

Interactive comment on “Revisiting paramagnetic relaxation enhancements in slowly rotating systems: how long is the long range?” by Giovanni Bellomo et al.

Carol Post (Referee)

cbp@purdue.edu

Received and published: 5 January 2021

The authors present a thoughtful study to examine paramagnetic enhancement of nuclear relaxation accounting for multiple spin effects using a complete relaxation-rate matrix analysis. The results are interesting, clearly presented, and substantiate the two conclusions of the study: first, that paramagnetic metal ions cannot be exploited for altering water proton relaxation in MRI contrast agents because the needed conditions for reorientation time of the macromolecule and the exchange time for water solvents are not within typical values; second, that intermolecular distances greater than 15 angstroms estimated from paramagnetic relaxation enhancements appear shorter

C1

than their actual values due to multiple-spin effects. This information provides important insight.

I have a few simple suggestions for the authors.

- Line 37: There were a number of groups who examined multiple-spin effects on cross-relaxation rates using a complete rate matrix at the same time as Borgias and James, 1989. It would be nice to reference some of the other papers as well, particularly one by Kaptein (e.g. Boelens and Kaptein, J Mag Res 1989; Olejniczak and Fesik J Mag Res 1986; co-workers and Gorenstein JACS 1990).

- Line 55 and elsewhere: The use of the phrase “the CORMA approach” sounds like the approach is unique to the CORMA program, but that is not the case. A more accurate phrase would be “the complete rate-matrix approach” or “the CORMA program.”

- Eq 1: I could not see the definition for sigma in the main text. Although the definition does appear in the supplement, it should appear with equation 1.

- Figure 1 and the description lines 92-100: The authors compare in fig 1a and 1c the apparent rates that would result from analyzing $M'(t)$ in comparison to the actual Solomon relaxation rate, eqn 2. It would be helpful for the reader to articulate in the figures and text “apparent relaxation rate” or somehow differentiate a rate estimated from $M'(t)$ versus the actual rates that appear in the rate matrix, eqn 1.

- line 91: it is mentioned that Led and coworkers reported deviations in distances determined from analysis of experimental magnetization decay. Can the authors make a direct comparison of the computed results (fig 1) with the experimental data? For example, the theoretical back-calculated distances in 1b with the experimental distances calculated from the experimental longitudinal relaxation rates? The question is whether estimates calculated using the complete rate matrix analysis gives better agreement with experiment than estimates from the Solomon equation.

Typographical corrections:

C2

- line 96: "Analogous behaviors are" should be "Analogous behavior is"
- line 98: "differ of orders" should be "differ by orders"
- line 170: "This occurs" is missing a subject noun. Perhaps "This contribution occurs" or "This transfer occurs"

Interactive comment on Magn. Reson. Discuss., <https://doi.org/10.5194/mr-2020-33>, 2020.