

Atmos. Chem. Phys. Discuss., referee comment RC2
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Comment on acp-2021-890

Anonymous Referee #2

Referee comment on "OH-initiated atmospheric degradation of hydroxyalkyl hydroperoxides: mechanism, kinetics, and structure–activity relationship" by Long Chen et al., Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2021-890-RC2>, 2021

The authors have conducted a detailed theoretical study on the OH-initiated atmospheric degradation of hydroxyalkyl hydroperoxides. For the resulting H-abstraction products RO₂ radicals, the subsequent reactions involving self-reaction, autoxidation and reaction with HO₂ radical and NO are taken into account. Such kind of studies are necessary for improving our understanding of VOC oxidation chemistry. I recommend this manuscript publication in ACP after the following minor revisions.

Specific Comments:

1. Authors discuss the transformation mechanism of HHPs. But there is no information on the concentration of HHPs (in forested regions?).
2. The lifetimes of distinct HHPs with respect to OH should be estimated under atmospheric conditions.
3. ΔE_a^\ddagger , ΔG_a^\ddagger and ΔG are employed in the manuscript, the author should explain the meaning of each item in detail.
4. Author should compare the barriers of the gas phase decomposition of HOCH₂OO radical with the barrier of self-reaction of HOCH₂OO radical. Kumar and Francisco reported the unimolecular decay of HOCH₂OO radical could be a new source of HO₂ radical (Angew. Chem. Int. Ed. 2015, 54, 15711-15714; J. Phys. Chem. A 2016, 120, 2677-2683).

5. Author should provide the pseudo first order rates for the reactions of distinct RO₂ radicals with HO₂ and NO under the urban, rural and forest environments.

6. In Fig. 2, the text (mentioned structural parameters) overlaps with the structures.