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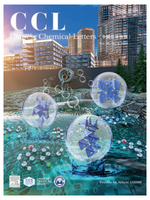

Water as a probe for the temperature-induced self-assembly transition of an amphiphilic copolymer

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ABSTRACT

The hydration state of amphiphilic block copolymers during the self-assembly transition is closely related to the structure and properties of copolymers. In this study, the temperature-induced self-assembly of copolymer poly(*N*,*N*-dimethylacrylamide)-poly(diacetone acrylamide) ($(PDMAA_{30}\text{-}PDAAM_{60})_2$) in aqueous solution was monitored by near-infrared spectroscopy with water as a probe. The wavelet packet transform was employed to improve the spectral resolution. The spectral information of hydrated water surrounding the hydrophilic PDMAA and hydrophobic PDAAM blocks was then extracted, revealing the significant roles of water in morphological transition of the copolymer from spherical to worm-like micelles. Specifically, water molecules interacting with N atoms and C=O groups of the hydrophilic block gradually decrease during the morphological transition, while hydrogen-bond structures NH−CO of the hydrophobic block gradually break, bringing more water molecules into contact with the hydrophobic block. This work provides a foundation for exploring the role of water molecules during the self-assembly transition of complex block copolymers.

Self-assembly is ubiquitous in biological systems, enabling protein folding, the formation of DNA double helix, and the construction of cell membranes. Inspired by their structure and functionality, a variety of amphiphilic compounds [1,2], particularly amphiphilic block copolymers [3,4], have emerged as progressive solutions to address difficulties in biology and materials science. When copolymers undergo external disturbances such as temperature and concentration, these molecules spontaneously form nanostructures such as spheres, worms-like, and vesicles, with applications in fields like drug delivery and gene transfer [5,6]. During the self-assembly process, water, as a common solvent, drives morphological transitions of copolymers [7-9]. Furthermore, the hydration state of self-assemblies largely determines their physicochemical properties [10,11]. Therefore, a deeper understanding of the role of water molecules surrounding block copolymers is of paramount important.

An analysis of water diffusion in a triblock copolymer PEO–PPO–PEO (where PEO is polyethylene oxide and PPO is polypropylene oxide) solution shows distinctive behavior: water molecules undergo normal diffusion in the hydrophilic PEO segment, but anomalous diffusion in the hydrophobic PPO segment [12]. Madathil *et al.* [13] investigated the impact of trace amounts of water on the aggregation behavior of a sulfonated pentablock copolymer (SPC) using small angle X-ray scattering, and observed that the introduction of trace water leads to a significant transition of the polymer from a disordered to an ordered state. This acceleration is attributed to the disruption of hydrogen bonds between sulfonic acid groups by trace water, enhancing the rapid morphological transformation in SPC. Additionally, a combination of experiments and simulations [14] unveiled that the poly(ᴅ,ʟ-lactide-*co*-glycolide)-*b*-poly(ethylene glycol)-*b*-poly(ᴅ,ʟ-lactide-*co*-glycolide) in water undergoes temperature-induced sol-gel transition, forming two states (gel I and gel II). Gel I is propelled by bridge structures among the coronas of micelles, while the formation of gel II is influenced by hydrophobic channels at the core-to-core location. Furthermore, Cho *et al.* [15] investigated the interaction between water and $PEO_{20}\text{-}PPO_{70}\text{-}PEO_{20}$ copolymer during morphological transitions. They found that the number of water molecules interacting with ether oxygen atoms increases during the transition from a loose (monomeric) to an aggregated (micellar) state, while this number decreases undergoing a sol-gel transi-

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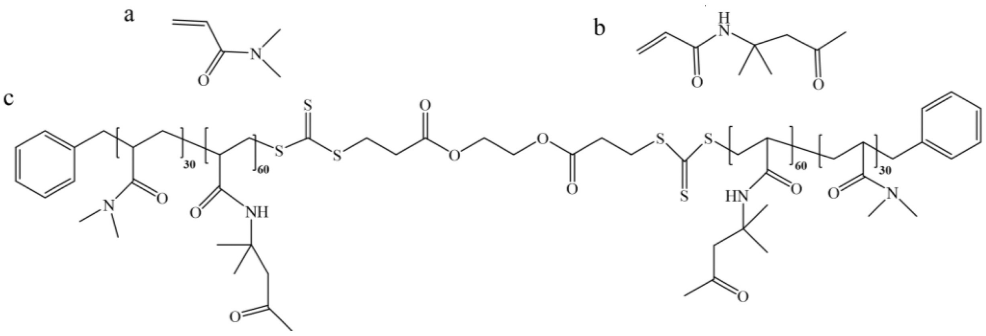

Fig. 1. Chemical structures of DMAA (a), DAAM (b), and (PDMAA$_{30}$-PDAAM$_{60}$)$_2$ (c).

tion. In summary, the self-assembly of copolymers is influenced by various factors, with water molecules playing diverse roles in this process. However, there is still an insufficient molecular-level understanding of how water induces self-assembly, particularly regarding the hydrogen bond structures formed between water and the hydrophilic/hydrophobic blocks in copolymers. To bridge this knowledge gap, our study focuses on the water-related hydrogen-bond structures in the poly(*N*,*N*-dimethylacrylamide)-poly(diacetone acrylamide) (PDMAA$_{30}$-PDAAM$_{60}$)$_2$ copolymer. We carried out near-infrared (NIR) spectroscopy to collect spectral information on water molecules during the temperature-induced self-assembly of the copolymer in aqueous solution (4-48 °C), aiming to elucidate the interplay between hydrogen-bond structures changes and morphological transitions of the copolymer.

NIR spectroscopy has proven to be a powerful technique for analyzing the structure of water and its interactions with solutes [16,17]. Leveraging the sensitivity of NIR spectra to both temperature and the variation of water structure, more detailed spectral information can be obtained [18]. Therefore, temperature–dependent NIR spectroscopy has been developed for analyzing different hydrogen-bonded water species in various systems. In other words, water can be used as a probe for sensing the molecular objects in aqueous solutions [19,20]. For example, the analysis of the morphology changes of poly(isopropylacrylamide) with temperature indicated that bridging water molecules connecting NH and CO groups in the polymer play a crucial role in maintaining the stability of the polymer in aqueous solutions [21]. During the gradual aggregation of low-concentration poly(*N*,*N*-dimethylaminoethyl methacrylate) with increasing temperature, it was observed that the disruption of water molecules with two hydrogen bonds can drive a transition of the polymer from a loose to a compact state [22]. Given the limited resolution of NIR spectra, chemometric methods are necessary for extracting effective information from the spectra [23,24].

N,*N*-Dimethylacrylamide (DMAA) and diacetone acrylamide (DAAM) were procured from Shanghai Macklin Biochemical Technology Co., Ltd. (PDMAA$_{30}$-PDAAM$_{60}$)$_2$ was synthesized *via* reversible addition-fragmentation chain transfer (RAFT) polymerization, where the hydrophilic PDMAA block and hydrophobic PDAAM block have a mean degree of polymerization (DP) at 30 and 60, respectively. Fig. 1 illustrates the structures of PDMAA and PDAAM monomers, as well as the copolymer (PDMAA$_{30}$-PDAAM$_{60}$)$_2$. The copolymer was prepared and provided by the group of Professor Longhai Guo at Beijing University of Chemical Technology. Their TEM results illustrate morphological transitions of the copolymer at various temperatures: spherical micelles at 4 °C, worm-like micelles at around 20 °C, and nearly ring-shaped worm-like micelles at approximately 37 °C [25]. The ultra-pure water is produced by Milli-Q^{TM} Advantage A10^{TM}, Merck Chemicals (Shanghai) Co., Ltd., China. The purity is 18.2 MΩ/cm (25 °C). Prepare a 15 wt% copolymer solution using ultra-pure water as the solvent and ensure complete dissolution by storing the solution in a refrigerator at 4 °C for subsequent analysis. DMAA-H$_2$O mixtures with H$_2$O mole fraction ranging from 10% to 90% with an increment of 10% and DAAM-H$_2$O mixtures with the concentration of DAAM from 1 wt% to 50 wt% with an increment of 2 wt% were prepared.

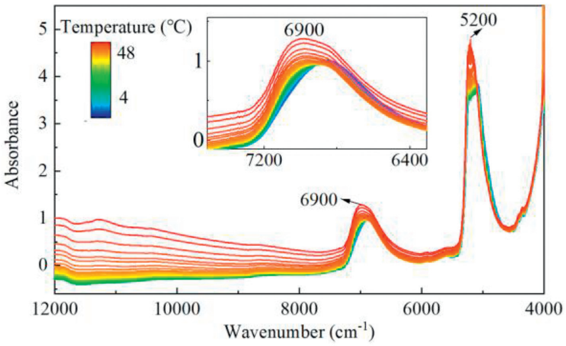

Fig. 2. NIR spectra of 15 wt% copolymer solution at 4–48 °C. The inset displays the enlarged spectra ranging from 7500 cm^{-1} to 6300 cm^{-1}.

All NIR spectra were measured using a Matrix F NIR spectrometer (Bruker, Germany) equipped with a 1 mm optical fiber probe immersed in 10 mL copolymer solution. The experimental temperature was controlled using a circulating water bath system (Thermo Fisher Scientific, China), recording spectra in the range of 12,000-4,000 cm^{-1} at a resolution of approximately 4 cm^{-1}. To enhance the signal-to-noise ratio, the scans were performed 64 times. The temperature control precision was ±0.01 °C. NIR spectra of copolymer solution were measured between 4 °C to 48 °C with a temperature interval of 1 °C. At each temperature, spectra were collected after stabilizing the sample for 15 min.

Wavelet packet transform (WPT) serves as an effective method for enhancing resolution [26]. Previous studies have indicated that [27], with a filter vanishing moment set to 4 and a decomposition level set to 7, the frequency component [5,2] significantly improves spectral resolution. Hence, the [5,2] component is selected for the subsequent analysis. All data were analyzed using MATLAB R2021b (The MathWorks, Inc., Natick, MA, USA).

Fig. 2 shows the NIR spectra of a 15 wt% copolymer solution from 4 °C to 48 °C. Two obvious peaks are observed around 6900 and 5200 cm^{-1}, associated with the information of bulk water [28]. The peak near 5200 cm^{-1} is over the range of the spectrometer. Thus, our analysis focuses on the broad peak at 6900 cm^{-1}, corresponding to the first overtone of the OH stretching vibration [29]. With increasing temperature, this peak gradually shifts towards higher wavenumbers due to the transition from strongly hydrogen-bonded water molecules to weakly hydrogen-bonded ones [30]. Additionally, sample transparency gradually reduces due to copolymer phase separation as the temperature rises, causing an increase

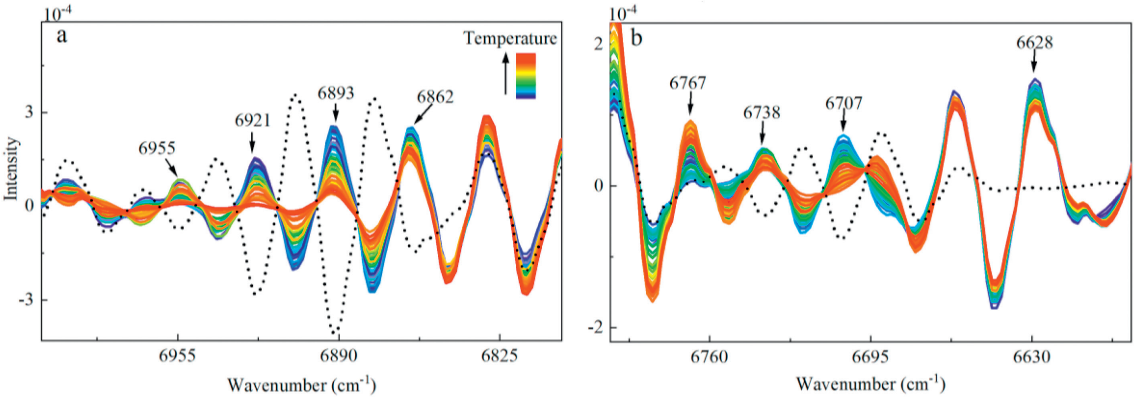

Fig. 3. High-resolution spectra of 15 wt% copolymer and bulk water (black dashed line) in regions of 7100-6800 cm^{-1} (a) and 6800-6600 cm^{-1} (b) at 4-48 °C.

in the baseline. Significantly, the spectral information of the first overtone of NH stretching vibration around 6600 cm^{-1} [31] is obscured by the strong water absorption peaks. The feature peaks of CH_2 groups near 8300, 7200, 6000 and 4500 cm^{-1} [32,33] were not further explored due to their weak absorption. Furthermore, detailed information on the interaction between water and the copolymer cannot be obtained due to the low spectral resolution.

WPT was employed to enhance spectral resolution. Figs. 3a and b present high-resolution spectra of the block copolymer solution and bulk water at temperatures ranging from 4 °C to 48 °C in the ranges of 7010-6800 cm^{-1} and 6800-6600 cm^{-1}, respectively. Eight obvious peaks appear in the copolymer spectra around 6955, 6921, 6893, 6862, 6767, 6738, 6707 and 6628 cm^{-1}, which are not observed in the bulk water spectrum, indicating these peaks are induced by the addition of the copolymer. Considering their wavenumber positions, the peaks potentially relate to the information of water molecules interacting with the copolymer or the NH groups of the copolymer.

Fig. 4 illustrates the intensity trends of these peaks as a function of temperature. The intensities of peaks at 6921, 6893, 6707, and 6628 cm^{-1}, as shown in Figs. 4a-d, underwent three similar stages with increasing temperature: a negligible change from 4 °C to around 19 °C (stage I), a sharp decrease between 19 °C and 36 °C (stage II), followed by a gradual plateau beyond approximately 36 °C (stage III). The results suggest that the copolymer maintains its morphology unchanged during stage I, undergoes significant morphological changes during stage II, and stabilizes again at stage III. This process may indicate that the copolymer undergoes temperature-induced self-assembly, with the transformation sequence as follows: the copolymer maintains a spherical morphology at 4 °C, transitions to a worm-like micelles around 19 °C, and gradually transforms into a ring-shaped worm-like micelles at approximately 36 °C. Subsequently, there is minimal change in morphology with temperature, indicating that the morphological transition has essentially been completed. Furthermore, these four peaks are already present when the copolymer exhibits a spherical morphology at 4 °C, indicating their association with this morphology. The spectral peak at 6767 cm^{-1} (Fig. 4h), which is absent during stage I, emerges during stage II with intensity gradually increasing, and stabilizes at stage III, indicating its association with the formation of worm-like micelles. These results indicated that these peaks play crucial roles during the morphological transition. For peaks at 6955 and 6738 cm^{-1} (Figs. 4e and f), their intensities show irregular changes with temperature, possibly due to peak overlap. Additionally, although the intensity of the 6862 cm^{-1} peak (Fig. 4g) linearly decreases with temperature, its correlation with the morphological transition is not pronounced. Subsequent investigations will focus on the characteristic peaks (6921, 6893, 6707, 6628 and 6767 cm^{-1}) closely correlated with the morphological transition, as in Figs. 4a-d and h.

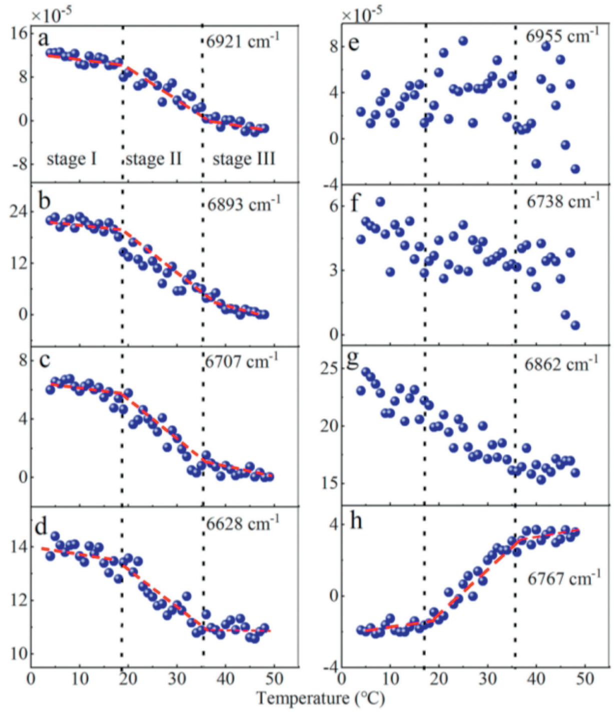

Fig. 4. Intensity variation of feature peaks at 6921 (a), 6893 (b), 6707 (c), 6628 (d), 6955 (e), 6738 (f), 6862 (g), and 6767 cm^{-1} (h) with temperature.

To further identify whether the peaks at 6921, 6893, 6707, and 6628 cm^{-1} are associated with the hydrophobic PDAAM block or hydrophilic PDMAA block, the following investigation was conducted. Due to the insolubility of PDAAM in water, the DMAA-H_2O mixture at 4 °C was analyzed to elucidate the interaction between water molecules and the PDMAA block. With the introduction of water molecules, only two peaks at 6921 and 6893 cm^{-1} appear among the four mentioned peaks, as shown in Fig. 5, which indicates that these two peaks result from the interaction between water molecules and DMAA. In addition, as the mole fraction of water increases, the intensity of these two peaks initially increases and then decreases, reaching a maximum when the mole fraction of water is approximately 0.5, as shown in Fig. 5 (insets a and b). This observation indicates that the molar ratio of H_2O to DMAA in the hydrogen bond structure of H_2O-DMAA is close to 1:1. Considering that the wavenumber of water peaks interacting with N is

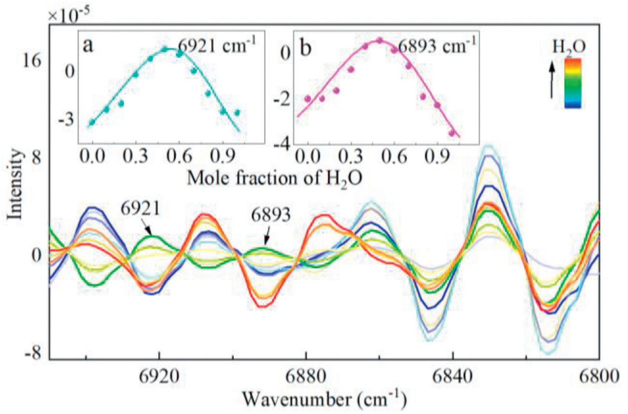

Fig. 5. High-resolution spectra of DMAA-H_2O mixture in the range of 6950-6800 cm^{-1}. The insets show the intensity variation of peaks at 6921 (a) and 6893 cm^{-1} (b) with the mole fraction of water.

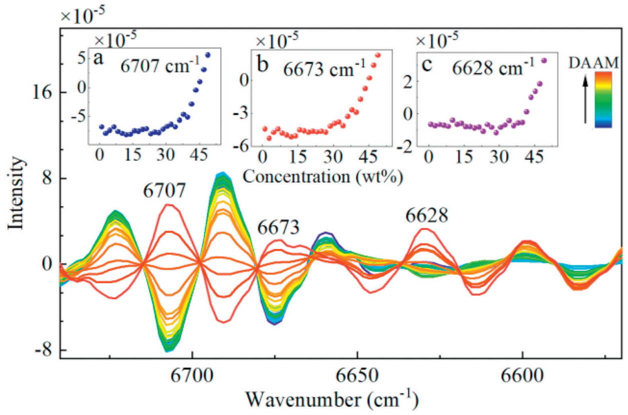

Fig. 6. High-resolution spectra of DAAM-H_2O mixture within the range of 6740-6570 cm^{-1}. The insets show the intensity variation of peaks at 6707 (a), 6673 (b), and 6628 cm^{-1} (c).

higher than those with C=O [27], the peaks at 6921 and 6893 cm^{-1} may be associated with spectral features of water in the H_2O–N and H_2O–C=O structures, respectively. Based on these findings, it is reasonable to believe that the peaks at 6921 and 6893 cm^{-1} may be associated with information of hydration water around the PDAAM block in the copolymer.

Based on the temperature-dependent intensity trend of these two peaks in Fig. 4, minimal changes are observed in the feature spectra of the hydration water around the PDAAM block when the copolymer is in a spherical state at stage I. This result suggests that the hydration environment remains undisturbed at this stage, indicating that the copolymer has not undergone a self-assembly morphological transition. Moving into stage II, a gradual dehydration of the PDAAM block occurs, leading to a reduction in the contact area between the PDMAA block and water molecules. This observation is consistent with the desolvation phenomenon observed in the morphological transition process of amphiphilic surfactants [34,35]. It is widely accepted that the self-assembled morphology of copolymers is commonly determined by the packing parameter P [36], as defined by the equation:

$$P = \frac{v}{a_0 l_c} \tag{1}$$

where v represents the area of the hydrophobic segment, a_0 is the optimal area of the head group, and l_c is the length of the hydrophobic chain. Generally, when $P < 1/3$, $1/3 < P < 1/2$, and $P > 1/2$, copolymers tend to adopt spherical, worm-like, and vesicular morphologies, respectively. Therefore, a reduction in the hydration of the hydrophilic head groups mentioned here leads to a decrease in α_0, resulting in an increase in P, which in turn causes the morphology of this copolymer to transition from spherical to worm-like or vesicular micelles. It is noted that the copolymers ultimately form ring-shaped worm-like micelles during the self-assembly process, rather than transitioning further to vesicles. This phenomenon is determined by the degree of polymerization of the hydrophilic and hydrophobic blocks of the copolymer. In stage III, the nearly unchanged spectral peaks of hydrated water signify that a stable environment surrounding the copolymer has once again been achieved, indicating the completion of the self-assembly transformation of the copolymer.

The investigation above has shown that only the two characteristic peaks at 6921 and 6893 cm^{-1} are present in the spectrum of water interacting with the PAMMA block. Therefore, it is speculated that the remaining two peaks at 6707 and 6628 cm^{-1} may contain information regarding the hydrophobic PDMAA block. It is widely recognized that the hydrophobic blocks in spherical morphology copolymers are aggregated through hydrogen bonding (NH···CO) [37], enclosing themselves within the core of the micelle without direct contact with water molecules. Therefore, it is speculated that 6707 and 6628 cm^{-1} likely correspond to the information of bonded NH groups. To validate the identity of this spectral peak, a similar investigation was carried out on the DAAM-H_2O mixture at 4 °C, considering the insolubility of PDMAA in water. Fig. 6 illustrates the high-resolution spectra of DAAM aqueous solutions at various concentrations in the region of 6740-6770 cm^{-1}. Three peaks at 6707, 6673, and 6628 cm^{-1} can be observed, potentially associated with NH groups in DAAM based on their wavenumbers. Furthermore, the intensity of these peaks exhibits a slow and then rapid increase with DMAA concentration (see insets a-c), consistent with the typical behavior of amide molecules, where the hydrogen-bond structure NH–CO dominates at higher concentrations [38]. The observation further supports the assignment of these peaks. Thus, it is reasonable to believe that the 6707 and 6628 cm^{-1} peaks are related to the NH groups of the copolymer. It should be noted that the absence of the spectral peak at 6673 cm^{-1} in the copolymer spectrum may be attributed to structural differences in solution between the DAAM and PDAAM blocks.

The declining intensity of the peaks at 6707 and 6628 cm^{-1} in the stage II of Fig. 4 suggests the progressive disruption of NH···CO structure of the hydrophobic block. This disruption results in increased extension of polymer chains and enhanced contact with water molecules [37]. As a consequence, the relative volume of the hydrophobic core increases, *i.e.*, a rise in parameter v in Eq. 1. Subsequently, the packing parameter P increases, signifying the occurrence of the self-assembly transition in the copolymer. Additionally, the nearly unchanged intensity of these spectral peaks in stages I and III signifies the initiation and completion phases of the morphological transformation.

For the 6767 cm^{-1} peak in Fig. 4, its intensity exhibits an increasing trend with temperature in the stage II, contrary to the variations of the peak intensity of the NH groups. Therefore, this peak is likely related to hydrated water surrounding the PDAAM block. The position of this peak closely aligns with the wavenumber (around 6760 cm^{-1}) at which water interact with molecules containing amide groups [39]. Hence, the spectral peak may be further associated with water molecules interacting with amide groups of the hydrophobic blocks.

In this study, the role of water molecules during the temperature-controlled self-assembly morphological transition of the copolymer $(\text{PDMAA}_{30}\text{-PDAAM}_{60})_2$ in aqueous solutions was investigated by near-infrared spectroscopy combined with a chemometric method. The results reveal a gradual decrease in water molecules bonded to N atoms and C=O groups of the hydrophilic PDMAA block with increasing temperature. This reduction results in a diminished contact area between the hydrophilic segment and water molecules, leading to an increase in packing parameter *P* and facilitating the morphological transition of the copolymer from spherical to worm-like and circular worm-like micelles. Additionally, the NH–CO structure in the hydrophobic PDAAM block gradually weaken as the temperature rises. This weakening allows more water molecules to surround the hydrophobic segment, causing an expansion in relative volume of hydrophobic segment and an increase in packing parameter *P*, thereby driving the morphological transition of the copolymer. In summary, the results presented herein demonstrate that hydrated water surrounding both the hydrophilic and hydrophobic segments play key roles in the morphological self-assembly of the amphiphilic block copolymer. These findings may provide new insights into the mechanisms of self-assembly morphology and guide the design of new amphiphilic block copolymers.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

Changlin Su: Writing – original draft, Validation, Methodology, Investigation. **Wensheng Cai:** Writing – review & editing, Supervision, Methodology, Conceptualization. **Xueguang Shao:** Writing – review & editing, Supervision, Methodology, Investigation, Funding acquisition, Conceptualization.

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