

Magn. Reson. Discuss., referee comment RC3  
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## **Comment on mr-2021-51**

Alexej Jerschow (Referee)

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Referee 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-RC3>, 2021

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This manuscript describes a search for quantum-rotor induced polarization effects in methyl groups of compounds similar to gamma picoline. The similarity is defined by having similar methyl-methyl distances and bond angle configurations. A number of identified compounds have been studied and the QRIP effect is either nonexistent or weak in them. This leads the authors to the conclusion that the molecular similarity criteria used are not sufficient to ensure the presence of this effect, and/or that nuances of the crystal structure are important for it to occur. The work therefore represents a negative result with regard to the initial hypothesis, while it does not preclude other factors and molecules being identified as displaying the QRIP effect in the future. A minor comment would be that clarity could be improved with regard to how narrow the initial hypothesis is. For example, is the concerted methyl rotation really the best way to insure the lowest amount of friction? Perhaps the authors may also wish to state that their study would indicate that it is not the case? Furthermore, I wonder whether relaxation effects could be of relevance here (e.g. through lattice dynamics / vibrations).