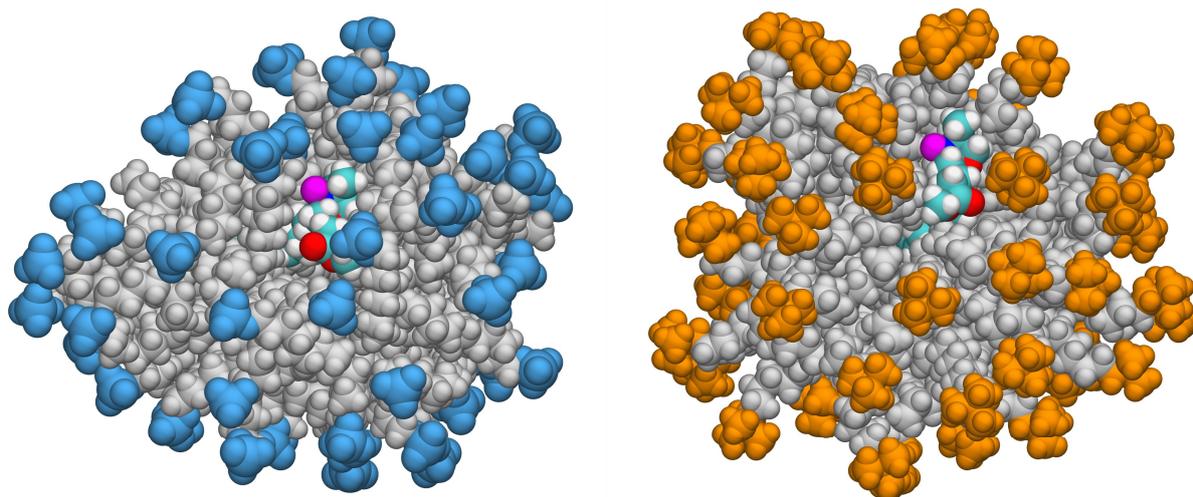
Acknowledgements

Appendix
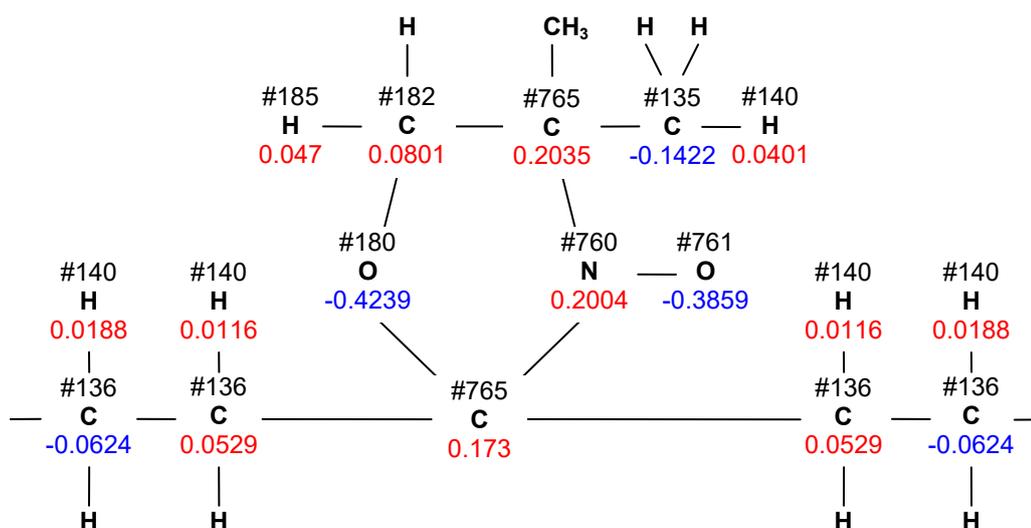
Figure A1. Atomic charges and types used in the potential model of MDS radical. The part with non-standard parameters is shown only.

Figure A2. Snapshots from MD trajectories showing typical MDS localization in SDS (left) and DTAB (right) micelles. For micelles, hydrocarbon core is colored gray and the headgroups are colored light blue or orange. The O˙ atom with unpaired electron is highlighted with pink.

References

1. Bahri M. A., Hoebeke M., Grammenos A., Delanaye L., Seret A. Investigation of SDS, DTAB and CTAB Micelle Microviscosities by Electron Spin Resonance. // Colloids Surf. A 2006. Vol.290, No.1–3. P.206–212.

2. Mchedlov-Petrossyan N. O., Vodolazkaya N. A., Yakubovskaya A. G., Grigorovich A. V., Alekseeva V. I., Savvina L. P. A Novel Probe for Determination of Electrical Surface Potential of Surfactant Micelles: N,N'-Di-n-Octadecylrhodamine. // J. Phys. Org. Chem. 2007. Vol.20, No.5. P.332–344.

3. Mchedlov-Petrossyan N. O. Protolytic equilibrium in lyophilic nanosized dispersions: differentiating influence of the pseudophase and salt effects. // Pure Appl. Chem. 2008. Vol.80, No.7. P.1459–1510.

4. Machado V. G., Stock R. I., Reichardt C. Pyridinium *N*-phenolate betaine dyes. // Chem. Rev. 2014. Vol.114, No. 20. P.10429–10475.

5. Lebedeva N., Bales B. L. Location of Spectroscopic Probes in Self-Aggregating Assemblies. I. The Case for 5-Doxylstearic Acid Methyl Ester Serving as a Benchmark Spectroscopic Probe to Study Micelles. // J. Phys. Chem. B 2006. Vol.110, No.20. P.9791–9799.

6. Lebedeva N., Zana R., Bales B. L. A Reinterpretation of the Hydration of Micelles of Dodecyltrimethylammonium Bromide and Chloride in Aqueous Solution. // J. Phys. Chem. B 2006. Vol.110, No.20. P.9800–9801.

7. Plieninger P., Baumgärtel H. A. 1H NMR Investigation Concerning the Insertion of Pyridinium N-Phenoxide Betaines into Micelles. // Liebigs Ann. Chem. 1983. Vol.5. P.860–875.

8. Tada E. B., Novaki L. P., El Seoud O. A. Solvatochromism in Cationic Micellar Solutions: Effects of the Molecular Structures of the Solvatochromic Probe and the Surfactant Headgroup. // Langmuir 2001. Vol.17, No.3. P.652–658.

9. Rakitin A. R., Pack G. R. Molecular Dynamics Simulations of Ionic Interactions with Dodecyl Sulfate Micelles. // J. Phys. Chem. B 2004. Vol.108, No.8. P.2712–2716.

10. Farafonov V. S., Lebed A. V. Developing and validating a set of all-atom potential models for sodium dodecyl sulfate. // J. Chem. Theory Comput. 2017. Vol.13, No.6. P.2742−2750.

11. Gao F., Yan H., Yuan S. Fluorescent Probe Solubilised in Cetyltrimethylammonium Bromide Micelles by Molecular Dynamics Simulation. // Mol. Simul. 2013. Vol.39, No.13. P. 1042–1051.

12. Mchedlov-Petrossyan N. O., Farafonov V. S., Cheipesh T. A., Shekhovtsov S. V., Nerukh D. A., Lebed A. V. In search of an optimal acid-base indicator for examining surfactant micelles: Spectrophotometric studies and molecular dynamics simulations. // Coll. Surf. A 2019. Vol.565. P.97–107.

Spectrophotometric studies and molecular dynamics simulations. // Coll. Surf. A 2019. Vol.565. P.97–107.

13. Farafonov V. S., Lebed A. V., Mchedlov-Petrossyan N. O. An MD simulation study of Reichardt's betaines in surfactant micelles: Unlike orientation and solvation of cationic, zwitterionic, and anionic dye species within the pseudophase. // Kharkiv Univ. Bull., Chem. Ser. 2018. Vol.30, No.53. P.27–35. https://doi.org/10.26565/2220-637X-2018-30-03

14. Farafonov V. S., Lebed A. V., Mchedlov-Petrossyan N. O. Examining solvatochromic Reichardt's dye in cationic micelles of different size via molecular dynamics. // Vopr. Khim. Khim. Tekhnol. 2018. Vol.5. P.62–68.

15. Mathias E. V., Liu X., Franco O., Khan I., Ba Y., Kornfield J. A. Model of Drug-Loaded Fluorocarbon-Based Micelles Studied by Electron-Spin Induced 19F Relaxation NMR and Molecular Dynamics Simulation. // Langmuir 2008. Vol.24, No.3. P.692–700.

16. Aliaga C., Bravo-Moraga F., Gonzalez-Nilo D., Márquez S., Lühr S., Mena G., Rezende M. C. Location of TEMPO derivatives in micelles: subtle effect of the probe orientation. // Food Chemistry 2016. Vol.192. P.395–401.

17. Giampaolo A. D., Cerichelli G., Chiarini M., Daidone I., Aschi M. Structure and solvation properties of aqueous sulfobetaine micelles in the presence of organic spin probes: a Molecular Dynamics simulation study. // Struct. Chem. 2013. Vol.24. P.945–953.

18. Kyrychenko A., Ladokhin A. S. Molecular Dynamics Simulations of Depth Distribution of Spin-Labeled Phospholipids within Lipid Bilayer. // J. Phys. Chem. B 2013. Vol.117, No.19. P.5875–5885.

19. Laudadio E., Galeazzi R., Mobbili G., Minnelli C., Barbon A., Bortolus M., Stipa P. Depth Distribution of Spin-Labeled Liponitroxides within Lipid Bilayers: A Combined EPR and Molecular Dynamics Approach. // ACS Omega 2019. Vol.4, No.3. P.5029–5037.

20. Stoica I. Force field impact and spin-probe modeling in molecular dynamics simulations of spin-labeled T4 lysozyme. // J. Mol. Model. 2005. Vol.11. P.210–225.

21. Oganesyan V. S., Chami F., White G. F., Thomson A. J. A combined EPR and MD simulation study of a nitroxyl spin label with restricted internal mobility sensitive to protein dynamics. // J. Magn. Reson. 2017. Vol.274. P.24–35.

22. Mukerjee P., Ramachandran C., Pyterl R. A. Solvent Effects on the Visible Spectra of Nitroxides and Relation to Nitrogen Hyperfine Splitting Constants. Nonempirical Polarity Scales for Aprotic and Hydroxylic Solvents. // J. Phys. Chem. 1982. Vol.86, No.16. P.3189–3197.

23. Grieser F., Drummond C. J. The Physicochemical Properties of Self-Assembled Surfactant Aggregates As Determined by Some Molecular Spectroscopic Probe Techniques. // J. Phys. Chem. 1988. Vol.92, No.20. P.5580−5593.

24. Vanquelef E., Simon S., Marquant G., Garcia E., Klimerak G., Delepine J. C., Cieplak P., Dupradeau F.-Y. R.E.D. Server: a web service for deriving RESP and ESP charges and building force field libraries for new molecules and molecular fragments. // Nucleic Acids Res. 2011. Vol.39. P.511–517.

В.С. Фарафонов, А.В. Лебедь. Нитроксильный спиновый зонд в ионных мицеллах: Молекулярно-динамическое моделирование.

Харьковский национальный университет имени В.Н. Каразина, химический факультет, пл. Свободы, 4, Харьков, 61022, Украина

Соединения с нитроксильным радикалом (NO˙) активно используются в качестве спиновых зондов для изучения организованных растворов, в том числе липидных мембран и мицелл. Их спектры электронного парамагнитного резонанса предоставляют информацию о составе среды, в частности, о содержании воды в ней. Однако, корректная интерпретация результатов измерений требует понимания микроскопических характеристик молекулярного зонда. В данной статье мы распространяем наши прежние исследования микроскопического состояния кислотно-основных и сольватохромных зондов на спиновые зонды. Мы со-общаем результаты молекулярно-динамического моделирования распространенного спинового зонда, метил-5-доксилстеарата, в мицеллах анионного (*н*-додецилсульфат натрия, ДСН) и катионного (*н*-додецилтриметиламмония бромид, ДТАБ) поверхностно-активных веществ. Локализация молекулы в

зонда в мицеллах обоих видов значительной разницы не выявлено, однако характеристики атома O˙ с неспаренным электроном существенно различаются: в частности, в мицеллах ДТАБ он менее гидратирован и образует меньше водородных связей с водой. Подобная ситуация наблюдается и для группы COO. Главной причиной этого установлено взаимодействие с катионными головным группами, которые экранируют атом O˙ и группу COO от воды. Эти наблюдения позволили пересмотреть точку зрения, что поверхностный слой мицелл ДТАБ в целом является менее гидратированным, чем таковой мицелл ДСН.

Ключевые слова: метил-5-доксилстеарат, додецилсульфат натрия, бромид додецилтриметиламмония, локализация, конформация, гидратация, водородная связь.

В.С. Фарафонов, О.В. Лебідь. Нітроксильний спіновий зонд в іонних міцелах: Молекулярно-динамічне дослідження.

Харківський національний університет імені В.Н. Каразіна, хімічний факультет, майдан Свободи, 4, Харків, 61022, Україна

Сполуки з нітроксильним радикалом (NO˙) активно використовуються як спінові зонди для дослідження організованих розчинів, у тому числі ліпідних мембран та міцел. Їх спектри електронного парамагнітного резонансу надають інформацію щодо складу середовища, зокрема, про вміст води в ньому. Втім, коректна інтерпретація результатів вимірювань потребує розуміння мікроскопічних характеристик молекулярного зонда. У даній статті ми поширюємо наші попередні дослідження мікроскопічного стану кислотно-основних та сольватохромних зондів в міцелах поверхнево-активних речовин на спінові зонди. Ми доповідаємо результати молекулярно-динамічного моделювання поширеного спінового зонда, метил-5-доксилстеарата, в міцелах аніонної (*н*-додецилсульфат натрію, ДСН) та катіонної (*н*-додецилтриметиламонію бромід, ДТАБ) поверхнево-активних речовин. Локалізація молекули в міцелах, її форма, склад локального оточення, гідратованість були обчислені та порівняні з наявними відповідними експериментальними даними. Між характеристиками молекулярного зонда в міцелах обох видів значної різниці не знайдено, проте характеристики атома O˙ з неспареним електроном є суттєво відмінними: зокрема, у міцелах ДТАБ він є менш гідратованим та утворює менше водневих зв'язків із водою. Подібна ситуація спостерігається і для групи COO. Головною причиною цього визначено взаємодію з катіонними головними групами, які екранують атом O˙ та групу COO від води. Ці знахідки дозволили переглянути точку зору, що поверхневий шар міцел ДТАБ в цілому є менш гідратованим, ніж такий міцел ДСН.

Ключові слова: метил-5-доксилстеарат, додецилсульфат натрію, бромід додецилтриметиламонію, локалізація, конформація, гідратація, водневий зв'язок.