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Supplementary Information

Structural Parameters of Lamellar Phases Formed by the Self-Assembly of Dialkyldimethylammonium Bromides in Aqueous Solution

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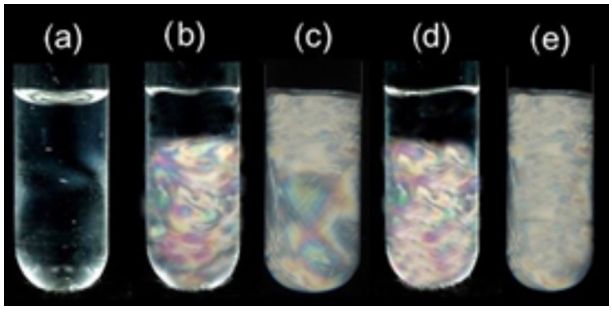

Figure S1. Samples observed under crossed polarizers: (a) 1.0% DDAB; (b) 10.0% DDAB; (c) 50.0% DDAB; (d) 10.0% DODAB; (e) 50.0% DODAB in water (all expressed as wt.% and observed at room temperature).

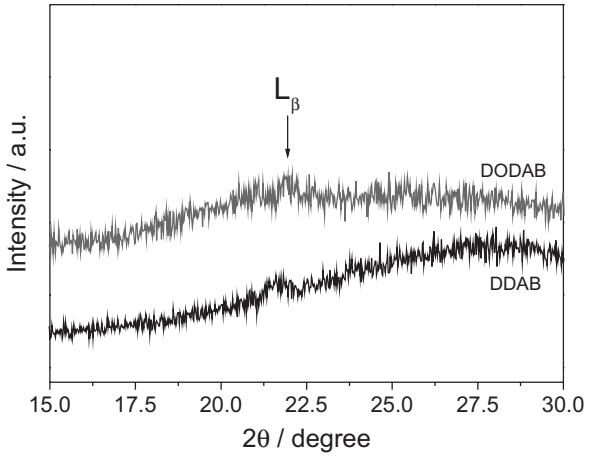

Figure S2. XRD data for 50.0% (a) DDAB; (b) DODAB samples above (45 °C) the T_m showing the absence of the gel phase diffraction peak.

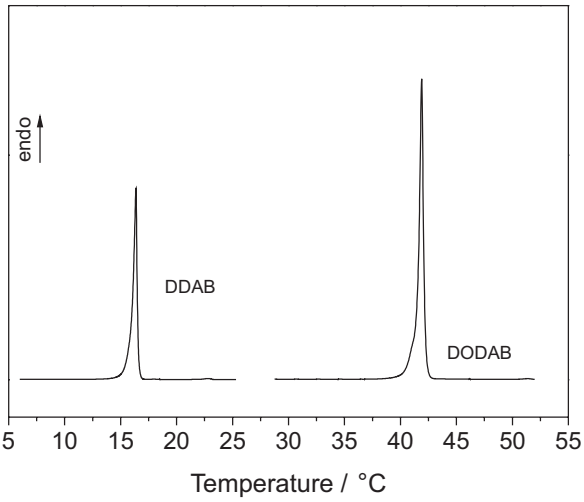

Figure S3. DSC thermograms for DDAB and DODAB vesicles showing a narrow peak for the gel-to-fluid phase transition. The T_m observed for DDAB vesicles was 16 °C.

Table S1. Transition temperatures (T_m), peak width ($\Delta T_{1/2}$) and transition enthalpies (ΔH), with standard deviation in parenthesis, for DDAB and DODAB vesicles

Amphiphile	T_m / °C	$\Delta T_{1/2}$ / °C	ΔH / (kJ mol^{-1})
DDAB[a]	16	0.5	4 (1)
DODAB[b]	42	0.5	41 (1)

[a]Didodecyldimethylammonium bromide (DDAB); [b]dioctadecyldimethylammonium bromide (DODAB).

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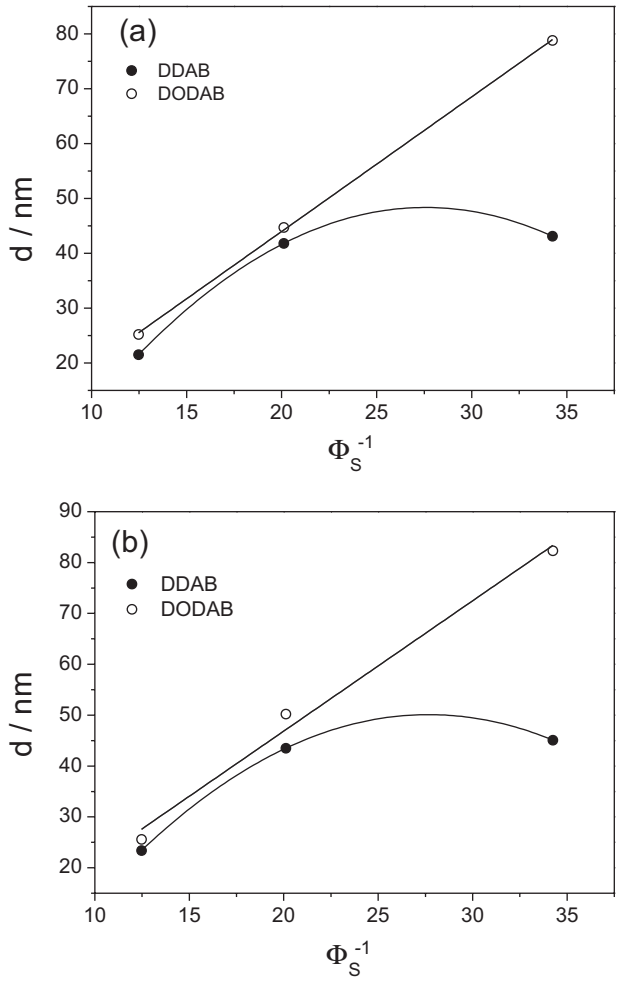

Figure S4. Repeat distance of bilayers (d) against the inverse of volumetric fraction of surfactant (Φ_S^{-1}) DDAB and DODAB at (a) 18 ºC; (b) 45 ºC.

Determination of the volumetric fraction of surfactants (Φs) in the samples

As described in the paper, the volumetric fraction of surfactant in the samples represents only the hydrophobic part of the surfactants composing the bilayers. The polar quaternary ammonium headgroups and the water are assumed to compose the aqueous phase. Thus, Φs can be calculated by the equation S1:

$$_S \quad \frac{V_{HC} \times \left(\frac{w_S}{M_S}\right)}{(V_{HC} + V_P) \times \frac{w_S}{M_S} + V_w \times \frac{w_w}{M_w}} \qquad (S1)$$

where:

V_{HC} = partial molecular volume of the surfactant alkyl chains;

V_P = partial molecular volume of the surfactant polar headgroups;

V_w = partial molecular volume of water;

W_S = weight fraction of surfactant in the sample;

w_w = weight fraction of water in the sample;

M_S = molecular weight of the surfactant used in the sample;

M_w = molecular weight of water.

The values used to calculate these parameters are listed in Table S2, based on the references 13, 36 and 41 cited in the paper.

Table S2. Molecular parameters used to calculate the volumetric fraction of surfactant in the samples prepared in this study

Parameter	DDAB[a]	DODAB[b]	Water
V_{HC}[c] / Å^3	702	1052	–
V_P[d] / Å^3	141	141	–
V_W[e] / Å^3	–	–	30
M[f] / (g mol^{-1})	462.63	630.95	18.02

[a]Didodecyldimethylammonium bromide (DDAB); [b]dioctadecyldimethylammonium bromide (DODAB); [c]V_{HC} = partial molecular volume of the surfactant alkyl chains; [d]V_P = partial molecular volume of the surfactant polar headgroups; [e]V_w = partial molecular volume of water; [f]M = molecular weight.

Determination of the cross-sectional area *per* surfactant (a_S) in DDAB and DODAB bilayers

According to the model proposed by White *et al*.[1] and successful used in previous reports of our group,[2] the area *per* surfactant (a_S) composing a bilayer can be simply calculated by the following equation S2:

$$a_S = \frac{2V_S}{d_{HC}} \qquad (S2)$$

where:

V_S = partial molecular volume of the surfactant ($V_S = V_{HC} + V_P$), defined in Table S2;

d_{HC} = bilayers thickness in the gel and fluid states, calculated for each surfactant according to equation 3 given in the manuscript.

References

1. White, S. H.; King, I. G.; *Proc. Natl. Acad. Sci. USA* **1985**, *82*, 6532.
2. Bernardes, J. S.; Norrman, J.; Piculell, L.; Loh, W.; *J. Phys. Chem. B* 2006, ***110***, 23433.