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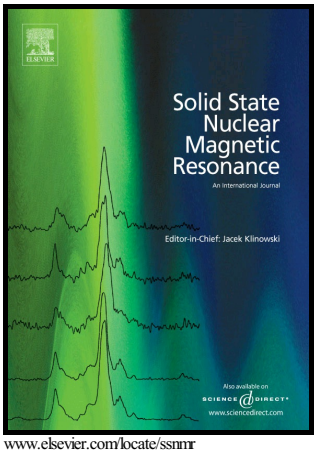

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^{1}H NMR Study of Water Molecules Confined in Nanochannels of Mordenite. Dedicated to the memory of Professor S. P. Gabuda (1936-2015)

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Abstract

Behavior of water molecules entrapped in nanochannels of zeolite mordenite has been investigated by ^{1}H NMR technique. The ^{1}H spectra and spin-lattice relaxation times in the laboratory and rotating frames, T_1 and $T_{1\rho}$, respectively, as well as the dipolar relaxation time T_{1D} have been measured in the temperature range from 96 to 351 K. Diffusion of water molecules along the channels was observed above ~ 200 K. While in bulk liquid the dipolar ordered state of nuclear spins is not formed owing to complete motional average of dipolar interactions, we show that such a state is observed for mobile molecules confined in a restricted geometry. At temperatures below ~140 K the relaxation was found to be mainly caused by interaction of ^{1}H nuclear spins with paramagnetic impurities. Complete lost of the fine structure of ^{1}H spectra above ~320 K is presumably caused by proton exchange. We show that the dipolar relaxation in mordenite is responsive to slow 180^0 reorientations of water molecules. The correlation times of nuclear and electron spin fluctuations were determined.

Keywords: Nanochannels, mordenite, NMR, relaxation, dipolar ordered state, molecular mobility.

1. Introduction

Physical properties of materials entrapped in nanosized cavities are of significant interest for both fundamental science and applications of nanoporous compounds. A variety of techniques is used to investigate the properties of such nanomaterials. One of them is nuclear