Supporting information
Parahydrogen induced polarization and spin order transfer in ethyl pyruvate at high magnetic fields

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1. Methods

**VP sample:** acetone or chloroform solution of 100 mM of VP, 5 mM [Rh]= [1,4-Bis(diphenylphosphino)butane](1,5-cyclooctadiene)rhodium(I) tetrafluoroborate (CAS= 79255-71-3, Merck). 1-13C-VP, 1-13C-VP-d3 and 1-13C-VP-d6 were synthesized according to Ref [1].

1 mL of the VP sample was loaded into a 10 mm heavy wall high-pressure NMR tube (513-7PVH-7, Wilmad-LabGlass).

**Hydrogenation.** Before hydrogenation, the tube with the VP sample was placed in a hot water bath of 55°C for 30 s. Then it was placed in the MRI and hydrogenation started within 10 s.

Hydrogenation is realized by flushing 90.5% pH2 at 10 bar through the solution. 100 PSI backpressure valve is connected to the outlet of the NMR tube. The solution was bubbled for 5-20 s, then SOT was applied after 2 s of settling down the liquid. 22 s and 7 s of hydrogenation time reported in the text is the sum of 20 s and 5 s of bubbling and 2 seconds of settling down.

Before all the following manipulations we measured one 13C spectrum using a 5° flipping angle. This was used to control hyperpolarization levels.

**Cleavage solution:** 1 mL of 1:1 distilled water to 1 M NaOH aqueous solution.

**Filters:**
- Particle filter Chromafil Xtra PET-20/25 0.20 μM
- Chloroform filter Tenax (Porous polymer absorber 60-0 mesh, Sigma 11982)

**ESOTHERIC parameters:**
- ESOTHERIC for 1-13C-EP-h8: $\tau_1 = 142$ ms, $\tau_2 = 28$ ms, $\tau_3 = 70$ ms, max theoretical polarization is 15.4%.
- ESOTHERIC for 1-13C-EP-d3: $\tau_1 = 165$ ms, $\tau_2 = 71$ ms, $\tau_3 = 100$ ms, max theoretical polarization is 57%.
- ESOTHERIC for 1-13C-EP-d6: $\tau_1 = \tau_3 = 166$ ms, $\tau_2 = 70$ ms, maximum theoretical polarization is 100%

**Polarizer MRI**

9.4 T high-resolution wide-bore micro-imager (9 cm bore, WB400, Avance NEO Bruker) with 25 mm 1H/13C imaging probe (MICWB40 RES 400 1H/13C 040/025 LLTR). We used following rectangular RF pulses for SOT: 1H-90° (75 W, 51.25 μs), 1H-180° (75 W, 102.5 μs), 13C-90° (200 W, 60 μs) and 13C-180° (200 W, 120 μs).

Before SOT, the spectrometer was shimmed and tuned using the same tube but without a capillary.

1H FLASH images of the tube filled with 1 mL chloroform are shown in Figure 4-A. 1H FLASH parameters were: 30 mm * 30 mm field of view, 384 x 384 matrix size, 1 mm slice thickness.

**Observation at 1 T benchtop NMR.**

1 T benchtop 1H/13C NMR spectrometers (Spinsolve Carbon, Magritek). The hyperpolarized spectra were acquired after 5° 13C excitation with a repetition time of 3 s. A thermal signal was acquired after the addition of 4 vol% Gd-contrast agent ([Gd], 1 mmol/mL, Gadovist, Bayer) using 90° 13C RF pulse, repetition time of 3 s, and 3600 scans.
2. ESOTHERIC in a three-spin system of $1^{-13}\text{C-EP-d6h2}$

![Diagram](image)

**Figure S1.** ESOTHERIC-Ref SOT applied to $1^{-13}\text{C-EP-d6h2}$: sequence itself (a), polarization isosurface as a function of $\tau_1$, $\tau_2$, and $\tau_3$ for $P=95\%$ (b), and effect of flipping angle deviation from nominal value on $P$ for $n=1$ (c), $n=5$ (d) with composite refocusing pulses ($\varphi_y2\varphi_x\varphi_y$) and $n=1$ (e), $n=5$ (f) with a single pulse refocusing ($\varphi_y2\varphi_x\varphi_y\rightarrow2\varphi_x$). The polarization of $99.7\%$ $1^{-13}\text{C-EP-d6}$ was reached at $\tau_1 = \tau_3 = 166\ms$, $\tau_2 = 70\ms$. The longest diameters of isosurface are 66 ms for $\tau_1$ and $\tau_3$, and 28 ms for $\tau_2$. To compensate for diffusion in the inhomogeneous magnetic field, multiple refocusing blocks are required; here calculations neglect diffusion, convection, and in homogeneous magnetic fields with ideal RF pulses. Note that a composite refocusing pulse is necessary to compensate for $B_1$ inhomogeneity and deviation of flipping angle from the nominal value (compare (d) and (e)). Although it seems that $n=1$ is superior to $n=5$ cases, the convection and diffusion in the inhomogeneous field is not included in the simulations and must be considered for better justification of the refocusing choice. The larger diagonals in c, d, e and f are $10^\circ$, $8.6^\circ$, $11.1^\circ$, $4.5^\circ$ for $\varphi(1\text{H})$ and $14.9^\circ$, $12.4^\circ$, $18.8^\circ$, $3.5^\circ$ for $\varphi(13\text{C})$. Only instantaneous (infinitesimally short) RF pulses were considered, hence the amplitude of gradients does not affect the RF-SOT.
3. ESOTERIC in a five-spin system of $^{13}$C-EP-$d3h5$

Figure S2. ESOTERIC-Ref SOT applied to $^{13}$C-EP-$d3h5$: sequence itself (a), polarization isosurface as a function of $\tau_1$, $\tau_2$, and $\tau_3$ for $P=50\%$ (b), and effect of flipping angle deviation from nominal value on $P$ for $n=1$ (c), $n=5$ (d) with composite refocusing pulses ($\varphi_y 2 \varphi_x \varphi_y$) and $n=1$ (e), $n=5$ (f) with a single pulse refocusing ($\varphi_y 2 \varphi_x \varphi_y \rightarrow 2 \varphi_x$). The polarization of 58% $^{13}$C-EP-$d3$ was reached at $\tau_1 = 165$ ms, $\tau_2 = 71.0$ ms, $\tau_3 = 100$ ms. The largest diagonals in at $\tau_1$, $\tau_2$, and $\tau_3$ directions are 112 ms, 48 ms, and 73 ms. To compensate for diffusion in the inhomogeneous magnetic field, multiple refocusing blocks are required; here calculations neglect diffusion, convection, and in homogeneous magnetic fields with ideal RF pulses. Note that a composite refocusing pulse is necessary to compensate for $B_1$ inhomogeneity and deviation of flipping angle from the nominal value (compare (d) and (e)). Although it seems that $n=1$ is superior to $n=5$ cases, the convection and diffusion in the inhomogeneous field is not included in the simulations and must be considered for better justification of the refocusing choice. The larger diagonals in c, d, and e are 17.6°, 16°, 20.2°, 7.6° for $\varphi(1H)$ and 22.7°, 22.7°, 27.7°, 22.3° for $\varphi(13C)$. Only instantaneous (infinitesimally short) RF pulses were considered, hence the amplitude of gradients does not affect the RF-SOT.
4. ESOTHERIC in a nine-spin system of $^{13}$C-EP-h8

Figure S3. ESOTHERIC-Ref SOT applied to $^{13}$C-EP-h8: sequence itself (a), polarization isosurface as a function of $\tau_1$, $\tau_2$ and $\tau_3$ for $P=13\%$ (b), and effect of flipping angle deviation from nominal value on $P$ for $n=1$ (c), $n=5$ (d) with composite refocusing pulses ($\varphi_y, 2\varphi_x, \varphi_y$) and $n=1$ (e), $n=5$ (f) with a single pulse refocusing ($\varphi_y, 2\varphi_x, \varphi_y \rightarrow 2\varphi_x$). The polarization of $15.4\%$ $^{13}$C-EP-h8 was reached at $\tau_1 = 142 \text{ ms}$, $\tau_2 = 28 \text{ ms}$, $\tau_3 = 70 \text{ ms}$. The largest diagonals in at $\tau_1$, $\tau_2$, and $\tau_3$ directions are 28 ms, 20 ms, and 54 ms. To compensate for diffusion in the inhomogeneous magnetic field, multiple refocusing blocks are required; here calculations neglect diffusion, convection, and inhomogeneous magnetic fields with ideal RF pulses. Note that a composite refocusing pulse is necessary to compensate for $B_1$ inhomogeneity and deviation of flipping angle from the nominal value (compare (d) and (e)). Although it seems that $n=1$ is superior to $n=5$ cases, the convection and diffusion in the inhomogeneous field is not included in the simulations and must be considered for better justification of the refocusing choice. The larger diagonals in c, d, and e are $16.5^\circ$, $14.5^\circ$, $10^\circ$, $4.1^\circ$ for $\varphi(\mathrm{H})$ and $26^\circ$, $30^\circ$, $34^\circ$, $12^\circ$ for $\varphi(\mathrm{C})$. Only instantaneous (infinitesimally short) RF pulses were considered, hence the amplitude of gradients does not affect the RF-SOT.
5. Hydrogenation of vinyl pyruvate

Figure S4. Repetition of hydrogenation. ESOTHERIC-Ref sequence (a) and $^{13}$C-integrals of the resulting $1^{13}$C-EP (product of $1^{13}$C-VP hydrogenation) in a consequent repetition of the polarization procedure as a function of bubbling time ($\tau_b$, B). Parameters: $\tau_1 = 142$ ms, $\tau_2 = 28$ ms, $\tau_3 = 70$ ms, $\tau_{G3} = 10$ ms, acquisition time is 1 s, hence the total duration of the experiment is $\tau_b + 1.2$ s which is equal to repetition time. Close to complete hydrogenation starts with $\tau_b = 10$ s.
6. Hydrogenation of $1^{-13}$C-vinyl pyruvate-$d6$

![Graph showing polarization of $1^{-13}$C-EP-$d6$ as a function of bubbling time.](image)

**Figure S5.** Polarization of $1^{-13}$C-EP-$d6$ as a function of bubbling time. ESOTHERIC-Ref(5) (Figure S4(a)) sequence with $\tau_1 = \tau_3 = 166$ ms, $\tau_2 = 70$ ms was used. Measured $T_1$ relaxation times of two protons coming from pH$_2$ were 10 s for CHD proton and 8 s for CHD$_2$ proton measured with T1IR sequence for one sample after hydrogenation with $\tau_b = 22$ s. The same sample was used to quantify here $^{13}$C polarization. The average $T_1$ of the hyperpolarized $^{13}$C was on average 26 s. Although complete hydrogenation is achieved only for $\tau_b > 12$ s the highest average polarization was achieved for $\tau_b = 7$ s and it was 17.4%, while for $\tau_b = 22$ s polarization was 6.5%.
7. Spontaneous cleavage of the sidearm in acetone

Figure S6. Hydrogenation in acetone-\textit{d6}. The presence of water in acetone results in slow cleavage of the sidearm. We measured the content of water (H$_2$O, HDO and D$_2$O) in acetone to be about 30 mM.
8. Distribution of $^1$H $B_1$ field in 5 mm BBFO probe along Z-axis

**Figure S7. $B_1$ field mapping for a 5 mm BBFO probe.** (A) Scheme of 5 mm NMR tube in the NMR probe (note that it is rotated 90°). Effective sensitive length of the BBFO probe is 23.6 mm. (B) Scheme of excitation-acquisition experiment where a gradient is switched on before excitation. Length of the pulse, $t$, was varied from 0 to 127.5 μs with the step of 0.5 μs. (C) One exemplary measurement (from top to bottom): NMR spectrum of 600 μL of H$_2$O:D$_2$O=9:1 in a high field NMR tube (524-PV-7) measured with the small flipping angle ($\varphi$) and gradient of 0.2% (top). Note that the single axis probe, and inbuilt Z-gradient system was used. Then each point of the phased spectrum was fitted with the sine decay function: $A \sin(\gamma B_1 t / 2\pi) e^{-t/\tau} + y_0$. Fitted parameters are given as: nutation frequency, $\gamma B_1$, duration of the 90°, $p_90$, pulse and amplitude, $A$. (D) Distribution of the angle: ECDF and PDF. Note the narrow distribution of the excitation angle for the small sample of 200 μL compared to 600 μL. For the experiment with 200 μL, the tube was moved to the middle of the coil.
9. ESOTHERIC efficiency in inhomogeneous B₁ field of 5 mm BBFO probe

Table S1. Effect of B₁ field inhomogeneity of 5 mm BBFO probe on SOT efficiency for EP-d6h2, EP-d3h5 and EP-h8. Four refocusing schemes were considered: single 180° refocusing pulse and composite pulse with number of refocusing elements n=1 and 5. The B₁ inhomogeneity for 200 μL sample is negligible for SOT efficiency. The same distribution was assumed for both ¹H and ¹³C B₁ fields. The used distributions are given on Figure S7D.

|                | Homogeneous B₁ | BBFO probe: 600 μL vs 200 μL distribution of B₁ |
|----------------|----------------|-------------------------------------------------|
|                | P₀ (%)         | n=1 [P, (P – P₀)/ P₀] | n=5 [P, (P – P₀)/ P₀] | n=1 [P, (P – P₀)/ P₀] | n=5 [P, (P – P₀)/ P₀] |
| **EP-d6h2**   |                |                                |                    |                                |                    |
| τ₁ = τ₂ = 166 ms, τ₃ = 70 ms | 99.7           | [96; -14.8%] vs [99.6; -0.1%]               | [65; -34%] vs [98; -1.7%] | [86; -14%] vs [99.6; -0.1%] | [86; -19%] vs [99; -0.7%] |
| **EP-d3h5**   |                |                                |                    |                                |                    |
| τ₁ = 165 ms, τ₂ = 71.0 ms, τ₃ = 100 ms | 58             | [48.5; -17.5%] vs [58; -1.3%]               | [44; -24%] vs [57.4; -0.5%] | [49.5; -14.5%] vs [58; -0.1%] | [47; -17.5%] vs [57.5; -2%] |
| **EP-h8**     |                |                                |                    |                                |                    |
| τ₁ = 142 ms, τ₂ = 28 ms, τ₃ = 70 ms | 15.4           | [12.3; -21%] vs [15.3; -0.2%]               | [9.5; -38%] vs [15; -1.6%] | [12.7; -18%] vs [15.4; -0.16%] | [12.2; -20%] vs [15.3; -0.16%] |
10. 10 mm NMR tube in 25 mm $^1$H/$^{13}$C imaging probe

Figure S8. Coronal (top) and axial (bottom) localizer (left) and FLASH (right) images of a 10 mm NMR tube in a 25 mm $^1$H/$^{13}$C probe at 9.4 T WB NMR. The 10 mm tube (Wilmad, 513-7PVH-7) was filled with 1 mL of acetone. The resulting sample size for 1 mL volume is 7 mm inner diameter (ID), and 25.6 mm height. Note that the $B_0$ field is not homogeneous on the top edge of the tube. In both cases, the field of view is 40 mm x 40 mm. This setting was used for all the experiments reported in the main text. This sample and setting were used to measure the $B_1$ map shown in Figure S11.
Figure S9. Coronal (top) and axial (bottom) localizer (left) and FLASH (right) images of a 10 mm NMR tube in a 25 mm $^1$H/$^{13}$C probe at 9.4 T WB NMR. The 10 mm tube (Wilmad, 513-7PVH-7) was filled with 1 mL of acetone. The resulting sample size for 1 mL volume is 7 mm inner diameter (ID), and 35.4 mm height. Note that the B$_0$ field is not homogeneous on the top edge of the tube. In both cases, the field of view is 50 mm x 50 mm. This sample and setting were used to measure the B$_1$ map shown in Figure S11.
11. $^1$H and $^{13}$C nutation curves for 25 mm $^1$H/$^{13}$C imaging probe

Figure S10. $^1$H (left) and $^{13}$C (right) nutation curves for the 1 mL chloroform-h measured with 25 mm $^1$H/$^{13}$C imaging probe (MICWB40 RES 400 $^1$H/$^{13}$C 040/025 LLTR). $^1$H power was 75 W and $^{13}$C power was 200 W. Experimentally, we used 50 μs and 60 μs 90° pulses for $^1$H and $^{13}$C respectively; 180° pulses had the same power and double amplitude as 90° pulses.
12. Distribution of $^1$H $B_1$ field in 25 mm $^1$H/$^{13}$C imaging probe along Z-axis

A) 25 mm $^1$H/$^{13}$C imaging probe

Sample sizes:
1. 1 mL, ID 7 mm, h=25.6 mm
2. 1.5 mL, ID 7 mm, h=35.4 mm

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B) Scheme of experiment

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C) Measurement:

$G=0.1\%$, 1 mL
$t=\text{Pulse}=[0, 1, ..., 199] \mu s$

$A \sin(\gamma B_1 t/2\pi)e^{-t/\tau} = \text{Fit}(t)$

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D) Angle distribution

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Figure S11. B, field mapping for a 25 mm $^1$H/$^{13}$C imaging probe. (A) Scheme of a 10 mm NMR tube (here 513-7PVH-7 was used) in the NMR probe (note that it is rotated $90^\circ$). (B) Scheme of excitation-acquisition experiment with the switch on gradient before excitation. Length of the pulse, $t$, was varied from 0 to 199 $\mu s$ with the step of 1 $\mu s$. (C) One exemplary measurement (from top to bottom): NMR spectrum of 1 mL acetone with the small flipping angle and gradient 0.1%. Note that here 3-axis 2.5 mic gradient system was used and only Z-gradient was applied. Then each point of the phased spectrum was fitted with the sine decay function: $A \sin(\gamma B_1 t/2\pi) e^{-t/\tau} + \gamma_0$. The fitted parameters are given as: nutation frequency, $\gamma B_1$, duration of the $90^\circ$, p90, pulse and amplitude, $A$. (D) Distribution of the angle: ECDF and PDF. Note the narrow distribution of the excitation angle for the small sample of 1 mL compared to 1.5 mL. Images of the samples are given on Figures S8 and S9. The centers of the samples were placed close to the isocenter of the magnet, gradient and RF-coil.
13. ESOTHERIC efficiency in inhomogeneous $B_1$-field of 25 mm $^1$H/$^{13}$C imaging probe

Table S2. Effect of $B_1$-field inhomogeneity of 25 mm $^1$H/$^{13}$C imaging probe on SOT efficiency for EP-$d6h2$, EP-$d3h5$ and EP-$h8$. Four refocusing schemes were considered: single 180° refocusing pulse and composite pulse with number of refocusing elements n=1 and 5. The same distribution was assumed for both $^1$H and $^{13}$C $B_1$-fields. The used distributions are given on Figure S11D.

| ESOTHERIC parameters | Homogeneous $B_1$ | 25 mm $^1$H/$^{13}$C imaging probe: 1.5 mL vs 1.0 mL distribution of $B_1$ |
|---------------------|------------------|--------------------------------------------------------------------------|
|                     | $P_0$ (%)        | $n=1 \frac{[P_0](P - P_0)}{P_0}$ vs $n=5 \frac{[P_0](P - P_0)}{P_0}$ | $n=1 \frac{[P_0](P - P_0)}{P_0}$ vs $n=5 \frac{[P_0](P - P_0)}{P_0}$ |
| EP-$d6h2$           | $\tau_1 = \tau_2 = 166$ ms, $\tau_3 = 70$ ms | 99.7 [86; -13.5%] vs [96.5; -3.2%] | [48; -51%] vs [78; -21%] | [85.4; -14%] vs [96; -4%] | [79.4; -20%] vs [94; -5%] |
| EP-$d3h5$           | $\tau_1 = 165$ ms, $\tau_2 = 71.0$ ms, $\tau_3 = 100$ ms | 58 [49; -17%] vs [55.7; -5%] | [38.5; -33%] vs [51; -11%] | [49; -15%] vs [55.5; -4%] | [47; -19%] vs [54.7; -5%] |
| EP-$h8$             | $\tau_1 = 142$ ms, $\tau_2 = 28$ ms, $\tau_3 = 70$ ms | 15.4 [11.6; -25%] vs [14; -8%] | [6; -60%] vs [11; -25%] | [12.4; -20%] vs [14.6; -5%] | [11.8; 22.5%] vs [14.3; 6.5%] |
14. Bruker pulse sequences

14.1. ESOTHERIC-Ref(1) with composite pulses

#include <Avance.incl>
#include <Grad.incl>
#include <Delay.incl>

"acqt0=p1*2/3.1416"
"p12=p1*2"
"p22=p2*2"
"p13=p1*5/90"
"d51=(d5-2*p22)/2" ; d5 is total tau1
"d52=(d6-2*p22)/2" ; d6 is total tau2
"d53=(d7-2*p22)/2" ; d7 is total tau3

1 ze
2 30m

d1
10m LOCKH_ON
30m pl1:f1
30m pl2:f2
50u UNBLKGRAD
10u gron1
< your hydrogenation procedure >
2u groff
300m gron2

(center (p1 ph2 p12 ph1 p1 ph2):f1
(p1 ph2):f1 ; L
1u groff
10mp gp3
5m BLKGRAD
(p13 ph2):f1
go=2 ph31
30m LOCKH_OFF mc #0 to 2 F0(zd)

exit
ph1=0
ph2=1
ph3=2
ph4=3
ph31=0

;pl1 : f1 channel - power level for pulse (default)
;pl2 : f2 channel - 90 pulse
;pl3 : power level for pulse (default)
;pl4 : channel - 90 pulse
;pl5 : total tau1
;pl6 : total tau2
;pl7 : total tau3
;gp1 : gradient during bubbling, large
;gp2 : gradient during SOT, tiny
;gp3 : gradient after L
14.2. ESOTHERIC-Ref(5) with composite pulses

#include <Avance.incl>
#include <Grad.incl>
#include <Delay.incl>
"acqt0=p1*2/3.1416"
"p12=p1*2"
"p22=p2*2"
"p13=p1*5/90"
"d51=(d5-2*p22)/10" ; d5 is total tau1
"d52=(d6-2*p22)/10" ; d6 is total tau2
"d53=(d7-2*p22)/10" ; d7 is total tau3
f: ze
2: 30m

d1
10m LOCKH_ON
30m pl1:f1
30m pl2:f2
50u UNBLKGRAD
10u gron1
< your hydrogenation procedure >
2u grof
300m gron2

(p1 ph2 p12 ph1 p1 ph2):f1 ; (p2 ph2):f2
(st (p1 ph2 p12 ph1 p1 ph2):f1)
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 1
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 2
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 3
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 4
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 5

(p1 ph2 p12 ph1 p1 ph2):f1
(st (p1 ph2 p12 ph1 p1 ph2):f1)
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 1
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 2
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 3
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 4
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 5

(p1 ph2 p12 ph1 p1 ph2):f1
(st (p1 ph2 p12 ph1 p1 ph2):f1)
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 1
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 2
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 3
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 4
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 5

(p1 ph2 p12 ph1 p1 ph2):f1
(st (p1 ph2 p12 ph1 p1 ph2):f1)
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 1
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 2
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 3
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 4
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 5

(p1 ph2 p12 ph1 p1 ph2):f1
(st (p1 ph2 p12 ph1 p1 ph2):f1)
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 1
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 2
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 3
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 4
(d51 p2 ph2 p22 ph1 p2 ph2 d51):f2 ; 5

(p1 ph2):f1 ; L
1u grof
10mp:gp3
5m BLKGRAD
(p13 ph2):f1
go=2 ph31
30m LOCKH_OFF mc #0 to 2 F0(zd)

exit
ph1=0
ph2=1
ph3=2
ph4=3
ph31=0
; p1 : f1 channel - power level for pulse (default)
; p1 : f1 channel - 90 pulse
; p2 : f2 channel - power level for pulse (default)
; p2 : f2 channel - 90 pulse
; d5 : total tau1
; d6 : total tau2
; d7 : total tau3
; gp1 : gradient during bubbling, large
; gp2 : gradient during SOT, tiny
; gp3 : gradient after L
14.3. ESOTHERIC-Ref(1) wo composite pulses

#include <Avance.incl>
#include <Grad.incl>
#include <Delay.incl>

"acq0=--p1*2/3.1416"
"p12=p1*2"
"p22=p2*2"
"p13=p15/90"
"d51=(d5-p22)/2" ; d5 is total tau1
"d52=(d6-p22)/2" ; d6 is total tau2
"d53=(d7-p22)/2" ; d7 is total tau3

f: =
2 30m
d1
10m LOCKH_ON
30m pl1:f1
30m pl2:f2
50u UNBLKGRAD
10u gron1

< your hydrogenation procedure >
2u groff
300m gron2
(p2 ph2):f2
(35m pl1:ph1):f1 (d51 p22 ph1 d51):f2 ; 1
(p2 ph4):f2
(d52 p22 ph1 d52):f2 ; 1

(35m pl1:ph1):f1 (p2 ph2):f2
(35m pl2:ph2):f1 (d53 p22 ph1 d53):f2 ; 1
(p1 ph2):f1 ; L
1u groff
10mp:gp3
5m BLKGRAD
(p13 ph2):f1
go=2 ph31
30m LOCKH_OFF mc #0 to 2 F0(zd)

exit
ph1=0
ph2=1
ph3=2
ph4=3
ph31=0
:pl1 :f1 channel - power level for pulse (default)
:pl1 :f1 channel - 90 pulse
:pl2 :f2 channel - power level for pulse (default)
:pl2 :f2 channel - 90 pulse
:d5 : total tau1
:d6 : total tau2
:d7 : total tau3
:gp1 : gradient during bubbling, large
:gp2 : gradient during SOT, tiny
:gp3 : gradient after L
14.4. ESOTHERIC-Ref(5) wo composite pulses

```c
#include <Avance.incl>
#include <Grad.incl>
#include <Delay.incl>
"acq0=p1/2*3.1416"
"p12=p1"2"
"p22=p2"2"
"p13=p15/90"
"d51=(d5-p22)/10" ;d5 is total tau1
"d52=(d6-p22)/10" ;d6 is total tau2
"d53=(d7-p22)/10" ;d7 is total tau3
1. ze
2. 30m
d1
10m LOCKH_ON
30m pl1:f1
30m pl2:f2
50u UNBLKGRAD
10u gron1
< your hydrogenation procedure >
2u groff
300m gron2
(p2 ph2):f2
(center (p12 ph1):f1 (d51 p22 ph1 d51):f2) ; 1
(center (p12 ph1):f1 (d51 p22 ph1 d51):f2) ; 2
(center (p12 ph1):f1 (d51 p22 ph1 d51):f2) ; 3
(center (p12 ph1):f1 (d51 p22 ph1 d51):f2) ; 4
(center (p12 ph1):f1 (d51 p22 ph1 d51):f2) ; 5
(p2 ph4):f2
(d52 p22 ph1 d52):f2 ; 1
(d52 p22 ph1 d52):f2 ; 2
(d52 p22 ph1 d52):f2 ; 3
(d52 p22 ph1 d52):f2 ; 4
(d52 p22 ph1 d52):f2 ; 5
(center (p1 ph1):f1 (p2 ph2):f2)
(center (p12 ph1):f1 (d53 p22 ph1 d53):f2) ; 1
(center (p12 ph1):f1 (d53 p22 ph1 d53):f2) ; 2
(center (p12 ph1):f1 (d53 p22 ph1 d53):f2) ; 3
(center (p12 ph1):f1 (d53 p22 ph1 d53):f2) ; 4
(center (p12 ph1):f1 (d53 p22 ph1 d53):f2) ; 5
(p1 ph2):f1 ; L
1u groff
10mp:gp3
5m BLKGRAD
(p13 ph2):f1
go=2 ph31
30m LOCKH_OFF mc #0 to 2 F0(zd)
```

exit
ph1=0
ph2=1
ph3=2
ph4=3
ph31=0
;pl1 : f1 channel - power level for pulse (default)
;pl2 : f1 channel - 90 pulse
;pl2 : f2 channel - power level for pulse (default)
;p2 : f2 channel - 90 pulse
;d5 : total tau1
;d6 : total tau2
;d7 : total tau3
;gp1 : gradient during bubbling, large
;gp2 : gradient during SOT, tiny
;gp3 : gradient after L
15. References

[1] R. Herges, A. Brahms, A. Pravdivtsev, T. Stamp, F. Ellermann, F. Sönnichsen, J.-B. Hövener, 2022, DOI 10.26434/chemrxiv-2022-xttst.