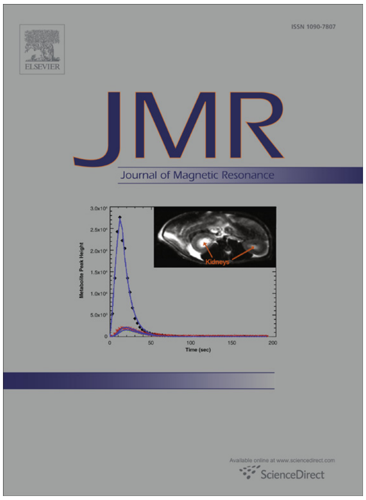

Parahydrogen discriminated PHIP at low magnetic fields.

I. Prina, L. Buljubasich, R.H. Acosta

PII: S1090-7807(14)00331-0
DOI: http://dx.doi.org/10.1016/j.jmr.2014.11.010
Reference: YJMRE 5555

To appear in: *Journal of Magnetic Resonance*

Received Date: 3 September 2014
Revised Date: 21 November 2014

Please cite this article as: I. Prina, L. Buljubasich, R.H. Acosta, Parahydrogen discriminated PHIP at low magnetic fields., *Journal of Magnetic Resonance* (2014), doi: http://dx.doi.org/10.1016/j.jmr.2014.11.010

Parahydrogen discriminated PHIP at low magnetic fields.

I. Prina[a], L. Buljubasich[a], R. H. Acosta*[a]

[a]FAMAF Universidad Nacional de Córdoba, IFEG CONICET, X5016LAE, Córdoba, Argentina

---

Abstract

Parahydrogen induced polarization (PHIP) is a powerful hyperpolarization technique. However, as the signal created has an anti-phase characteristic, it is subject to signal cancellation when the experiment is carried out in inhomogeneous magnetic fields or in low fields that lack the necessary spectral resolution. The use of benchtop spectrometers and time domain (TD) analyzers has continuously grown in the last years and many applications are found in the food industry, for non-invasive compound detection or as a test bench for new contrast agents among others. In this type of NMR devices the combination of low and inhomogeneous magnetic fields renders the application of PHIP quite challenging. We have recently shown that the acquisition of *J*-spectra in high magnetic fields not only removes the anti-phase peak cancellation but also produces a separation of thermal from hyperpolarized signals, providing Parahydrogen Discriminated (PhD-PHIP) spectra. In this work we extend the use of PhD-PHIP to low and inhomogeneous fields. In this case the strong coupling found for the protons of the sample renders spin-echo spectra that have a great complexity, however, a central region in the spectrum with only hyperpolarized signal is clearly identified. This experimental approach is ideal for monitoring real time chemical reaction of pure PHIP signals.

Keywords: Hyperpolization, Low Field, NMR spectroscopy, J-Spectra, CPMG, PHIP

---

1. Introduction

Hyperpolarization techniques have become relevant tools in the Nuclear Magnetic Resonance (NMR) community. In particular, Para-Hydrogen Induced Polarization (PHIP) is a relatively new technique which has significantly grown in the last two decades. Traditionally, NMR has dealt with the detection of nuclear spins in thermal equilibrium with an external magnetic field, resulting in a signal proportional to the small population difference, determined by a Boltzmann distribution, between the eigenstates of the Zeeman interaction Hamiltonian. One way to improve the NMR sensitivity consists in the direct hydrogenation of non-saturated compounds with molecular hydrogen enriched in its para-state (p-H_2) prior to the NMR experiment. In 1986, C. R. Bowers and D. P. Weitekamp reported a method to obtain large nuclear-spin polarization by exploiting the state of parahydrogen during a hydrogenation reaction [1]. The first results, where the reaction occurs in the presence of the same magnetic field of the NMR experiments, confirmed the predictions and inspired the acronym PASADENA (Parahydrogen And Synthesis Allow Dramatically

---

Email address: `racosta@famaf.unc.edu.ar` (R. H. Acosta*)