

Interactive comment on “Paramagpy: Software for Fitting Magnetic Susceptibility Tensors Using Paramagnetic Effects Measured in NMR Spectra” by Henry William Orton et al.

Anonymous Referee #1

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The paper presents Paramagpy, a new software for the fitting of magnetic susceptibility tensors with especial attention to biomolecules labelled with paramagnetic metal ions that simultaneously display PCS, PRE, RDC and CCR effects. The description of the program is good and deep enough to understand how it works.

The software is robust and stable. I was able to run some examples and it produces the expected results not showing any instabilities. It is normal for the first versions to present some bugs but for the moment I didn't find any. The software also resist the introduction of errors in the input files in a way that it automatically ignores data lines with incorrect format. The documentation files are helpful and of good quality with a

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complete set of examples.

They claim, as the biggest advantage of this software with respect to the previous ones, that Paramagpy can use CCR effects to improve the calculation. In Fig. 4 they show one example where they compare the results taking and not taking into account CCR effects but only the correlation plot is presented without any statistical analysis. As the effect seems to be important I think that a statistical analysis of the improvement offered by this new approach should be presented with some examples, which they already have. For example, just showing the Pearson correlation coefficients (R) or Q-factors with and without CCR. In addition they could explain in which cases the consideration of cross-correlated relaxation can have a strongest effect on the tensor prediction.

They also say that the software includes some additional options for PCS and PRE calculations not offered by PyParaTools, the other program that can integrate PCS, RDC and PRE effects in the calculations. It would be nice if they specify which are these options.

Another advantage of Paramagpy claimed by the authors is that the algorithm used can overcome some of the local minima problems of Numbat and PyParaTools, as it is done by Rosetta, where they split the problem into its linear and non-linear parts to avoid local minima.

In summary, Paramagpy is a good software that can properly calculate magnetic susceptibility tensors. It supports multiple models and multiple datasets for the calculations, with a good GUI but it requires some statistical analysis to probe the advantages of the novelties included in the software. I think this point is important, not only to justify the assertions they make but to show how and when this approach actually improves the calculations.

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