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Reply on RC3

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-AC3, 2021

"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."

We agree with that summery.

"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? Perhpas the authors may also wish to state that their study would indicate that it is not the case?"

We agree that also mechanisms other than pairwise concerted rotation of two face-to-face methyl groups are not the only and possibly not even the best way to lower the rotational barrier of methyl rotation in a crystalline environment. Further candidates include a gear-like coupling of two adjacent methyl groups (which, however, we did not observe in any real molecule), and phonon modes of the molecular crystal, which could couple to the rotational motion of a methyl. We also added that statement into the final discussion.

"Furthermore, I wonder whether relaxation effects could be of relevance here (e.g. through latttice dynamics / vibrations)."

That is a good point: Cross relaxation is an essential part of the QRIP theory as proposed by Levitt et al. Competing relaxation pathways would quench the effect. We added a short remark into the final discussion.