Photo-chemically induced dynamic nuclear polarization detected by zero and ultra-low field NMR

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Nuclear magnetic resonance (NMR) is a powerful technique to study molecular structure, dynamics and interactions, and to perform imaging. The main drawback of the method is low sensitivity. Nuclear spins are usually polarized by a strong magnetic field (up to 20 T), still resulting in just a small spin polarization of order of 10⁻⁵. One way to boost the NMR signal is to perform chemically induced dynamic nuclear polarization (CIDNP). This allows to increase spin polarization by up to three orders of magnitude.

Spin polarization by CIDNP occur in those cases where chemical reactions depend on the nuclear spin states and is described by so-called radical pair mechanism. Formation of the short-living radical pairs result in sorting of the nuclear spin states between recombination products of the radical pairs [1]. Apart from hyperpolarization CIDNP also allows to study the short-living radicals in a solution and their kinetics, measure electron g-factors in the radicals, and determine the hyperfine constants, which characterise the spin-spin electron-nuclear interaction.

Recently, a method to detect the NMR spectra at zero and ultra-low fields (ZULF) was developed [2]. Meanwhile, CIDNP has a strong dependence on the magnetic field [1]. At zero field there is no quantization axis available and in order to generate a hyperpolarized nuclear spin order the system should contain at least two coupled nuclear spins in the RP. In this case CIDNP can be used to produce nuclear singlet order corresponding to the population imbalance between the ST states of the nuclear spins. The singlet order of a heteronuclear spin pair is the initial state for ZULF NMR detection.

Here we present our most recent results of studying CIDNP by ZULF NMR in the system of ortho-benzoquinone and tetraphenylporphyrin. In this system the RPs between the two compounds can be produced by shining a green light (515 nm), the light excites electrons in the porphyrin and it interacts with benzoquinone [3]. This should become a first observation of ZULF CIDNP NMR, which potentially also does not require usage of the prepolarizing magnetic fields.

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