

RELAXATION OF PARAHYDROGEN-ENABLED STATES USING VARIABLE FIELD NMR SPECTROSCOPY

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Relaxation in Nuclear Magnetic Resonance (NMR) spectroscopy is a widely studied phenomenon. In addition to its practical implications for experimental duration, analysis of relaxation mechanisms allows characterisation of structure, crystal morphology and molecular dynamics. Difference in nuclear relaxation is also utilized as sophisticated contrast in Magnetic Resonance Imaging (MRI) [1].

Nuclear spin order relaxes depending on external factors such as magnetic field strength, temperature as well as internal factors such as viscosity, molecular size, nuclear interactions. Some nuclear spin-order displays exceptionally long lifetimes. For instance, nuclear magnetization converted to so-called singlet order can decay orders of magnitude longer enabling a better storage of spin-polarization in the system [1-3].

This is particularly relevant for Parahydrogen-Induced Polarization (PHIP) technique. PHIP experiments involve chemical reactions between substrates and parahydrogen gas in which 100% of nuclear spins are entangled in the nuclear singlet state. Therefore, slow relaxation leads to better accumulation of highly polarized substrates and influences practical utility of the method [2].

In this study, the relaxation properties of a compound containing three alkene groups at different magnetic fields are analysed by comparing longitudinal relaxation times T_1 to the nuclear singlet lifetimes T_s . The singlet state is acquired between the two cis-protons of the alkene group. The increasing relaxation contrast at low-fields suggests that for these derivatives PHIP experiments may be better performed at lower fields but predominantly relaxation is driven by ¹H dipolar interactions. Therefore, efficient PHIP experiments using similar molecular system may take a considerable advantage of isotope labelling to achieve higher efficiency for PHIP applications.

[1] M. H. Levitt, "Chapter 1: Long-lived States in Nuclear Magnetic resonance: An Overview," in *New Developments in NMR*, 2020, pp. 1-32, doi: 10.1039/9781788019972-00001.

[2] L. Dagys, B. Ripka et al., "Geminal parahydrogen-induced polarization: accumulating long-lived singlet order on methylene proton pairs," *Magnetic Resonance*, vol. 1, no. 2, pp. 175–186, Aug. 2020, doi: 10.5194/mr-1-175-2020.

[3] G. Stevanato et al., "A Nuclear Singlet Lifetime of More than One Hour in Room-Temperature Solution," *Angewandte Chemie*, vol. 127, no. 12, pp. 3811–3814, Feb. 2015, doi: 10.1002/ange.201411978.