

Advances in High-Field DNP and EPR

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In recent years several hyperpolarization methods boosting NMR sensitivity attained much attention. Dynamic nuclear polarization (DNP) is one of these methods, transferring the much higher Zeeman polarization of unpaired electron spins onto nuclear spin systems by resonant microwave excitation of paramagnetic DNP agents. This method, already discovered in the 1950's, attracted new attention after it has been demonstrated that significantly enhanced NMR signals could also be achieved at high magnetic fields as used nowadays for most NMR applications¹. Encouraged of this work performed on solid state samples we started to investigate the potential of DNP on liquid state samples at high magnetic fields². Unexpected large polarization transfer from organic radicals to solvent protons could also be detected in liquids³, which can be rationalized by fast local dynamics between the DNP agent (radical) and target (solvent) molecule⁴. Experimental requirements, polarization transfer mechanism and potential applications of this method will be illustrated and discussed.

Pulsed EPR methods allowing to measure distances in the 1-8 nm range with very high precision become more and more popular to obtain long range restraints in macromolecular biological systems⁵. So far mostly nitroxide spin labels covalently attached to the biomolecule are used as paramagnetic spin probes. Here we will show the performance of the PELDOR (Pulsed Electron Electron Double Resonance) experiment on a manganese-nitroxide model compound, demonstrating that at high magnetic fields such experiments can be successful performed and quantitatively interpreted. This is especially interesting for biological applications, where naturally occurring magnesium ions can be replaced by manganese.

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