

Magn. Reson. Discuss., author comment AC1
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Reply on RC1

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-AC1>, 2021

"Although the results are largely negative, I do think that this study deserves to be in the scientific literature, since it demonstrates that either gamma-picoline and the few other compounds that show a strong QRIP possess some very subtle structural feature that has escaped detection by the authors in their detailed study, or possibly that the crystal structure is not the determining factor after all. For example some subtlety of the phonon spectrum might be responsible, although I confess that I have not much of an idea where to look. Nevertheless, I do suggest that in their conclusions, the authors might at least speculate on the possibility that molecular and crystal structures are not the determining factor for this phenomenon after all.

In summary this is a worthwhile study, and should be published, even though ..."

We are glad to learn that the referee finds our work publishable although our results are largely negative. We also thank for the suggestion to add a speculation into the final paragraph whether the discussion of the crystal structure is sufficient to understand the phenomenon of QRIP.

"A few small things should be corrected. It is not quite true that "only the methyl groups of a few substances seem to allow for the effect". Very weak QRIP effects have also been observed in 17O water-endofullerene (doi.org/10.1103/PhysRevLett.120.266001). "

Ref added.

"The authors cite Ludwig et al. (PNAS, 2010) as having studied QRIP, but the attribution of the described effects to QRIP have been disputed (doi.org/10.1016/j.jmr.2017.12.009). "

We excluded the reference by Ludwig et al. 2010 and instead added the more suitable review by Meier 2018.

"I was surprised to see that the article cited as Roy 2013 has a completely incorrect list of authors. That error suggests that all references should be rechecked carefully. "

We corrected that Ref and rechecked all other refs.

"A compilation of the studied molecular systems in one place would be helpful. In some cases one has to trawl through the text to find what a certain number refers to. "

A table with all the investigated compounds has been added to the begin of the results chapter.

"I do not feel that providing the X-ray structural data of some of the compounds is worthwhile in the main text (figures 7, 8). The MAS spectra of the MOFs also do not seem worthy of display in the main manuscript, especially since the QRIP results were negative. "

We shifted these Figs to the Supplement.

"On the other hand, the authors cite neutron scattering data which shows a tunneling splitting, but never provide this data at all. Personally, I would be more interested in seeing that."

The data are given in the Supplement.