UDK 548.523

MELAMINE CYANURATE PHASE SHIFTS AS A FUNCTION OF LOCAL CONCENTRATION

Timralieva A.A. (ITMO University), Nesterov P.V. (ITMO University), Shilovskikh V.V. (ITMO University), Nebalueva A.S. (ITMO University)

Scientific Supervisor- Prof. Dr. Skorb E.V.

(ITMO University)

Abstract. There is a new trend in the drug delivery area that leads to the supramolecular assemblies application as a "capsule shell". X-Ray diffraction study of melamine cyanurate assembly shows the high sensitivity of the structure to the local concentrations of individual compounds that confirm the possibility of active molecules incapsulation into melamine cyanurate structure.

Nowadays there several challenges in the drug delivery area. One of the most important requirements to modern methods of drug delivery is reversive encapsulation of an active molecular into a "shell". The capsule should be harmless for the human body, controlled-damaged and at the same moment stable till the active molecules come to the set point. One supposed to use supramolecular assemblies as the "shells" for drug delivery according to their structural characteristics.

Melamine cyanurate is one of the most wide-spread supramolecular assemblies. Molecules of cyanuric acid and melamine are linked by hydrogen bonding into rosettes. The energy of hydrogen bonding is relatively low, and the structure forming of melamine cyanurate does not require any individual molecules changing. Melamine cyanurate rosettes based on distributed hydrogen bonding are also packed into two-dimensional layers. These layers are linked by hydrophobic bonding.

According to X-Ray diffraction (XRD) analysis, it was observed that the crystallinity of the melamine cyanurate assembly is dependant on the local concentration of components. The calculated crystallinity of melamine cyanurate is in a range from 52% to 84%. The crystallinity of the melamine cyanurate highly depends on the synthetic method and the intensity of the compounds mixing.

In the case of highly intensive mixing and the equidistribution of compounds in the synthetic cell, the local concentrations of individual compounds can be under almost total control. In the research different ratio of melamine and cyanuric acid were varied.

The well-known structure of melamine cyanurate provided to compare obtained XRD data from different powder sets with literature datum. The most intensive and stable for every powder set peak is on 28° that relates to lattice space. One of the reflexes is also stable as it defines the plane that appeared according to the hydrogen bonding between individual molecules. Compounds ratio far from 1:1 shows the disappearing of several reflections that confirm relative lattice slip.

The high sensitivity of melamine cyanurate to the ratio of individual compounds may lead to local orientant doping. Currently, it is supposed to use some dyes molecules as these orientants that also leads to the incapsulation of and bioactive molecules.

Timralieva A.A.	Signature
Skorb E.V.	Signature