Relaxation rate enhancement of ^{1}H due quadrupolar ^{14}N nuclei – general vs. perturbation approach

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Nuclear Magnetic Resonance relaxometry is a rich source of information on dynamical and structural properties of condensed matter. Of special importance are field cycling relaxation experiments which provide spin-lattice relaxation rates over a frequency range covering three orders of magnitude, typically from 10 kHz to 20 - 40 MHz for ^{1}H. The broad range of frequencies allows detecting motional processes of different time scales by a single experiment.

When the system, beside of protons, consists of quadrupole nuclei, in some cases (e.g. relatively slow dynamics) one may observe field-specific ^{1}H relaxation rate enhancement, referred to as quadrupolar peaks. The peaks result from quadrupolar interactions and appear at fields where proton resonance frequency overlaps one of the quadrupole nucleus transition frequencies. From the positions of the peaks one can determine parameters of the quadrupole coupling (the coupling constant and electric field gradient asymmetry parameter – the fingerprint of molecular structure), while it shapes reflect local dynamics of the system.

Here we compare two approaches for analysis of the relaxation enhancement of ^{1}H due to the presence of quadrupole nuclei ^{14}N: the general approach based on Stochastic Liouville Equation formalism and the perturbation approach. We show, that the simplified approach is valid only for certain motional conditions, that is as long as the product $\omega_Q \tau > 20$ or $\omega_Q \tau < 0.5$ (where ω_Q stands for the quadrupolar coupling constant in angular frequency units, while τ represents correlation time of rotational dynamics responsible for the fluctuations of quadrupole interactions). These findings may useful when considering appropriate model for the description of data for biological systems, for example proteins or tissues.

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