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CALCULATION OF DIPOLAR CORRELATION FUNCTION IN SOLIDS WITH INTERNAL MOBILITY

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Investigation of thermally activated molecular internal motions in solids is an important application of nuclear magnetic resonance (NMR) method. At the present time there are a great number of papers describing calculations of different NMR values measured in solids with internal mobility. Almost all of these values are governed by the dipolar correlation function:
, where

$$a_{ij}(t') = R_{ij}^{-3}(t')[1-3\cos^2\theta_{ij}(t')]$$

are the values, which describe dipolar interactions between nuclear magnetic moments.

In the present work a general equation for the dipolar correlation function, to be used to analyze various kinds of internal motions, described by two or three correlation times τ_{ck} (k= 1,2,3) has been obtained. For the case of two types of internal motion this correlation function has the form:

$$h(t) = < M_2 > + (\overline{\overline{M_2}} - < M_2 >)\cdot\exp(-\frac{t}{\tau_{c1}}) + (\overline{M_2} - < M_2 >)\cdot\exp(-\frac{t}{\tau_{c2}})$$
$$+ (M_2 + < M_2 > - \overline{M_2} - \overline{\overline{M_2}})\cdot\exp[-(\frac{1}{\tau_{c1}} + \frac{1}{\tau_{c2}})t$$

Here M_2 is the NMR second moment for rigid lattice; $\overline{M_2}$ is the second moment of motionally narrowed NMR line by the first dynamic process; $\overline{\overline{M_2}}$ is the second moment of motionally narrowed NMR line by the second dynamic process; M_2 is the second moment of motionally narrowed NMR line by the first and second dynamic processes.

The expression obtained for the dipolar correlation function has been used to analyze the experimental temperature dependences of different NMR measured values: second moment like: spin-lattice relaxation times; amplitude of solid echoes signals.