

Magn. Reson. Discuss., author comment AC2
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Reply on RC2

Corinna Dietrich et al.

Author comment on "The relation between crystal structure and the occurrence of quantum-rotor-induced polarization" by Corinna Dietrich et al., Magn. Reson. Discuss., <https://doi.org/10.5194/mr-2021-51-AC2>, 2021

"While this represents a negative finding, it is still a rather conclusive one, and suited for publication in Magnetic Resonance."

We are glad that also this reviewer considers our ms worth to be published.

"I have the following suggestions for the manuscript:

- In the abstract, the authors write that "a high tunnel frequency is favorable". This should in my view be rephrased to "is required". After all, if the tunnel frequency is small, there is no quantum rotation, and - consequentially - no QRIP will be observed."

Thanks, we changed that statement accordingly.

"- It may be confusing to readers who are not very familiar with the effect, that a free rotor shows a large tunneling splitting. Indeed, in the limit of free rotation, there should be no tunneling. It would therefore be valuable to point out that the tunneling splitting is defined as the difference between the first two rotational states, and it is the population differences across these states that give rise to QRIP."

We added that statements into the introduction.

"- The authors find a small, but significant tunneling splitting in compounds 8 and 12, but do not explicitly report details on their attempt to observe QRIP in this compound. Was such an attempt made? What was the concentration after dissolution? Is ¹³C labelling possible? Perhaps it is worth pointing out, that larger molecules will also tend to "loose" quantum-rotor-induced polarization more quickly due to their longer correlation times."

We indeed did perform three dissolution experiments on compound 8 and two dissolution experiments on compound 12. According to your suggestion we added some more details to the text and included the hint at the longer correlation times. The possibility of ¹³C

labelling was added to the conclusion.

"- The authors report on MAS QRIP experiments. How have these actually been conducted? QRIP requires equilibration at 4 Kelvin even in the most favourable cases. Have the authors performed such a temperature jump experiment with MAS? If yes, it would be prudent to give the details of temperature vs. time. A key parameter would be, after all, the time required to ramp the temperature from 4 K to say 30 K. If no such experiment has been conducted, the MAS data will be completely inconclusive with respect to QRIP, and should not be shown in the manuscript."

The experimental details are given in chapter 2.2. We added the information about the temperature (4.2 K helium temperature to room temperature in the magnet).

"Finally, the manuscript is very well written overall, but the jubilee's spelling in the special issue statement should be checked."

We corrected the spelling of the name of the jubilee.