Adiabatic approach to polarize ^{15}N nuclei with SABRE at high magnetic fields

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Parahydrogen induced polarization (PHIP) is a well-established tool to dramatically enhance weak nuclear magnetic resonance (NMR) signals in NMR-spectroscopy and imaging (MRI). A version of PHIP, termed Singal Amplification by Reversible Exchange (SABRE) is based on the reversible interaction of parahydrogen and substrate molecules with an organometallic complex. To perform SABRE in a high magnetic field it is necessary to irradiate the sample using radiofrequency (RF) pulses with adiabatic amplitude modulation on ^{1}H and ^{15}N nuclear channels.

In our work we analyze SABRE pulse sequences in a high magnetic field (9.4 T) and optimize experimental parameters such as: RF-pulse amplitudes and frequencies, RF-pulse amplitude switching profile. We also propose a new approach for the calculation of RF-pulse amplitude switching profiles based on the SABRE spin dynamics calculation. Such calculation considers both - the presence of spin relaxation and reversible chemical exchange of parahydrogen and substrate with the SABRE complex by means of the Liouville equation. We demonstrate experimentally that in some cases our approach for calculation RF-amplitude switching profile leads to almost three-fold increase in ^{15}N hyperpolarization efficiency as compared to linear and constant adiabaticity amplitude switching. The proposed optimization procedure of the experimental SABRE parameters allowed us to achieve ^{15}N NMR-signals enhancement of 4000.

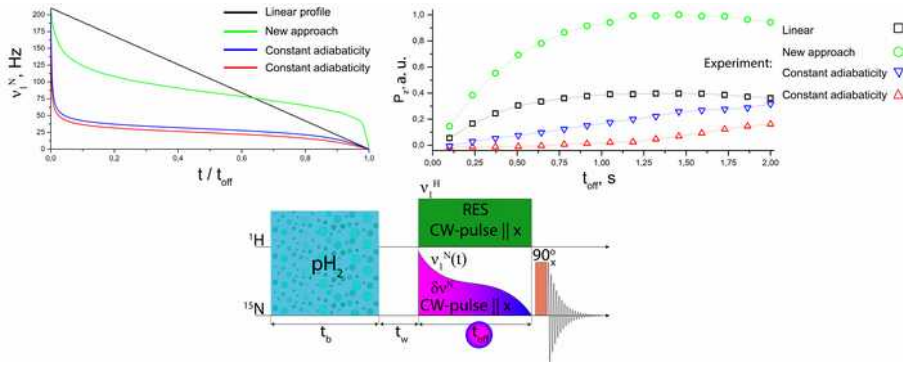

Fig. 1. ^{15}N polarization in high-filed SABRE pulse sequence (bottom). Left picture corresponds to the RF-amplitude switching profiles, right picture – ^{15}N polarization for different switching profiles

We acknowledge support from the Russian Ministry of Education and Science (Contract No. 075-15-2021-580)