Magn. Reson. Discuss.,
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Open Access MAGNETIC RESONANCE Discussions

Interactive comment on "Geminal Parahydrogen-Induced Polarization: Accumulating Long-Lived Singlet Order on Methylene Proton Pairs" *by* Laurynas Dagys et al.

Anonymous Referee #2

Received and published: 20 July 2020

Dagys et al. conducted an interesting NMR study of a ruthenium-catalyzed geminal hydrogenation reaction producing overpopulated singlet spin order in a methylene group. By intelligent design of the pulse sequences and pH2 bubbling intervals, the authors studied the kinetics of the buildup and decay of the singlet order and zz- spin order in the intermediate of the hydrogenation reaction. This allowed them to extract relevant chemical and relaxation parameters and, in general, presented an elaborated strategy for the analysis of the reaction intermediates for the future experiments utilizing pH2. The work is well conducted, and the results are presented clearly. The paper without a doubt deserves publication in the Open Magnetic Resonance. The only puzzling fact is more than a factor of 2 difference between Ts measured at room temperature and at

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Discussion paper

PHIP conditions. The authors mention temperature as a potential reason for discrepancy... Would it be possible to conduct a singlet state lifetime measurement with the synthesized molecule at elevated temperature to support this statement?

I also suggest citing the following review relevant in the context of the interplay between chemical kinetics and spin dynamics in experiments utilizing pH2:

K. V. Kovtunov, E. V. Pokochueva, O. G. Salnikov, S. F. Cousin, D. Kurzbach, B. Vuichoud, S. Jannin, E. Y. Chekmenev, B. M. Goodson, D. A. Barskiy, I. V. Koptyug, Chem. Asian J. 2018, 13, 1857.

Otherwise, the paper is ready for publication.

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