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Magn. Reson. Discuss., community comment CC1
https://doi.org/10.5194/mr-2021-39-CC1, 2021

Comment on mr-2021-39 from the NMR Dept., Institute of Macromolecular Chemistry, Prague

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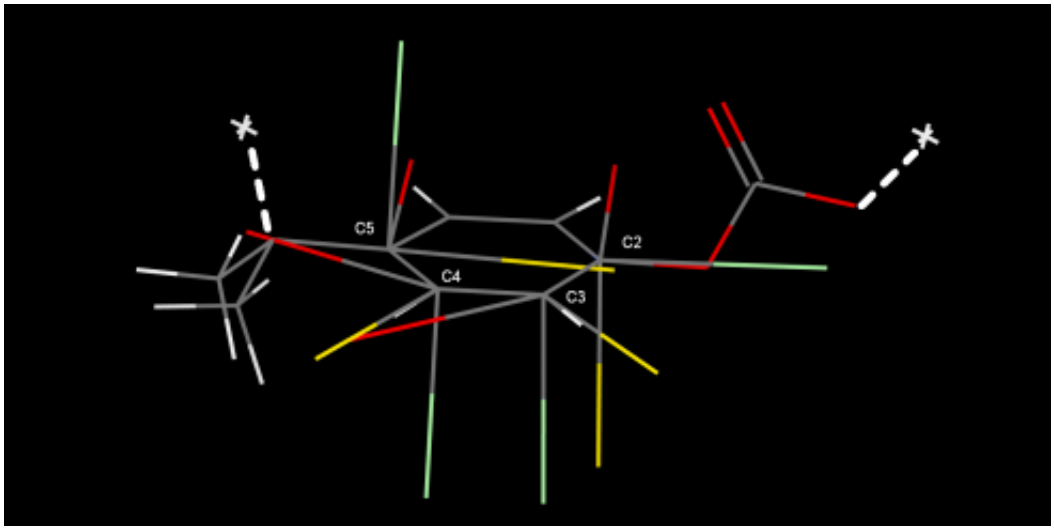
Community comment on "Efficient polynomial analysis of magic-angle spinning sidebands and application to order parameter determination in anisotropic samples" by Günter Hempel et al., Magn. Reson. Discuss., https://doi.org/10.5194/mr-2021-39-CC1, 2021

With Dr. Brus we thought I might contribute here today. The reason is I've been recently looking at orientations of some ^{13}C chemical shielding tensors, so it didn't take me long to verify the orientations shown in the paper in Figure 6 agree, expectedly, with those predicted by the periodic density functional theory based calculations for crystalline 4,4'-isopropylidenediphenyl-bis(phenyl carbonate) whose structure is available from the CCDC as #1141365. Using the CASTEP 16.1 code I've optimized the structure with the PBE functional and computed the chemical shielding tensors applying the GIPAW-PBE approach, as in a number of our publications. The computation took less than one hour using 72 cores of an up-to-date computer at https://metavo.metacentrum.cz/. The orientations are visualized in the picture that I attach below, and are color coded with yellow for "x_1" in the paper, red for "x_2", and green for "x_3" (the white dashed lines point towards the fragments which were omitted for clarity; please be sure to note the atom numbering in both pictures). I processed the data for this visualization using our INFOR code (https://doi.org/10.1016/j.cplett.2016.05.027). Anyway I attach MAGRES file which can be used with, for instance, https://www.ccpnc.ac.uk/magresview/magresview/magres_view.html?JS software (I now checked it correctly opened). I hope that helps.

What I particularly liked about this paper was the discussion of ambiguities at page 3, as we tackled various chemical shift tensor definitions in the context of protons in https://www.mdpi.com/1420-3049/24/9/1731 and other occasions.

Should you have any related questions, just send me an email: czernek@imc.cas.cz



Please also note the supplement to this comment:
https://mr.copernicus.org/preprints/mr-2021-39/mr-2021-39-CC1-supplement.zip