

Dynamics of solid proteins by means of Nuclear Magnetic Resonance Relaxometry

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Fast Field-Cycling relaxometry is an NMR technique used to determine the spin-lattice relaxation rates (R_1) of samples as a function of resonant frequency (or, equivalently, magnetic field strength). When studied over wide range of frequencies, $R_1(\omega)$ (the relaxation dispersion profile) provides information on molecular dynamics of the system under investigation.

Due to the presence of ^{14}N nuclei in the structure of amide groups, ^1H spin-lattice relaxation dispersion profiles of proteins are described in terms of a sum of homonuclear ^1H - ^1H and heteronuclear ^1H - ^{14}N contributions. Standard quantitative analysis relies on formulae including power-laws or Cole-Davidson spectral density functions for the homonuclear contribution and Lorentzian or Gaussian functions for the heteronuclear counterpart [1,2]. In the present studies we make an attempt to describe the relaxation dispersion profiles of proteins by employing: 1) multi rotational-like dynamics for ^1H - ^1H interactions and 2) quadrupolar relaxation enhancement of ^1H relaxation originating from ^1H - ^{14}N dipole-dipole interactions [3, 4].

Thorough quantitative analysis of relaxation data obtained for solid proteins: elastin, lysozyme and albumin shows, that the homonuclear contribution to the NMRD profile can be described in terms of three rotational-like dynamical processes occurring on a different time scales, ranging from μs to ns, and frequency independent term A. Despite structural differences between the investigated systems, the parameters characterising ^1H - ^1H dipolar interactions (coupling constants and correlation times), ^1H - ^{14}N couplings (^1H - ^{14}N distances and ^1H - ^{14}N bond orientations) and ^{14}N quadrupolar interactions (coupling constants, asymmetry parameters) are similar.

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