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ABSTRACTS

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CQ-12P/10 **Transport phenomena and solid-state NMR**

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The investigations of the transport phenomena or thermally activated molecular and atom internal motions in solids are important applications of nuclear magnetic resonance (NMR) method. In this report we consider the problem of the ^1H NMR lineshape in solids contained the mobile water molecules. It is well -known that ^1H NMR spectrum of a water molecule contains the two lines at frequency $\nu_0 \pm \nu$ (ν_0 is the Larmor frequency) [1]. If there are n magnetically nonequivalent water molecules in the solid and motions of the water molecules absent the ^1H NMR spectrum contains in general case n Pake's doublets at frequencies $\nu_0 \pm \nu_j$ and amplitudes p_j. If the water molecules are moved between these n magnetically nonequivalent positions the NMR spectrum is narrowed and at high temperature the averaged NMR spectrum is observed [2]. The temperature interval at which $2\nu_j \approx \nu_C$ (ν_C is the correlation frequency characterizing the motion of the water molecule) is the most interesting interval since the transformations of NMR lineshape in this interval are the most sensible to the microscopic mechanism of the water mobility.

For the temperature transformation of the ^1H NMR lineshape of the moving water molecules we obtained the following equation

$$I(\Delta) = A[f(\Delta) + f(-\Delta)] \ , \tag{1}$$

where $\Delta = \omega - \omega_0$, A is constant and

$$f(\Delta) = \mathrm{Re}\frac{g(i\Delta)}{1 - \nu_C \cdot g(i\Delta)} \ . \tag{2}$$

In Eq.(2)

$$g(i\Delta) = \sum_{j=1}^{n} p_j \frac{1}{\sqrt{2\pi\sigma^2}} \int_0^{\infty} \frac{d\nu}{\nu_C + i(\nu + \Delta)} \cdot \exp\left(-\frac{(\nu - \nu_j)^2}{2\sigma^2} \right) . \tag{3}$$

If $\sigma = 0$ and $n = 2$, $p_1 = p_2 = 1/2$ from Eqs. (1) – (3) it follows the well-known result [3]. However this results to leave out of account the magnetic dipolar interactions between nuclei of the different water molecules (intermolecular interactions). Usually these interactions are included in consideration by introduction the phenomenological parameter T_2 [4,5]. However in this model the parameter T_2 is not depended on temperature and so one is not reflects the observed averaging of the intermolecular interaction at the mobility of the water molecules. In contrast to these approaches, the equations (1) – (3) correctly account as intramolecular so intermolecular dipolar interaction of the mowing water molecules.

[1] J.E.Pake, J.Chem.Phys., **16**, 327 (1948)

[2] N.A.Sergeev, O.V.Falaleev, S.P.Gabuda, Phys. Solid State **11**, 2248 (1969).

[3] A.V.Sapiga, N.A.Sergeev, Crystal Research and Technology, **36**, 875 (2001).

[4] N.A.Sergeev et al., J.Struct.Chem. **22**, 83 (1981).

[5] A.V.Sapiga, N.A.Sergeev, Mol.Phys.Rep, (Poland), **29**, 60 (2000).