

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

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Referee comment on "Residual dipolar line width in magic-angle spinning proton solid-state NMR" by Matías Chávez et al., Magn. Reson. Discuss.,  
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This is a very well written paper about an interesting and key topic in solid-state NMR, namely understanding the spinning-frequency dependence of  $^1\text{H}$  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  $^1\text{H}$  spins with different  $^1\text{H}$  chemical shifts. Experimental  $^1\text{H}$  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, 3<sup>rd</sup> 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