

# Structures of lamellar liquid crystals formed by the self-association of double chain cationic surfactants in water

**Guilherme Augusto Ferreira (PG) and Watson Loh (PQ)\***

\*wloh@iqm.unicamp.br

Instituto de Química, Universidade Estadual de Campinas, Campinas, SP.

Palavras Chave: surfactants, colloids, liquid crystals, lamellar phases, self-assembly

## Introdução

The dialkyldimethylammonium bromides are a class of double chain cationic surfactants which possess great scientific interest [1]. Herein the lamellar phases originated from self-assembling of two surfactants, didodecyldimethylammonium (DDAB) and dioctadecyldimethylammonium (DODAB) bromides, were investigated to clarify the phase behavior and to highlight the dynamic processes involved, at a molecular level, in the structural properties of the lamellar phases. For this purpose, mixtures of both surfactants in water were prepared in the range of concentration from 1,0 to 85,0% (w/w) and characterized by SAXS analyses.

## Resultados e Discussão

The SAXS curves for several concentrations of samples prepared with DDAB and DODAB confirmed the association into the ordered lamellar  $L_\alpha$  (fluid) and  $L_\beta$  (gel) phases. The swelling curves (Fig. 1) for samples prepared with both surfactants show that upon dilution, the swelling of lamellar phases formed by DDAB and DODAB display a different behavior.

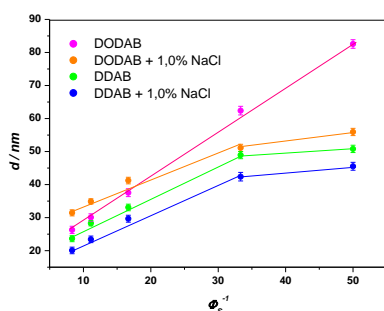


Fig. 1 – Interlamellar distance ( $d$ ) against the inverse of volumetric fraction of surfactants ( $\Phi_s^{-1}$ ) DDAB and DODAB in the absence and presence of salt (discussed below).

By extrapolation of swelling curves it's possible to obtain the bilayers thickness. The values found were  $2,41 \pm 0,06$  nm for DODAB, suggesting interdigitation of carbonic chains, and  $2,30 \pm 0,04$  nm for DDAB, being this last in accordance with literature [2]. We propose that the structural

properties investigated are strongly influenced by electrostatic forces acting on the system. It is known that DODAB bilayers possess higher surface charge density than those formed by DDAB molecules. Therefore, at low temperatures, due to unfavorable close contacts between the charged ammonium headgroups, the alkyl chains of DODAB are forced to interdigitate in order to condense the tail groups while keeping the neighboring headgroups apart. Characterization of samples formulated above the transition temperature to the fluid phase confirmed this hypothesis (Fig. 2) as can be noted by the increase of bilayers thickness.

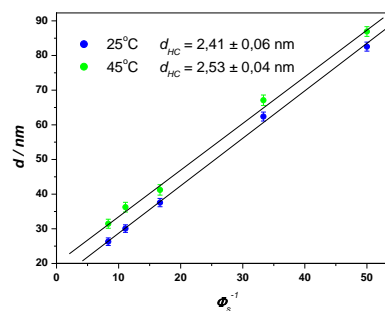


Fig. 2 – Interlamellar distance ( $d$ ) against volumetric fraction of surfactants ( $\Phi_s^{-1}$ ) DDAB and DODAB at 25 and 45° C.  $d_{HC}$  represents the bilayers thickness.

From the ion correlation effects [3], we propose that the higher swelling of DODAB bilayers is due to the osmotic pressure of the solvent trying to balance the chemical potential of water inside and outside of bilayers. Characterization of samples formulated with NaCl confirmed the hypothesis (Fig. 1)

## Conclusões

Both surfactants DDAB and DODAB self-assemble into lamellar liquid crystalline phases, which structural properties, such as swelling and thickness of bilayers, can vary with length of alkyl chains and can be strongly influenced by the electrostatic forces.

## Agradecimentos

CNPq, LNLS (SAXS beamline)

<sup>1</sup>Wu, F. G.; Yu, Z. W.; Ji, G. *Langmuir*, **2011**, *27*, 2349.

<sup>2</sup>Grillo, I.; Penfold, J.; Tucker, I.; Cousin, F. *Langmuir*, **2009**, *25*, 3932.

<sup>3</sup>Segad, M.; Jonsson, B.; Akesson, T.; Cabane, B. *Langmuir*, **2010**, *26*, 5782.