SUPPORTING INFORMATION

for

Clinical-Scale Batch-Mode Production of Hyperpolarized Propane Gas for MRI

Oleg G. Salnikov,^{a,b} Panayiotis Nikolaou,^c Nuwandi M. Ariyasingha,^d Kirill V. Kovtunov,^{a,b} Igor V. Koptyug,^{a,b} and Eduard Y. Chekmenev^{d,e}*

^a International Tomography Center, SB RAS, 3A Institutskaya St., Novosibirsk 630090, Russia

- ^b Novosibirsk State University, 2 Pirogova St., Novosibirsk 630090, Russia
- ^c Vanderbilt University Institute of Imaging Science (VUIIS), Department of Radiology, Vanderbilt
- University, Nashville, Tennessee 37232-2310, United States
- ^d Department of Chemistry, Integrative Biosciences (Ibio), Wayne State University, Karmanos
- Cancer Institute (KCI), Detroit, Michigan 48202, United States
- ^eRussian Academy of Sciences, Leninskiy Prospekt 14, Moscow 119991, Russia



Figure S1. Scheme of experimental setup for batch-mode production and NMR detection of hyperpolarized propane gas.



Figure S2. Scheme of experimental setup for continuous mode production and NMR detection of hyperpolarized propane gas.



Figure S3. (a) Reaction scheme of pairwise addition of parahydrogen to propylene to form hyperpolarized propane. (b) ALTADENA ¹H NMR spectra of continuously flowing HP propane gas

before (blue trace) and after (red trace) the catalyst employment in cyclopropane hydrogenation. Conditions: catalyst mass = 118 mg, T = 100 °C, P = 90 psig, gas flow rates 480 sccm for propylene and 960 sccm for p-H₂.



Figure S4. (a) Reaction scheme of pairwise addition of parahydrogen to propylene to form hyperpolarized propane. (b) ALTADENA ¹H NMR spectra of continuously flowing HP propane gas before (blue trace) and after (red trace) the catalyst employment in cyclopropane hydrogenation. Conditions: catalyst mass = 280 mg, T = 130 °C, P = 90 psig, gas flow rates 480 sccm for propylene and 960 sccm for p-H₂.



Figure S5. Enlarged version of the second image from the series of MRI HP propane images shown in Figure 4a.



Figure S6. Corresponding image of thermally polarized neat water phantom for comparison with series of HP propane images shown in Figure 4a.