

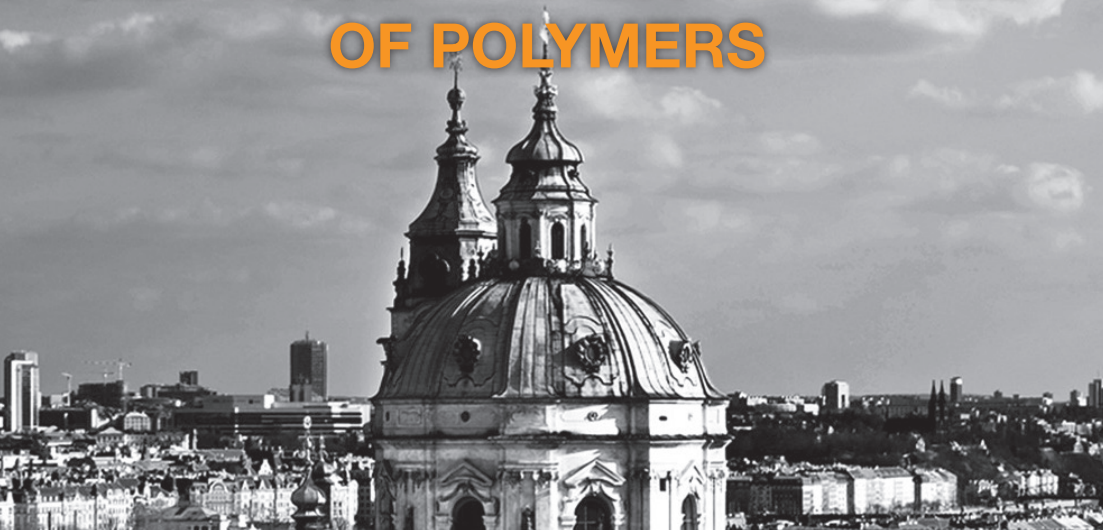
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SELF-ASSEMBLY IN THE WORLD OF POLYMERS



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PRAGUE MEETING
ON MACROMOLECULES

BOOK OF ABSTRACTS AND PROGRAMME

SELF-ORGANIZATION PROCESSES IN LECITHIN-BILE SALT MIXTURES: COMPUTER SIMULATIONA. Markina^a, V. Ivanov^a, P. Komarov^b, A. Khokhlov^a, S.-H. Tung^c^a*Moscow State University, Moscow, Russian Federation*^b*Institute of Organoelement Compounds RAS, Moscow, Russian Federation*^c*National Taiwan University, Taipei, Taiwan*

Problems of self-organization of biological surfactants have attracted increasing interest due to a wide range of practical applications. There are two main classes of surfactants: phospholipids and bile salts. Phospholipids, zwitterionic surfactants, typically form a bilayer or vesicles in aqua solutions and reverse micelles in organic solvents, such as hexane or cyclohexane, for example. Bile acids are also amphiphilic molecules, their main feature is facial morphology with polar and nonpolar surfaces [1].

We have performed computer simulation of three-component systems consisting of lecithin, bile salt and solvent, which may be water or an organic solvent, and studied the structure of molecular aggregates. We found that formation of "worm-like" micelles is observed in hexane- lecithin solution with increasing bile salt concentration (Fig. 1). Addition of bile salts into the aqueous lecithin solution also induces formation of elongated structures with ellipsoidal or cylindrical shape. Aggregates morphology in lecithin - bile salts mixture could be affected by inorganic salt. We believe that the formation of long flexible worm-like micelles can be the reason for the experimentally observed viscosity increase.

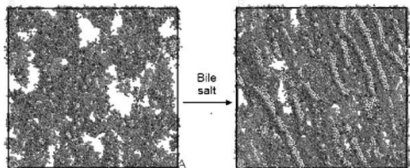


Fig.1. Structures formed in the hexane - lecithin solution by increasing bile salt concentration.

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