

Interactive comment on “Aqueous Reactions of Organic Triplet Excited States with Atmospheric Alkenes” by Richie Kaur et al.

Anonymous Referee #2

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In this very ambitious study, the authors measured the kinetics of oxidation of a series of alkenes by the triplet excited state of benzophenone, which they use as a model compound for triplet excited states in atmospheric waters. They then looked for correlations between the kinetic data and various properties of the alkenes, some of which were derived using density functional theory (DFT) calculations. They found a fairly good correlation between the rate constants and the one-electron oxidation potential for the alkenes, and used that to develop a quantitative structure-activity relationship (QSAR). They used the QSAR, and more DFT calculations, to infer triplet oxidation rates for several biogenically derived alkenes. Finally, they perform some estimates of the potential importance of triplet chemistry in atmospheric waters. I recommend publication in ACP after some minor points are addressed.

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Minor comments:

- It is not mentioned in the main text how many times each kinetic experiment was repeated - I only knew this after looking at Table S1
- Can the authors discuss and provide some estimate of the error/uncertainty for the parameters derived from the DFT calculations? How does this impact the discussion of the outliers for the QSAR?
- I note from Table S1 that several different reference probes were used. The reason for this should be discussed. The reference rates and the uncertainty in those rates should be listed/discussed. Were the uncertainties included in the reported uncertainties in k , and considered in the development of the QSAR?
- Just a suggestion: Fig. 4 and some of the discussion of these calculations could be moved to the SI, since the article is already quite dense with information and this line of inquiry was ultimately inconclusive.
- A little more information about the atmospheric lifetime calculations should be provided. Are you considering repartitioning of the OVOCs between the gas and aqueous phases as the reaction proceeds? Or are the calculated rates basically initial rates?

Interactive comment on Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2018-1259>, 2018.

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