

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 new and quite comprehensive software for the analysis of paramagnetic effects. It can be considered as a follow-up of the quite popular programme Numbat, with a lot of extra possibilities. The theoretical background seems thorough. This software will be quite useful for the community and the work seems sound, so publication is recommended. Two points could be considered:

(1) As was pointed out also in the public discussion, taking an average of structures from an ensemble could be a simplification. NMR ensembles usually represent experimental uncertainty, which should be reflected in the uncertainty of the paramagnetic

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parameters derived for this ensemble.

(2) The standard Q-value definition is used here. We have introduced an alternative definition (Q_a), with the sum of the absolute experimental and calculated values in the denominator rather than only the experimental values. The standard definition results in a bias in cases where the deviation between calculated and experimental data is large. This is relevant in particular for PRE data that can vary strongly with small changes in distance. In cases where the experimental PRE is much larger than the calculated, the Q value is low, in cases where the experimental value is low and the calculated high, the Q value is high, thus biasing the results toward fitting the low PREs better than the high ones.

$$Q(a) = \sqrt{\frac{(\sum (exp - calc)^2)}{(\sum (|exp| + |calc|)^2)}}$$

Example: Exp: 100 Calc: 10 Q = 0.81 $Q_a = 0.669$ Exp: 10 Calc: 100 Q = 0.81 $Q_a = 0.669$ This was published in J. Am. Chem. Soc. 2010, 132, 1, 241-247, <https://doi.org/10.1021/ja9064574>. For PCS the absolute number bars were added, because these values can also be negative, contrary to PREs. Also the subscript (a) was added later for clarity. In cases where the experimental and calculated values are similar, Q and Q_a are equivalent, with $Q = 2 \times Q_a$. The authors could consider whether the Q_a is a better alternative for the Q factor.

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