

Realization of ^1H spin polarization of 40% at room temperature

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Dynamic Nuclear Polarization (DNP) is a means of transferring spin polarization from electrons to nuclei. As a method for enhancing bulk nuclear spin polarization, DNP has been successfully applied to areas ranging from fundamental physics to materials science, biology, and medical science. The conventional DNP, which is used radical as a polarizing agent, is carried out in the strong magnetic field and at cryogenic temperature (e.g. 3.35 T and 1.4 K) to polarize electron spins in the order of 10%.¹⁾ One approach for overcoming the limitation of the experimental conditions is to use non-thermalized electron spins instead. DNP with electron spins in the photo-excited triplet state (triplet-DNP) can achieve hyperpolarization independent of the magnetic field strength and temperature.²⁾ We employed pentacene as a polarizing agent, which has an electron spin polarization of 73%, and *p*-terphenyl as a host material because of its stability at room temperature and large pentacene capacity.

In this study, we focused on realizing the highest ^1H spin polarization at *room temperature*. The finally achievable nuclear spin polarization with triplet-DNP is determined by the balance between the spin-lattice relaxation time of the nuclear spin (^1H in this report) and the speed of the polarization transfer.

In order to suppress the spin-lattice relaxation time³⁾, we used pentacene-*d*₁₄ as the polarizing agent (Fig. 1(a)). The triplet electrons played the role of a polarizing agent as well as contributed to ^1H spin-lattice relaxation through a perturbation of the local field of the ^1H spins in the vicinity. In addition, we synthesized *p*-terphenyl-2',3',5',6'-*d*₄ (Fig. 1(b)). The ^1H spin-lattice relaxation in *p*-terphenyl-*h*₁₄ was mainly due to the pendulum motion of the central benzene ring, which modulates the local dipolar field of the ^1H spins in and near the central ring.⁴⁾

A high-repetition-rate laser system was developed to increase the speed of polarization transfer, and it consists of two Neodymium-doped Yttrium Aluminum Garnet (YAG) lasers with wavelengths of 1064 nm and 1319 nm and LiB₃O₅ crystal for sum-frequency generation.⁵⁾ The wavelength, pulse width, repetition rate, and output power were 589 nm, 126 ns, 3 kHz, and 1 W, respectively.

Using a single crystal of *p*-terphenyl-*d*₄ doped with pentacene-*d*₁₄ and the new laser, we conducted the triplet-DNP in 0.65 T and at room temperature. The buildup curve is shown in Fig. 1(c). 40% of ^1H spin polarization was obtained in 15 minutes, which corresponded to the 20,000-fold enhancement under the same conditions.

Hyperpolarization techniques using photo-excited triplet electrons can be used to simplify DNP experiments. The NMR sensitivity of samples that prefer ambient temperatures can be boosted significantly.³⁾ Bulk nuclear hyperpolarization in such low magnetic fields is also desirable to achieve the polarized target for RI beams⁶⁾ and the polarized filter for neutron beams.⁷⁾

References

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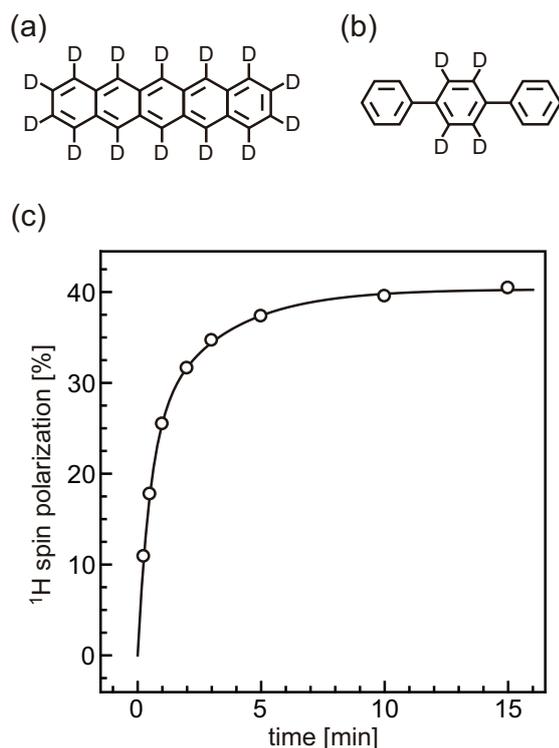


Fig. 1. (a) pentacene-*d*₁₄. (b) *p*-terphenyl-2',3',5',6'-*d*₄. (c) Polarization buildup curve. The polarizations were estimated by comparing the intensities of the hyperpolarized signals and the thermal intensities in 0.6 T at room temperature.

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