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ENCAPSULATION OF SMALL ORGANIC MOLECULES IN SUPRAMOLECULAR ASSEMBLIES OF MELAMINE BARBITURATE

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Abstract. Supramolecular organic assemblies are promising systems for the encapsulation of small organic and drug-like molecules. In this work, we have shown the possibility of the inclusion of Rhodamine 6G moiety in the melamine barbiturate supramolecular structure and provided some insights into the process of early stages of melamine barbiturate supramolecular assemblies formation.

Dye molecules (such as fluorescein, rhodamine 6G, Congo red, etc.) are used as drugs-like substances. It was shown previously that melamine barbiturates are capable of forming the highly ordered supramolecular assemblies that can encapsulate some amount of small organic molecules (like dyes). Therefore, the relevance of this work lies in the creation of systems capable of encapsulating drugs and their use in the targeted delivery of drugs.

This study aims to investigate the processes of encapsulation of rhodamine 6G dye in the supramolecular structures of melamine barbiturate: at the early stages of nucleation and during crystal growth in aqueous solutions. Thus, the objectives of the study are to simulate solutions of melamine barbiturate with dyes with different concentrations and ratios of substances (including cases of a supersaturated solution) by the methods of Molecular Dynamics, as well as to consider the thermodynamics of self-assembly processes of melamine barbiturate with rhodamine 6G dye utilizing methods of quantum chemistry.

In the course of the work, the methods of computational chemistry were used: classical molecular dynamics and quantum chemistry. The method of classical molecular dynamics was used to obtain data on the nucleation process of supramolecular assemblies of melamine and barbituric acid with the inclusion of the rhodamine 6G, quantum mechanical methods were used to consider the benefits of the formation of supramolecular systems of melamine and barbituric acid with the rhodamine 6G.

It was shown that rhodamine 6G is included in the supramolecular assemblies of melamine barbiturate. In the process of nucleus formation, the assemblies of melamine and barbituric acid with themselves, as well as melamine-barbituric acid dimers were observed. Associates of barbituric acid with itself were formed mainly in layers, but melamine-melamine and melamine-barbituric acid dimers were forming mostly planar structures. Moreover, both methods showed that rhodamine 6G is slightly better associated with barbituric acid than with melamine. Also, it was shown that dye moiety serves as a nucleation centre. The results of this work will make it possible in the future to obtain the most effective supramolecular systems capable of encapsulating small organic molecules and drug-like substances.

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