Electronic Supplementary Material (ESI) for Chemical Science.

Supporting Information

Efficient Cross-effect Dynamic Nuclear Polarization without Depolarization in High-resolution MAS NMR

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1. EPR analysis

Table SI 1. Results from the fit of the CW 285 GHz EPR TEMTriPol-1 spectrum with two components with two different values of the exchange interaction.

Component	J	α	β	γ	**Weight**
#1	10 MHz	-37°	102°	45°	0.6
#2	80 MHz	214°	105°	5°	0.4

2. Effect of the value of T_{1n} in the simulations

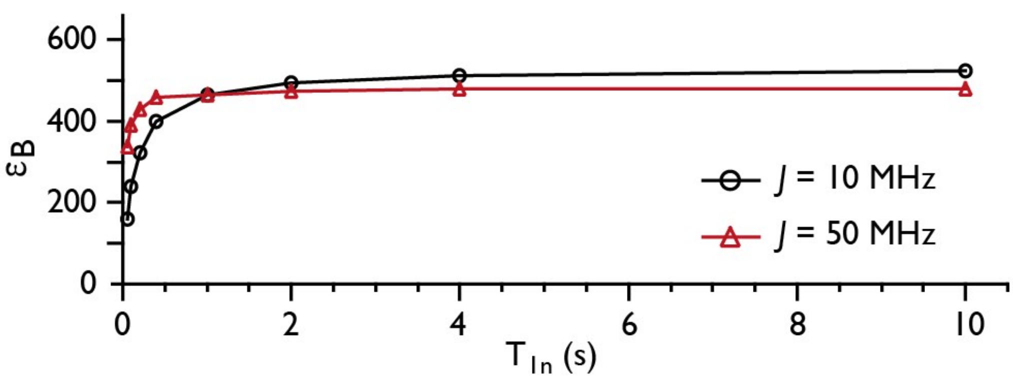

Figure SI 1. Evolution of ϵ_B as a function of the nuclear relaxation times for two different exchange interaction values $J_{a,b}/2\pi$ = 10 MHz (black circles), $J_{a,b}/2\pi$ = 50 MHz (red triangles) for $B_0 = 18.798$ T, $\omega_{\mu w}/2\pi$ = 527.1 GHz corresponding to the optimal positive DNP position, and a MAS frequency of 8 kHz.

3. Depolarization and the electron-electron coupling strength

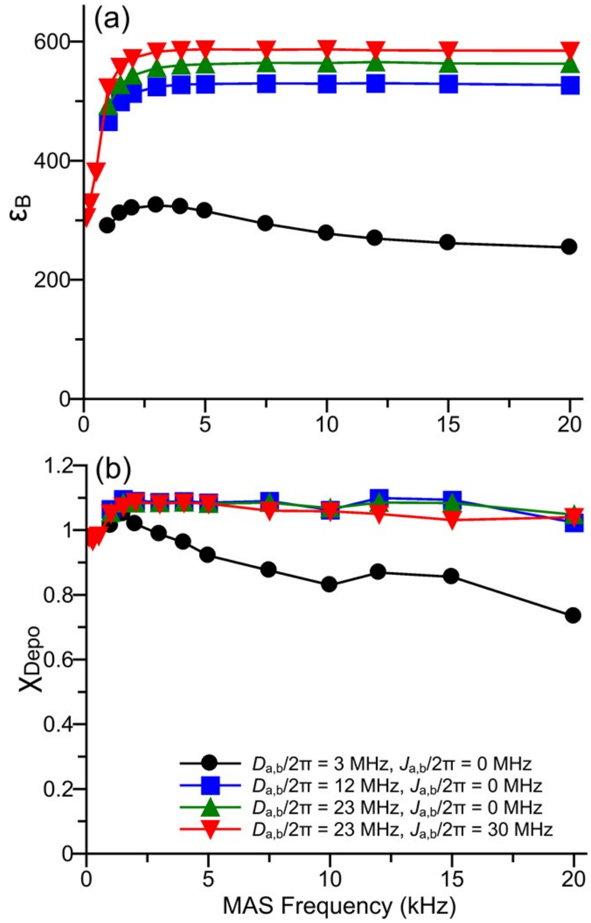

Figure SI 2. Simulations of the MAS dependence of the theoretical enhancement factor ε_B (a) and of the depolarization factor χ_{depo} (b) for different dipolar couplings and $D_{a,b}$ and exchange-interaction ($J_{a,b}$): $D_{a,b}/2\pi$ = 3 MHz (black circles), $D_{a,b}/2\pi$ = 12 MHz (blue squares), $D_{a,b}/2\pi$ = 23 MHz (green up-pointing triangles) and $J_{a,b}/2\pi$ = 0 MHz for all, $D_{a,b}/2\pi$ = 23 MHz and $J_{a,b}/2\pi$ = 30 MHz (red down-pointing triangles). B_0 = 9.394 T and $\omega_{\mu w}/2\pi$ = 263.45 GHz.

4. ^{13}C-^{13}C correlation on NA cellulose at 18.8 T

Table SI 2. Chemical Shifts of cellulose I_{α} and I_{β} taken from Kono *et al.* [1]

Allomorph	δ/ppm	atom
Cellulose I_{α}	106.9	C1
	91.6	C4
	90.8	C4
	76.5	C3
	76.2	C3
	74.4	C5
	73.6	C2
	72.6	C2,5
	67.1	C6
Cellulose I_{α}	107.6	C1
	105.9	C1
	90.6	C4
	90.0	C4
	76.8	C3
	76.0	C3
	74.2	C5
	73.0	C2,5
	67.5	C6
	66.9	C6

1. H. Kono, S. Yunoki, T. Shikano, and M. Fujiwara, 2002, 7506–7511.