Prof. Yu Huang
State Key Laboratory of Loess Science,
Institute of Earth Environment, Chinese Academy of Sciences, Xi'an, 710061, China
Tel./Fax: (86) 29-62336261
E-mail: huangyu@ieecas.cn

Mar. 24, 2026

Dear Prof. Arthur Chan,

Revision for Manuscript egusphere-2025-4646

We thank you very much for giving us the opportunity to revise our manuscript. We sincerely appreciate your comments and suggestions on the manuscript entitled "**Mechanistic investigations of the formation of multifunctional products from the multi-generation ·OH oxidation of styrene**". We have carefully revised the manuscript according to your comments. All revisions are highlighted in blue for clarity. The response letter is attached at the end of this cover letter.

We hope that the revised manuscript can meet the requirement of *Atmospheric Chemistry & Physics*. If there are any further modifications or revisions, please do not hesitate to contact us.

Looking forward to hearing from you as soon as possible.

Best regards,

Yu Huang

Comments of Editor

The abstract remains very narrow in scope and do not meet the last criterion in the author guidelines: "importance and implications of the results". Right now the last sentence is "The volatility of the oxidation products significantly decreases with increasing the number of ·OH oxidation steps." This statement is too narrow and does not explain the broader impacts of this work.

Response: Based on the Editor's suggestion, the abstract has carefully revised in the revised manuscript.

Abstract: Styrene is a highly reactive aromatic hydrocarbon that has been identified as a key secondary organic aerosol (SOA) precursor. Recent laboratory chamber experiments have identified C_7 and C_8 series compounds as the main components of SOA in the photooxidation of styrene. However, their molecular structures and formation pathways remain largely uncharacterized. Herein, the formation mechanisms of multifunctional products from the multi-generation ·OH oxidation of styrene are studied using the quantum chemistry methods. The calculations show that the first generation RO_2 radicals can either proceed unimolecular decomposition to yield benzaldehyde (C_7H_6O), or undergo bimolecular reactions with HO_2·/NO to form the first generation closed-shell C_7- and C_8-products, hydroperoxide 1^{st}-ROOH ($C_8H_{10}O_3$), benzaldehyde, and organic nitrate 1^{st}-$RONO_2$ ($C_8H_9NO_3$). For the second generation ·OH oxidation, OH-addition reaction occurring at the *ortho*-site of 1^{st}-ROOH and 1^{st}-$RONO_2$ has a significant dominance. The *ortho*-OH-addition products can proceed through two O_2-addition steps and a cyclization process to produce the peroxide bicyclic peroxy radicals (BPR). BPR can further react with HO_2·/NO to form the second generation closed-shell C_8-products, hydroperoxide 2^{nd}-ROOH ($C_8H_{12}O_8$), organic nitrate 2^{nd}-$RONO_2$ ($C_8H_{10}N_2O_{10}$), and other multifunctional products, in which the first two products have fractional yields of 41.4% and 4.8%, respectively. For the third generation ·OH oxidation, OH-addition occurring at the C=C double bond of 2^{nd}-ROOH and 2^{nd}-$RONO_2$ has the lowest barrier. The major third generation closed-shell C_8-products are the multifunctional hydroperoxides and organic nitrates. These findings carry important implications for advancing our understanding of the chemical composition and formation mechanisms of aromatic SOA.