The Henryk Niewodniczański
Institute of Nuclear Physics
Radiospectroscopy Division
ul.Radzikowskiego 152, 31-342 Kraków, Poland
tel.: +48 (12) 637-02-22
fax: +48 (12) 637-54-41
qamts99@alf.ifj.edu.pl

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Measurement of molecular reorientations by NMR solid – echo method

P. Bilski[1], N. A. Sergeev[2], J. Wąsicki[1]

[1]Faculty of Physics, Adam Mickiewicz University, Poznań, Poland

[2]Institute of Physics, University of Szczecin, Szczecin, Poland

The effects of nonzero pulse widths on the solid-echo signals in solids with molecular motions have been investigated. It has been shown that in the slow - motion region $(M_2\tau_c^2 \approx 1)$ the amplitude of the echo signal $(90^0 - \tau - 90^0_{90} - t)$ is reduced and the maximum of the echo signal is shifted to the end of the second pulse. Comparison of the developed theory with experimental results obtained on polycrystalline C_6H_6 and NH_4Cl demonstrates good agreement between them.

Using the following correlation function for the dipolar magnetic field:

$$h(|t|) = \overline{M_2} + \Delta M_2 \exp\left(-\frac{|t|}{\tau_c}\right) \tag{1}$$

and calculating the integrals

$$\begin{aligned} F(t,t_2\tau,t_1) = \frac{1}{4}\int_0^{t_1} dt''\int_0^{t_1} h(t'',t')dt' + \int_{t_1}^{\tau-t_1} dt''\int_0^{t_1} h(t'',t')dt' + \int_{t_1}^{\tau-t_1} dt''\int_{t_1}^{\tau-t_1} h(t'',t')dt' \\ - \int_{t-\tau-t_2}^{t} dt''\int_0^{t_1}(h(t'',t')dt' - 2\int_{t-\tau-t_2}^{t} dt''\int_{t_1}^{\tau-t_1} h(t'',t')dt' + \int_{t-\tau-t_2}^{t} dt''\int_{t-\tau-t_2}^{t} h(t'',t')dt', \end{aligned} \tag{2}$$

we obtain the following expression for the solid – echo signal:

$$(t,t_2,\tau,t_1) \approx \frac{\hbar\omega}{kT}\exp\left\{-\frac{1}{2}\langle\overline{M_2}\rangle\left[t-\left(2\tau+t_2-\frac{t_1}{2}\right)\right] - \langle\Delta M_2\rangle\tau_c^2 R(t,t_2,\tau,t_1,\tau_c)\right\} \tag{3}$$

where

$$\begin{aligned} R(t,t_2,\tau,t_1,\tau_c) = -\frac{7}{4} + \frac{t}{\tau_c} - \frac{3t_1}{4\tau_c} - \frac{t_2}{\tau_c} - \frac{1}{4}\exp(-\frac{t_1}{\tau_c}) - \exp(-\frac{t_2}{\tau_c}) - \frac{1}{2}\exp(-\frac{t}{\tau_c}) \\ + \exp(-\frac{\tau-t_1}{\tau_c}) - \frac{1}{2}\exp(-\frac{t-t_1}{\tau_c}) + \exp(-\frac{\tau+t_2}{\tau_c}) + \exp(-\frac{t-\tau}{\tau_c}) + \exp(-\frac{t-\tau-t_1}{\tau_c}). \end{aligned} \tag{4}$$

In Eq.(4) τ_c is correlation time of the molecular motion; t_1 and t_2 are the widths of the first and second RF pulses; τ is the time interval between the RF pulses and this is the time between the beginnings of the first and second pulses; t is the time where NMR signal is observed and this time is measured from the beginning of the first pulse; $\Delta M_2 = M_2 - \langle M_2\rangle$ where M_2 is the second moment of NMR line in „rigid" lattice of polycrystalline sample, $\langle M_2\rangle$ is the second moment of motionally narrowed NMR line ($\tau_c^{-1} \rangle\rangle M_2^{1/2}$).

From Eq.(3) it follows that at $\langle M_2\rangle\tau_c^2 \rangle\rangle 1$ (the case of rigid lattice) and $\langle M_2\rangle\tau_c^2 \langle\langle 1$ (the case of motionally narrowed NMR line) the maximum of solid - echo signal is observed at $t_e = 2\tau + t_2 - \frac{t_1}{2}$ [1-3]. If we consider the delta – function approximation for the RF pulses and put in Eq.(4) $t_1 = t_2 = 0$ we obtain from Eq.(3) the known result [4]. From analysis of Eq.(3) it follows that in the slow – motion regime $(\langle M_2\rangle\tau_c^2 \approx 1)$ the amplitude of the echo signal is reduced and the maximum of the echo signal is shifted to the end of the second pulse.

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