

Magn. Reson. Discuss., author comment AC2
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Reply on RC1

Nino Wili et al.

Author comment on "Reverse dynamic nuclear polarisation for indirect detection of nuclear spins close to unpaired electrons" by Nino Wili et al., Magn. Reson. Discuss., <https://doi.org/10.5194/mr-2022-12-AC2>, 2022

Thank you for your comments. We will address all points in the revised manuscript, but I will give some preliminary answers here already for the sake of discussion.

1. Indeed the NOVEL condition will be difficult to fulfill at higher fields. However, the method might also work with other DNP sequences, for example, the adiabatic solid effect (<https://doi.org/10.1021/acs.jpcclett.0c00654>). If the NOVEL condition cannot be fulfilled, it should be possible to use an amplitude modulation scheme where the modulation frequency is part of the resonance condition. We (and other co-authors) recently showed this for the case where the available power is even higher than than the NOVEL case (<https://arxiv.org/abs/2203.07023>), but it should also be possible for the case of lower power - at the expense of a lower scaling factor. Since the first transient of the NOVEL transfer is already reached after a few hundred ns, modulated sequences with a lower scaling factor, but better bandwidth might turn out to be beneficial after all.

2. The chirp pulses were only used as hyperfine-decoupling during the waiting time T. They provide efficient and easy-to-setup inversion. No chirps were used for the DNP steps. We expect that the partial excitation will have the same influence as in other EPR sequences, namely that of orientation selection (i.e. only some orientations will be excited).
The experiment should still work in principle.

3. We expect this to work in principle for nitroxides (but experiments will have to be done). One particular problem in Q-band might be the nitrogen hf-coupling, which for some orientations might coincide with the proton Larmor frequency. It is not entirely clear at the moment (to me personally) how this affects the resonance conditions and the DNP transfer.

4. This is indeed the case, and I apologize for the omission of some experimental details. This will be provided in the revised manuscript

5. The periodic inversion pulses for hyperfine decoupling are used during the waiting time T. We will clarify this either in the figure caption or in an additional sequence diagram.

