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Mobility of molecules and diagram of the state of a glyceryl monooleate-water system according to NMR data

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Abstract

Transverse relaxation and self-diffusion of molecules in a glyceryl monooleate (monoolein)-D2O system was studied using pulsed 1H NMR in a range of water concentrations from 10 to 30 wt % and a range of temperatures from 20 to 90°C. It was noted that self-diffusion is described by one or two self-diffusion coefficients, depending on the temperature and concentration of water, while NMR-relaxation has a complex form. It was determined that with a reduction in the transverse magnetization, a component that has a form similar to Gaussian and relaxation times of 70 to 250 j, s is observed at certain temperatures and concentrations of water, confirming the formation of structures in which glyceryl monooleate molecules (GM) are characterized by anisotropic rotational mobility. It was demonstrated that the ranges of the concentrations of water and temperature in which this component is observed correspond to liquid-crystalline phase for lamellar and inverse hexagonal structural organizations of lipids, according to the state diagram obtained by X-ray diffraction. In the state diagram areas corresponding to micellar and cubic structures (characterized by the isotropic rotation of GM molecules in the time scale of NMR), multiexponential decays of magnetization with average relaxation times were noted in the range of 10 to 200 ms. A number of features were discovered with the use of NMR: specimens always contain structures with isotropic rotational mobility in the presence of structures characterized by anisotropic rotational mobility; a change in the fraction of the structures with anisotropic rotational mobility takes place slowly over 5-15 K, not abruptly. Our conclusions regarding the polymorphism of a GM-D2O system in the presence of anisotropic structures was confirmed by an analysis of the transverse NMR relaxation in an egg phosphatidylcholine-D2O system, for which the presence of only lamellar liquid-crystalline structure is confirmed by 31P NMR. © Pleiades Publishing, Ltd., 2011.

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Keywords

Glyceryl monooleate, H NMR study, Magnetization, Self-diffusion, State diagram, Transverse relaxation