Synthesis and Aggregation Behavior of Jellyfish-Shaped Triazine Hexamer Quaternary Ammonium Chloride Surfactant

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Abstract: A novel jellyfish-shaped triazine hexamer quaternary ammonium chloride surfactant (TH₁₂QC) was synthesized, which consisted of one triazine spacer group and six long flexible hydrophobic chains. The molecular structure and aggregation behavior of TH₁₂QC was investigated by nuclear magnetic resonance (NMR), surface tension, electrical conductivity, dynamic light scattering (DLS), transmission electron microscope (TEM), etc. The results show that the jellyfish-shaped TH₁₂QC has better surface activity and lower surface tension than traditional ionic and Gemini surfactants in aqueous solution. There are two inflection points in the curve of conductivity versus concentration of the TH₁₂QC aqueous solution, which correspond to the critical aggregation concentration (CAC) and the critical micelle concentration (CMC) respectively. The existence of CAC indicates that there is a pre-aggregation process before TH₁₂QC forms micelles. The results of DLS and TEM show that network pre-aggregation, spherical aggregation and dense spherical aggregation were observed in different concentration of TH₁₂QC aqueous solution, and the electrostatic equilibrium of the system subtly depends on the concentration of the solution. In addition, intramolecular and intermolecular hydrogen bonding is also an important factor. This study provides a method for studying the aggregation behavior and morphology of oligomeric surfactants with rigid spacer groups.

Key words: quaternary ammonium surfactant, aggregation behavior, surface tension, critical micelle concentration
meric and traditional surfactants and concluded that the benefits of oligomeric surfactant such as the lower critical micelle concentration (CMC) and the denser interface layer both on air-liquid and in air-solid. These benefits might result from their easier formation of micelles and excellent adsorption properties. As the degree of oligomerization changed, the viscosity of the system altered systematically. In order to develop the surfactant with lower CMC, the research on surfactants with higher degree of oligomerization has attracted more and more scholars’ attention in recent years.

Yoshimura et al.\textsuperscript{13} prepared and characterized a series of trimeric cationic quaternary ammonium surfactants with different hydrophobic chain lengths such as 3CntrisQ and 12-s-12-s-12. The research showed that with the increasing of hydrophobic chain length, the ability of surfactant to reduce the interfacial tension of solution is significantly improved. At the same time, they also discussed the self-assembly behavior which depends on solution concentration. For trimeric surfactants, with the increase of alkyl chain length, the aggregation behavior of micelles in water was changed significantly including network-like, spherical-like and worm-like aggregation, which had not been observed in corresponding Gemini surfactant.

In addition, Fan et al.\textsuperscript{14, 15} studied a series of interesting surfactants combined by liner or star-shape spacer, including trimeric and tetrameric surfactant. In their study, the influence of both liner and star-shape spacer on the surfactant with flexible topological structure was studied. The self-assembly behavior of oligomeric surfactants at different interfaces, including air/water, water/solid and aqueous solutions, was explored. However, there are few relative reports about cationic surfactant with relatively higher oligomeric degree, and the reports on the morphology of micelles are limited to the formation of worm-like or chain-like structure which formed by oligomeric surfactant with flexible spacer group. The morphology about micellar aggregation formed by oligomeric surfactants with rigid spacer group is rarely reported.

In this paper, a novel kind of jellyfish-shaped triazine hexamer quaternary ammonium chloride (TH\textsubscript{12}QC) surfactant with six long hydrophobic chains and one rigid triazine spacer groups was synthesized, and the surface activity and aggregation behavior of TH\textsubscript{12}QC was discussed through surface tension, electrical conductivity, emulsifying property, dynamic light scattering (DLS), transmission electron microscope (TEM), etc. The chemical structure of TH\textsubscript{12}QC is shown in Fig. 1. It is named jellyfish-shaped surfactant because its aggregation form is similar to the jellyfish with six antennae at a certain concentration. The results discussed in this paper will prove to be a powerful complement to the research on aggregation and self-assembly behavior of this oligomeric surfactant, and will be more conducive to solving dispersion problems in nanomaterial preparation due to its excellent surface activity.

2 Experimental Procedures

2.1 Materials

All chemicals were reagent-grade commercial materials and used without further purification. Melamine and trimethylamine were obtained from Aladdin Biochemical Technology Co., Ltd. (Shanghai, China). Epichlorohydrin and N,N-Dimethyl dodecyl tertiary amine were obtained from Lianshui Xinyuan Biotechnology Co., Ltd. (Huai’an, China). N,N-dimethylformamide, \(n\)-hexane, dimethylbenzene, acetone, absolute ethanol, petroleum, octane ether, \(n\)-nonane and \(n\)-dodecane were purchased from Sinopharm Chemical Reagent Co., Ltd. (Beijing, China).

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{molecular_formula.png}
\caption{Molecular formula and structure diagram of TH\textsubscript{12}QC.}
\end{figure}
2.2 Synthesis of 1,1',1''',1''''',1'''''-(1,3,5-triazine-2,4,6-triyl) tris (azanetriyl) hexakis (3-chloropropan-1-ol)

Triethylamine (2.8 mL, 0.0201 mol) and melamine (5.000 g, 0.0397 mol) was dissolved in the N,N-dimethylformamide (31.000 g, 0.4241 mol) in a three-necked flask at room temperature under nitrogen atmosphere. Epichlorohydrin (31.500 g, 0.3405 mol) was slowly dropped into the flask with the drop acceleration of 5 drops/min. The mixture was heated to 105°C and refluxed for 48 hours at 105°C, when the process of dropping was completed. The solution was concentrated on a rotary vacuum evaporator, then the residual solid was washed once with the hexane, then twice recrystallization with the acetone. A brown solid product of residual solid was washed once with the hexane, then twice recrystallization with the acetone. The product was dried under vacuum at 65°C. TH₁₂QC as a brown solid was synthesized according to Scheme 1, and the yield was 65.2%. The ¹H NMR and ESI-MS date of the product in this process is shown in Fig. 2.

As shown in Fig. 2(a), δ7.27 (s, 1D, CDCl₃), δ5.31 (s, 6H, OH), δ4.63 (d, 6H, CH), δ3.22 (m, 24H, CH₂N⁺), δ3.30 (s, 36H, CHₓN⁺), δ2.11 (d, HCHCH₂), δ1.29 (m, 12H, N + CH₃CH₂), δ1.26 (m, 96H, CH₃(CH₂)₂), δ0.88 (m, 18H, CH₃CH₂). In addition, it can be seen from Fig. 2(b) that there is an obvious peak at the value of m/z of 291.29. The molecular weight (M) of TH₁₂QC is 1963.71, and this hexameric surfactant has six positive charges, so the peak at the value of m/z of 291.29 is consistent with the theoretical m/z peak of hexamer [M – 6Cl⁻] 291.46. In order to further study the molecular structure of the product, the element analysis was carried out. The analytical results of element C, H, N, O and Cl in the product are 63.32%, 11.28%, 9.85%, 4.81% and 10.74%, respectively. The theoretical values of element C, H, N, O and Cl in TH₁₂QC are 64.29%, 11.41%, 8.57%, 4.89% and 10.84%, respectively. The practical data is very close to the theoretical data, which further confirms that the product is mainly hexamer. The results of ¹H NMR, ESI-MS and element analysis show that the product is the target product TH₁₂QC.

![Scheme 1 Synthetic procedure of TH₁₂QC.](image)

**Scheme 1** Synthetic procedure of TH₁₂QC.
2.4 Electrospray Ionization Mass Spectrometry Measurement (ESI-MS)

Electrospray ionization mass spectrometry (ESI-MS) of TH_{12}QC surfactant samples were analyzed by LCT time of flight mass spectrometer (Micromass, America). The measurement condition was set to positive ion mode (ESI^+), the ion source temperature of ion source and desolvent were set as 80°C and 120°C, respectively. The conical hole voltage and the capillary voltage was 60V and 3.3 kV, and the scanning range was 50~1000 m/z.

2.5 Surface Tension Measurement

Wilhelmy hanging plate method was used to measure the relationship between the surface tension (\(\gamma\)) and the concentration (C) of TH_{12}QC aqueous solution with JK99C Automatic Surface Tension Instrument (Zhongchen, Shanghai, China). The sampling period was settled as 150s, and the system temperature was controlled at 25 ± 0.5°C. 50 ml of well dissolved TH_{12}QC aqueous solution was dropped in crystallizing dish. Results displayed as an average with error bars corresponding to standard deviation obtained for n = 3 independent experiments.

The surface excess concentration (\(\Gamma\)) in mol m\(^{-2}\) and the area occupied by each surfactant (A) in cm\(^{-1}\) could be measured according to Gibbs adsorption isotherm equations (Equation 1 and Equation 2):

\[
\Gamma = - \left( \frac{d\gamma}{dC} \right) \left( \frac{1}{kT} \right)
\]

\[
A = \frac{1}{N\Gamma}
\]

Where \(\gamma\) represents surface tension and C is the concentration of surfactant, R is the gas constant (8.31 J K\(^{-1}\) m\(^{-3}\)), N is the Avogadro constant (6.02 \times 10^{23}), T is the absolute temperature and the value of I (the number of species at the interface for which the concentration varies with the surfactant concentration) is considered to be 7.

2.6 Electrical Conductivity Measurement

The DDSJ-308A conductivity meter (INESA Scientific Instrument Co., Ltd, Shanghai) was used for the measurement about the relationship between electrical conductivity (\(\kappa\)) and different concentration (C) of TH_{12}QC aqueous solution. The identical DJS-1D platinum plate with the electrode constant of 0.971 was used for this measurement. The system was equipped with circulating water and the temperature was controlled at 25 ± 0.5°C. During the experiment, 50 ml distilled water was used to dissolve a series of appropriate amount of TH_{12}QC. \(\kappa\) was recorded when the conductivity meter indicator no longer fluctuated. Every experiment was conducted three times at same concentration of TH_{12}QC and data were averaged by three measurements.

2.7 Transmission electron microscopy (TEM)

Micrographs of TH_{12}QC aggregations were obtained using the JEOL JEM-2100 (HR) transmission electron microscope at an operating voltage of 200 kV. A drop (20 \(\mu\)L) of the solution of TH_{12}QC was dropped onto a carbon coated copper grid (200 mesh) and allowed to stand for 5 minutes to form a thin liquid film on the copper grid, which was then dried under an infrared baking lamp.

2.8 Dynamic Light Scattering (DLS)

Sample of the TH_{12}QC was measured on the NanoBrook 90Plus Particle Size Analyzer (Brookhaven, America), which was equipped with a high power 35 mW red diode laser (wavelength = 640 nm), and the scattering angle was settled as 90°. The measurements were performed at 25.00 ± 0.01°C. The samples with 0.026 to 10.36 mM concentration were placed in quartz cell previously washed with Hellmanex III 3%. Each sample was measured three times, with an average of 15 scans per time. By using the cumulant analysis of autocorrelation function, the polydispersity.
and the average hydrodynamic diameter (z-average) of the samples were determined.

3 Results and Discussion

3.1 The Krafft point and surface activity of TH12QC

The clear solution of 0.1 wt% TH12QC is prepared in the heating state then stored in the refrigerator at \( \sim 5\,^\circ\text{C} \) for at least 24 hours. Conductivity method was used to determine the Krafft Temperature (\( T_k \)) of TH12QC. Under constant stirring, the change of conductance (\( \kappa \)) was measured with the gradual rising of temperature. At this temperature range, solution is always clear, and the value of conductivity changes almost nothing. Accordingly, the \( T_k \) of TH12QC is lower than 5\,^\circ\text{C}, and \( T_k \) of TH12QC is too low to be observed. The reason is that there are six hydrophilic hydroxyl groups and six quaternary salt cations in the molecular stuture of TH12QC, which endows TH12QC with superior solubilities.

One of the important properties of surfactants is that they can significantly reduce the surface tension of aqueous solutions. The value of CMC can indicate the activity of surfactant, and it is often measured by surface tension method and conductivity method\(^{12}\). The surface tension and the electrical conductivity are plotted as a function of TH12QC concentration as shown in Fig. 3 and Fig. 4. TH12QC molecule has six long alkyl hydrophobic chains and rigid spacer group in its center, which make it stretch like jellyfish. These structural characteristics give it unique interface properties.

As seen from Fig. 3, with the increase of concentration of TH12QC solution, the surface tension of this system decreases significantly, but the rate of surface tension decrease is not exactly the same in the research range of TH12QC concentration. The CMC from the break point in Fig. 3 is 0.195 mM. The slope of the curve becomes smooth behind this point, and surface tension (\( \gamma \)) is closing to 35.2 mN/m. TH12QC also is compared with the cationic surfactant C12TAB which has the same length of alkyl chain. The result shows that the \( \gamma_{\text{max}} \) of TH12QC is also lower than C12TAB (38.6/38.9 mN/m)\(^{13}\). This ability to decrease surface tension implies that the molecule of TH12QC may be forced to align more regularly at the air-water interface due to the role of spacer group.

As shown in Fig. 4, Electrical conductivity measurement has been applied to study the surface activity of the surfactant. The CAC (\( C_1 \)) and CMC (\( C_2 \)) values of TH12QC can be determined from the breakpoints. By differentiating the curve of electrical conductivity, the values of these points are identified as 0.0624 mM and 0.197 mM, which extremely close to the value of CMC from surface tension curve. The reason for the slight difference between the CMC values measured by the two methods is the existence of non-surface-activity premicellar aggregates. The similar conclusion has been reported in other works\(^{14, 28}\). Herein, we define the values of critical aggregation concentration and critical micelle concentration are 0.0624 mM and 0.195 mM in this work. The reason that the first point could not be observed in measurement of surface tension and might be attributed to the extremely slight solution concentration. However, in TH12QC aqueous solution, the slight transformation which attributes to the presence of intermolecular aggravation behavior could be observed by the electronic conduction curve.

![Fig. 3](image3.png) Variations of surface tension (\( \gamma \)) of the TH12QC aqueous solution with the concentration (\( C \)) at 25.0 °C. The red line is the corresponding differential curve.

![Fig. 4](image4.png) Variations of electrical conductivity (\( \kappa \)) of the TH12QC aqueous solution with the concentration (\( C \)) at 25.0 °C. The red line is the corresponding differential curve.
The differences of TH$_{12}$QC from other traditional cationic surfactants are described in Table 1. As shown in Table 1, compared with C$_{12}$TAB and 12-3-12-4-12-3-12, surface excess concentration ($\Gamma$) of TH$_{12}$QC is larger, indicating that the triazine ring as spacer groups can effectively overcome the charge repulsion between the monomers, and the branched chains of triazine ring linking are arranged more orderly and densely at the water/air interface. Even though triazine rings of TH$_{12}$QC are rigid and cannot to achieve ideal folding and torsion, TH$_{12}$QC still exhibits superior interfacial aggregation ability than 12-3-12-4-12-3-12 with the similar rigid structure. However, the area occupied by each surfactant molecular (A) of TH$_{12}$QC is not larger than that of C$_{12}$TAB, which may be due to the change of TH$_{12}$QC morphology with the increase of solution concentration. When the solution is extremely diluted, the molecular chain of TH$_{12}$QC stretches sufficiently. With the change of concentration, the molecular morphology of TH$_{12}$QC doesn’t keep a single stretching state any longer, and the molecules of TH$_{12}$QC begin to aggregate, and the branched chain attracts and entangles with each other.

Generally speaking, surfactants with hydrophilic groups can be better dissolved in water. Interestingly, for tetramer surfactant AD-8 with rigid spacer group, AD-8 has a lower CMC than 12-3-12-4-12-3-12, which may be due to the change of TH$_{12}$QC morphology with the increase of solution concentration.

3.2 Ionization and aggregation capacity about TH$_{12}$QC

According to Fig. 4, the curve shows the relationship between electrical conductivity ($\kappa$) and concentration ($C$) of TH$_{12}$QC aqueous solution, presents nonlinear relation between conductivity and concentration at a lower concentration range, as the predict of Kohlrausch’s law. It is obvious that with the increasing of concentration, this curve presents a nonlinear relationship between $\kappa$ and $C$ and displays its two inflection points that correspond CAC and CMC, accordingly. As described in Table 1, CAC and CMC of TH$_{12}$QC aqueous solution are determined as 0.0624 mM and 0.195 mM, respectively. For ionic surfactant molecules in solution, the presence of electrostatic repulsion of the same charges often makes it difficult to approach each other. Although electrostatic repulsion still exists in the system, six branched chains are connected on ring type spacer group of TH$_{12}$QC. Electrical conductivity of solution is mainly affected by the dissociation and association of TH$_{12}$QC in solution, and this process can be divided into the following stages.

Table 1 Physicochemical Properties of C$_{12}$TAB$^{(13)}$, 2RenQ$^{(16)}$, 12-2-12$^{(17)}$, 3C$_{10}$NAc-Tz$^{(18)}$, 3C$_{10}$NAc-Tz$^{(17)}$, 12-3-12-4-12-3-12$^{(11)}$, AD-8$^{(19)}$ and TH$_{12}$QC.

| Surfactant        | CAC  [mM] | CMC  [mM] | $\gamma_{\text{max}}$ [mN m$^{-1}$] | $10^6\Gamma$ [mol m$^{-2}$] | A  [nm$^2$/molecule] |
|-------------------|----------|----------|-------------------------------------|----------------------------|-----------------|
| C$_{12}$TAB       | –        | 14$^a$, 16$^b$ | 38.6$^a$, 38.9$^b$                   | 3.42                       | 0.49            |
| 2RenQ             | –        | 0.90$^a$  | 21.4$^b$                            | 2.31                       | 0.72            |
| 12-2-12           | –        | 0.97$^a$  | 32.4$^a$                            | –                          | 0.1             |
| 3C$_{10}$NAc-Tz   | –        | 0.19$^a$  | 32.9$^a$                            | 3.54                       | 0.47            |
| 3C$_{10}$Ac-Tz    | –        | 0.0110$^a$ | 28.6$^a$                            | 4.84                       | 0.34            |
| 12-3-12-4-12-3-12 | –        | 0.06$^a$  | –                                   | 1.30                       | 0.64            |
| AD-8              | –        | 6$^a$     | –                                   | –                          | –               |
| TH$_{12}$QC       | 0.0624$^a$ | 0.195$^a$ | 35.2$^a$                            | 4.04                       | 0.41            |

$^a$ Surface tension method. $^b$ Electrical conductivity method.
maximum slope can be seen, which indicates that TH$_{12}$QC has strong dissociation ability in this region. As a salt molecule, a single TH$_{12}$QC dissociates into a positive hydrophilic and hydrophobic acid radical ion and a negative chloride ion in water.

The slope of the conductivity curve decreases slightly when the concentration is between CAC and CMC. This indicates that the degree of dissociation of TH$_{12}$QC molecule decreases in this concentration range, which may be due to the relatively high concentration of TH$_{12}$QC aqueous solution, the increase of the number of molecules in the system, and the enhancement of intermolecular force. In addition, with the increase of molecular density, alkyl chains attract each other and form hydrophobic networks, which results in the formation of non-polar hydrophobic micro-regions and hinders the dissociation of TH$_{12}$QC molecules. The ionization process is still continuing as the concentration increases because isolated TH$_{12}$QC molecules still exist in the system, and dissociation may occur at the edge of the network structure. In the other side, for those TH$_{12}$QC molecules which at the edge of network structure can bind well with water molecule, and still dissociate. But those TH$_{12}$QC molecules in the network structure are protected by the non-polar region, thus more difficult to dissociate.

When the concentration exceeds the CMC, the curve has a noticeable change that its slope reduces. The presence of isolated TH$_{12}$QC molecules still exist in the system, and dissociation may occur at the edge of the network structure. In the other side, for those TH$_{12}$QC molecules which at the edge of network structure can bind well with water molecule, and still dissociate. But those TH$_{12}$QC molecules in the network structure are protected by the non-polar region, thus more difficult to dissociate.

In order to investigate the change of TH$_{12}$QC aggregate size with concentration, Tyndall effect of TH$_{12}$QC aqueous solution with different concentration was measured, and the results are shown in Fig. 5. Results of the Tyndall effect shows that at extremely low concentration region (C = 0.013 mM, 0.026 mM, C < CAC), the incident laser light scatters weakly and the Tyndall effect exists slightly. At this time, the solution is colloid. It indicates that at this concentration, even if TH$_{12}$QC molecules is not achieving large-scale aggregation, the slight Tyndall effect confirms that the micro-particles (R$_a$ < λ) produced by pre-aggregation begin to occur in the solution. Obviously, with the increase of solution concentration, the Tyndall effect becomes more and more obvious, and the size of micelle aggregations in this size range becomes larger and larger.

In order to determine the existence and the behavior change of aggregations, DLS analysis is performed in this work (Fig. 6). It should be noted that when the sample concentration is 0.026 mM the R$_a$ of the aggregate is large extremely, reaching 2433.2 nm. This is because the principle of DLS is to measure the diffusion coefficient to measure the size of aggregates indirectly, and the strong

\[ \alpha_1 = \frac{(d\kappa/dC)_{CAC}}{(d\kappa/dC)_{C<CAC}} \]

\[ \alpha_2 = \frac{(d\kappa/dC)_{CMC}}{(d\kappa/dC)_{C<CAC}} \]

The value of \( \alpha \) can better identify and explain the relationship between \( \kappa \) and \( C \) about TH$_{12}$QC. The \( \alpha_1 \) and \( \alpha_2 \) of TH$_{12}$QC are 0.98 and 0.76, respectively. These values are close to the results of previous research. The results show that TH$_{12}$QC molecule as a quaternary ammonium salt can be well dissociated at very low concentration, and the significant change of \( \alpha \) indicates that the environmental polarity around TH$_{12}$QC molecule is changed, implying that the morphology of TH$_{12}$QC molecular aggregation changes. Micellar ionization degree (\( \alpha \)) also confirms the existence of above different dissociation stages.

3.3 Size and morphology about TH$_{12}$QC

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![Fig. 5](image-url) Tyndall effect of the TH$_{12}$QC aqueous solution with the different concentration (C) at 25°C. Concentration of TH$_{12}$QC in each image: 0 mM, 0.013 mM, 0.026 mM, 0.148 mM, 0.355 mM, 2.96 mM, 5.92 mM, and 14.8 mM (from left to right).
The intermolecular attraction effect will provide larger measurement results. Combining with the result of the Tyndall effect, it is easy to find that the molecules of TH_{12}QC have already formed many pre-aggregations in extremely dilute solutions with concentration below the CAC. When the concentration is lower than CAC, oligomeric surfactants prefer to form such premicellar aggregate structure. It is attributed to the polarity effect of both hydroxyl and quaternary ammonium salts and electrostatic attraction between TH_{12}QC molecules. Results from the data of the relative intensity demonstrate, when the solution concentration approaches CAC, the main size distribution range of TH_{12}QC changes from \( R_h = 323.7 \text{ nm} \) to \( R_h = 680.8 \text{ nm} \), which indicates that small pre-aggregations begin to bind with each other.

Furthermore, it can be seen that a new distribution interval appears when the concentration of solution is between CAC and CMC. The main \( R_h \) distribution interval of TH_{12}QC is not changed significantly. It can be concluded that the network pre-aggregations of TH_{12}QC molecule disintegrate at this concentration, and begin to form more intensively denser micellar aggregations, which is described in Fig. 6. However, the third interval of \( R_h \) distribution appears when the concentration increases to a higher concentration region (\( C > \text{CMC} \)). It can be assumed that when the solution concentration reaches the higher region (\( C > \text{CMC} \)), TH_{12}QC molecules are close to each other and begin to entangle with each other which leads to the appearance of spherical micellar aggregations or other denser structures. Moreover, these spherical micelles can form larger aggregations, the main distribution interval of aggregations moves to the higher region as shown in Fig. 6.

To confirm the morphology and aggregation behavior of TH_{12}QC micelles changing with aqueous concentration, observation of TEM is performed. TEMs of TH_{12}QC with different concentration are illustrated in Fig. 7. The projection effect of TEM is similar to that of Liao et al. As the concentration increases, the aggregation morphologies of TH_{12}QC micelles change obviously. When the concentration is below CAC, network pre-aggregations of TH_{12}QC molecule can be observed as shown in Fig. 7(a). When the concentration is close to CMC, micelles tend to form irregular aggregations rather than exist alone as shown in Fig. 7(b). When the concentration is beyond CMC, TH_{12}QC micelles transfers to form spherical aggregation eventually as shown in Fig. 7(c) and (d), and this can be inferred that the density of micellar aggregation is raised up significantly. Considering all the above conclusions, the change of TH_{12}QC molecular morphology with concentration is illustrated in Fig. 8.

**4 Conclusions**

The above results show that the hexamer-branched cat-ionic quaternary ammonium salt surfactant TH_{12}QC has been synthesized. The two characteristic concentration points of TH_{12}QC which include critical aggregation concentration (CAC) and critical micelle concentration (CMC) are determined, it can be inferred that TH_{12}QC molecules and micelles have different aggregation behavior in solution. The surface tension of water is reduced significantly due to the high density of hydroxyl groups and long hydrophobic chains. However, because the volume of TH_{12}QC
molecule is relatively larger, a single molecule occupies a large area at the interface, and the existence of rigid triazine ring spacer group makes it less affinity to the oil phase of alkanes. Because of its ability to form dense intermolecular hydrogen bonding and intramolecular hydrogen bonding, also because of the electrostatic attraction between negative hydroxyl groups and positive quaternary ammonium salt groups, pre-aggregates are forming before the critical concentration of aggregation (CAC). With increasing solution concentration, TH12QC molecules begin to connect with each other to form network aggregates, and there are two distribution regions of size of micellar hydrodynamic radius. When the concentration of solution is higher than CAC, with the densities of hydrogen bonding and electrostatic gravitational increasing, the stretched condition of TH12QC molecular chains begin to contract to the center, so the morphology of network aggregates changes and spherical aggregates begin to form. Simultaneously, there are two types of micelle aggregates in the solution. When the solution concentration is higher than CMC, eventually, spherical aggregates begin to adsorb each other and form large spherical assemblies. At this time, there are three distribution regions of micelle aggregates in the solution. Jellyfish- Shaped triazine surfactant TH12QC enriches the oligomeric surfactant system with rigid spacer groups which as the centre of the topological structure and provides more reference materials for the study of micelle morphology of oligomeric surfactants.

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