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Application of Redfield relaxation theory onto a 5/2 spin system and comparison to NQR relaxation measurements

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Motivation and Introduction

Nuclear Quadrupole Resonance Spectroscopy (NQRS) is a chemically and structurally very sensitive spectroscopy method that is probing high spin ($I > 1/2$) nuclei in solid samples without the need of an external magnetic field. Using RF pulse sequences, the technique has the potential to fully determine the transitions of a spin ensemble regarding their relaxation properties. The relaxation behaviour allows gaining insight into molecular dynamics. Also, the spatial symmetry and the quadrupolar coupling strength of the intramolecular electric field gradient at the position of the probed nucleus can be derived experimentally; these parameters determine the frequency positions of the nuclei's spin transitions.

The semiclassical BWR (Bloch, Wangsness, Redfield) theory for spin relaxation allows for a description of the relaxation behaviour of NQR transitions.

Method

Presented will be a simplified application of Redfield's relaxation theory to 5/2 spin nuclei. From the spin density distribution only the transverse single quantum transitions will be considered to find expressions for the lineshapes of the two corresponding transition frequencies. As a starting point, the quadrupolar Hamiltonian in the principal axis system is used.

As dynamical model for the EFG fluctuations, an exponentially decaying autocorrelation function for the stochastic Hamiltonian is assumed. So, the variation of the fluctuating EFG, which is generated by the molecular dynamics around the nucleus, is described by a characteristic time τ_C and the variance $\overline{\omega^2}$.

Experimental

NQRS experiments are carried out using two complementary RF-pulse spectrometer systems; the self-constructed „ConCradle" and the commercial system „Scout" from Tecmag, Inc. (Texas). The available RF coils cover a range of 20 MHz up to 150 MHz and can be thermalized around body temperature or in liquid nitrogen. Both systems are placed in a shielding chamber to protect the measurements from RF spur signals. For T_1 and T_2 relaxation time measurements pulse sequences well known in the NMR community are used, as for example spin echo and inversion recovery.