Magn. Reson. Discuss.,
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Open Access MAGNETIC RESONANCE Discussions

Interactive comment on "Study of electron spectral diffusion process under DNP conditions by ELDOR spectroscopy focusing on the ^{14}N Solid Effect" *by* Marie Ramirez Cohen et al.

Anonymous Referee #1

Received and published: 4 March 2020

This manuscript reports on the influence of the ^{14}N solid effect on electron spectral diffusion profiles measured at nitroxide radical concentrations relevant for dynamic nuclear polarization. The authors approach the problem by combining considerations on spin dynamics with an empirical parametrized fitting model. This approach leads to an improvement compared to simulations disregarding the ^{14}N solid effect and, indeed, at 20 mM concentration to reasonable agreement with experimental results. At an intermediate concentration of 10 mM, the model turns out to be simplistic. This is useful work, which improves understanding of electron spectral diffusion at high nitroxide radical concentrations. I recommend publication in Magnetic Resonance after minor revision that takes into account the following suggestions:

1. It is very awkward to report and use a nitroxide g tensor g = [2.0065, 2.0037, 1.9997], which is certainly wrong. The values reported earlier by Florent et al. were (almost) in line with expectations from numerous other reports and from quantum-chemical computations. The sentence quoting a "systematic error of 4 mT in the determination of the external magnetic field" is ambiguous, as it does not tell whether the error applies to Florent et al. or to the present work (it is the present work). You should be able to check this by using the proton Larmor frequency from ELDOR-detected NMR for calibration. It may not be necessary to repeat all computations (the anisotropy is correct, the absolute error too small to influence these simulations), but the issue should be reported in a clear way.

2. Please explain why T_M can serve as a lower limit for T_{2mw} (page 11, line 13, and wouldn't $T_{2\rho}$ be a better choice?). This is not obvious to me.

3. You claim (page 19, line 2) that the weaker ^{14}N signals on the negative side of the allowed transition are presumably due to co-alignment of ^{14}N and ^{1}H hyperfine tensors. Did you test this?

4. You appear to cite every paper on W-band ELDOR-detected NMR on nitroxides (page 4, line 7/8), except for the very first one (DOI: 10.1016/S0009-2614(98)00765-9)

Typos:

Page 4, line 29: space missing between "0.6" and "mm"

Page 9, caption Figure 2: there is a surplus red "[** small m]"

Page 11, line 24: "signals reveal very weak signals" is awkward (signals are very weak)

Page 12, line 7: "three-spin calculation" (delete surplus "s")

Page 12, line 15: "we added reintroduced" should only read "we added"

Page 12, line 20: "on for the different forbidden transitions" shouldn't this read "one for each of the forbidden transitions"?

Page 14, line 2: “see Fig. 3” (not 2)

Page 15, line 15: notorious Microsoft Word box for a symbol in front of “20-70 MHz”

Page 16, caption Fig. 3: spaces missing between “0” and “MHz” as well as between “100” and “MHz”

Page 22, line 3: Reference with superscript 7 should be in Name, Year format

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