

Magn. Reson. Discuss., referee comment RC1
<https://doi.org/10.5194/mr-2021-45-RC1>, 2021
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Comment on mr-2021-45

Anonymous Referee #1

Referee comment on "Residual dipolar line width in magic-angle spinning proton solid-state NMR" by Matías Chávez et al., Magn. Reson. Discuss.,
<https://doi.org/10.5194/mr-2021-45-RC1>, 2021

This is a very well written paper about an interesting and key topic in solid-state NMR, namely understanding the spinning-frequency dependence of ^1H solid-state NMR lineshapes under magic-angle spinning (MAS). Specifically, exact numerical simulations are compared to predictions from second- or third-order Floquet theory effective Hamiltonian expressions. In this way, subtle effects relating a change from a $1/\text{spinning frequency}$ to $1/\text{spinning frequency}^2$ dependence as well as small shifts in the lineshape centre of gravity are explored, notably considering the usual case of ^1H spins with different ^1H chemical shifts. Experimental ^1H MAS NMR spectra up to 160 kHz MAS are also presented for ortho-phospho-L-serine showing the same shifts in the lineshape centre of gravity are well explained by the theoretical predictions.

Minor improvements

Fig. 4 caption, 3rd line: deviations which become

Fig. 6 explain the straight lines in the caption

Fig. 8 avoid repeat of blue and red in c to avoid confusion with colours used in b: how about green and orange instead?

Can the SI use S1 etc labels for page numbers, sections, Tables and Figures.

SI Figure 2: line 4, space between set and between