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Structure of complexes of poly-γ-benzyl-L-glutamate with water and dioxane molecules studied by IR spectroscopy and quantum chemical calculations

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Abstract

© 2014 Pleiades Publishing, Ltd. The structure of supramolecular complexes of poly-γ-benzy--L-glutamate (PBG) with water and dioxane molecules during sorption from pure liquids and their binary mixtures is studied by IR spectroscopy and quantum chemical calculations. It is shown that the sorption sites of water and dioxane in PBG are different in nature. Water molecules are bound in the monomeric form to the carbonyl groups of the ester moieties of the side chains and the helical backbone of the peptide to form complexes with two hydrogen bonds. Dioxane molecules are sorbed in a large amount in the region of the side chains of PBG, causing their repacking with preservation of the helicity of the polypeptide backbone. Under simultaneous sorption of water and dioxane vapors, the binding of the latter increases the number of water molecules bound to the carbonyl groups of PBG. In this case, there is also an additional absorption of water molecules on the oxygen atoms of dioxane molecules. Calculations have shown that in the most probable configuration of the complexes, the water molecule simultaneously forms hydrogen bonds with the carbonyl groups of the side chain and the peptide backbone. Dioxane molecules do not penetrate to the peptide groups of helical backbone of PBG due to steric hindrance and are localized in the region of the benzyl moieties of the side chains; such complexes are stabilized by weak CH...O interactions.

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Keywords

14-dioxane, DFT, hydration, IR spectroscopy, poly-γ-benzyl-L-glutamate