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Comment on mr-2021-23

Vladimir Zhivonitko (Referee)

Referee comment on "Determination of hydrogen exchange and relaxation parameters in PHIP complexes at micromolar concentrations" by Lisanne Sellies et al., Magn. Reson. Discuss., https://doi.org/10.5194/mr-2021-23-RC3, 2021

This paper describes an original and interesting approach for obtaining important kinetic (as well as relaxation) parameters of the reversible H_2 exchange between an asymmetric Ir complex and parahydrogen at micromolar concentration range. These parameters can be widely used for optimizing SABRE experiments and achieving the highest possible level of reliability and sensitivity in parahydrogen-based hyperpolarization applications related but not limited to dilute biofluids and natural extracts. The approach is based on acquiring data by a repetitive and controlled bubbling of parahydrogen followed by pulse sequences of two types with selective excitations/refocusing of hydride resonances and H_2 resonance. The results are very well presented in the paper, and the next review round is not needed.

In addition to the suggestions of the other reviewers, the following really minor improvements could be considered: (1) In several places, a previously reported 1000-fold magnetization enhancement is mentioned. Of course, the authors are aware that signal enhancements are field dependent, so when quoting the enhancement, maybe it is good to specify the field strength used in that publications. (2) I couldn't find any information about positions of H_A and H_X hydrides for the studied isoquinoline complex. This is probably the first publication with Ir-mtz and isoquinoline. Among other matters, adding ppm values for H_A and H_X is quite important for understanding why the bandwidths of 500 Hz and 2000 Hz were chosen, especially, in the case of the open and filled reburp pulses. (3) In addition, authors may think to mention that Eqns. 1 and 2 can be coupled by the presence of cross-correlated relaxation terms. This will lead to a more complicated form of solutions in Eqns. 3-9. At the same time, for the studied asymmetric complex this effect most likely is weak and can be neglected. (4) The last two pulses in the sequence Fig.2b are sort of special because they represent combined selective excitation/refocusing of both H_2 and the high-field hydride resonances. These pulses could be marked somehow in the figure to show this difference.