

SOCIETA' ITALIANA
DI BIOFISICA
PURA E APPLICATA

SIBPA

GRUPPO NAZIONALE
DI CIBERNETICA E
DI BIOFISICA, CNR

GNCB

Camogli 6 - 8 Ottobre 1983

ATTI

VI Congresso SIBPA-VII Congresso GNCB

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A cura di F. Conti e S. Vallerga

A STUDY ON THE PHASE DIAGRAMS OF TWO-COMPONENT PHOSPHOLIPID BILAYERS; PHOSPHATIDYLCHOLINE (PC)/ PHOSPHATIDYLETHANOLAMINE (PE) MIXTURES.

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Abstract - To calculate the phase diagrams of PC/PE mixtures, a generalization of the Priest (1) phenomenological model has been used. A new excess free energy term in the state function has been proposed to consider the two-component phospholipid bilayers where both the chain lengths and the polar heads of the components can be different.

With this proposed state function, the phase diagrams of different experimentally studied PC/PE mixtures have been constructed. Complete miscibility was obtained when the components had the same chain length. $L_E > L_C$ gave a peritectic system while for $L_E < L_C$ an eutectic system was originated.

Experimental data from different sources were compared to the theoretical calculations.

Introduction - The lipid composition of biological membranes is complex. This could be connected with the necessity to provide the correct micro-environment for the membrane-bound proteins.

At the moment little is known about the physiological meaning of the different head groups of the phospholipids and their mixing behaviour.

Considering that the phase properties and the function of the lipid membranes are directly related, we have developed a model to study the phase transition properties of a two-component system where both the chain length and the polar heads of the components can be different. Based on Landau phenomenological theory (2) of phase transition, a simple model for binary mixtures of lecithin (PC) homologues, when the lipid components have the same head

group but the chain lengths are different, has been developed by Priest (1). The model contains only two parameters which can be fitted independently.

Starting from this model we have determined the parameters for one component bilayers of PE homologues and taking into consideration the hydrogen bondings between the polar heads of PE molecules, a new excess free energy term in the state function of binary mixtures was constructed.

Theory - The free energy function of PC/PE binary mixtures has been considered similar to that of two-component lecithin bilayers (eq. 18, Ref. 1). Thus,

$$\begin{aligned} \frac{G(X_E, S)}{2RT} = & X_E \frac{F_E(S)}{RT} + (1-X_E) \frac{F_C(S)}{RT} + \\ & + \frac{1}{2} X_E \ln X_E + \frac{1}{2} (1-X_E) \ln(1-X_E) + \\ & + \Delta U \cdot X_E + \frac{(\sigma |\Delta L| + \gamma)}{RT} \left(\frac{1}{2} - S \right) X_E \cdot \\ & \cdot (1 - X_E) \end{aligned} \quad - 1 -$$

where $\Delta L = L_E - L_C$ and X_E is the mole fraction of PE component. The first two terms represent the free energy functions of one-component PE and PC bilayers respectively (3) while the third and fourth terms are the entropy of mixing. The difference in chemical potential (ΔU) between the two components of the mixture is also considered and the last term account for the experimental fact that PC/PE mixtures of same length components are not ideal ones, i.e. the excess free energy does not vanish when $\Delta L = 0$.

As it has been previously shown (3), the excess free energy reflects the difference of the nearest neighbour interaction energies between the same and different components.

