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ABSTRACTS

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DQ-10/17 **MARKOVIAN AND NON-MARKOVIAN PROCESSES
OF MOLECULAR MOBILITY AND NMR OF MINERAL NATROLITE**

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The mineral natrolite ($\text{Na}_2\text{Al}_2\text{Si}_3\text{O}_{10}\cdot 2\text{H}_2\text{O}$) is the typical channel-type compound with porous structure (zeolite). It has been established by NMR method that there are two different kinds of the water molecular motion. The molecular motion of the first kind is the 180° flip motion and the second one is the diffusion of the water molecules [1]. From NMR data it follows that water molecules diffuse along the vacancies whose positions coincide with the regular positions of water molecules. The chemical and structurally equivalence of water molecules suggests that the diffusive jumps of water molecules may be characterised by the same correlation time τ_c . However, this suggestion does not agree to observed temperature transformations of the NMR spectra (see figure).

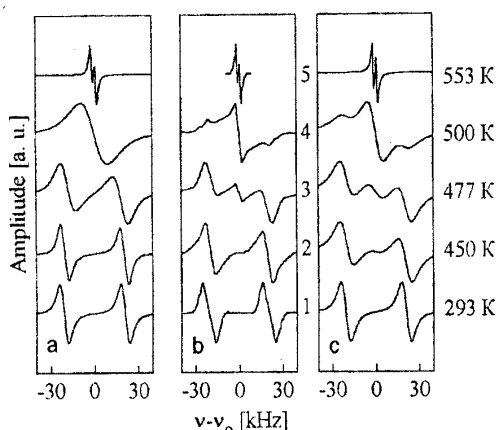


Fig.: The temperature dependencies of the ^1H NMR spectrum of natrolite for the case when vector \mathbf{B}_0 lies in $[110]$ direction: (a) theoretical NMR spectra obtained for the model of homogeneous diffusion of water molecules with the activation energy $E_a=73$ kJ/mole; (b) experimental NMR spectra; (c) theoretical NMR spectra obtained for the normal distribution of the activation energy ($E_a=73$ kJ/mole and $\sigma_E=4.2$ kJ/mole).

From comparison of the experimental and simulated NMR spectra it can be concluded that the model of the normal static distribution of the activation energy may be considered as a preferable model for the diffusion of the water molecules in the natrolite.

References

- [1] A.V.Sapiga, N.A.Sergeev, *Cryst. Res. and Techn.*, v.36, n.8-10 (2001) pp.875-883.
- [2] H.Sillescu, *J. Chem. Phys.*, **54** (1971) 2110; *J. Chem. Phys.*, **104** (1996) 4877.
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In order to explain the observed temperature transformations of the ^1H NMR spectra we have considered two models of water molecular mobility. At first we assumed that the molecular diffusion in natrolite is not characterised by the single correlation time. We assumed that a distribution of the correlation time τ_c is due to a static distribution of the activation energy E_a and the distribution function of E_a is the normal distribution. The second model is the model of non-Markovian mobility of water molecules [2]. We assumed that there are dynamic fluctuations in the activation energy E_a . The non-Markovian process was obtained using composite two-dimensional Markov process from which the non-Markovian process is obtained as a projection from the composite process by integration over all "nonobservable" states [3].