Computer Simulations of the Electric Interactions between the Phospholipid Head-Groups and Ionic Admixtures in the Membrane Surface

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Some phospholipids (e.g. lecithin) form a system of electric dipoles on the membrane surface layer. In the case of lecithin the positive dipole charge is located on the choline and the negative one on the phosphoric molecule group. These dipoles are arranged almost parallel to the membrane surface. Taking the dipole membrane structure as a base for further investigations, a computer model of the electrostatic interaction between the dipole system and the ionic admixture was investigated. The model presumes hexagonal centered or a rectangular flat geometry of the 121 dipoles distribution. The dipoles may rotate freely around round the motionless symmetry axis perpendicular to the system surface. The initial state is given by fixing the geometry of the dipole matrix and ionic admixture distribution. Subsequently this system underwent a computer simulation which consisted of a calculation of resultant force moments acting on each dipole caused by other dipoles and ions. These force moments lead the system to the equilibrium state (minimum of the binding energy). The minimum energy value of the dipoles system depends on concentration and charge of the admixtured ions. The results of repeated simulations indicate that the system achieve the least of all binding energy (the most stable equilibrium state) at 1.5% concentration of admixtured ions in case of ion charge equal to 1Q (where Q denotes arbitrary unit of ion charge) and at 2.5% concentration of admixtured ions in case of ion charge equal to 2Q. The calculated results are in a good agreement with the experimental.