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The cross-correlation effects in relaxation of quadrupolar nuclei in the multipolar spin systems

A theoretical treatment of the longitudinal and transverse nuclear magnetic relaxation of quadrupolar nuclear in multipolar spin systems in the presence of quadrupolar-chemical shift anisotropy interference is presented for any spin.

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Summary

The relaxation theory of Bloch-Wangsness-Redfield [1] has been used widely for interpretation of the data in solid-state and high resolution NMR relaxation experiments. However, there are difficulties in extracting dynamic information on some systems in the presence of nuclear spins with $I > 1/2$. These difficulties associated with tremendous calculator work for obtaining matrix representation of relaxation superoperator for multipolar spin systems and with the complexity of solving the relaxation equations for spin density matrix. The restriction of basis set for relaxation superoperator in mutlipolar spin system may lead to loss of the relevant physical observables induced by the relaxation . Such situation arises if the interference interactions give the contributions in the relaxation.

In the present paper a theoretical treatment of the longitudinal and transverse nuclear magnetic relaxation of quadrupolar nuclear of any spin in multipolar spin systems is proposed in the operator representation without preliminary selection of basis set in the presence of quadrupolar-chemical shift anisotropy interference, based on the second order time dependent perturbation theory [2]. The operator representations are particularly attractive since they permit us to avoid dealing with individual matrix elements.

The main equations for longitudinal and transverse relaxation of quadrupolar nuclear in multipolar spin system were derived if the relaxation is defined by chemical shift anisotropy, quadrupolar interactions and mixed fluctuations. The theory was applied to study of a relaxation and a line shape of quadrupolar nucler of spin $S=1, 3/2, 3$ in anisotropic molecular system in the presence of Q-CSA cross-correlation and in dipolar coupled spin system IS ($I=1/2, 1$). The effects of high rank multipoles on lineshape and longitudinal relaxation of $S=3$ spin system were studied in the presence of Q-CSA cross-correlation. It was found that quadrupolar interaction induced magnetic multipolar the same evenness but Q-CSA inteference interaction course multipolar rank higher on one. The necessity of quantitative estimates of the values of Q-CSA cross-correlation contributions requires working out of new methods of exciting of particular types of coherence, and the methods for their registration. We also discuss the possibility of the application of traditional schemes for the excitation of multiquantum coherence for spin systems with quadrupolar nuclei.

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