Liquid State Dynamic Nuclear Polarization at High Magnetic Field

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Funding Grants: G.S. Boebinger (NSF DMR-1157490, NSF DMR-1644779); S. Hill (CHE-1229170); S. Wi (CHE-1808660)

Liquid-state Nuclear Magnetic Resonance is a commonly used tool in chemistry, biology and medicine to identify and characterize molecules, but it suffers from low sensitivity. Dynamic Nuclear Polarization (DNP) can increase the sensitivity, but it is challenging in the liquid state and particularly at high magnetic fields, where the the challenge is worth addressing because NMR resolution increases with increasing magnetic field.

In this study we demonstrate a significant gain in sensitivity (as high as seventy-fold) in the liquid state using the scalar Overhauser effect (a form of DNP) at 14.1T in a large sample volume, while also demonstrating the higher resolution from high magnetic fields.

We used the newly-commissioned 14.1T liquid DNP magnet system, developed in-house at the MagLab, to demonstrate large enhancements in ^{13}C magnetic resonance signals for ^{13}C located in several molecules (see Table 1).

The strong scalar liquid DNP effect observed is limited to specific molecules, but it demonstrates the dipolar Overhauser effect, which can be universally applied to many molecules. *The dipolar effect is particularly strong for small molecules used in studies of metabolomics (medical), natural products (biology), and molecular dynamics (chemistry), thus advancing a wide variety of applications.*

Facilities and instrumentation used: 14.1 T liquid DNP magnet system in the EMR and NMR facilities

Citation: T. Dubroca, S. Wi, J. van Tol, L. Frydman and S. Hill, *Large volume liquid state scalar Overhauser dynamic nuclear polarization at high magnetic field,* Phys. Chem. Chem. Phys. **21** 21200-21204 (2019); 10.1039/C9CP02997D

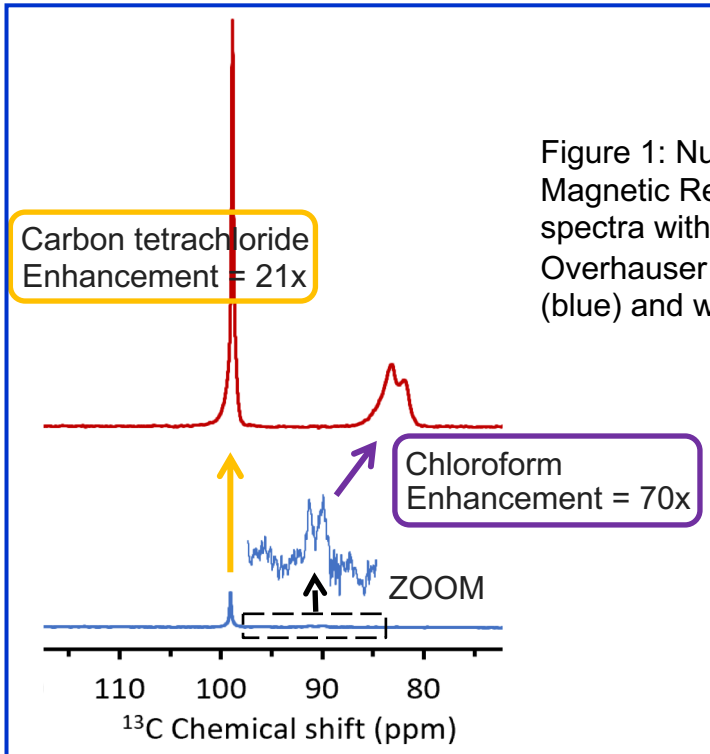

Figure 1: Nuclear Magnetic Resonance spectra without scalar Overhauser effect (blue) and with it (red).

Target molecule	Enhancement peak height ratios	Enhancement peak area ratios
Carbon tetrachloride	21 ± 1	20 ± 1
Deuterated chloroform	52 ± 1	70 ± 2
Chloroform	70 ± 7	88 ± 2
Phenylacetylene-2-^{13}C	35 ± 6	33 ± 1
n-Pentane-d_{12} (solvent)	1 ± 0.05	1 ± 0.05

Table 1: Sensitivity enhancements for various molecules.