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STRUCTURAL FEATURES OF REVERSE AOT MICELLES IN WATER/CYCLOHEXANE: MOLECULAR DYNAMICS STUDY

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A study of the structural features of reverse micelles of Na AOT (sodium bis(2-ethylhexyl) sulfosuccinate) molecules in cyclohexane with an aqueous core was carried out using the molecular dynamics method. Reverse AOT micelles are formed in three-component systems containing a non-polar solvent, water, and AOT molecules at certain concentration ratios, expressed as w = [H_2O]/[AOT]. A strong hydrogen bond between water molecules and AOT was found at the concentration w=6. For the first time, a sharp decrease in hydrogen bonding between water molecules and AOT at w=7 was shown, caused by a difference in the packing of AOT molecules and the collective dynamics of water molecules in the micelle core. The calculated results are in good agreement with experimental data from other authors. It is shown that, along with the methods of vibrational spectroscopy and dynamic light scattering, the molecular dynamics method is also informative for determining the structural characteristics of supramolecular structures and analyzing the collective dynamics of water molecules.

Keywords: *Molecular dynamics method; Reverse micelles; Hydrogen bonding*
PACS: 82.70.Uv; 47.11.Mn; GROMACS 5.1.3

INTRODUCTION

The formation of reverse AOT micelles with an aqueous nano-core [1] is of particular interest, as these systems serve as a medium for the growth of nanoparticles of various types [2, 3], organic molecules [4-6], biomolecules [7], and metal nanoparticles [8, 9]. Information on the stability of reverse micelle solutions, the shape of reverse micelles, their size distribution, and the properties of water in the core of reverse micelles has been obtained using small-angle X-ray [9] and neutron scattering [10], nuclear magnetic resonance [6], infrared spectroscopy [3, 6, 11], UV-vis spectroscopy [4], Raman spectroscopy, dielectric spectroscopy [12], methods of dynamic [13] and static light scattering [14], ultrafiltration [15], conductivity [16], and density measurements [17-19], as well as other physical methods. The difficulty of obtaining detailed molecular-level information on the structure of reverse micelles is that, unlike other complex organic structures, reverse micelles are self-assembled exclusively in solutions, which does not allow for X-ray analysis or the use of high-resolution microscopy [20]. Therefore, molecular dynamics is one of the main methods for studying supramolecular systems with a large number of degrees of freedom.

The aim of this work is the molecular dynamics investigation of the self-organization of reverse micelles of AOT molecules in the cyclohexane + water system and the study of structural properties and types of interactions depending on the variation of parameter w.

METHOD OF MOLECULAR DYNAMICS

The self-organization of reverse AOT micelles with a change in the molar ratio of water and surfactant (w = [H_2O]/[AOT] (Fig. 1) was studied using the GROMACS (Groningen Machine for Chemical Simulations) software package [21], version 5.1.3.

To describe water, the SPC/E (Extended Single Point Charge) interaction potential was used [22], which was successfully applied in other studies [23-31]. TIP3P water model is used in these molecular dynamics simulations to accurately capture hydrogen bonding behavior in this micellar system.

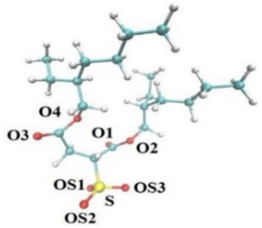

Figure 1. Chemical structure AOT

Systems were chosen in such way that the number of AOT and cyclohexane molecules were constant, and the number of water molecules corresponded to the concentration range w=0.25÷11 presented in Table 1. For cyclohexane and AOT (Figure 1), the all-atom force field potential CHARMM27 [32] was chosen, as it describes well the formation of reverse micelles in other solutions [33] and clusters [34]. A cubic cell with periodic boundary conditions and a cut off radius of 1.2 nm were applied. Other parameters and detail procedure of NPT ensemble are presented in our previous work [24]. The equilibrium systems were prepared for 30 ns with a time step of

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2 fs (Figure 2). Only the last 5 ns of the runs were used for data analysis. For the velocity autocorrelation function, the equilibrium system was rerun for the next 15 ps.

Table 1. Number of molecules in the system as a function of w = [H_2O]/[AOT] concentration.

Number of molecules			
w	cyclohexane	water	AOT
0	1000	0	95
0.25	1000	24	95
0.5	1000	47	95
1.0	1000	95	95
2.0	1000	189	95
3.0	1000	284	95
4.0	1000	379	95
5.0	1000	473	95
6.0	1000	568	95
7.0	1000	662	95
8.0	1000	757	95
9.0	1000	852	95
10.0	1000	946	95
11.0	1000	1041	95

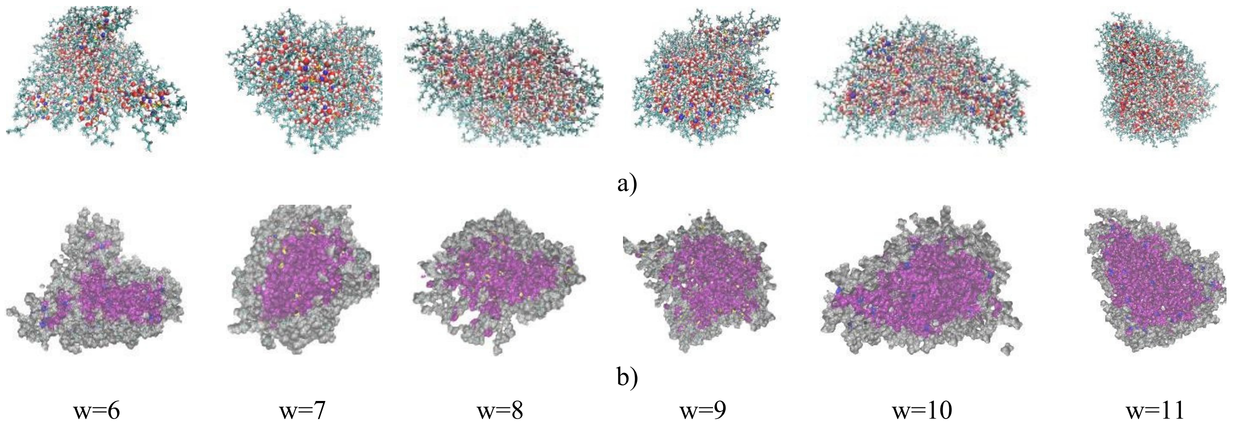

Figure 2. Formed micelles in concentration range 6÷11 of w = [H_2O]/[AOT]

RESULTS AND DISCUSSION

Figure 3 presents the number of hydrogen bonds at various water/AOT concentrations (w), illustrating two main types of interactions: between the SO^- anionic group of AOT and water molecules, and between water molecules themselves. At low concentrations (w=1 and w=2), these two interaction types are roughly equal in number, suggesting a balance between AOT-water and water-water bonding. However, starting at w=3, a shift occurs with water molecules forming significantly more hydrogen bonds with each other than with AOT, at a ratio of approximately 2.5:1. This shift indicates the formation of a more cohesive water network within the micellar core, as the available water molecules begin interacting primarily with each other rather than with the surfactant. This structural change suggests that, as the water content grows, water molecules cluster into a stable pool, altering the micelle's internal arrangement.

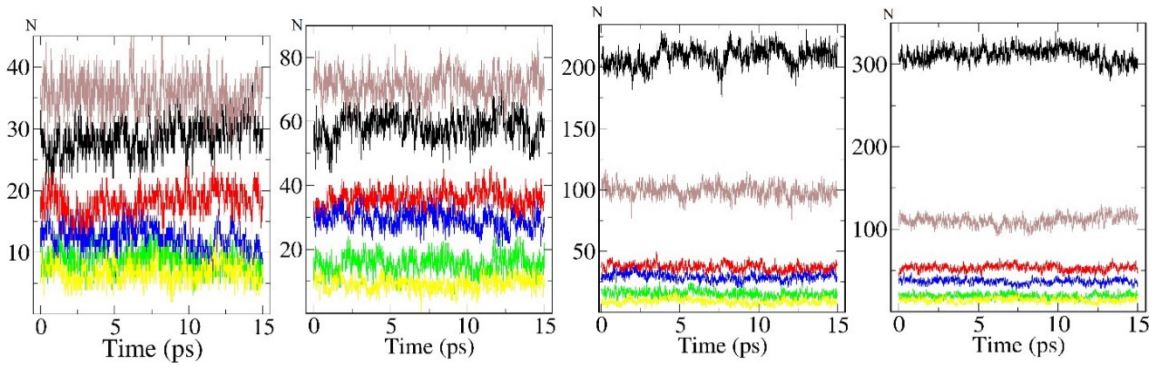

Figure 3. Number of hydrogen bonds in the system as a function of water/AOT concentration, shown from left to right: w=1, w=2, w=3, w=4. Different types of hydrogen bonds are presented: between water molecules and: molecules calculated as the centre of mass of molecules (black); hydrophilic part of SO^- (brown); O1 atom of AOT molecule (red); O2 atom of AOT molecule (green); O3 atom of AOT molecule (green); O4 atom of AOT molecule (yellow)

As shown in Figure 4, at higher concentrations (w=6 and w=7), the number of hydrogen bonds between the SO^- group and water remains stable, but a sharp increase in water-water interactions occurs. This increase enhances the internal hydrogen-bonded network among water molecules, contributing to a more robust water framework within the micelle and impacting the overall structure. Additionally, for higher concentrations (w≥7), we observe a distinct pattern where interactions between specific oxygen atoms on AOT (O1 and O3) and water increase, while those involving O2 and O4 decrease. This pattern suggests a reorganization of the surfactant layer around the expanding water core. The repacking of AOT molecules likely facilitates this structural shift, helping to stabilize the enlarged core. These findings support a mechanism of micelle elongation under high hydration, as previously reported in studies describing the transition from spherical to cylindrical shapes in micelles at elevated water content.

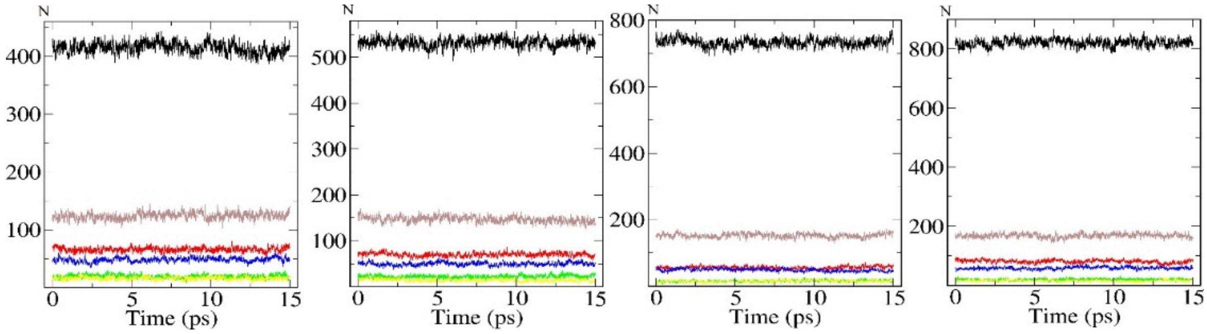

Figure 4. Number of hydrogen bonds in the system as a function of water/AOT concentration, shown from left to right: w=5, w=6, w=7, w=8. The types of hydrogen bond are shown in Figure 2.

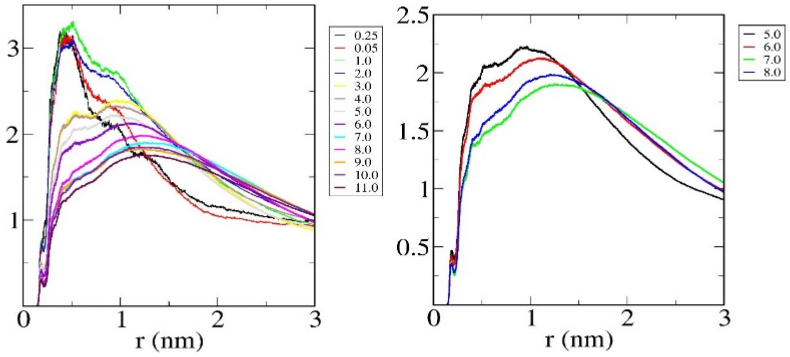

Figure 5. Radial distribution function between water molecules and AOT (calculated as the centre of mass of molecules).

Figure 5 provides further structural insight through the radial distribution function (RDF) between water and AOT molecules. At low water content (w=0.25÷2), RDF peaks are observed at 0.5 nm and 1.2 nm, indicating that water molecules are closely associated with AOT, suggesting a compact micellar core. However, as concentration increases to w=3÷6, the intensity of the first RDF peak diminishes, reflecting the shift toward water-water hydrogen bonding within the growing core. For concentrations w=7 and above, the peaks shift further towards longer distances, indicating that the micelle is adjusting to a larger, less compact core. This structural adaptation results in a looser AOT packing, consistent with the formation of elongated micelles as the water pool expands.

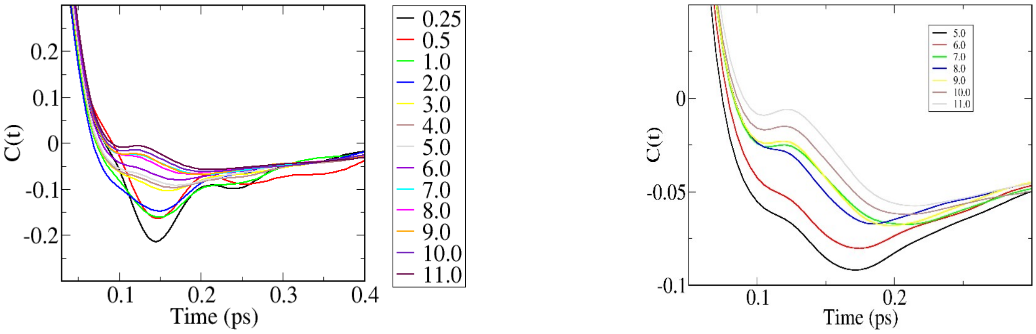

Figure 6. Autocorrelation velocity function for the water oxygen atom

The autocorrelation velocity function of the water oxygen atom (Figure 6) highlights dynamic changes across concentrations. At low concentrations (w=0.25÷2), we observe a distinct minimum around 0.15 picoseconds and a slight maximum at approximately 0.2 picoseconds, indicating restricted motion of water molecules due to strong interactions with the AOT head groups. With increasing concentration (w=3÷6), this minimum becomes blurred, signaling that the water core has become more stable and continuous, allowing for greater water mobility. At higher concentrations (w≥7), the velocity function shifts, with the minimum appearing at around 0.1 picoseconds and the maximum at about 0.12 picoseconds. This shift signifies increased fluidity and longer-range interactions within the water core, consistent with structural elongation of the micelle [35].

In summary, at low water concentrations, hydrogen bonding is primarily between AOT and isolated water molecules, supporting a compact micellar core. As water content rises, the formation of a stable hydrogen-bonded water network within the core prompts a structural shift in the micelle, with AOT molecules rearranging around the expanded core. This progression from isolated water molecules to a cohesive water network causes the micelle to elongate, consistent with experimental observations of shape transitions in AOT micelles as hydration increases [35]. These findings illustrate how hydrogen bonding dynamics drive structural adaptations within reverse AOT micelles, influencing both the shape and internal dynamics of the micellar system as water concentration changes.

CONCLUSIONS

The study of the structural characteristics of reverse micelles in cyclohexane solution with an aqueous core has been carried out using the method of molecular dynamics. In micelles, there is a strong interaction between surfactant molecules and water, which leads to the rearrangement of water molecules and changes in micelle shape. It was shown that during the transition from w=5.6 to w=7, a difference in the packing of surfactant molecules and the water core is observed, which is related to the dynamics of water molecules. The calculation of hydrogen bonds in the system, the radial distribution function between surfactant molecules and water, as well as the autocorrelation velocity function for the water oxygen atom, showed a deviation for w=7. This deviation is related to the minimal interaction of surfactant molecules with water and compensation of Coulomb and Van der Waals forces, as well as the dielectric susceptibility of water observed in similar systems [15, 19]. The results based on data analyses reveal that at w=6, a strong hydrogen bond appears between the hydrophilic group of AOT and water, and at w=7, the strength of the hydrogen bond changes drastically, indicating that the micelle changes its shape. This fact is also confirmed by other authors [14, 35]. Thus, there is a significant increase in the interaction of water with the polar groups of AOT, leading to structural changes in micelles. With a further increase in www, the content of the aqueous pseudophase and the interaction of polar groups of surfactant molecules with water molecules determine the size of nanoparticles obtained in micelles.

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СТРУКТУРНІ ОСОБЛИВОСТІ ОБРОТНИХ МІЦЕЛ АОТ У ВОДІ/ЦИКЛОГЕКСАНІ: МОЛЕКУЛЯРНО-ДИНАМІЧНЕ ДОСЛІДЖЕННЯ

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Методом молекулярної динаміки проведено дослідження структурних особливостей зворотних міцел молекул Na AOT (біс(2-етилгексил)сульфосукцинат натрію) у циклогексані з водним ядром. Зворотні міцели AOT утворюються в трикомпонентних системах, що містять неполярний розчинник, воду та молекули AOT при певних співвідношеннях концентрацій, виражених як w = [H2O]/[AOT]. Виявлено сильний водневий зв'язок між молекулами води та AOT при концентрації w=6. Вперше було показано різке зменшення водневих зв'язків між молекулами води та AOT при w=7, викликане різницею в упаковці молекул AOT та колективною динамікою молекул води в ядрі міцели. Результати розрахунків добре узгоджуються з експериментальними даними інших авторів. Показано, що поряд з методами коливальної спектроскопії та динамічного розсіювання світла метод молекулярної динаміки також є інформативним для визначення структурних характеристик супрамолекулярних структур та аналізу колективної динаміки молекул води.

Ключові слова: *метод молекулярної динаміки; зворотні міцели; водневий зв'язок*