

DETECTION OF J-COUPPLING USING ATOMIC MAGNETOMETER

RELATED APPLICATIONS

[0001] This application is the national phase application of International application number PCT/US2010/030897, filed Apr. 13, 2010, which claims priority to and the benefit of U.S. Provisional Application No. 61/168,795, filed on Apr. 13, 2009, which is hereby incorporated by reference in its entirety.

STATEMENT OF GOVERNMENT SUPPORT

[0002] This invention was made with government support under Contract No. DE-AC02-05CH11231 awarded by the U.S. Department of Energy and with support from the National Institute of Standards and Technology, a non-regulatory agency within the U.S. Department of Commerce. The government has certain rights in this invention.

BACKGROUND OF THE INVENTION

[0003] The present invention relates to the field of nuclear magnetic resonance and, more particularly, to the field of detection of J- or scalar coupling.

[0004] Nuclear magnetic resonance (NMR) endures as one of the most powerful analytical tools for detecting chemical species and elucidating molecular structure. The fingerprints for identification and structure analysis are chemical shifts, nuclear Overhauser effects, and scalar couplings of the form $J_{I_1 I_2}$. The latter yield useful information about molecular spin topology, bond and torsion angles, bond strength, and hybridization. NMR experiments are conventionally performed in high magnetic fields, requiring large, immobile, and expensive superconducting magnets. However, detection of NMR at low magnetic fields has recently attracted considerable attention in a variety of contexts, largely because it eliminates the need for superconducting magnets. Additional advantages of low and zero field NMR include extremely homogeneous fields (both spatially and temporally) for narrow lines and the appeal of measuring small contributions to the Hamiltonian in the absence of a much larger Zeeman interaction.

[0005] One-dimensional and two-dimensional spectroscopy (see, S. Appelt, H. Kuhn, F. W. Häsing, B. Blümich, Chemical analysis by ultrahigh-resolution nuclear magnetic resonance in the Earth's magnetic field, *Nat. Phys.* 2 (2006) 105-109; and J. N. Robinson et al., Two-dimensional NMR spectroscopy in Earth's magnetic field, *J. Magn. Res.* 182 (2006) 343-347, respectively) have been demonstrated in the Earth's magnetic field using inductive detection. J-resolved spectra have been detected with superconducting quantum interference device (SQUID) magnetometers in $\sim\mu\text{T}$ fields (see, R. McDermott et al., Liquid-state NMR and scalar couplings in microtesla magnetic fields, *Science* 295 (2002) 2247-2249). Atomic magnetometers have been used to perform one-dimensional spectroscopy (see, I. M. Savukov, M. V. Romalis, NMR detection with an atomic magnetometer, *Phys. Rev. Lett.* 94 (2005) 123001; I. M. Savukov, S. J. Seltzer, M. V. Romalis, Detection of NMR signals with a radio-frequency atomic magnetometer, *J. Magn. Res.* 185 (2007) 214-220; and M. P. Ledbetter et al., Zero-field remote detection of NMR with a microfabricated atomic magnetometer, *Proc. Natl. Acad. Sci. (USA)* 105 (2008) 2286-2290) and for remote detection of magnetic resonance imaging in low mag-

netic fields. Nuclear magnetic resonance in a zero-field environment has been detected indirectly using field cycling techniques (see, D. B. Zax, A. Bielecki, K. W. Zilm, A. Pines, Heteronuclear zero-field NMR, *Chem. Phys. Lett.* 106 (1984) 550-553; and D. B. Zax, A. Bielecki, K. W. Zilm, A. Pines, D. P. Weitekamp, Zero field NMR and NQR, *J. Chem. Phys.* 83 (1985) 4877-4905). However, this practice does not remove the requirement for a superconducting magnet.

Low Field Nuclear Magnetic Resonance

[0006] Nuclear magnetic resonance (NMR), conventionally detected in multi-tesla magnetic fields, is a powerful analytical tool for the determination of molecular identity, structure, and function. With the advent of prepolarization methods and alternative detection schemes using atomic magnetometers or superconducting quantum interference devices (SQUIDS), NMR in very low- (\sim earth's field), and even zero-field, has recently attracted considerable attention. Despite the use of SQUIDS or atomic magnetometers, low-field NMR typically suffers from low sensitivity compared to conventional high-field NMR.

[0007] NMR^{1,2} in low or zero magnetic field has long been viewed as a curiosity due to the low nuclear spin polarization, poor sensitivity of inductive pickup coils at low frequencies, and the absence of site-specific chemical shifts.

[0008] Despite the use of atomic magnetometers or SQUIDS, low-field NMR using samples thermally prepolarized in a permanent magnet typically suffers from low signal-to-noise ratio compared to inductively-detected high-field NMR, in part because of the low polarization available from thermalization in a permanent magnet.

[0009] While parahydrogen induced polarization (PHIP) has been investigated in a variety of magnetic fields, ranging from the earth's field to high field, observation of the resulting NMR signals has always been performed in finite magnetic field.

SUMMARY OF THE INVENTION

[0010] An embodiment of a method of detecting a J-coupling of the present invention includes providing a polarized analyte adjacent to a vapor cell of an atomic magnetometer and measuring one or more J-coupling parameters using the atomic magnetometer. According to an embodiment, measuring the one or more J-coupling parameters includes detecting a magnetic field created by the polarized analyte as the magnetic field evolves under a J-coupling interaction.

BRIEF DESCRIPTION OF THE DRAWINGS

[0011] The present invention is described with respect to particular exemplary embodiments thereof and reference is accordingly made to the drawings in which:

[0012] FIG. 1 illustrates a system 100 for detecting J-coupling in accordance with an embodiment of the present invention.

[0013] FIGS. 2A and 2B provide graphs that show the response of an atomic magnetometer to test fields of varying frequency and the noise floor of the magnetometer, respectively.

[0014] FIGS. 3A and 3B provide graphs of a raw signal and a Fourier transform of the raw signal, respectively, which were obtained with a sample of ¹³C enriched methanol following an excitation pulse with area $B_1 T_p (\gamma_H - \gamma_C) = 2.4$ rad.