Universal features of ^{1}H relaxation in proteins and quadrupolar relaxation enhancement

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Nuclear Magnetic Resonance (NMR) relaxometry is considered as powerful methods providing information about molecular dynamics and structure. In this work NMR relaxometry has been applied to a series of solid proteins: elastin, lysozyme and albumin in order to inquire into their dynamical properties. The data have been analyzed in terms of a "semi-phenomenological" model – *i.e.* decomposed into three relaxation contributions described by Lorentzian spectral densities associated with dynamical processes referred to as slow, intermediate and fast ones. It has turned out that despite structural differences the correlations times for each "dynamical fraction" are very close. The structural differences are reflected by the corresponding dipolar relaxation constants which shown an interesting pattern.

^{1}H relaxation in proteins results from two relaxation pathways provided by ^{1}H-^{1}H and ^{1}H-^{14}N dipole-dipole interactions, respectively. The last contribution gives rise to qudrupole relaxation enhancement effects often referred to as "quadrupole peaks". This effect manifests itself as a frequency-specific increase of the ^{1}H spin-lattice relaxation rate. From the positions of the "quadrupole peaks" one can straightforwardly determine parameters of ^{14}N quadrupole coupling (the coupling constant and asymmetry parameter) which reflect the value of the electric field gradient tensor at the position of ^{14}N and hence are a fingerprint of the molecular structure. The shape of the "quadrupole peaks" is a very important source of information on the molecular motion provided a proper theoretical model has been used for its analysis. Thus, the second part of this talk will be devoted to a comparison of a model of quadrupolar relaxation enhancement based on the second-rank perturbation theory [1] and a model based on the Stochastic Liouville Equation [2]. The validity range and limitations of the perturbation approach will be discussed in detail.

1. P.H. Fries, E. Belorizky, *J. Chem. Phys*. **143**, 044202, 2015
2. D. Kruk, A. Kubica, W. Masierak, A.F. Privalov, M. Wojciechowski, W. Medycki, *Solid State NMR* **40,** 114, 2011

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