Supplemental Material

Effect of Paraffin Oil on the Cubic Phase of Hydrated Monoolein.

Materials

Monoolein (MO, 1-oleoyl-rac-glycerol, lot # M239-029-L, 356.54 g/mole) was purchased from Nu Chek Prep Inc. (Elysian, MN). Paraffin oil (lot # 341107) was from Hampton Research (Laguna Niguel, CA). Water (resistivity > 18 MΩ·cm) was purified by using a Milli-Q Water System (Millipore Corporation, Bedford, MA) consisting of a carbon filter cartridge, two ion exchange filter cartridges and an organic removal cartridge.

Sample preparation

A stock consisting of 50 %(w/w) paraffin oil in MO was prepared by weighing equal quantities of the two components into a vial, heating to 40^{o}C to melt the MO followed by vortex mixing. The stock was diluted further with molten MO to obtain the desired concentrations of oil in MO. Hydrated MO/paraffin oil samples at 50 %(w/w) water and of total mass 20 – 30 mg were prepared at room temperature (~23°C) using a home-built syringe mixer (Cheng *et al.*, 1998). The aqueous dispersions were transferred to 1 mm quartz capillary tubes (Hampton Research, Laguna Niguel, CA) and flame-sealed using a propane/oxygen torch (Smith Equipment, Watertown, SD). A bead of 5-minute epoxy (Devcon, Danvers, MA) was applied to protect and ensure the integrity of the flame seal.

X-ray diffraction

X-ray diffraction measurements were performed for phase identification and microstructure characterization using a rotating anode x-ray generator (Rigaku RU-300 operating at 45 kV and 250 mA) producing Ni-filtered Cu K_α radiation (wavelength $\lambda = 1.5418$ Å) as described in Cherezov *et al.*, 2002. Sample-to-detector distance was 335 mm as measured using a silver behenate standard (Blanton *et al.*, 1995). Capillaries were placed in a home-built sample-holder with space for seven samples (Zhu & Caffrey, 1993) and were continuously translated at a rate of 3 mm/min back and forth along a 3 mm section of the sample to average the contributions to total scattering from different parts of the sample and to minimize possible radiation damage effects (Cherezov *et al.,* 2002). The temperature inside the sample holder was regulated by two thermoelectric Peltier effect elements controlled by a computer feedback system. Measurements were performed at 20.0 ± 0.05^{o}C. Typical exposure time was 30 min.

Results

At low concentrations, paraffin oil caused the lattice parameter of the cubic-Pn3m phase to drop. At 5 %(w/w) oil, it induced inverted hexagonal (H_{II}) phase formation. The latter persisted with a constant lattice parameter of ~62.5 Å up to 20 %(w/w) oil. At 50 %(w/w) paraffin oil, the system existed in a liquid-like phase characterized by a diffuse band centered at 81 Å. The results are consistent with a partitioning of the paraffin oil into the apolar compartment of the lyotropic mesophase. This relieves packing energy at the chain termini and allows the system to express its intrinsic curvature by forming the H_{II} phase. At the highest concentrations used, the oil presumably dissolves the lipid and, when combined with water, forms a liquid dispersion.

Table 1. Effect of paraffin oil on the phase identity and microstructure of monoolein at 20°C and 50 %(w/w) water.

Concentration of paraffin oil, %*	**Phase Identity**	**Structure parameter, Å**
0	Cubic-Pn3m	104.9 (d_{100})
1	Cubic-Pn3m	102.2 (d_{100})
2.5	Cubic-Pn3m	98.7 (d_{100})
5	Cubic-Pn3m + H_{II}	95.0 (d_{100}); 62.2 (d_{10})
10	H_{II}	62.7 (d_{10})
20	H_{II}	62.4 (d_{10})
50	Liquid (most likely)	81

*Calculated as [100 (mass paraffin oil) / (mass paraffin oil + mass MO)]

References

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