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Physicochemical properties and bioactivity studies of synthesized counterion coupled (COCO) gemini surfactant, 1,6-bis(*N*, *N*-hexadecyldimethylammonium) adipate

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ABSTRACT

In the present investigation, we report the surface activity, micellar, thermodynamic properties and bioactivity studies of synthesized counterion coupled (COCO) gemini surfactant, 1,6-bis(*N*,*N*-hexadecyldimethylammonium) adipate (16-6-16). In aqueous solution, the CMC (critical micelle concentration) of 16-6-16 was measured by electrical conductivity, surface tension, dye solubilization and fluorescence measurements techniques. The surface activities and surface properties of the COCO gemini surfactant, 16-6-16 were evaluated. The CMC as well as A_{min} (the minimum area per surfactant molecule at the air/water interface) decrease and the Γ_{max} (the maximum surface excess concentration at the air/water interface) increases with increasing the temperature. We also report the thermodynamics of 16-6-16 and evaluated Gibbs energies. The aggregation number (N_{agg}) of 16-6-16 is reported. The bioactivity studies of 16-6-16 showed to be nontoxic, biocompatible and having good antibacterial activity.

1. Introduction

Surfactants are a special class of compounds which are amphiphilic in nature and having important physicochemical properties at interfaces as well as in bulk solution [1–3]. Generally, they are composed of two distinct parts, one polar and the other nonpolar, incompatible with each other. In aqueous environment, above their *critical micelle concentrations* (*CMC*), some amphiphilic molecules e.g., surfactants [1–6], amphiphilic drugs [7–18], etc. can form a kind of self-organized molecular assembly, which can be called as *micelles* [1–18]. The interests in micelle solutions stems from their potential as functional molecular assemblies for use in many fields of pure and applied sciences as they can be used as models for several biochemical and pharmacological systems, and is advantageous in different industrial areas, like pharmaceuticals, cleaning, paint, emulsion, oil recovery, catalysis, microreactor, cosmetics, etc. [1–3,19,20].

The gemini (or dimeric) surfactants are surfactants which are made up of two amphiphilic moieties connected at the level of the head groups (or very close to the head groups) by a spacer group [1,21–28]. In gemini surfactants, there are two hydrophilic groups and two hydrophobic groups per molecule are present where as in conventional surfactants, the single hydrophilic and single hydrophobic group per molecule are present [1,21–28]. There are many unique properties which made the gemini surfactants superior to those of their single-chain counterparts. For example, remarkably low CMCs; much higher efficiency, in regard to reducing surface tensions; unusual aggregation morphologies; and better wetting, solubilizing, and foaming properties, etc.) and make them potentially useful in many applications (e.g., in soil remediation, enhanced oil recovery, drug entrapment and release, and the construction of high-porosity materials, etc.). Overall, the greater efficiency and effectiveness of gemini surfactants over comparable conventional surfactants make them more cost-effective as well as environmentally desirable [1,21–28].

The purpose of this work was to synthesize the class (counterion coupled, COCO) of gemini surfactants and to study their surface and solution properties. In the present investigation, we report the synthesis, surface activity, micellar, thermodynamic properties and bioactivity of counterion coupled (COCO) gemini surfactant, 1,6-bis(*N*,*N*-

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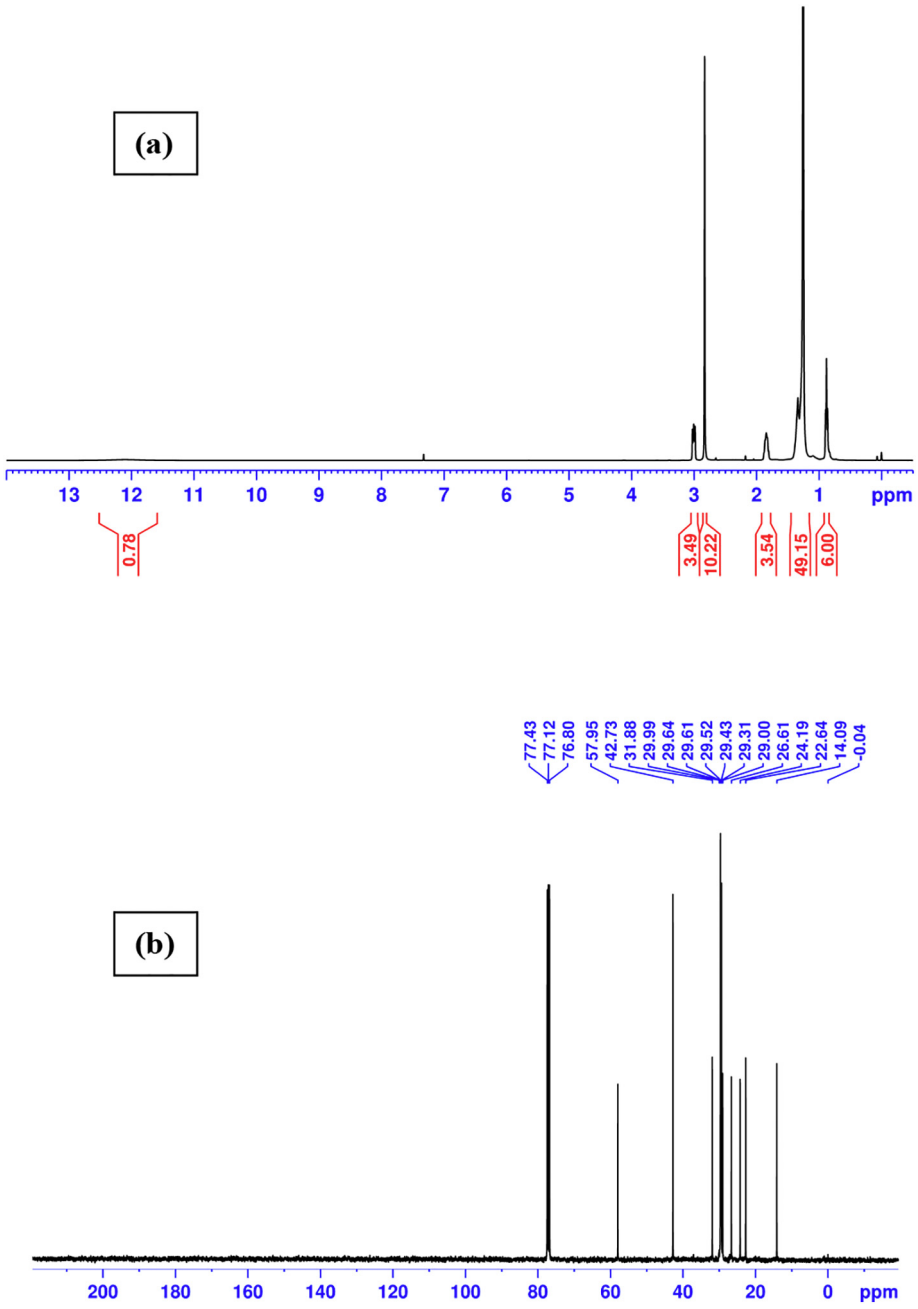

Fig. 1. ^{1}H NMR (a) and ^{13}C NMR (b) spectra of counterion coupled (COCO) gemini surfactant, 1,6-bis(*N*,*N*-hexadecyldimethylammonium) adipate (16-6-16).

hexadecyldimethylammonium) adipate (16-6-16). The aim of the study is to obtain information about the physicochemical characterization of the COCO gemini surfactant, 16-6-16 in aqueous solution. The cocogems are promising candidates in various applications, especially in drug delivery. The study is important from both the basic and applied research point of view.

2. Experimental

2.1. Materials

Adipoyl chloride (98%, Aldrich, USA), *N*,*N*-dimethylhexadecylamine (≥95%, Aldrich, USA), Sudan III (≥99%, Sigma, USA), pyrene (≥99%, Sigma, USA) and cetylpyridinium chloride, CPC (≥99%, Sigma, USA) were used as received. The COCO gemini surfactant, 16-6-16 was synthesized and purified. Milli-Q water (sp. cond. = 1–2 μS·cm^{-1} at 298.15 K) was used as the solvent throughout the experiment.

2.2. Methods

2.2.1. Synthesis and characterization of counterion coupled (COCO) gemini surfactant (16-6-16)

The counterion coupled (COCO) gemini surfactant, viz., 1,6-Bis(*N*,*N*-hexadecyldimethylammonium) adipate (16-6-16) was synthesized by adopting the following procedure: