PHOTO-SABRE Polarization on *trans*-Azobenzene using Parahydrogen under Light

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Parahydrogen can be used to hyperpolarize nuclear spins allowing enhancement of signals in nuclear magnetic resonance and magnetic resonance imaging by up to five orders of magnitude. This method is applicable when a pairwise hydrogenation reaction occurs; the singlet spin order (population imbalance between the singlet and triplet states of the spin pair) of parahydrogen can be transferred into and redistributed across the nuclear spin system of the target molecule. Of particular interest are reversible hydrogenation reactions happening in catalytic complexes: in this case a dihydrogen molecule H_2 that is dissolved in a solution can reversibly bind to a metal center, typically stabilized iridium ion. It is possible to transfer its nuclear spin order to another target molecule that binds to the same complex simultaneously with the hydrogens. The method is called SABRE (Signal Amplification By Reversible Exchange),[1] and it enables the polarization of a wide variety of substrates, including important biomarkers that can be used as contrast agents for bio-imaging.

Azobenzene is an interesting molecule which exists in two isomeric forms, trans-ABZ and cis-ABZ. The stable form trans-ABZ can be easily converted to cis- form by light irradiation, the amount of cis-ABZ is determined by wavelength of the light. Recently [2] it was shown that cis-ABZ can be polarized in SABRE process, but trans-ABZ was not polarized.

Here we present a study on PHOTO-SABRE of cis- and trans-azobenzene under light illumination at ultralow magnetic field. We have detected strong ^{15}N and ^{1}H polarization of trans-azobenzene and measured decay time of strong polarization in field range from 100 nT to 9.4 T. During SABRE process also long-lived states (LLS) of cis- and trans- $^{15}N_2$-azobenzene populates. We have optimized conditions for the LLS population and measured relaxation rate of LLS in trans-$^{15}N_2$-azobenzene which can be up to 17 minutes [3].

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[1] R.W. Adams et al., Science **2009**, *323 (5922)*, p. 1708.

[2] K.F. Sheberstov et al., *Chem. Phys. Chem.* **2021**, *22 (14)*, p. 1527.

[3] K.F. Sheberstov, H.M. Vieth, H. Zimmermann, B.A. Rodin, K.L. Ivanov, A.S. Kiryutin, A.V. Yurkovskaya, *Sci. Rep.* **2019**, *9 (1)*, p. 20161.