

**DIFFERENT STATES OF WATER
IN α -, β -, AND γ -CYCLODEXTRIN HYDRATES**

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α -, β - and γ -cyclodextrins (CDs) are unique macromolecules that have a hydrophobic inner cavity and a hydrophilic outer surface. They are so-called molecular containers that are able to hold the molecules of the "guest" substance in their inner cavity forming inclusion complexes with a variety of organic and inorganic molecules or fragments of molecules. Cyclodextrins in the complex protect the "guest" molecule from damage by various reactive molecules and this contributes to their wide application in the pharmaceutical industry to increase the solubility of substrates and create long-acting drugs; in the food industry to stabilize low-stable molecules and protect the "guest" molecules from oxidation, steric rearrangements, hydrolysis, racemization and enzymatic degradation. The solid phase of cyclodextrins is almost always a hydrate, and therefore the formation of inclusion complexes is a process of complete or partial replacement of water molecules in CDs hydrates with guest molecules. Thus, quantitative thermodynamic characteristics of dehydration processes ($\Delta_{\text{deh}}H^\circ$, $\Delta_{\text{deh}}S^\circ$, $\Delta_{\text{deh}}G^\circ$), which are practically absent in the literature by now, are very relevant for obtaining a variety of CDs inclusion complexes.

A new approach to the study of dehydration processes is proposed, which is mainly performed in closed volume by a static method with a membrane-gauge manometers [1], which previously showed its promise in the study of supramolecular compounds [2]. The $p_{\text{H}_2\text{O}}-T-x$ (molar fraction of water in CD hydrate) dependences obtained under equilibrium conditions provide information about the available phase transitions and the composition of the phases involved in them. The thermodynamic characteristics of the dehydration processes calculated from the experimental data will be used to quantify the binding energies of water molecules with the CD-framework.

As a result of this work, general patterns and specific differences in the chemical bonds of water with the frameworks of α -, β - and γ -cyclodextrins were revealed, which is valuable information for the targeted synthesis of new materials.

1. Davydova E.I., Sevastianova T.N., Suvorov A.V., Timoshkin A.Y. // *Coord. Chem. Rev.* 2010. V. 254. P. 2031–2077. <https://doi.org/10.1016/j.ccr.2010.04.001>

2. Zelenina L.N., Chusova T.P., Sapchenko S.A., Gelfond N.V. // *Russian Journal of Inorganic Chemistry.* 2023. V. 68. P. 174-180. <https://doi.org/10.1134/S0036023622602343>

This work was supported by Russian Science Foundation (grant № 24-23-00237).