Abstract

Investigation of the structure and dynamics of natrolite by using nuclear magnetic resonance methods

Mateusz Wojciech Paczwa

Department of Solid State Physics, Institute of Physics, Faculty of Mathematics and Physics, University of Szczecin, Wielkopolska 15, 70 - 451 Szczecin

The PhD thesis presents results of structure investigation of natural zeolites based on natrolite and internal dynamic water molecules and sodium cations which are located in channels. All research has been conducted by using nuclear magnetic resonance methods (NMR - Nuclear Magnetic Resonance).

The first chapter consists of the theoretical part and is dedicated to a description of zeolites - structure, ways of classification, microporous properties and their application. Zeolites are a distinct group of minerals from a aluminosilicate family and constitute one of the most important groups of microporous materials. Zeolites are crystalline solids materials with regular microporous structure that is made of three-dimensional framework with silicon and alumina tetrahedrons with cavities and channels inside where cations and water molecules may reside. This microporous structures have very interesting physical and chemical properties like ion exchange, catalysis, adsorption and separation.

The second, third and fourth chapter constitute the main point of the thesis and concern the analysis and an interpretation of experimental results of a study of the natrolite by using NMR spectroscopy methods. The paper focuses on the natrolite ($Na_2Al_2Si_3O_{10}\cdot 2H_2O$), that has the smallest size of channels compared to other well known zeolites. Furthermore an important feature of natrolite, because of its practical application, is that as a natural mineral it can be relatively easy to obtain and modify. The experimental part will present experimental absorption NMR spectra of ^{1}H, ^{23}Na, ^{27}Al, ^{29}Si nuclei in case of static samples and experimental absorption MAS NMR spectra of ^{1}H, ^{23}Na, ^{27}Al, ^{29}Si nuclei for spinning samples at the magic angle ($54{,}74^{\circ}$) with respect to the direction of the magnetic field (Magic

Angle Spinning spectroscopy) for rotating frequencies in a wide range of temperatures from 180 K to 400 K; temperature dependence of spin - lattice relaxation times of ^{1}H, ^{23}Na, ^{27}Al nuclei in a laboratory T_1 and a rotating $T_{1\rho}$ reference system and temperature dependence of dipole relaxation times T_{1D} of ^{1}H nuclei. The following NMR spectroscopy methods were used: solid - echo method, decoupling and without decoupling method, spin - locking method and etc.

A theoretical interpretation of the experimental results is presented in detail in the paper. Structural parameters determined on the basis of NMR spectra were compared to theoretical parameters that were obtained based on different theoretical models and literature data. Motion parameters for proper magnetic nuclei are also determined and presented based on temperature dependence of relaxation processes: activation energy and their dispersion that are crucial in the analysis of microscopic mechanism of motion of ions and water molecules. A study of motions of water molecules in nano - channels of the natrolite and understanding dynamical processes like diffusion and reorientation of water molecules is an interesting aspect of the paper.