

Interactive comment on "Towards resolving the complex paramagnetic NMR spectrum of small laccase: Assignments of resonances to residue specific nuclei" by Rubin Dasgupta et al.

Anonymous Referee #3

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Dasgupta et al. present a well-conceived technical study that seeks to resolve the paramagnetic NMR spectrum of the trinuclear copper centre in the small laccase from S. coelicolor. I judge their analysis and interpretation to be sound and correct. The work reported appears to be a follow-on to work reported by the same authors in Biophys. J. 119, 9-14, 2020. To an outsider in this area, it would be useful to have some explicit discussion about how this previous report links into the present work.

Having read referees 1 and 2 reports I agree with their assessment and the changes they have requested, the Table of chemical shift and assignments would be a useful addition. In line with their views and comments I am also positive about this work.

C1

Picking up on referee 2 comments; Abstract, line 11. The authors appear to imply that the efficiency of the kinetically challenging task of reducing molecular oxygen is linked to mobility of active site residues? What is the evidence for this? Is this related to the sentence in the Introduction on line 60? It appears to me that the authors are attempting to correlate dynamics versus catalytic reactivity. Whilst there may well be a case for this, I am not aware that this applies in the present case. The observation of ligand dynamics in the first coordination sphere in a metalloenzyme is interesting, but how does this fit with the entatic state view?

Line 63, characterisation of.... Line 102, three pairs of...

Interactive comment on Magn. Reson. Discuss., https://doi.org/10.5194/mr-2020-31, 2020.