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Structural Aspects of Pressure Effects on Infrared Spectra of Mixed-Chain Phosphatidylcholine Assemblies in D_2O[†]

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ABSTRACT: The barotropic behavior of D_2O dispersions of 1-stearoyl-2-caproyl-*sn*-glycero-3-phosphocholine, C(18):C(10)PC, a highly asymmetric phospholipid in which the length of the fully extended acyl chain at the *sn*-1 position of the glycerol backbone is twice as long as that at the *sn*-2 position, has been investigated by high-pressure Fourier transform infrared spectroscopy. This asymmetric phosphatidylcholine bilayer at room temperature displays a pressure-induced phase transition corresponding to the liquid-crystalline → gel phase transition at 1.4 kbar. A conformational ordering of the lipid acyl chains is observed to take place abruptly at the transition pressure of 1.4 kbar. However, the lamellar lipid molecules and their acyl chains remain to be orientationally disordered in the gel phase until the applied pressure reaches 5.5 kbar. In the gel phase of fully hydrated C(18):C(10)PC, the asymmetric lipid molecules assemble into mixed interdigitated bilayers with perpendicular orientation of the zigzag planes among neighboring acyl chains. The role of excess water played in the interchain structure and the behavior of excess water and bound water under high pressure are also discussed.

It is well recognized that in biological membranes all of the component lipids are amphipathic in nature and that phospholipids are a major class of membrane lipids. In general, phospholipids consist of a pair of long acyl chains and a compact polar headgroup composed of a phosphate moiety and the esterified alcohol. These amphipathic phospholipid molecules spontaneously assemble into multiple arrays of two-dimensional lamellar structure called liposomes in excess water. If the chain length difference between the *sn*-1 and *sn*-2 acyl chains of the phospholipid molecule is large, the asymmetric phospholipids in liposomes can be packed at $T < T_m$ into an interdigitated mode [for a review, see Huang and

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Mason (1986)]. Among the various detected interdigitated modes, the mixed interdigitation is perhaps most unique, since the acyl chains in the bilayer core are observed to exhibit interdigitations at temperatures both above and below T_m (McIntosh et al., 1984; Hui et al., 1984).

1-Stearoyl-2-caproyl-*sn*-glycero-3-phosphocholine, or C(18):C(10)PC, is the first asymmetric phospholipid species which has been shown by X-ray diffraction to self-assemble into lamellae with a mixed interdigitated packing mode at $T < T_m$ (McIntosh et al., 1984; Hui et al., 1984; Mattai et al., 1987). In this packing mode, the methyl terminus of the C(10) chain is packed end to end, at the bilayer center, with the methyl terminus of the C(10) chain from another lipid molecule in the opposing bilayer leaflet, while the longer C(18) chain from the two leaflets spans the entire hydrocarbon width of the bilayer. The mixed interdigitated gel bilayer is thus characterized by having the area per phospholipid molecule at the lipid/water interface encompass three acyl chains. moreover, C(18):C(10)PC molecules in the bilayer are also demonstrated to be packed in a partially interdigitated mode at $T > T_m$ (McIntosh et al., 1984; Hui et al., 1984; Mattai et al., 1987).

Although the general structural feature of the mixed interdigitated bilayer comprised of pure C(18):C(10)PC is now well-known (Huang & Mason, 1986), it is not clear whether the plane of the long C(18) chain zigzag carbon–carbon backbone in the bilayer core is perpendicular or parallel to the plane of the short C(10) chain zigzag carbon–carbon backbone. Moreover, the orientation of chain–plane between two adjacent molecules in the mixed interdigitated bilayer also remains to be determined. In this paper, we have continued our structural studies of C(18):C(10)PC lamellae. Specifically, we examined the effect of high pressure on the C(18):C(10)PC lamellae in D_2O by FT-infrared spectroscopy. Our spectroscopic studies on the barotropic behavior of C(18):C(10)PC provide additional information concerning the lipid structure and dynamics. In particular, the relative orientations of acyl chains for C(18):C(10)PC packed in the mixed interdigitated mode are now presented in this paper.

MATERIALS AND METHODS

The methods of preparation and purification for the C(18):C(10)PC lipid have been given in detail elsewhere (Xu & Huang, 1987; Mason et al., 1981). Lipid dispersions in 70 and 10 wt % D_2O were prepared for infrared spectroscopic experiments by heating the lipid/D_2O mixture in a closed vial to ~60 °C followed by vortexing. After immediate freezing of the samples in dry ice, the heat/votex/freeze cycle was then repeated twice. Homogeneous samples were then placed at room temperature, together with powdered α-quantz, in a 0.37 mm diameter hole on a 0.23 mm thick stainless steel gasket mounted on a diamond anvil cell as described previously (Siminovitch et al., 1987a,b; Wong et al., 1985; Wong & Mantsch, 1985).

Infrared spectra of the samples were measured on a Bomem Model DA 3.02 Fourier transform spectrophotometer with a liquid nitrogen cooled mercury–cadmium telluride detector. The infrared beam was condensed by a sodium chloride lens system onto the sample in the diamond anvil cell. For each spectrum 512 scans were coadded at a spectral resolution of 4 cm^{-1}. Data reduction was performed with software developed in this laboratory. Pressures were determined from the frequency shift of the 695-cm^{-1} infrared phonon band of α-quartz (Wong et al., 1985). The details for the pressure measurement have been given elsewhere (Siminovitch et al., 1987a,b; Wong et al., 1985; Wong & Mantsch, 1985).

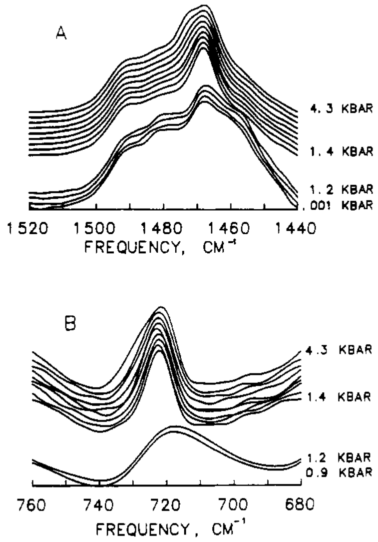

FIGURE 1: Stacked contour plot of infrared spectra of fully hydrated C(18):C(10)PC in the CH_2 bending region from 0.001 to 4.3 kbar (A) and in the CH_2 rocking region from 0.9 to 4.3 kbar (B). Pressure increment is 0.3–0.4 kbar.

RESULTS AND DISCUSSION

Infrared spectra of asymmetric mixed-chain C(18):C(10)PC bilayers in 70 and 10 wt % D_2O have been measured as a function of pressure up to 50.4 and 55 kbar, respectively. Dramatic changes in the infrared spectrum of fully hydrated (70 wt % D_2O) C(18):C(10)PC are induced by external pressures at 1.4 and 5.5 kbar. Considerable differences in the infrared spectra and their pressure profile between partially hydrated (10 wt % D_2O) and fully hydrated (70 wt % D_2O) C(18):C(10)PC are observed in the present work.

Liquid-Crystalline to Gel Phase Transition As Induced by External Pressure at 1.4 kbar. A series of stacked contours of infrared spectra for fully hydrated C(18):C(10)PC (70% D_2O) in the CH_2 scissoring region (1440–1520 cm^{-1}) and the CH_2 rocking region (680–760 cm^{-1}) are presented in panels A and B of Figure 1, respectively, as a function of external pressure. At low pressures (<1.4 kbar), a broad infrared band peaked at 1467 cm^{-1} is observed. This band corresponds to the CH_2 bending mode of the lipid methylene chain (δCH_2), and the shape of the broad feature is characteristic of the lipid methylene chain in the liquid-crystalline state (Siminovitch et al., 1987a). Also shown in Figure 1A at low pressures are the low-field shoulder at ~1455 cm^{-1} and the overlapping bands at 1470–1510 cm^{-1}. They correspond to the asymmetric CH_3 bending mode of the chain terminal methyl groups and the headgroup choline methyl groups, respectively. In contrast, the infrared spectrum of C(18):C(10)PC lamellae in the 1440–1520-cm^{-1} region is dramatically changed at 1.4 kbar. The δCH_2 band becomes much narrower; the CH_3 bending bands of both chain terminal methyl groups and headgroup choline methyl groups are much weaker (Figure 1A). These spectral features observed at 1.4 kbar are displayed typically by phospholipid lamellae in the gel phase (Siminovitch et al., 1987a,b; Wong & Mantsch, 1985). The results obtained in the spectral region of 1440–1520 cm^{-1} thus indicate that fully hydrated C(18):C(10)PC lamellae undergo a liquid-crystalline to gel phase transition as the external pressure reaches 1.4 kbar.

The spectral change in the CH_2 rocking mode region (680–760 cm^{-1}) at 1.4 kbar shown in Figure 1B is completely consistent with the results obtained from the CH_2 scissoring region (1440–1520 cm^{-1}). At low pressure (<1.4 kbar), the

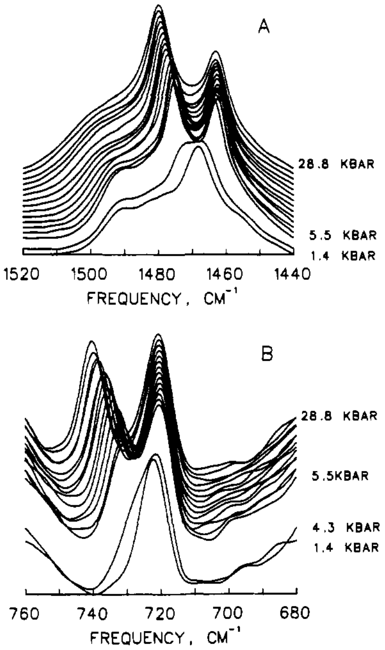

FIGURE 2: Stacked contour plot of infrared spectra of fully hydrated C(18):C(10)PC in the CH_2 bending region (A) and in the CH_2 rocking region (B) from 1.4 to 28.8 kbar. Pressure increment above 3.3 kbar is 1–1.7 kbar.

broad band peaked at ~718 cm^{-1}, corresponding to the CH_2 rocking mode of the methylene chain (γCH_2), is characteristic of the lipid acyl chain in the highly disordered liquid-crystalline phase (Siminovitch et al., 1987a,b). At 1.4 kbar, the γCH_2 band shifts discontinuously to a higher frequency of 722 cm^{-1} and becomes much narrower, a characteristic displayed by phospholipid lamellae in the gel phase. The results obtained in the 680–760-cm^{-1} spectral region thus indicate that a pressure-induced phase transition from the liquid-crystalline state to the gel state takes place at 1.4 kbar for fully hydrated C(18):C(10)PC lamellae.

Correlation Field Components of δCH_2 and γCH_2 Bands. When the acyl chains of phospholipids in the plans of the bilayer are orientationally highly restricted with close packing in an orthorhombic subcell lattice, their infrared spectra in the scissoring (δCH_2) and the rocking (γCH_2) regions give rise to characteristic splitting called correlation field splitting, resulting in two component bands (Wong et al., 1988). The barotropic behavior of the δCH_2 and γCH_2 bands of fully hydrated C(18):C(10)PC lamellae is depicted in Figures 1 and 2. No correlation field splitting of either the δCH_2 or the γCH_2 mode can be observed at pressures below 4 kbar. However, at 4.3 kbar, a correlation field component $\delta' CH_2$ at 1472 cm^{-1} begins to develop (Figure 1A). The magnitude of the component band increases with increasing pressure, and it becomes fully developed at 5.5 kbar (Figures 2A and 3A). Similarly, a well-resolved correlation field component for the γCH_2 band at ≈730 cm^{-1} is observed at 5.5 kbar (Figure 2B). These results thus indicate that in the pressure range of 1.4–5.5 kbar the orientational fluctuations of gel-state C(18):C(10)PC decrease with increasing pressure, and at 5.5 kbar the orientational fluctuations as well as the twisting and torsional motions of the zigzag planes of the acyl chains are completely damped, resulting in a highly ordered gel phase. Moreover, the fully developed correlation field splitting observed at 5.5 kbar implies that the acyl chains of fully hydrated C(18):C(10)PC at this high pressure are laterally packed in an orthorhombic subcell lattice in which the zigzag plane of the *sn*-1 acyl chain is nearly perpendicular to the zigzag plane of the *sn*-2 acyl chain within each molecule and between neighboring molecules.

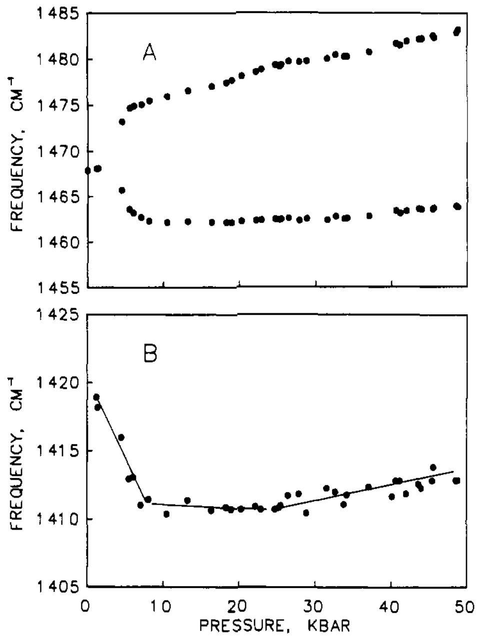

FIGURE 3: Pressure dependences of the frequencies of the δCH_2 mode of the acyl chains (A) and the δCH_2 mode of the αCH_2 groups (B).

Frequencies of the internal modes of molecules are usually observed to increase with increasing external pressure due to the pressure-enhanced intermolecular anharmonic interactions (Wong, 1987). On the other hand, a decrease in the frequency of the vibrational mode of a specific functional group in a molecule can occur with increasing external pressure (pressure-induced softening); such a decrease in frequency can be taken as evidence to indicate that the intermolecular interaction at this functional group is weakened by pressure as a result of pressure-induced structural deformation near the functional group. Figure 3B shows the pressure dependence of the CH_2 bending frequency of the αCH_2 groups which are the C(2) methylene units of the acyl chains. This frequency decreases considerably with increasing external pressure in the pressure range of 0.001–5.5 kbar. As discussed earlier, in this same pressure range the orientational ordering at C(18):C(10)PC is observed to increase with increasing pressure, and the pressure-induced ordering is completed at 5.5 kbar. Consequently, the pressure-induced softening of the αCH_2 bending mode in this pressure range can be taken as evidence to suggest that the orientational ordering process involves a structural yielding of the acyl chains near the interfacial region, which results in weaker interchain interactions among the neighboring αCH_2 groups as pressure increases.

Mixed Interdigitated Gel Phase in the Pressure Range up to 28.8 kbar. After the pressure-induced orientational ordering process is completed, a "valley" between the two correlation field component bands of the CH_2 scissoring (Figure 2A) or rocking (Figure 2B) modes becomes a prominent spectroscopic feature for the pressure-induced gel phase of fully hydrated C(18):C(10)PC. This pronounced "valley" is indicative of the interdigitated bilayer structure in the gel phase since it has also been observed in the interdigitated gel phases of 1-palmitoyl-*sn*-glycero-3-phosphocholine, 1,3-dipalmitoyl-*sn*-glycero-2-phosphocholine, and 1,2-di-*O*-hexadecyl-*sn*-glycero-3-phosphocholine after the orientational fluctuations of the chains in these gel phases are completely damped [Siminovitch et al. (1987b,c) and references cited therein]. Thus, the present infrared spectra confirm the presence of an

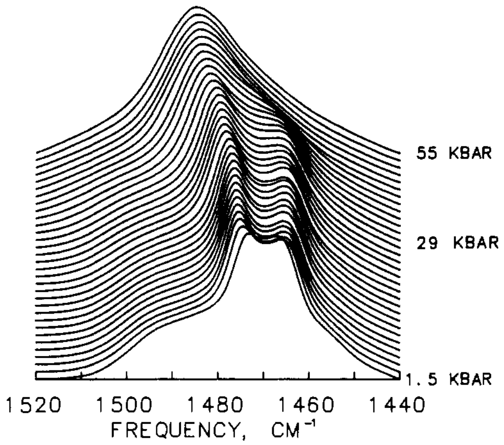

FIGURE 4: Stacked contour plot of infrared spectra of partially hydrated C(18):C(10)PC in the CH_2 bending regions from 1.5 to 55 kbar. Pressure increment is 1–2 kbar.

interdigitated bilayer structure in the gel phase of fully hydrated C(18):C(10)PC induced by an external pressure of 1.4 kbar. This interdigitated structure in the gel phase of fully hydrated C(18):C(10)PC has been characterized by earlier X-ray diffraction studies (Hui et al., 1984; McIntosh et al., 1984). The C(18):C(10)PC bilayer in the interdigitated gel state is called the mixed interdigitated bilayer in which the long C(18) acyl chain from opposing monolayers is interdigitated fully across the entire hydrocarbon width of the bilayer, while the short C(10) acyl chain of one lipid molecule packs end to end with the short C(10) acyl chain of another lipid molecule in the opposing bilayer leaflet.

The present results show that the mixed interdigitated structure is present not only in the temperature-induced gel phase but also in the pressure-induced gel phase. Moreover, in the plane of the mixed interdigitated gel phase, the neighboring zigzag planes of the acyl chains are intra- and intermolecularly near perpendicular to each other in the two-dimensional packing lattice.

Effects of Water on Interchain Structure. The infrared spectra of partially hydrated C(18):C(10)PC (in 10 wt % D_2O) in the δCH_2 region are plotted in Figure 4 as a function of pressure. These spectra and their pressure profile are comparable with those of fully hydrated symmetric diacylphosphatidylcholines (Siminovitch et al., 1987a,b; Wong & Mantsch, 1985) and differ considerably from those of the fully hydrated C(18):C(10)PC shown in Figure 2A. The pronounced "valley" between the correlation field component bands of δCH_2 observed in the fully hydrated C(18):C(10)PC and other interdigitated systems (Siminovitch et al., 1987a,c) is absent in the infrared spectra of partially hydrated C(18):C(10)PC (Figure 4). Moreover, the magnitude of the correlation field splitting of the partially hydrated sample is much smaller (Figure 4), and thus, correlation interactions are much weaker in this sample. Consequently, the mixed interdigitated bilayer structure detected in the fully hydrated C(18):C(10)PC (70% D_2O) is no longer present in the partially hydrated sample. This is consistent with the interchain structure of partially hydrated C(18):C(10)PC (<10% H_2O) based on the X-ray diffraction data (Tardieu et al., 1982; McIntosh et al., 1984). In this structure, the shorter decanoyl chains of C(18):C(10)PC molecules in one leaflet of the bilayer pack tail to tail with the longer stearoyl chains of C(18):C(10)PC molecules in the opposing leaflet to form dimers; this packing is now referred to as partially interdigitated gel structure (Huang & Mason, 1986). In each dimer, half of the long acyl chain orients parallel to the long chain of the neighboring molecule. Moreover, the perpendicular orientation between the acyl chains of neighboring dimers does not extend to the full bilayer width in this partially interdigitated packing (Huang & Mason, 1986). Consequently, correlation field interactions are weaker, and thus, the magnitude of correlation field splitting is smaller in this partially interdigitated C(18):C(10)PC.

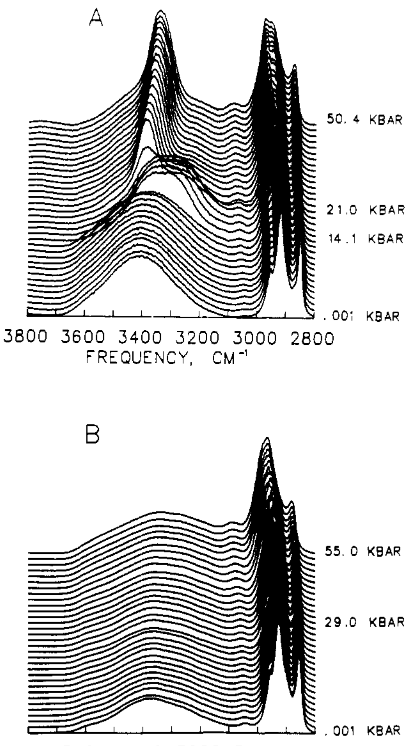

FIGURE 5: Stacked contour plot of infrared spectra of fully hydrated (A) and partially hydrated (B) C(18):C(10)PC in the frequency region 2800–3800 cm^{-1}. Pressure increment is 1–1.7 kbar for (A) and 1–2 kbar for (B).

Water transforms into ice VI and ice VII at 12–14 and 21 kbar, respectively (Wong & Moffatt, 1987). The uncoupled OH stretching infrared band of water near 3400 cm^{-1} is extremely broad. It shifts to lower frequency and becomes a broad doublet in ice VI and becomes very sharp in ice VII (Wong & Moffatt, 1987). Figure 5A shows the pressure effects on the infrared spectrum of fully hydrated C(18):C(10)PC in the frequency region 2800–3800 cm^{-1}. The bands in the frequency region 2800–3000 cm^{-1} are due to the CH stretching modes of the lipid molecules, and the bands near 3400 cm^{-1} are due to the uncoupled OH stretching mode, νOH. As seen in Figure 5A, the broad νOH band of water changes to that of ice VI at 14 kbar and to that of ice VII at 21 kbar. Therefore, the excess water in fully hydrated C(18):C(10)PC exhibits the same characteristics as free water, which transfers into ice VI and ice VII at 14 and 21 kbar, respectively. It is interesting to note that in fully hydrated C(18):C(10)PC the phase transitions of the excess water do not affect the interchain structure of the lipid molecules as evident from the absence of spectral changes in the infrared spectrum of the lipid vibrational modes at the critical pressures of water/ice VI and ice VI/ice VII transitions (Figures 2, 3, and 5A).

Figure 5B shows the pressure effects on the infrared spectrum of the νOH band of the partially hydrated C(18):C(10)PC (10 wt % D_2O). The νOH band in this sample appears as a broad band in the pressure range from 0.001 to 55 kbar. No significant change in the νOH band is observed at the critical pressures of the pressure-induced transitions among water, ice VI, and ice VII. These results indicate that all the water molecules in this partially hydrated sample are bound to lipid molecules and the bound water molecules do not take part in the pressure-induced phase transitions from water to ice VI and ice VII. The νOH band of the bound water is also observed in the infrared spectra of fully hydrated sample (Figure 5A), especially at pressures above 21 kbar where the sharp ice VII νOH band is on top of the broad νOH band of bound water (Figure 5A).

In the mixed interdigitated gel bilayers of the fully hydrated C(18):C(10)PC, each choline headgroup encompasses three acyl chains, in contrast to two for the partially interdigitated gel bilayers in 10 wt % D_2O. Consequently, without excess water to fill up the space betweens neighboring headgroups, voids are present in the headgroup region in the mixed interdigitated structure, and thus, this structure becomes unstable. Therefore, in partially hydrated C(18):C(10)PC, the mixed interdigitated structure does not exist due to the lack of excess water in this system.

CONCLUSIONS

The following conclusions can be drawn from the results of the present high-pressure infrared spectroscopic investigation.

(1) A phase transition from the liquid-crystalline phase to the gel phase in fully hydrated C(18):C(10)PC lamellae is induced by external pressure at 1.4 kbar and room temperature.

(2) In the liquid-crystalline phase of fully hydrated C(18):C(10)PC lamellae, the conformation of the acyl chains is highly disordered due to the presence of a large number of gauche bonds on the acyl chains. Moreover, the orientations of the acyl chains as well as the lipid molecules along the chain axis are also highly disordered due to large-angle reorientational fluctuations of the molecules and twisting and torsion motions of the acyl chains.

(3) In the gel phase above 1.4 kbar, the conformation of the acyl chains becomes more ordered, and the acyl chains are nearly fully extended. However, in this gel sphase the orientations of the acyl chains and the lipid molecules are still quite disordered until the pressure reaches 5.5 kbar, where reorientational fluctuations of the lipid molecules and twisting and torsion motions of the acyl chains are completely damped by external pressure. During the orientational ordering process in the pressure range 1.4–5.5 kbar, a structural yielding of the acyl chains near the interface region takes place.

(4) High-pressure infrared spectroscopic investigation in the present work confirms the presence of the interdigitated interchain structure in the gel phase of fully hydrated C(18):C(10)PC in the pressure range up to 28.8 kbar. The orientations of neighboring acyl chains between the long and the short acyl chains within each interdigitated lipid pair as well as between the long acyl chains of neighboring interdigitated lipid pairs are nearly perpendicular to each other.

(5) One of the criteria for the formation of the mixed interdigitated bilayer structure in C(18):C(10)PC is the presence of excess water. The function of this excess water for the stabilization of the mixed interdigitation is to occupy the space between neighboring headgroups. Without excess water, the mixed interdigitated structure becomes unstable, and the interchain packing changes to that of the partial interdigitation in which each headgroup encompasses only two acyl chains, and thus, the area of the headgroup is comparable with the cross-sectional area of the sum of two acyl chains without voids in the headgroup region.

(6) In fully hydrated C(18):C(10)PC, the behavior of excess water is similar to that of pure water which undergoes a series of pressure-induced phase transitions from water to ice VI and ice VII. On the other hand, bound water molecules do not take part in these pressure-induced phase transitions.

(7) Although the presence of excess water is required to form the mixed interdigitated structure in C(18):C(10)PC, the pressure-induced phase transitions of the excess water exhibit an insignificant effect on the mixed interdigitated packing of the C(18):C(10)PC lamellae.

Registry No. C(18):C(10)PC, 78119-50-3; D_2, 7782-39-0.

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