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Dr. F. Ann Walker, *Associate Editor*
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Ms No: ja0749005
Title: "Spectroscopic and Quantum Chemical Studies on Low-Spin $\text{Fe}^{\text{IV}}=\text{O}$ Complexes: Fe-O Bonding and Its Contributions to Reactivity"

Dear Ann,

We have revised our Ms No. ja0749005 according to all of the suggestions of reviewer 5 and have considered and addressed the comments of reviewer 4. Please find attached the replies to both reviewers. In particular, we have completely rewritten the discussion section to make our logic flow clearer to reviewer 4. However, as I indicated in our earlier correspondence, he/she is not being reasonable in his/her anonymous comments. Our purpose of studying model complexes is to gain insight into reactivity, both of the models and the related enzymes. We have been able to accomplish this in this study and believe this belongs (tightly and clearly) in the primary literature.

To reiterate my reply to the three points summarized in your cover letter:

- 1) We have clarified wording choices and tightened the discussion. In the opinion of reviewer 5, the paper "is extremely well written".
- 2) We have rewritten the discussion section to clarify the connection between the model complexes studied here and the biologically relevant enzyme intermediates. This is a tight chain of arguments, relevant to the data and not beyond the scope of this study.
- 3) The spectroscopic data on the transition energies provide the evaluation of the quality of the DFT calculations here, not vice versa.

I think this is an important paper in experimentally defining the frontier molecular orbitals responsible for the reactivity of $\text{Fe}^{\text{IV}}=\text{O}$ species and hope you and the reviewers agree.

Best regards,

Ed