

surfactant and lipid systems. The basis of the power of these techniques is that only the nuclei, which are at resonance, will be directly observed. This allows observation of selected parts and facets of the system, usually by making use of the constituent nuclei of the components (i.e., no perturbation of the system by incorporated foreign "probe" molecules). Substitution of protons by deuterium atoms either in the aqueous fraction or in the lipid component has relatively minor and predictable effects on the system's behavior and has been used to great advantage (5-18) in the investigation of bilayer phases formed by lipids and surfactants in the presence of water.

Unlike the more commonly encountered hydrogen (^1H) and carbon (^{13}C) nuclei, the deuterium (^2H) nucleus has a spin quantum number, $I = 1$, with an associated quadrupolar moment. This means that there are three nondegenerate nuclear spin energy levels (Fig. 2). In an isotropic environment in which the effects of electric field gradients at the nucleus are averaged to zero, a single resonance is observed. The presence of electrical field gradients in an axially symmetric field, however, leads to changes in the spin energy levels (see Fig. 2), which leaves the $m = 0 \rightarrow +1$ and $m = -1 \rightarrow 0$ transitions with different energies. This has the effect of producing two absorption peaks at resonance separated by a frequency difference $\Delta\nu$, the size of which depends on the size of the interaction with the electrical field gradient as

$$\Delta\nu = 3/4 \chi (3\cos^2\theta - 1) \quad [1]$$

where χ is the quadrupolar coupling constant that has a value of 167 kHz for deuterium attached to carbon (19) and θ is the angle between the principal axis, being the vector of the C-D bond and the magnetic field. The case of the nucleus interacting with a field gradient of axial symmetry has been shown to be applicable to those normally studied in lamellar surfactant and lipid systems.

In molecules containing several deuterium atoms, a doublet splitting will be observed for each atom, reflecting the degree of dynamic freedom that atom has in the molecule. Assignment of splittings to particular deuterium atoms in a molecule must be done by observation of selectively deuterated molecules. Deuterium NMR may, therefore, be used to probe the dynamic structure of the chains, as a function of position, composition of phase, and temperature. An *order profile* of the lipid chains, defined by the order parameter, S_{CD} , can be derived from the quadrupolar splittings (Eq. 2) of the ^2H nuclei in the different segments.

$$\Delta\nu = 3/4 \chi |S_{\text{CD}}| \quad [2a]$$