

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

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This manuscript describes an open-source software (Paramagpy) which promises to be very useful for the analysis of the NMR data of paramagnetic systems, because able to account for all paramagnetic effects (PCSs, pRDCs, PREs and CCRs) and to relate them to the pdb structure of a protein. The relevant equations describing the paramagnetic effects are reported according to the most recent formulations and the main functionalities of the program are clearly described.

The manuscript is recommended for publication. The following suggestions are provided with the aim to clarify to the readers some aspects that may not appear fully

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clear.

1) Could the authors analytically show that the Eqs. 17-21, 24-27 for the Curie-dipolar cross correlated relaxation (section 5) provide the well-known equation by Ghose-Prestegard (J. Magn. Reson. 1997, 128, 138) in its conditions of validity (isotropic susceptibility tensor)?

2) When indicating that the multiple models in a solution NMR ensemble can be used to fit the data (section 7), a warning should be provided that ensemble averaging of the paramagnetic data may be incorrect because the NMR family reports on the experimental uncertainty of the structural model, and not on the real conformational ensemble sampled by the system.

Interactive comment on Magn. Reson. Discuss., <https://doi.org/10.5194/mr-2019-3>, 2019.

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