α-GEL FORMATION ABILITY OF MONOHEXADECYL PHOSPHATE NEUTRALIZED BY L-ARGININE

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The aqueous phase diagram of monohexadecyl phosphate neutralized by L-arginine (C16MP- Arg, Figure 1) was studied using analytical techniques including differential scanning calorimetry (DSC), small/ wide-angle X-ray scattering (SWAXS) measurements, Fourier transform infrared spectroscopy (FT-IR), and ^{1}H nuclear magnetic resonance (NMR) spectroscopy. We found that the mixture could form an α-gel over wide ranges of concentrations and temperatures (Figure 2). The α-gel was thermodynamically stable at 25°C (below the phase transition temperature for hexagonal or lamellar liquid crystals), and did not transform to coagel for at least one year. This behavior is unique among anionic surfactant systems. Thus, the balance between hydrophilic and hydrophobic volumes is a key factor for determining whether a stable α-gel can be obtained. In this system, the relatively large volume of Arg relaxed the alkyl chains of C16MP and prevented their crystallization.

We also characterized the behavior of water in the C16MP-Arg α-gel system. An increased water concentration resulted in an increase in the d-spacing of the lamellar bilayers (Figure 3) as well as an increased wavenumber for the O-H stretching vibration peak. In addition, the melting enthalpy increased with increasing water concentration, while freezing was not observed below a water concentration of 20 wt%. These results suggest that the overall properties of water changed as a function of its concentration in the sample. ^{1}H-NMR spin-spin relaxation time (T_2) measurements further suggest that the protons of water and C16MP-Arg can be classified into three components (low-, middle-, and high-T_2 components) as a function of the temperature and concentration. The low-T_2 component mainly arose from the protons of C16MP-Arg alkyl chains, and its mobility increased with increasing temperature. The high-T_2 component arose from the protons of water. The water behaved as "bound water" for the C16MP-Arg headgroups at –30°C and a water concentration of 20 wt%, and the mobility increased with increasing temperature and water concentration. These changes suggest that an increased water concentration results in an increased amount of water being incorporated between the C16MP-Arg lamellar bilayers as well as in spaces surrounded by α-gel domains.

We anticipate that the results of this study will be useful in cosmetics and personal care industries.

References
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J. Oleo Sci., 67, 851-857 (2018).
2)   K. Tanaka, Y. Hirai, T. Suzuki, M. Akamatsu, K. Sakai,
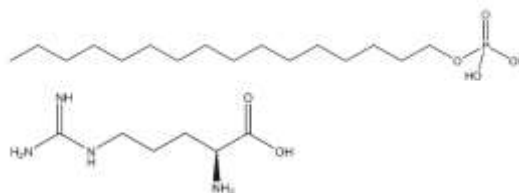H. Sakai, *J. Oleo Sci.,* 68, 225-231 (2019).

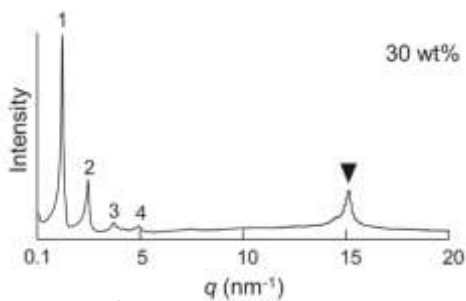Figure 1 Molecular structures of C16MP and L-arginine

Figure 2 SWAXS pattern of the C16MP-Arg + water system at 30 wt% concentration.
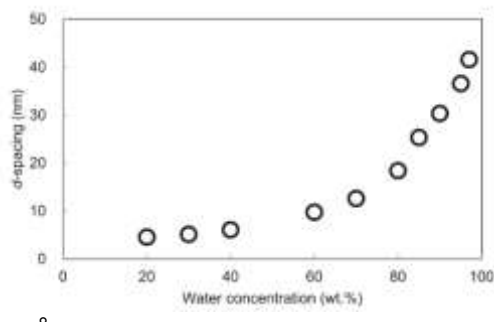

Figure 3 Long-range d-spacing values as a function of water concentration