Abstract

Title: Fast Dynamic Processes in Solution Studied by NMR Spectroscopy

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Abstract: Nuclear magnetic resonance (NMR) spectroscopy is capable to deliver a detailed information about the dynamics on molecular level in a wide range of time scales, especially if accompanied by suitably chosen theoretical tools. In this work, we employed a set of high-resolution NMR techniques to investigate dynamics processes in several weakly interacting molecular systems in solution.

Van der Waals interactions play an important role in inclusion complexes of cryptophane-C with chloroform or dichloromethane. The complex formation was thoroughly investigated by means of ^{1}H and ^{13}C NMR experiments along with the quantum-chemical density functional theory (DFT) calculations. We characterized kinetics, thermodynamics, as well as fine details of structural rearrangements of the complex formation.

Internal dynamics of oligo- and polysaccharides presents a considerable challenge due to possible coupling of internal and global molecular motions. Two small oligosaccharides were investigated as test cases for a newly developed integrated approach for interpreting the dynamics of the molecules with non-trivial internal flexibility. The approach comprised advanced theoretical tools, including stochastic modeling, molecular dynamics (MD) simulations, and hydrodynamic simulations.

A biologically important bacterial O-antigenic polysaccharide from *E. Coli* O91 was addressed employing selective isotope labeling and multiple-field ^{13}C relaxation experiments. The complex dynamics of the polysaccharide is characterized by the conformational motion of the exocyclic groups of the sugars, superimposed to the breathing motion of the polymeric chain.

Hydrogen bonding is another major non-covalent interaction. Dilute solutions of ethanol were chosen as a model of liquid systems containing extensive hydrogen-bonded networks. We developed a new methodology consisting of NMR diffusion measurements, DFT calculations, and hydrodynamic modeling and utilized it to determine average size of the molecular clusters of ethanol at given conditions.

Keywords: Nuclear magnetic resonance, Dynamics, Ethanol, Cryptophanes, Saccharides