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ABSTRACTS

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DQ-10/23 NMR METHOD USED FOR INVESTIGATION OF WATER MOBILITY IN POROUS CRYSTAL

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Traditional NMR investigations of molecular mobility in a solid state are based on study of temperature dependence of second moment (M_2) and determination of activation energy. The methods of study of molecular mobility are basing on analysis of local magnetic field tensor which molecular motion averaging is now widely used [1,2]. However from the analysis of NMR line-shape in monocrystals is possible to obtain the additional information about type of mobility, paths of diffusion and distribution of correlation time [3]. For this purpose it is necessary to study the NMR-line shape in the temperature range, in which a width of NMR spectrum will be comparable to molecular motion frequency ($\nu_c \sim M_2^S$). But some features modifications of NMR line-shape in solid state have remained not study till now, that restricts application of a method NMR for a research of a molecular motion.

It is shown that the form of spectrum is determined by effects of frequency exchange in a temperature range of Pake doublets' averaging. For example, the decrease of doublet splitting and broadening of doublet components in the temperature range of slow motions ($\nu_c \leq M_2^S$) are largely determined by frequency exchange. Earlier this change of doublet splitting was explained by influence of vibration motion of water molecule [4]. However, vibration motion of water molecules can only partially explain apparent changes of spectra in the range of slow motions. Sometimes the composite spectrum observed in the temperature range of slow motions ($\nu_c \approx M_2^S$) was explained as a result of frequency exchange and distribution of correlation times. The distribution of correlation times is result of a nonuniform distribution of water vacancies in neighbor position and complicated potential landscape, or presence nonequivalent paths for diffusion with different barriers. In the report the influence of vibration motion and regular diffusions on the NMR-line shape is discussed. The examples of analysis of spectrums in same zeolites (natrolite, edingtonite) are given.

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