

Specialized Colloque AMPERE 2003



NMR and EPR of Broad-Line Solids

*Dedicated to Professor Robert Blinc
on the occasion of his 70th birthday*

Book of Abstracts



Bernardin, Portorož

Slovenia

September 8 - 12, 2003



INFLUENCE OF MOLECULAR MOTIONS ON THE NQR ECHOES

N.A.Sergeev^a, A.M.Panich^b, M.Olszewski^a^aInstitute of Physics, University of Szczecin, 70-451 Szczecin, Poland^bPhysics Department, Ben-Gurion University, P.O.B. 653, Beer Sheva 84105, Israel
pan@bgumail.bgu.ac.il

In thiourea - C_2Cl_6 inclusion compound, the guest molecules are entrapped within the unidirectional, non-intersecting tunnels of a hydrogen-bonded thiourea network and pack within van der Waals contact of each other. Hahn echo measurements show that spin-spin relaxation time T_2 is nearly temperature independent at 20-55 K. Higher temperature yields a significant shortening of the echo decay on heating (Fig.1).

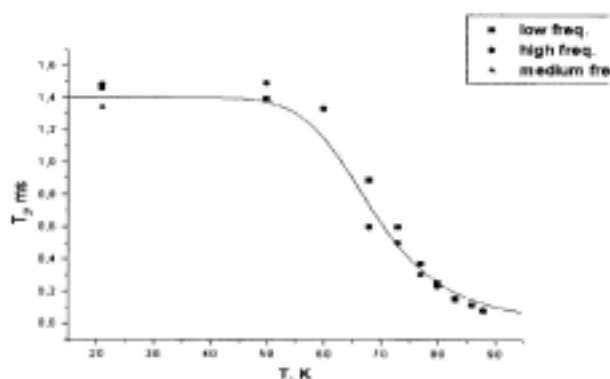


Fig. 1. Triangles, squares and circles correspond to three peaks of broad ^{35}Cl NQR spectrum received by a frequency-sweep technique

However, we show that due to the dipole-dipole interaction of mobile nuclear spins in the slow motion limit, the thermal fluctuations can lead to the shortening of the echo decay with increased temperature. Taking into account this mechanism, our calculation leads to an expression:

$$T_2^{-1} = T_{2X}^{-1} + \left(\frac{\Delta M_2}{12\tau_c}\right)^{1/3} \quad (1)$$

Here ΔM_2 is the difference of the second moments of ^{35}Cl NQR spectra of the rigid lattice and of mobile molecular groups, T_{2X}^{-1} is a temperature independent term.

The solid line in Fig. 1 is a theoretical curve calculated using Eq.(1) and $\tau_c = (10^{-14} s) \cdot \exp(18.3 kJ \cdot mol^{-1} / RT)$ obtained from spin-lattice relaxation data [1]. The best fit between theory and experiment is found for $T_{2X} = 1.4$ ms and $\sqrt{\Delta M_2} = 8$ kHz. As it is seen from Fig. 1, satisfactory agreement between theoretical and experimental curves is obtained.

[1] Panich A.M., Semenov A.R., Chekhova G.N., Krieger Yu.H., Goren S.D., *Solid State Commun.*, **110**, 363 (1999).