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Discussions

Interactive comment on "ssNMRlib: a comprehensive library and tool box for acquisition of solid-state NMR experiments on Bruker spectrometers" *by* Alicia Vallet et al.

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Replying to: "1. The setup was tested on AVIII and NEO consoles. The authors should comment, if or how their setup and pulse sequences are compatible with AVII consoles. Despite the fact that the support for AVII consoles is declining, they are still widespread within the NMR community."

Our reply: We have developed NMRlib on AVIII, and successfully tested it on NEO consoles. We do not think that it currently works on AVII, nor how much effort it would be to make it work on AVII. Note that Trent Franks writes in his comment (see SC2): "In my experience, this approach would be back-compatible with AVII systems with just

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a little bit of work, if it doesn't already work, especially if the guts are mostly in python."

Replying to: "2. How about compatibility on a spectrometer work station running Microsoft Windows OS?"

Our reply: We only can give a similar response than to point 1. As our spectrometers are all equipped with LINUX workstations, we only have experience with this environment. Therefore, we recommend to install a Linux computer, to make NMRlib available on a spectrometer.

Replying to "3. Obviously, frequency units are more intuitive in the NMR perspective. However, from a technical point of view the use of power levels in Watts alerts the user more than using frequency units, as the nutation by X kHz can require very low or very high power, depending on the 90âŮę pulse length. Can the authors comment on how their safety check traps this potential risk? "

Our reply: We considered the options of checking either Watt or kHz. We finally opted for kHz for two reasons: (i) the probe specifications provided by the manufacturer are generally in kHz. One would find on such a specification sheet, e.g. the one of our 1.3 mm probe: "the probe can provide >170 kHz For pulse lengths up to 50 ms". How this translates to Watt depends on the setup. We, thus, thought that it is more general to provide a table with kHz power limitations. (ii) the existing "Power Check" feature that is by default enabled in Topspin checks already for Watt power levels. The peak power level that the Power Check verifies is probe-specific, and defined by the Bruker engineer during installation or hardware control. The check in kHz is an additional layer, on top of the Power Check. The kHz calculation depends on the correct calibration of the reference pulse lengths (p21, p22, p23). If those are incorrectly set, the calculation will go wrong, and NMRlib would calculate possible too high power levels (in Watt). We partly capture such a scenario by also doing safety checks on p21, p22, and p23. If those pulse lengths are odd, then the safety check alerts the user.

Replying to : "4. Along these lines, the authors implemented safety measures by checking for overshooting RF power for specific pulse elements. However, RF limits are given here in units of kHz, which might be risky as the absolute power integral is crucial. The authors should add more details on how exactly the safety checks are implemented as it is still unclear to the reader by which criteria the margins are set. "

Our reply: The safety check feature goes through all the parameters of a given experiment and compares the values to those provided in a table. This table is listed in a file, and the user can check, edit, and chnage those values. The python script that does the safety check is experiment-specific, because the parameters used in a given experiment are different from one pulse sequence to the next. As stated above, the safety check, operating in kHz rather than Watt, would only have a problem if the reference pulses, from which power levels (e.g. for CP) are calculated, are wrong. For example, if the reference 90 degree pulse length p21 is mis-set 2 times too long, the calculation would indicate that at that power level (plw2) the obtained RF field is 2 times lower than what it really is. Accordingly, the calculation of a power level for a CP, which is based on this reference pulse, would have as a result a too high power (in Watt). This might possibly cause problems. We circumvent the problem by checking also whether the reference power levels are in a reasonable range. We do not claim that this safety check is 100% safe. Nonetheless, they turn out to remove a vast majority of problems. We are open to suggestions how to improve the safety check feature! We have now added an entire section to the updated Supporting Information, which explains in more detail how the safety checks work.

We have attached the new part of the Supporting Information to this message.

Replying to question 5., related to the implication of Bruker in this process:

Our reply: In principle we agree that it would be best if Bruker did this work, or if they integrated this library, and ensured its continuity over time. We have indeed discussed with Bruker, and while they are generally interested, it is a very slow and time-consuming process to get Bruker practically involved in such a development. As an aside, currently Topsolids lacks largely the 1H-detected bio-ssNMR experiments, currently. While it is not clear how Bruker's tools will evolve, we think that it makes sense to just move forward and make this tool freely available to the academic community. In conclusion, it is a nice attempt and the authors introduce some new assignment experiments, however, the setup is only a minor advancement compared to already existing tools. In my view, joining forces with Bruker would be much more fruitful in terms of an universal solution for the NMR community.

We thank the reviewer for the overall positive assessment.

Please also note the supplement to this comment:
https://mr.copernicus.org/preprints/mr-2020-25/mr-2020-25-AC3-supplement.pdf

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