DPPC bilayer thickness and surface area in unilamellar liposomes: SANS results obtained by contrast variation

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Unilamellar liposomes from DPPC (1,2-dipalmitoylphosphatidylcholine) and perdeuterated DPPC-D62 in aqueous dispersions (1 wt. % of lipid) were prepared by extrusion through two filters with 500 Å pores.Their small-angle neutron scattering (SANS) curves at three different ^2H_2O molar fractions in H_2O (1.0; 0.7 and 0.5) were measured on the YuMO spectrometer in the region of scattering vector $q \hat{I} <0.006;0.383> Å^{-1}$. All six SANS curves were fitted simultaneously by Minuit using the following model: The bilayer was divided into 5 parts: the central region consisting of CH_3 groups of lipid acyl chains, two regions containing the rests of acyl chains and two polar regions containing the polar headgroups. The coherent neutron scattering length density ρ was homogeneous within each region. Besides the lipid, the bilayer contained N_L water molecules per lipid in the polar region, the value of ρ of this water increased linearly up to the bilayer – aqueous phase interface. The liposomes were supposed to be polydisperse hollow spheres with the inner R_i and outer R_o radii; R_o-R_i=d_L is the bilayer thickness, R_{mean} the mean liposome radius and σ_R the dispersion of Gaussian distribution of radii. The YuMO resolution function was taken into account by the Gaussian distribution in q. Using the known water and DPPC molecular component volumes in the bilayer, the following values were obtained at 50°C: d_L=48.56 Å, polar region thickness d_P=9.4 Å, lipid surface area A_L=61.31 Å^2 and N_L=8.50. The (R_{mean}±σ_R) values varied between 287.5±99.9 Å and 336.5±136.1 Å, except of 265.9±246.3 for DPPC-D62 in 70 % ^2H_2O.