Synthesis of Cationic Novel Bolaform Surfactant and Effect of Alkyl Group Chain Length on Polar Head Group

1. Propane-1,3-bis(trimethylammonium bromide)

and

Propane-1,3-bis(triethylammonium bromide)

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Abstract: Surfactants are a class of chemical compounds with unique properties, structure of which is consisted of hydrophobic and hydrophilic parts. This double structure gives rise to their unique behaviors in various conditions. Bolaforms are organic molecules compounds of two charged groups which are connected via a linear poly methylen chain. Bolaforms' surfactants don't work as well as conventional surfactant (having a head group and one alkyl chain) in reducing surface tension. Bolaforms are absorbed in water – air interface, however, their effectiveness in terms of reducing water surface tension is not considerable compared to common surfactants. In this paper, synthesis of two kinds of bolaforms with the same spacer length and different heads is investigated. The structural formula for synthesized kinds is as follows: bolaform A with structural formula $Br^{-}(CH_3)_3N^{+}(CH_2)_3\ N^{+}(CH_3)_3\ Br^{-}$ with methyl side branches in head group and bolaform B with structural formula of $Br^{-}(CH_3\ CH_2)_3N^{+}(CH_2)_3\ N^{+}(CH_3\ CH_2)_3Br^{-}$. IR and NMR identification techniques approves obtained product. Using surface tension measurement device it can be observed that synthesized bolaforms has high CMC; in other words, bolaform's surfactants with short spacer play electrolytic role.

Keywords: Cationic Novel Bolaform, Electrolytic

1. Introduction

Surfactant molecules self-associate in aqueous solution because the reduction of the hydrocarbon-water interface is energetically favored; the critical concentration at which aggregation occurs reflects the balance between the hydrophobic interaction of the hydrocarbon parts of surfactant molecules and the hydration and electrostatic repulsive effects of hydrophilic

head groups[1]. The bis (quaternary ammonium) surfactants have been shown to be more potent bactericidal agents than the corresponding monoquaternary Surfactants. Moreover, these surfactants are very interesting from the fundamental point of view. Indeed their structure can be considerably modified by acting on the length and nature both of polar head groups. It is then interesting to check how such changes affect the micellar properties of these surfactants (critical micelle concentration (CMC), micelle ionization degree, aggregation number, etc.) and their ability to comicellize with the corresponding single chain quaternary ammonium surfactants and other surfactants and to try to associate their biological activity to their structure. The Bolaform surfactants seem to differ in several ways from the normal unipolar surfactants. First, their CMC values are much higher, the size of their micelles is smaller, and the degree of ionization of their micelles is larger than that for a unipolar surfactant with a hydrocarbon chain having the same number of carbon atoms. Second, the Bolaform surfactants generally form a folded, wicket-like conformation at the air-aqueous solution interface. Third, the hydrophobic alkyl chain of an Bolaforms surfactant may assume a different conformation in aqueous solution [2].

2. Experimental Section

Materials: Triethylamine for synthesis (Fluka), Ethanol Absolute (Merck)-1,3 dibromo propane (Merck), Trimethylamine solution 31-35 wt. % in ethanol (~4.2 M) sigma-aldrich was prepared.
Methods*:* The Bolaform surfactants are synthesized in the following way: Triethylamine was added in large excess to 1,3 dibromo propnae and the mixture was kept under vigorous stirring at 55C for five days. The obtained white powder was recrystallized three times from ethanol to obtain 1,3-bis (triethylammonium bromide)[3]. we can also add 1,3 dibromo propnae directly to Trimethylamine solution 31-35 wt. % in ethanol (~4.2 M) and obtain white powder after three times recrystallized in ethanol and then the product is called propane 1,3-bis (trimethylammonium bromide). In this study, propane 1,3-bis (trimethylammonium bromide) and propane 1,3-bis (triethylammonium bromide) are called A and B, respectively.

3. Results and Discussion

^{1}H NMR (500 MHz, D_2O):

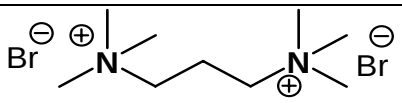
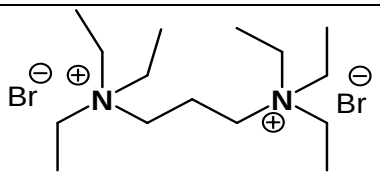
δ: 3.30 (18H, S), 3.2 (4H, triplet), 2.17 (2H, multiplet) for A bolaform.

δ: 1.25 (18H, triplet), 3.28 (12H, quartet), 3.24(4H, triplet), 2.17 (2H, multiplet) for B bolaform

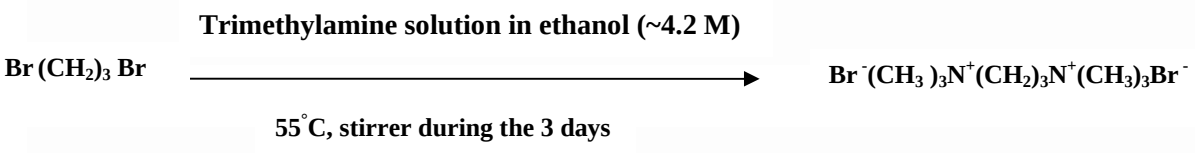
IR Spectroscopy: Another method to identical structure of bolaforms is IR spectroscopy.These kinds of bolaforms have absorbance water**.** Figure 1 shows the spectra of bolaform with 12 length spacer.

Surface Tension Measurement: Surface tension measurements were carried out at 298.15 K by the ring method using a Sigma 700 tensiometer under atmospheric pressure. Surface tension diagram of bolaforms are shown in the Figure 2 and 3.

Table 1. Characterization of Novel Bolaform Surfactants

Bolaform names	**structure**	**Melting point**
propane 1,3 bis (trimethylammonium bromide)		250°
propane 1,3 bis (triethylammonium bromide)		245°

Synthesis method for Bolaform A is as follows:



Synthesis method for Bolaform B is as follows:

IR and NMR identification techniques approve obtained product. Bolafroms synthetic are highly attracted to water, and are water absorbent. Figure 1 shows IR spectra of these surfactants.

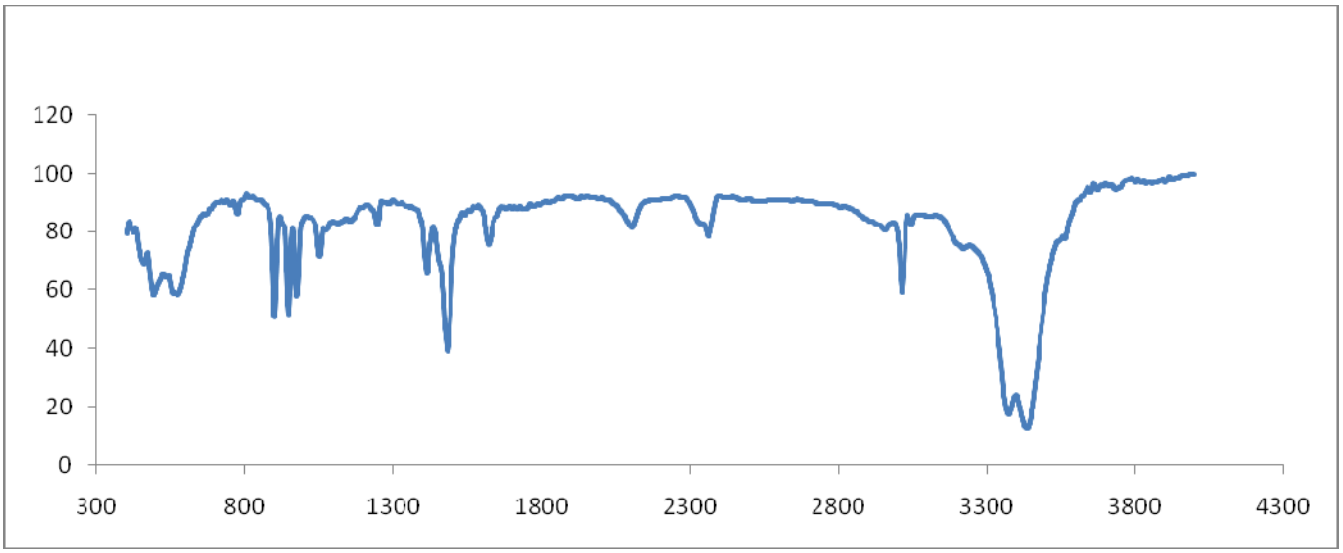


Figure 1.IR spectra of bolaform A

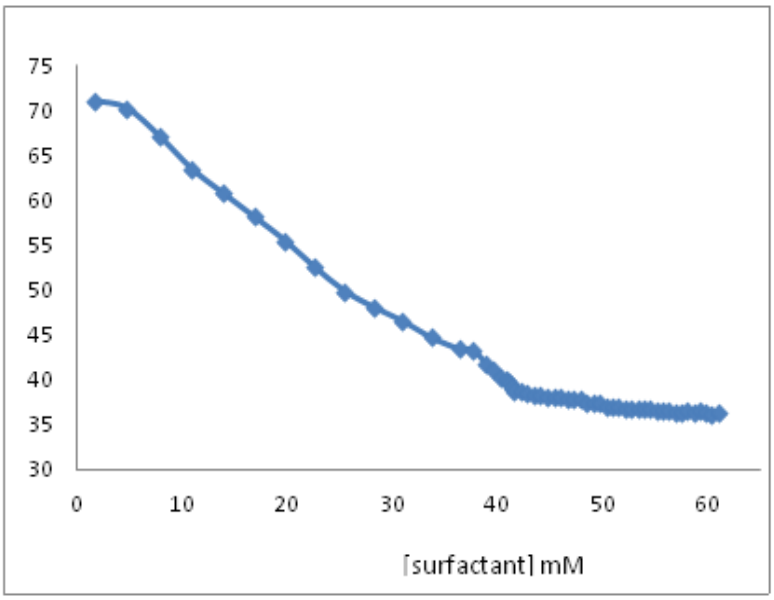


Figure2.surface tension diagram of bolaform B

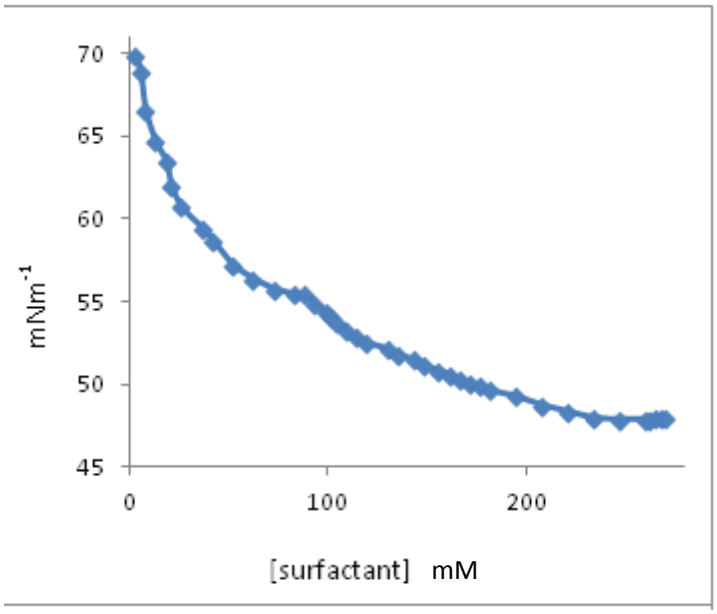


Figure 3.surface tension diagram of bolaform A

4. Conclusions

Using surface tension measurement device, it can be observed that synthesized bolaforms have high CMC; in other words, bolaform's surfactants with short spacer play electrolytic role. Bolafrom surfactant A and B show more electrolytic properties and cause to reduction of surface tension in surfactant mix. Generally if length spacer is short, bolaforms make vesicle in bulk. CMC of bolaform A is higher than the bolaform B. Results indicate that bolaforms have behavior similar to conventional surfactants in many respects. Bolaforms form micelle in higher concentrations because of two polar head groups, while bolaforms provide interesting biological properties. Bolafrom surfactants are highly attracted to water, and are water absorbent. Alkyl groups play important role in surface tension measurement and decrease CMC. Ethyl groups are more water absorbent than the methyl group in polar head group of bolaform surfactants. In order to increase purity of bolaforms surfactant with ethyl Substituted in head group, we should repeat recrystallization processes several times. So bolaforms with methyl groups in polar head groups have more purity and have low water absorbance.

References

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