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ABSTRACTS

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NON-MARKOVIAN PROCESSES OF MOLECULAR MOTIONS IN SOLIDS

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Motions of molecules or molecular groups in solids are considered as a stochastic process in majority of theories analyzing influence of the molecular dynamics on the NMR [1]. In condensed matter only the components in a configuration space are usually taken into account [1,2]. However it is not always reasonable. Reorientations or diffusion of molecular groups are often connected with the large structural fluctuations in solid dynamics. This leads

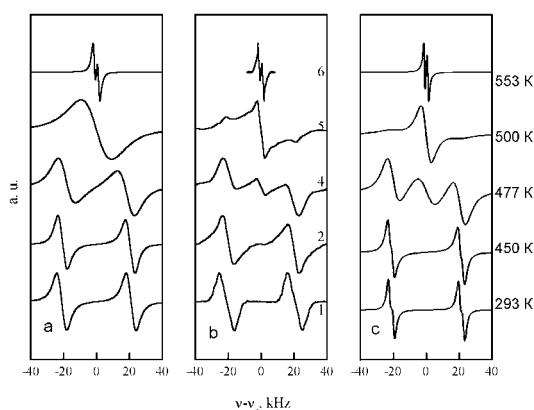


Fig.: The temperature dependence of the ^1H NMR spectrum of natrolite for the case when vector B_0 lies in $[110]$ direction: (a) theoretical NMR spectra obtained for the model of homogeneous diffusion of water molecules with the activation energy $E_a=73$ kJ/mole; (b) experimental NMR spectra; (c) theoretical NMR spectra obtained for the non-Markov model of water molecular motions with fluctuations driven by dichotomic noise ($E_a=73$ kJ/mole and $\sigma=4,2$ kJ/mole).

with temperature.

The numerical methods have been used to analyze temperature dependencies of NMR line when the fluctuations have a more complicated and real character. The Orstein-Uhlenbeck process (diffusion, stationary, Gaussian, Markov process) has been used to describe changing of activation energy with time.

References:

- [1] A. Abragam, *The Principles of Nuclear Magnetism*, Clarendon Press, Oxford, 1961.
- [2] N.G. van Kampen, *Stochastic Processes in Physics and Chemistry*, North-Holland, Amsterdam, 1981.
- [3] H. Sillescu, *J. Chem. Phys.*, 104, 4877 (1996).
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to the creation of additional “non-observable” states. In that case the non-Markovian models can be useful. It has been made use of the procedure of the creation of non-Markovian process, connected with the projection from a higher-dimensional Markov process by integrating over all “non-observable” variables [3].

In case of non-Markovian molecular motions we assume that the activation energy fluctuates and causes the transformation of transition probability matrix into the stochastic matrix. Then master equation changes into the stochastic equation. It has been shown in [4] that the simple fluctuations driven by a bitable process of telegraphic type, called dichotomic noise (DN) may very well explain the observed temperature dependence of NMR spectra in the mineral natrolite. Markov model of the water molecules diffusion with single correlation time can not correctly describe behavior of these spectra