Supporting Information For

Relaxation Dynamics of Nuclear Long-Lived Spin States in Propane and Propane-d$_6$ Hyperpolarized by Parahydrogen

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1. Experimental setup for NMR spectroscopy at 1.4 T

Scheme S1. Experimental setup for NMR spectroscopy using a bench-top 1.4 Tesla NMR spectrometer. This experimental setup is composed of three parts: custom-built parahydrogen generator, propane polarizer stages similar to those in Scheme 1, and a bench-top 1.4 T Nanalysis (NMR Pro 60) NMR spectrometer.

Low-field NMR setup to study HP propane relaxation at 1.4 T
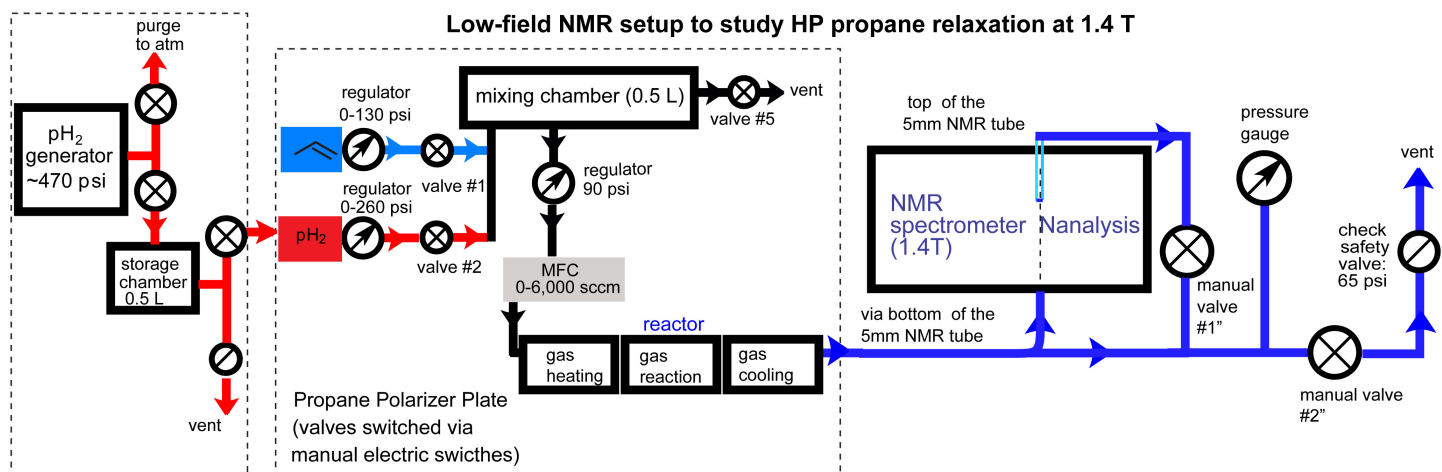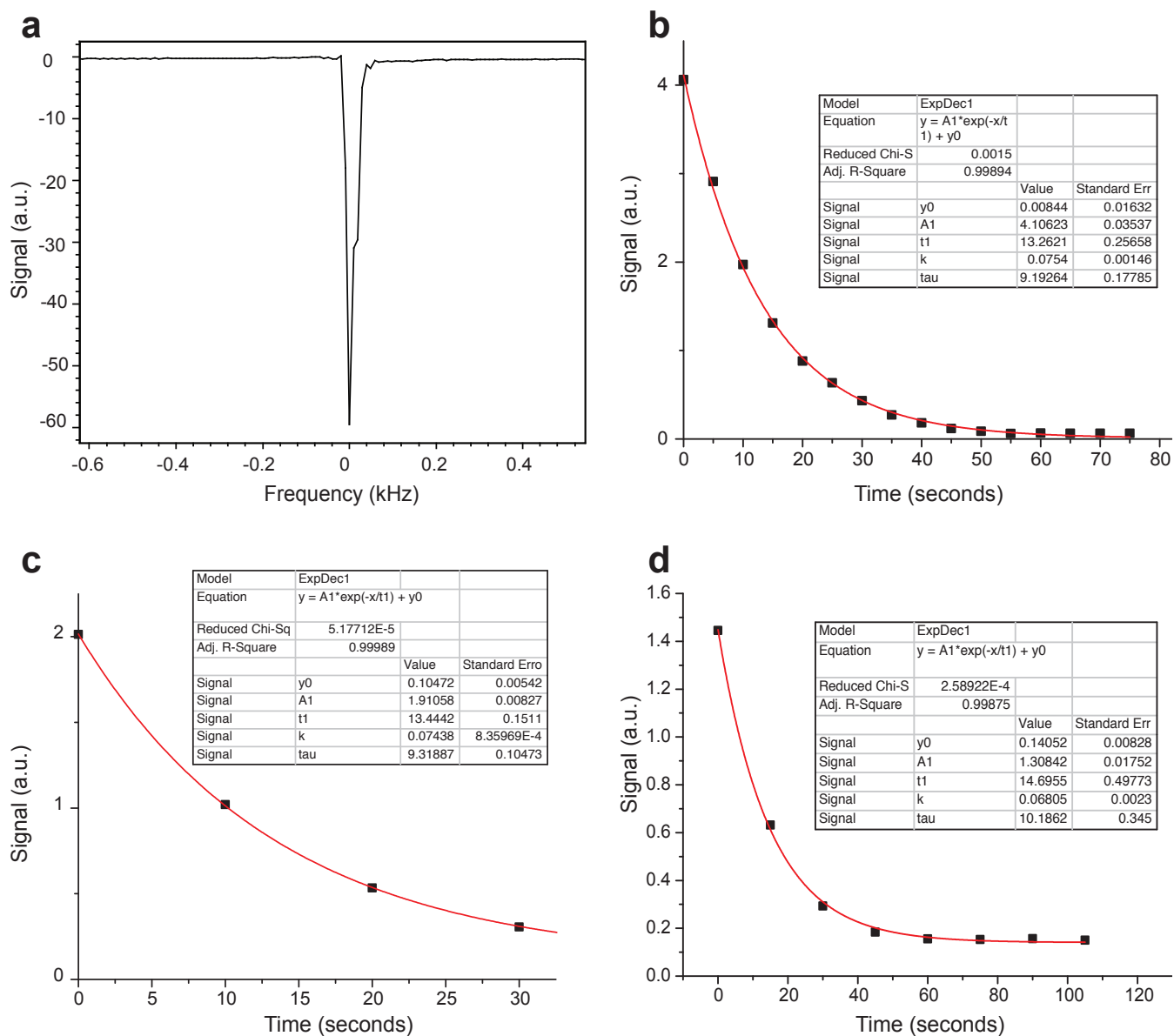
2. Additional Figures and Tables

Figure S1. a) An example of a ^{1}H spectrum of condensed HP propane obtained during the condensation studies performed using the 0.0475 T spectrometer setup, with some changes to gas collection as described in the experimental section. Note that since the spectrum is obtained using SLIC excitation, the polarization levels cannot be determined precisely, because the efficiency of SLIC conversion of pseudo-singlet overpopulation into observable magnetization is well below 100%. b), c), and d) are signal decay curves of the liquefied HP propane with time using RF SLIC pulses (duration of each pulse is 200 ms) applied every 5 s (b), 10 s (c) and 15 s (d) --note the effective T_{LLS} values obtained vary when different durations of SLIC pulse is employed because of the polarization loss induced by the RF pulse excitation, which was not taken into account. Note the effective values of T_{LLS} correspond to the lower limit value of the actual T_{LLS} (see the main text for details).
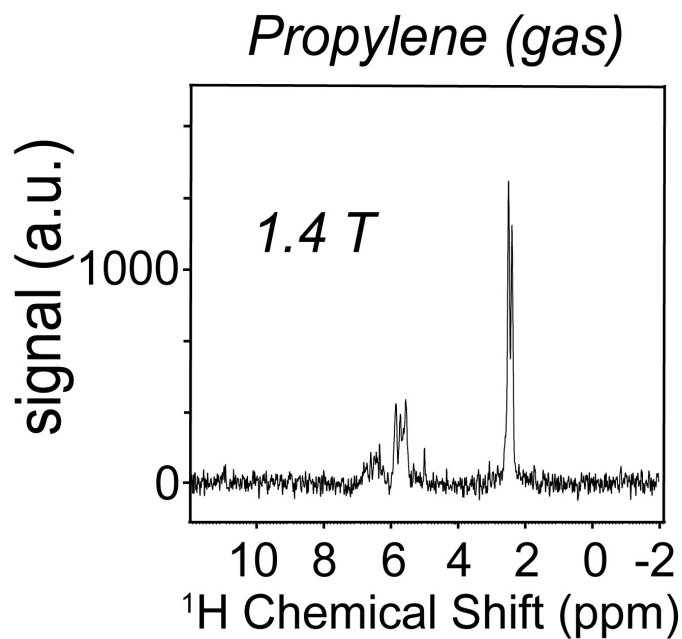
Figure S2. The thermally equilibrated proton NMR spectrum of propylene recorded using the 1.4 T NMR spectrometer.
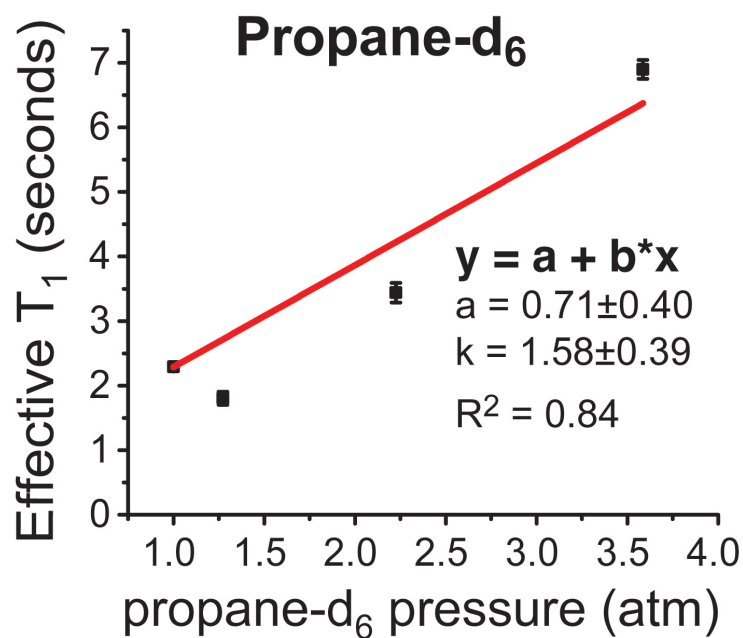

Figure S3. The exponential decay constants (effective T_1) for HP propane-d_6, which were obtained using the sequence described in Scheme 2c.

Table S1. Effective T_{LLS} values and corresponding error bars for the partial-SLIC excitation experiment described in Figure 6a of the main text. The data were acquired using a 1:1 mixture of propylene and pH_2 at 38 psi (or 3.6 atm) backpressure using otherwise-identical experimental conditions as those used to obtain the data in Figure 4b of the main text. The data set with "0" SLIC pulse duration corresponds to the 3.6 atm data point from Figure 4b of the main text. The effect of SLIC excitation on the remaining pseudo-singlet spin order pool is not taken into account in our simulations.

SLIC pulse duration in Figure 6a (milliseconds)	SLIC pulse application repetition time (TR) (milliseconds)	Effective T_{LLS} value (seconds)	Effective T_{LLS} error (seconds)
"0"	N/A	8.4*	0.6*
50	540	8.1	0.3
100	550	6.9	0.4
200	560	6.3	0.4
400	730	5.1	0.1
600	950	4.8	0.1
800	1170	5.4	0.1
1200	1610	5.3	0.1
1600	2030	5.0	0.1

* note this "0" value corresponds to a different measurement, when the sample chamber was refilled before each data point of the decay curved was taken using the pulse sequence shown in Figure 3b.