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Elucidating the effect of additives on the alkyl chain packing of a double tail cationic surfactant

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ABSTRACT

Hypothesis: Some low molecular weight additives can strongly influence the phase behavior of aqueous surfactant systems, and this offers an important handle to control the properties of surfactant solutions and thus to optimize the stability and performance of various formulations.

Experiments: The surfactant dioctadecyldimethylammonium chloride (DODAC) self-assembles into two lamellar phases in water, the gel phase (L_{β}) and the liquid crystalline phase (L_{α}). Here, we present approaches to tune the gel-to-liquid crystalline transition temperature (T_m) with the use of additives. The effects of urea, sodium butyrate and butyric acid on the packing behavior of DODAC were determined. The surfactant phases were characterized using polarized optical microscopy (POM), differential scanning calorimetry (DSC), and small/wide angle X-ray scattering (SWAXS).

Findings: All three additives - urea, sodium butyrate and butyric acid yield a single and stable lamellar phase. Urea and sodium butyrate have only minor effects on T_m , butyric acid gives a large decrease as it stabilizes the L_{α} phase with respect to the L_{β} phase. From the bilayer thickness of the gel phase an interdigitated or tilted packing of the surfactant molecules is suggested. The addition of sodium butyrate gives a highly interdigitated gel structure and resulted in the transition from lamellar liquid crystal to an isotropic L_3 phase.

1. Introduction

Amphiphilic molecules, such as surfactants and polar lipids, can be used for many novel health-care and personal-care applications as solution behavior modifiers [1-5]. Since the first investigations by Kunieda and Shinoda [6] on the solution behavior of long di-alkyl quaternary ammonium salts, there has been much work done to understand the properties of the bilayer structures that dominate the phase diagrams of the binary surfactant-water systems [3, 7-9]. Two types of lamellar structures are found for these systems – the lamellar gel phase (L_{β}) with highly ordered alkyl chains with little conformational

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