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Magn. Reson. Discuss., referee comment RC1
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Comment on mr-2021-33

Ville-Veikko Telkki (Referee)

Referee comment on "^{129}Xe ultra-fast Z spectroscopy enables micromolar detection of biosensors on a 1□T benchtop spectrometer" by Kévin Chighine et al., Magn. Reson. Discuss., https://doi.org/10.5194/mr-2021-33-RC1, 2021

The manuscript describes the first application of 129Xe Hyper-CEST method with a low field NMR spectrometer. The authors prove the feasibility of the experiments by comparing ultrafast Z-spectra of a solution including a mixture of two different cryptophane cages measured at 11.7 and 1 T. They show that bound Xe signal is observable even at 19 um concentration at 1 T. The manuscript describes lots of useful practical information related to the low-field experiments; for example, they tuned a Magritek Spinsolve Carbon spectrometer to Xe frequency by adjusting the temperature of the magnet, and they demonstrate also an alternative way of tuning by wrapping a copper foil around the sample. Furthermore, they compare experimental observations with the spectral simulations. The manuscript is very well written.

I recommend a minor revision based on the comments below.

Fig. 2 is not referred in the manuscript text, please refer.

Page 4: Sentence “This was expected as the magnet, of the Halbach type, delivers an horizontal static magnetic field, and thus xenon crosses areas of null field during its transfer” is bit illogical, because the horizontal direction of the magnetic field does not automatically mean that field is zero during the transfer of the sample. Do you mean that

the fringe field on top of the instrument is close to zero?

Section 2.3: It would be interesting to see a comparison of the SNR values of the dissolved Xe peak in the spectra measured at 11.7 and 1 T (SNRs determined from the spectra shown in Fig. 3) to have an idea about the order of magnitude, how much lower the sensitivity at 1 T is. I understand that this value is dependent on many instrumental and sample transfer related factors, but still I would be curious to see the values.

Fig. 5: as the authors discuss in the text, the profile is affected by the spatially dependent spin density, as the gradient is perpendicular to the sample tube, and the coil excitation-detection profile. The authors might discuss about the possibility for the spin-density and coil excitation-detection profile correction as described, e.g., in Ahola, Nat. Commun. 2017, 6, 8363.

The shapes of the simulated spectral lines in Fig. 8 are quite difficult to see due to overlapping lines, could the plot be modified?

The authors might consider adding the script of the ultrafast Z-sequence to the supporting information of the manuscript.