MAGNETIC RESONANCE
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Discussions

Magn. Reson. Discuss., community comment CC1
https://doi.org/10.5194/mr-2021-29-CC1, 2021

Comment on mr-2021-29

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Community comment on "Improved NMR transfer of magnetization from protons to half-integer spin quadrupolar nuclei at moderate and high magic-angle spinning frequencies" by Jennifer S. Gómez et al., Magn. Reson. Discuss., https://doi.org/10.5194/mr-2021-29-CC1, 2021

There has been increasing interest in CPMAS from 1H to half-integer quadrupolar nuclei in order to materilize the high 1H DNP enhancement through efficienct spin diffusion for detecting quadrupolar nuclei. This work is practically useful to this effort in addtion to proximity information by optimizing the pulse sequences. They have chosen gamma-alumina as the sample system which has fairly large shift dispersion at 800 MHz field. The proton homonuclear coupling is relatively weak as compared to rigid orgainic molecules. They have also chosed 20 and 62.5kHz spinning speeds and typical rf fields that 3.2mm and 1.3mm probes can achieve. From previous publication, the authors also have added adibatic pulses to improve the offset performance and some moodifications to the blank rotor period to reduce the 1H T2 loss. There is no doubt that they have improrved the performance, but I am not sure if this optimization is generally applicable to other samples and spin systems. My particular concern is strong 1H homonuclear coupling. It is correct that the first-order 1H homonuclear term is not 'recoupled' for the selected heteronuclear recoupling sequences. What about the high-order homonuclear terms that causes the short T2 especially at not-so-high spinning speeds? My observation is 1H T2 under the recoupling is often very short, thus can have strong effect to the performances. I wonder if the authors could provide some 1H T2 infomation under the recoupling sequence, say as compared to regular spin-echo T2 decay. In addtion, is it possible to program the experiment to avoid the blank rotor period to rotor during the CT p-pulse by simultaneous pulses.

I would be interetsed in the overall transfer efficiency. It seems very low based on the S/N. Of course, only a small portion of gamma-alumina has 1H in its vicinity. It would help to know where the main loss comes from for future improvement.

I would like to commend this work on the through description of symmtry based recoupling and search for recoupling sequences that are optimal for CPMAS with practically feasible spinning speed and rf field for 3.2mm and 1.3mm probes.

The first citation on PRESTO,p2l65, should include paper from the original paper from Levitt's group.