

Supporting information for

Lyotropic liquid crystalline phases formed in ternary mixtures of *N*-alkyl-*N*-methylpyrrolidinium bromide/1-decanol/water

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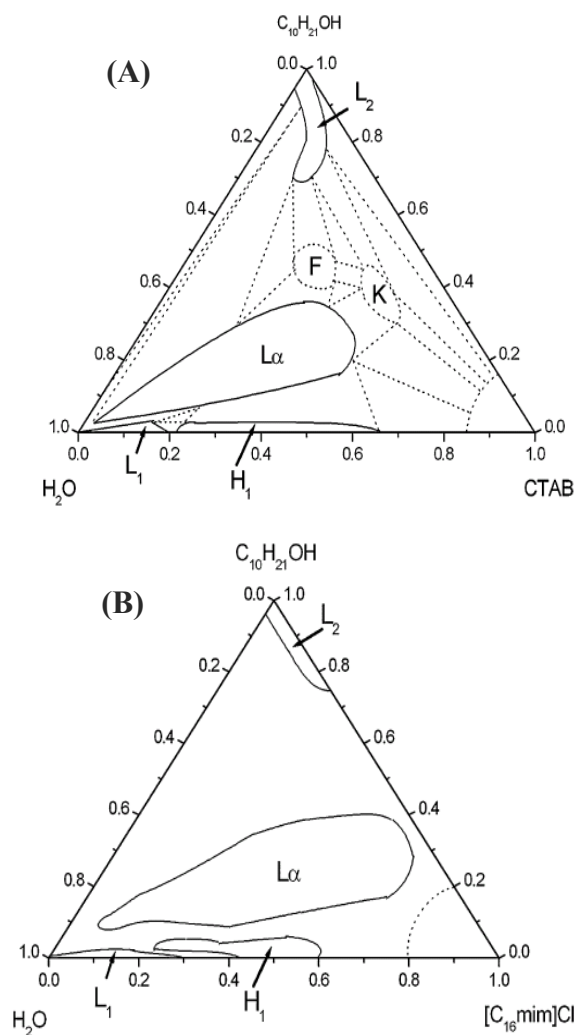


Figure S1 (A) Phase diagram for the ternary system of C₁₆TAB-C₁₀H₂₁OH-H₂O [29]. Codes for phases: L₁, isotropic H₂O solution; L₂, isotropic C₁₀H₂₁OH solution; H₁, hexagonal; L_α, lamellar; F, reversed hexagonal; K, reversed phase with a non-hexagonal rod-structure. (B) Phase diagram for the ternary system of [C₁₆mim]Cl, C₁₀H₂₁OH, and H₂O at 25°C [21]. Codes for phases: L₁, isotropic H₂O solution; L₂, isotropic C₁₀H₂₁OH solution; H₁, hexagonal; L_α, lamellar.

Table S1 Structural parameters for the liquid crystalline phases in the
 C_n MPB– $C_{10}H_{21}OH$ – H_2O ($n = 12, 14, 16$) systems

C_n MPB	12						14						16						
	Φ_s (%)	Φ_o (%)	Φ_w (%)	$d_L(d_{II})$ (Å)	d_w (Å)	a_s (Å ²)	Φ_s (%)	Φ_o (%)	Φ_w (%)	$d_L(d_{II})$ (Å)	d_w (Å)	a_s (Å ²)	Φ_s (%)	Φ_o (%)	Φ_w (%)	$d_L(d_{II})$ (Å)	d_w (Å)	a_s (Å ²)	
$L\alpha$	L α -1	18.40	6.47	75.13	20.96	12.70	19.95	17.89	7.11	75.00	24.50	12.63	19.86	13.79	6.20	80.01	26.57	14.32	20.66
	L α -2	14.82	5.19	79.99	20.46	14.09	20.45	13.80	5.51	80.69	23.58	14.45	20.57	11.76	5.10	83.13	26.20	15.64	21.46
	L α -3	12.19	4.68	83.13	19.73	15.60	21.14	12.27	5.21	82.52	22.90	15.56	21.01	11.08	3.82	85.10	25.75	17.37	22.18
phase	L α -4	11.16	3.73	85.11	19.23	16.96	21.65	10.68	4.29	85.03	22.34	16.82	21.63	8.09	3.58	88.33	24.85	19.80	22.98
	H _I -1	6.46	0.65	92.89	14.11	29.17	28.17	6.44	0.67	92.89	16.46	31.83	27.75	3.13	0.57	96.30	20.04	47.63	26.37
	H _I -2	7.82	0.60	91.58	14.53	28.34	27.28	7.27	0.61	92.12	16.58	30.99	27.83	4.62	0.61	94.77	19.04	39.13	27.70
phase	H _I -3	9.56	0.62	89.82	14.59	26.75	27.16	8.80	0.62	90.58	16.86	29.73	27.33	6.48	0.64	92.88	17.63	32.36	29.63
	H _I -4	11.78	0.57	87.63	14.75	25.31	27.08	10.84	0.64	88.52	17.08	28.35	26.97	8.24	0.23	91.19	16.07	24.51	31.48

Theory for calculation of structural parameters of liquid crystalline phase

The lattice parameters D (distance between the centers of adjacent cylinders), and d (lamellar periodicity) of the hexagonal and lamellar liquid crystalline phases were obtained according to eq. (1) and (2), respectively¹.

$$q_{(h,k)} = (4\pi / \sqrt{3}D) \cdot (h^2 + k^2 - hk)^{1/2} \quad (1)$$

$$q_{(l)} = (2\pi / d) \cdot l \quad (2)$$

where $q_{(h,k)}$ and $q_{(l)}$ are the scattering vectors corresponding to the scattering peaks observed in the SAXS spectra for the hexagonal and lamellar phase, respectively, h , k , l are Miller indexes, and a_0 is the lattice parameter.

From the results of SAXS, several structural parameters characterizing the structure of the liquid crystalline phase could be calculated as follows.

For hexagonal liquid crystalline, the radius of cylinder unit (d_H) could be obtained using Eq. (3)²:

$$d_H = D \cdot \left(\frac{2}{\sqrt{3}\pi} \cdot (\phi_S + \phi_O) \right)^{1/2} \quad (3)$$

where ϕ_S and ϕ_O are the volume fractions of surfactant (C_n MPB) and oil (1-Decanol).

The volume fraction of surfactant ϕ_S in the ternary mixture is calculated by Eq. (4)³:

$$\phi_S = \frac{W_S / \rho_S}{W_S / \rho_S + W_O / \rho_O + W_W / \rho_W} \quad (4)$$

where W_S , W_O , and W_W are the weight fraction of C_n MPB, 1-decanol and water, respectively, and ρ_S , ρ_O , and ρ_W are the densities of C_n MPB, 1-decanol and water, respectively. The density of C_n MPB is obtained using a pycnometer as reported previously⁴, and the reference solvent is ethyl acetate ($\rho = 0.8944 \text{ g}\cdot\text{cm}^{-3}$). The densities of C_{12} MPB, C_{14} MPB, and C_{16} MPB are 1.1961, 1.1696, and 1.1538 $\text{g}\cdot\text{cm}^{-3}$, respectively.

Furthermore, the thickness of water channel (d_W) is given by

$$d_w = D - 2d_H \quad (5)$$

The area per molecule of C_n MPB at the hydrophilic/hydrophobic interface in the hexagonal phase could be given by

$$a_s = \frac{2V_L \cdot \phi_s + \phi_o}{d_H \phi_s} \quad (6)$$

where V_L is the volume of the hydrophobic part of the surfactant, calculated according to the Tanford equation⁵:

$$V_L (\text{\AA}^3) = 27.4 + 26.9N \quad (7)$$

N denotes the number of carbon atoms of the hydrophobic chain of the surfactant.

For lamellar liquid crystalline phase, the thickness of hydrophobic domain (d_L) could be obtained as

$$d_L = (\phi_s + \phi_o) \cdot d \quad (8)$$

While the thickness of the water layer (d_w) is given by

$$d_w = d - d_L \quad (9)$$

Furthermore, the area per molecule for C_n MPB in the hydrophobic/hydrophilic interface is given by

$$a_s = \frac{2V_L \cdot \phi_s + \phi_o}{d_L \phi_s} \quad (10)$$

References

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