Motional narrowing of the ₂H NMR spectra near the chain melting transition of phospholipids/D₂O mixtures

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Abstract. The reduction in spectral splitting, or motional narrowing, of the deuterium spectra of D_2O /phospholipid mixtures near the main chain melting phase transition was studied for palmitoyloleoylphosphatidyl-choline (POPC), palmitoyloleoylphosphatidylethanolamine (POPE) and equimolar mixtures of the two at 10% hydration. For POPC the splitting was about 1700 Hz in both the fluid and gel phases, dropping to zero near the phase transition (as reported previously). For POPE the splitting remained approximately constant above the phase transition. Below the phase transition the spectrum showed a single broad line whose linewidth varied between 100 Hz and 800 Hz. This was interpreted as being due to small domains of water within a weakly hydrated crystal. POPC:POPE (1:1) samples exhibited motional narrowing behaviour similar to that for POPC except that the splitting above the phase transition was approximately twice that below the transition. The relatively broad temperature range (~20 K) of the transition is explained using a simple physical model involving lipid fluctuations near the phase transition.

Key words. $_{2}$ H NMR – D $_{2}$ O – Motional narrowing – Gel-fluid phase transition – Phospholipids – Low hydration