Title: Dynamics of hydrogen bonded networks viewed by NMR spectroscopy

Author: Petr Dvořák

Department: Department of Low Temperature Physics

Supervisor: doc. RNDr. Jan Lang, Ph.D., Department of Low Temperature Physics

Abstract:

This work describes especially experimental studies of dynamic processes in common polar solvents such as water and ethanol. The nuclear magnetic resonance (NMR) technique was used - primarily measurements of NMR relaxations and measurements of self-diffusion coefficients using NMR. Three main topics were addressed. The first one deals with chemical exchange in mixtures of light and heavy water. Within this topic, a methodology for the preparation of ultra-pure samples was developed and a suitable method for suppressing radiation damping was proposed. Then the final samples were prepared, and the relaxation data were measured. Three models of chemical exchange were discussed. The second topic deals with correction of the Stokes-Einstein relation so that it can also be used for determination hydrodynamic radii of small molecules and clusters. This correction was made by comparing the measured diffusion coefficients of the model molecules with the calculated diffusion coefficients using hydrodynamic simulations. The third topic deals with the relaxivity of magnetic nanoparticles. New potential contrast agents for magnetic resonance imaging based on iron oxide nanoparticles were studied.

Keywords: NMR, relaxation, chemical exchange, water, diffusion