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MAGNETIC RESONANCE
Discussions

Interactive comment on "Origin of the Residual Linewidth Under FSLG-Based Homonuclear Decoupling in MAS Solid-State NMR" *by* Johannes Hellwagner et al.

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*It will be interesting to see how compensated cycles perform (even though the contribution the line width is marginal) for super-cycled FSLG/PMLG schemes where the effective axis is more along the z-axis. Does the supercycling minimise the third-order effect in any way or RF inhomogeneity?

The reason why we analyzed the performance of the basic FSLG sequence was the fact that the theoretical description is simpler than the one for the super-cycled versions and we wanted to be able to compare theory, experiments and simulations in order to gain as much insight as possible. Therefore, we did not yet look at super-cycled

implementations and cannot give a definite answer to this question. We would prefer not to speculate about the effects of super cycling on these broadening mechanisms.

*The compensated schemes push the spectrum to lower ppm values. Is it totally right that transient compensated schemes yield spectra with absolute values of the frequency? For instance, in Figure 6, the shift is uniform, and unless one has the reference, it is impossible to say which gives the absolute values right. And if the reference is fixed, for a given spectrometer, under given conditions, the shift is always the same, unless the higher-order terms come into play for this as well. That is not very clear in the text.

The transient compensation leads to two effects that make the experiment more reproducible and the chemical shifts less arbitrary. The first is the better balancing of the forward and backward nutation in the FSLG experiment due to a better match of the rf-field amplitudes under phase ramps with positive and negative slopes. This part was actually missing and has been added to the manuscript (line 317) as "... to be due to the better compensation of the effective nutation over a full FSLG cycle and the additional ...". The second reason is the better elimination of fictitious fields as stated on line 318. This will not lead to absolute chemical shifts because the transient compensation is not perfect and especially the forward and backward nutation in the FSLG experiment will always produce some small residual effective nutation but this contribution is minimized by the transient compensation. We have changed the conclusions on line 435 to a more cautious formulation: "Removal of phase transients and adaption of the pulse sequence led to more predictable results in terms of chemical-shift scaling and smaller variations of the shift on the frequency axis.". We hope that this change makes it clearer that absolute frequency calibration is not possible even with transient compensation.

*The spectrum obtained with the compensated scheme, Figure 6, has certain artifacts like a shoulder for the NH_3+, any comments.

We are not sure what the source of the shoulder is. The NH3 line of the compensated spectrum is slightly narrower and it could originate from some structure that starts to become visible. It could also be due to an artefact that shifts to a different spectral position in the compensated spectra. Since we do not know, we would prefer not to speculate about it.

*Any comments on the performance of these schemes at higher MAS, higher than 60 kHz. Also in the introduction when slow to medium MAS frequencies are mentioned, perhaps it is good to indicate what the frequencies are.

We have added a number to the text on line 33 to quantify the slow to medium MAS frequencies by adding "(slower than 60 kHz)". The exact number is debatable but we think that starting at 60 kHz averaging by MAS leads to some resolution in proton spectra. We have not looked at fast MAS experimentally and cannot comment on the performance under such conditions.

*Certain inconsistencies, I believe, like definition of $\tau_i (i = 1to4)$ on pages 6 and 7, for instance.

textcolorblueWe have added more references to "A. Garon, R. Zeier, S.J. Glaser, Visualizing operators of coupled spin systems, Phys. Rev. A. 91 (2015)" where the three-spin spherical tensor operators are defined. The caption of Fig. 1 was amended with the sentence: "For a definition of the three-spin spherical-tensor operators, see Ref. (Garon et al., 2015)." and after the expressions for the operators in the main text on line 155 we added: "... tensor operators where we follow the definition and notation introduced in Ref. (Garon et al., 2015).". We hope that this clarifies this point.

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