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EVOLUTION OF THE SHAPE OF QUADRUPOLE PEAKS – FROM SOLID TO DISSOLVED PROTEINS

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Quadrupole Relaxation Enhancement (QRE) is a complex, quantum – mechanical phenomenon, which is observed in systems including at least one nucleus possessing a quadrupolar moment ($S > 1/2$) coupled to another nuclei (typically ^1H) by dipole-dipole interactions. When time modulations of the dipole-dipole coupling is slow enough i.e. on the time scale of the molecular dynamics in solids, the proton magnetization can be taken over by ^{14}N nuclei. This which manifests itself as a local (frequency specific) enhancement of the relaxation rate of protons (quadrupole peaks). The studies are focused on a detailed quantum-mechanical analysis of this effect for a series of systems of progressively faster dynamics: from solid proteins to their water solutions. The shapes of the quadrupole peaks change with the hydration level of proteins and their comprehensive analysis gives insight into global motions of protein domains.

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