Liwen Yang et al. “SIM-HOM (version 1.0): A Mechanistic Module for the formation of highly oxygenated organic molecules from Isoprene, Monoterpene and Sesquiterpene evaluated with ADCHAM (version 1.0)”

Paul Wennberg

This is a very welcome effort to build a mechanistically informed module that can capture the formation of highly oxygenated molecules in the oxidation of biogenic alkenes initiated by OH and ozone. The authors have used MCM and other compiled mechanisms that provide detailed gas phase oxidation insights and added pathways that describe HOM formation from autoxidation and RO2+RO2 chemistry. They use a set of simulations from CLOUD to benchmark the compiled mechanism both with single and mixed alkene starting mixtures. The mechanism has significant skill and will substantially advance our ability to simulate the production of HOMs and the associated aerosol in many regions of the world.

Response: We thank the reviewer for positive and constructive evaluation of our work. We appreciate the concise and accurate summary of our study, as well as the recognition of these key improvements we have made in developing a mechanistically detailed module for simulating HOM formation during the oxidation of biogenic alkenes. We address the reviewer’s specific comments in detail below.

In our response, original comments from reviewers are in black, our response is in blue and revised texts in the manuscript are in green.

I recommend publication in close to the current version. I ask the authors, however, to consider providing a more complete description of what chemistry drives the HOM formation – I suspect that perhaps the ‘top ten’ pathways provide most of the HOM production in each system and it would be helpful for future investigations to have this quantified here.

Response: We thank the reviewer for this constructive suggestion. We agree that identifying the dominant processes leading to HOM formation would be valuable for future studies. However, we find it difficult to implement this analysis in a clear and mechanistically meaningful way within the framework of the current model. In our

simulations, HOM formation does not arise from a small number of isolated pathways, but rather from a highly coupled sequence of reactions. Many reactions, such as the initial oxidation steps or early autoxidation processes, do not directly produce HOM but strongly influence the composition of the radical pool and the probability of subsequent HOM-forming reactions. Their contribution to HOM formation is therefore indirect but still essential, which makes it challenging to rigorously define and rank discrete "pathways" that drive HOM production.

To illustrate this complexity, we performed a simple sensitivity test in which key autoxidation steps prior to HOM formation in the monoterpene- and sesquiterpene-dominated O_3 oxidation systems were selectively suppressed. Specifically, we set the rate coefficients of three RO_2 autoxidation steps to zero individually and examined the resulting change in simulated HOM concentrations. When the autoxidation steps leading to RO_2 species with O = 4 and O = 6 were suppressed, the simulated HOM concentrations decreased substantially. In contrast, suppressing the autoxidation step leading to RO_2 with O = 5 resulted in an increase in HOM concentrations. In the mechanism, the RO_2 species with 5 O atoms originate from the autoxidation of alkoxy radicals (RO) formed in earlier RO_2 reactions. When this autoxidation channel is removed, the system may appear to shift the radical budget toward alternative RO_2 + RO_2 reactions that produce RO radicals, which can subsequently undergo further oxidation and contribute to HOM formation. Due to the limited availability of experimental constraints for pure isoprene systems, we did not perform the same sensitivity test for the isoprene mechanism.

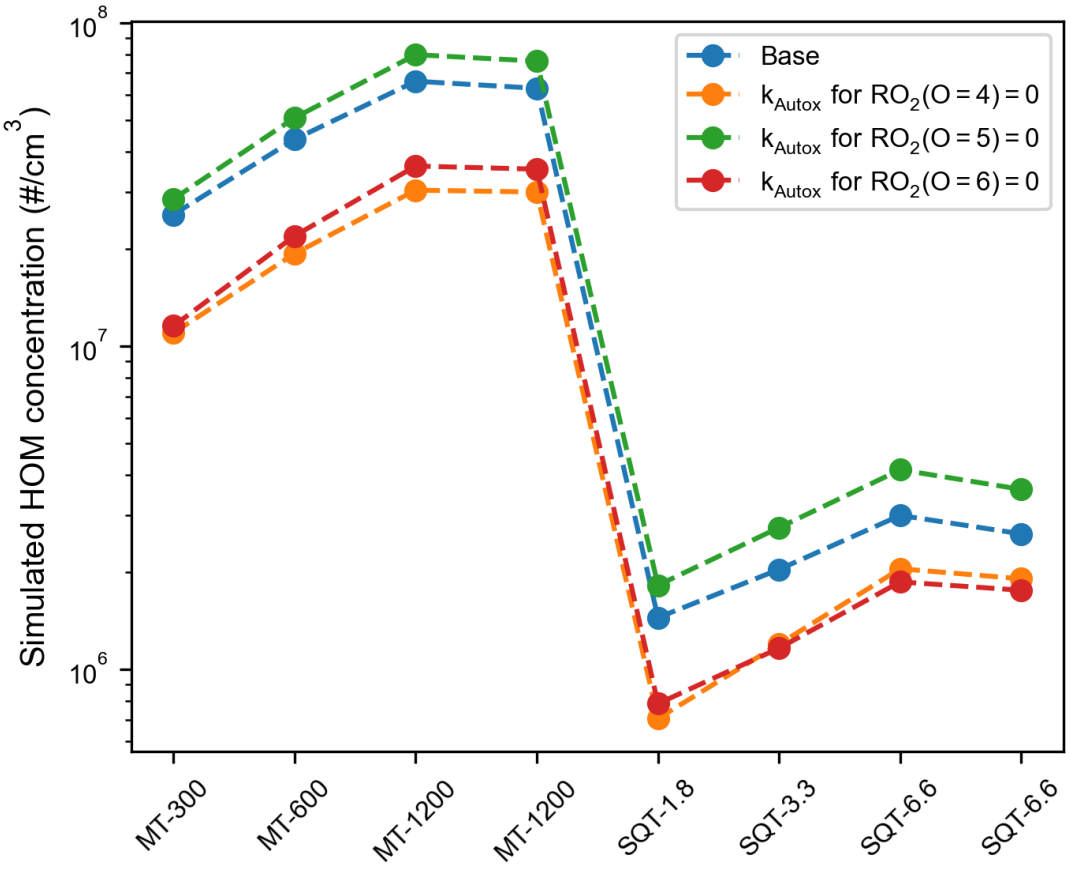

Fig R1. Modelled HOM concentrations during monoterpene and sesquiterpene ozonolysis experiment. The different model results are from the model sensitivity tests with different autoxidation settings.

This example illustrates that even reactions occurring prior to HOM formation can influence HOM yields in non-linear ways by altering the balance between RO_2, RO, and subsequent autoxidation processes. As a result, the contribution of individual reactions cannot always be interpreted independently, and the concept of a small set of dominant linear pathways may not fully capture the behavior of the coupled radical system.

In addition, the relative importance of individual reactions is strongly condition-dependent, for example with respect to NO concentration, precursor type, and oxidant regime. A ranking derived under a specific set of conditions may therefore not be generally applicable. Conducting individual sensitivity analyses for the very large

number of reactions included in the mechanism would also be computationally demanding and may not necessarily lead to a physically interpretable ranking of pathways. For these reasons, we believe that providing a robust and generally meaningful "top pathway" analysis is difficult within the scope of the present study. Nevertheless, we appreciate the reviewer's suggestion and consider that the development of systematic pathway analysis tools for complex HOM chemistry would be a valuable direction for future work.

For the RO2 + RO2 chemistry my sense, based on Murphy et al., 2025 (https://pubs.rsc.org/zh-tw/content/articlepdf/2025/ea/d5ea00106d), is that the dimer formation branching ratio is generally ~10%. Even for simple alkanes (e.g. ethane RO2), this seems the case. To the extent that this is true, the major question is just the rate coefficients for these RO2+RO2 reactions. Given that addition of a functional group (e.g. HOCH2CH2OO vs CH3CH2CH2OO) has such a rate enhancement, I am curious whether such enhancements are additive in your mechanism (e.g. does adding a carbonyl and an alcohol or acid yield 100x rate – see for example Ziola and Ziemann - J Phys Chem A. 2025 Feb 13; 129(6):1688-1703). I would also ask the authors to provide evidence for the statement (ln314) "Likewise, reactions between two non-autoxidizable RO2 are not included due to their low propensity to form accretion products". Finally, in the monoterpene RO2 section, please add a reference to Kenseth, 2023 where you cite Peräkylä et al., 2023. [https://www.science.org/doi/10.1126/science.adi0857]

Response: **(1) On additivity of functional group effects (carbonyl, alcohol, acid, etc.)**

We thank the reviewer for raising this important mechanistic question and for pointing to Ziola and Ziemann (2025). **In the current version of SIM-HOM, we do not assume additive rate enhancements based on the number or type of functional groups (e.g., carbonyl + alcohol leading to 100× enhancement). Instead, we parameterize RO_2 + RO_2 rate coefficients according to overall oxidation state and molecular size (i.e., number of carbon and oxygen atoms), without explicitly resolving individual functional group.**

In practice, this representation is conceptually similar to a functional-group-based description but expressed in a simplified form: the number of oxygen atoms (nO) is used as a proxy for the degree of functionalization rather than explicitly tracking specific functional groups. This choice reflects the current limitations in available structure–reactivity relationships for RO_2 radicals, resulting the substantial increasing uncertainty from explicit group-based scaling, and the significant computational cost such a treatment would impose in large chemical mechanisms.

Accordingly, more highly oxygenated (i.e., more autoxidized and generally larger) RO_2 radicals are assigned higher $RO_2 + RO_2$ rate coefficients, whereas less oxygenated radicals are assigned lower values. Specifically, for isoprene-derived RO_2, $k_{(RO_2 + RO_2)}$ is set in the range of $1*10^{-12}$–$8*10^{-12}$ cm^3s^{-1}; for monoterpene-derived RO_2 radicals, $1*10^{-12}$–$1.5*10^{-11}$ cm^3s^{-1}; and for sesquiterpene-derived RO_2 radicals, $5*10^{-12}$–$1.5*10^{-11}$ cm^3s^{-1}. We have clarified this assumption explicitly in the revised manuscript to avoid any misunderstanding that a functional-group additivity framework is applied.

(2) On the assumed dimer branching ratio for dimer formation

We agree that recent literature, including Murphy et al. (2025), suggests that the effective branching ratio toward accretion (ROOR-type) products is often on the order of ~10%, even for relatively simple alkyl peroxy radicals. In SIM-HOM, however, we do not prescribe a fixed dimer branching ratio. In the model configuration, considering computational limitations, $RO_2 + RO_2$ accretion reactions are treated independently from other reaction channels. Accretion reactions are implemented explicitly, representing reactions between autoxidizable RO_2 and several major non-autoxidizable RO_2 species in each system. All other $RO_2 + RO_2$ pathways are treated as permutation reactions. Consequently, the effective branching ratio for ROOR formation is not prescribed as a constant value in the model.

In our implementation, $RO_2 + RO_2$ reactions leading to closed-shell monomers are assigned rate coefficients in the range of 1×10^{-12} to 1.5×10^{-11} cm^3s^{-1}, whereas $RO_2 + RO_2$ reactions leading to HOM dimers are assigned rate coefficients in the range of 1×10^{-14} to 1.5×10^{-12} cm^3s^{-1}. As a result, the effective branching ratio toward ROOR

formation in the model is typically on the order of ~10%. Because these ROOR products arise from bimolecular RO_2 + RO_2 reactions, the specific ROOR species formed depend on the identities of the reacting RO_2 precursors.

(3) On the exclusion of reactions between two non-autoxidizable RO_2

In SIM-HOM, dimer formation is restricted to reactions involving at least one highly oxygenated (HOM-type) RO_2 radical. Reactions between two non-autoxidizable (i.e., low-oxygen, non-HOM-forming) RO_2 radicals are therefore not treated as explicit accretion product formation pathways. Instead, they are represented within a pseudo-unimolecular loss framework against the total RO_2 pool, leading to closed-shell monomer products.

This treatment does not imply that reactions between two non-autoxidizable RO_2 radicals are incapable of forming ROOR accretion products. Rather, they are not explicitly considered because the primary purpose of SIM-HOM is to represent the HOM formation. This simplification is motivated by several considerations. First, experimental evidence indicates relatively low formation rates of ROOR products from low-oxygen RO_2 radicals under atmospheric conditions (Berndt et al., 2018). Second, from a mechanistic perspective, the formation of HOM accretion products containing at least six oxygen atoms typically requires the two precursor RO_2 radicals to collectively contain at least eight oxygen atoms. Consequently, ROOR formation relevant for HOM chemistry is expected to preferentially occur between highly oxygenated, autoxidizable RO_2 radicals and more abundant RO_2 radicals that do not undergo autoxidation.

In the revised manuscript, we have clarified that reactions between two non-autoxidizable RO_2 radicals are represented within the generic RO_2 loss scheme rather than being fully excluded. We also explicitly state that accretion product formation is limited to reactions involving HOM-type RO_2 radicals and have added literature support for the reduced accretion efficiency of non-autoxidizable RO_2 radicals.

(4) Additional reference request (monoterpene RO_2 section)

We thank the reviewer for this suggestion and have added a citation to Kenseth et al.,2023, alongside Peräkylä et al., 2023, to appropriately acknowledge recent advances in monoterpene RO_2 chemistry and accretion product formation.

Line 311-332: Autoxidizable RO_2 radicals, due to their higher degree of functionalization, exhibit faster dimerization rates (Berndt et al., 2018). Non-autoxidizable RO_2 radicals, which are generally present at higher concentrations, can serve as reaction partners in these bimolecular reactions. Reactions between two autoxidizable RO_2 are not explicitly represented, due to their extremely low concentrations, which makes their contribution to dimer formation negligible. Likewise, reactions between two non-autoxidizable RO_2 are not treated as explicit accretion product formation pathways due to their products are probably not HOM. Instead, these reactions remain represented within the generic RO_2 loss framework of the RO_2 pool, where they contribute to closed-shell monomer formation through the pseudo-unimolecular reaction scheme. In this way, the total RO_2–RO_2 reaction flux among all RO_2 species is still accounted for, while only those combinations most relevant for HOM dimer formation are treated explicitly.

$RO_2 + RO_2$ rate coefficients are assigned according to the overall oxidation state and molecular size of the RO_2 radicals, using the number of oxygen atoms as a proxy for the degree of functionalization. This approach is consistent with the parameterization described above, where more highly oxygenated and generally larger RO_2 radicals are assumed to exhibit higher reactivity in $RO_2 + RO_2$ reactions. SIM-HOM uses $RO_2 + RO_2$ reaction rates leading to closed-shell monomer products in the range of 1×10^{-12} to 1.5×10^{-11} cm^3s^{-1} and $RO_2 + RO_2$ reactions leading to HOM dimers in the range of 1×10^{-14} to 1.5×10^{-12} cm^3s^{-1}. This choice reflects the generally smaller branching fraction of the accretion channel relative to the formation of monomer products. As a result, the effective branching ratio toward accretion products in the model is typically on the order of ~10%, consistent with recent experimental and theoretical studies (Murphy et al., 2025; Berndt et al., 2018). Because these dimers arise from explicit bimolecular

reactions, the identities of these products are determined by the specific pair of reacting RO_2 precursors.

Ref:

Berndt, T., Mender, B., Scholz, W., Fischer, L., Herrmann, H., Kulmala, M., and Hansel, A.: Accretion Product Formation from Ozonolysis and OH Radical Reaction of α-Pinene: Mechanistic Insight and the Influence of Isoprene and Ethylene, Environ. Sci. Technol., 52, 11069-11077, 10.1021/acs.est.8b02210, 2018.

Murphy, S. E., Crounse, J. D., Poulsen, A. S., Lipson, J. E., Kjaergaard, H. G., and Wennberg, P. O.: Accretion product formation in the self- and cross-reactions of small β-hydroxy peroxy radicals, Environ. Sci. - Atmospheres, 5, 1312-1325, 10.1039/d5ea00106d, 2025.

To my knowledge, however, there is no evidence that acyl peroxy radicals yield such ROOR and I would like to understand what this mechanism suggests as CH3C(O)OO is both one of the most ubiquitous (PAN decomposition) and reacts at 1/10 the collision rate. This is especially important during nighttime with NO3 addition to biogenic alkenes will produce RO_2 in a low radical environment.

Response: We thank the reviewer for raising this important question regarding the potential role of acyl peroxy radicals in ROOR formation. While experimental evidence remains limited for small acyl peroxy radicals such as $CH_3C(O)OO$, previous mechanistic studies have suggested that acyl-containing RO_2 radicals formed in the oxidation of biogenic VOCs can participate in $RO_2 + RO_2$ reactions leading to peroxide dimers. For example, Zhang et al. (Zhang et al., 2015@PNAS) proposed reaction pathways in which acyl peroxy radicals produced during monoterpene oxidation can form ROOR-type dimers through $RO_2 + RO_2$ reactions.

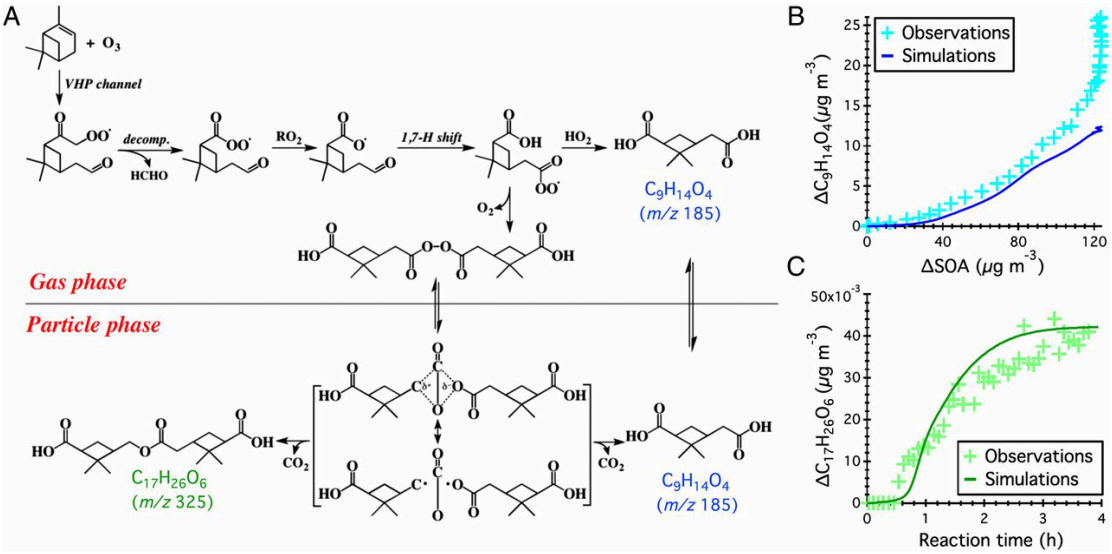

Figure R2. (A) Proposed gas- and particle-phase mechanism for the formation of the dimer $C_{17}H_{26}O_6$ and pinic acid ($C_9H_{14}O_4$). Model simulations (solid line) and experimental observations (plus sign) of the growth dynamics of (B) $C_9H_{14}O_4$ and (C) $C_{17}H_{26}O_6$. (Zhang et al., 2015)

In the present model, we do not introduce a specific or separate parameterization for acyl peroxy radicals. Instead, they are treated within the general RO_2 + RO_2 reaction framework applied to all organic peroxy radicals. In other words, the mechanism does not assume any enhanced or distinct ROOR-forming behavior for acyl peroxy radicals compared with other RO_2 species. As a result, their contribution to ROOR formation in the model is determined solely by their abundance and the generic RO_2 + RO_2 reaction parameterization.

We agree with the reviewer that small acyl peroxy radicals such as $CH_3C(O)OO$, which can be produced from processes such as PAN decomposition, are expected to have different kinetic characteristics and may not efficiently form ROOR. In the present mechanism, accretion product formation is mainly associated with large multifunctional RO_2 radicals produced during VOC oxidation and autoxidation. These RO_2 radicals contain substantially more carbon atoms and functional groups and are therefore considered the dominant precursors of ROOR-type dimers. Small RO_2 radicals, including simple acyl peroxy radicals, are not expected to contribute significantly to ROOR formation in the model. We have clarified this point in the

revised manuscript to avoid the impression that such small RO_2 species are treated as efficient ROOR precursors.

Ref:

X. Zhang, R.C. McVay, D.D. Huang, N.F. Dalleska, B. Aumont, R.C. Flagan, & J.H. Seinfeld, Formation and evolution of molecular products in α-pinene secondary organic aerosol, Proc. Natl. Acad. Sci. U.S.A. 112 (46) 14168-14173, https://doi.org/10.1073/pnas.1517742112 (2015).

Finally, I would suggest that although NOx is not considered in the current model it would be helpful to include in the "future work" some commentary on whether NO3 chemistry with biogenics is likely to be important source of HOMs and which alkenes you would recommend be studied in more detail. For example, I think one of the first demonstrations the ROOR formation from NO3 addition is important for SOA was Sally Ng's study in 2008 that illustrated that this pathway was likely responsible for all the SOA formed in an isoprene chamber study - https://acp.copernicus.org/articles/8/4117/2008/acp-8-4117-2008.html. I'd recommend citing this study in the introduction as well

Response: We thank the reviewer for this constructive suggestion. We agree that discussing the potential importance of NO_3 chemistry with BVOCs for HOM formation would significantly strengthen the "Future Work" section, and we will add a dedicated paragraph addressing this aspect. We also cited the chamber study by Sally Ng and co-workers (Ng et al., 2008) in the introduction.

Regarding the potential of NO_3 reactions to serve as an important source of HOMs, current literature suggests that the answer is compound-dependent. For isoprene, NO_3 oxidation appears to be substantially more efficient in forming HOMs than O_3 or OH oxidation. Reported HOM molar yields from isoprene + NO_3 are ~1.2% (Zhao et al., 2021), whereas corresponding yields from isoprene + O_3 and isoprene + OH are much lower, ~0.01% and ~0.03%, respectively (Jokinen et al., 2015). These comparisons suggest that, under nighttime or high-NO_3 conditions, isoprene + NO_3 chemistry could

represent a disproportionately important source of HOMs relative to other oxidants. We will therefore explicitly identify isoprene as a high-priority candidate for future NO_3–BVOC mechanistic development within SIM-HOM.

For sesquiterpenes, available laboratory data indicate HOM yields of ~1.7–1.8% (e.g., Jokinen et al., 2016, Boreal Env. Res.; Richters et al., 2016, ES&T), supporting the view that large, highly substituted alkenes are efficient precursors of HOMs. Although most existing yield data are derived from O_3 or OH oxidation, multiple double bonds suggest that NO_3 addition could also promote rapid autoxidation and potentially efficient dimer formation. We will therefore highlight sesquiterpenes as another important class warranting detailed NO_3-focused investigation.

For monoterpenes, however, existing studies indicate that HOM formation from O_3 oxidation (2.9–7%, Ehn et al., 2014; Kirkby et al., 2016) and OH oxidation (~1.2%, Kirkby et al., 2016) is already substantial. This indicates that, unlike isoprene, NO_3 chemistry is less likely to represent a uniquely dominant HOM source for monoterpenes, although it may still contribute under specific nocturnal conditions. Nevertheless, it is important to note that NO can exert nonlinear effects on HOM formation (Nie et al.,2023). Such nonlinear NO influences on RO_2 chemistry and HOM production have already been discussed in previous mechanistic studies, including the PRAM framework. We will therefore clarify in the revised manuscript that, while NO_3 chemistry may not dominate monoterpene oxidation, its interaction with RO_2 chemistry could still influence HOM formation under certain atmospheric conditions. We will clarify this compound-dependent perspective in the revised manuscript.

Overall, we agree with the reviewer that inclusion of NO_3–BVOC chemistry is an important next step. In the revised manuscript, we will cite Ng et al. (2008) to contextualize the role of NO_3-initiated ROOR formation, and (ii) expand the “Future Work” section to discuss, in a structured manner, the relative importance of NO_3 oxidation for isoprene, sesquiterpenes, and monoterpenes, and to prioritize specific alkenes (particularly isoprene and selected sesquiterpenes) for future mechanistic development and model integration.

Line 72-76: Additionally, RO2-RO2 can result in the formation of HOM monomers, where two RO2 react to produce two new molecules, often with one less oxygen atom than their precursors. RO2-RO2 reactions can also form HOM dimers (Heinritzi et al., 2020; Berndt et al., 2018; Ng et al., 2008), which are less volatile than HOM monomers and play a pivotal role in NPF and SOA formation.

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Line 611-621: In particular, the potential contribution of NO_3-initiated oxidation to HOM formation is not yet represented in the current version of the model. Recent studies suggest that the importance of NO_3 chemistry is strongly compound-dependent. For example, laboratory measurements indicate that HOM yields from isoprene + NO_3 reactions (~1.2%) (Zhao et al., 2021) are substantially higher than those from isoprene oxidation by O_3 or OH (Jokinen et al., 2015), implying that NO_3 chemistry may represent an important nighttime source of HOMs from isoprene. For larger BVOCs such as sesquiterpenes, their multiple double bonds and high reactivity may also favor rapid autoxidation following NO_3 addition, potentially leading to efficient HOM formation. In contrast, monoterpenes already exhibit substantial HOM production through O_3 and OH oxidation (Ehn et al., 2014; Kirkby et al., 2016), suggesting that NO_3 chemistry may play a less dominant role, although it could still contribute under certain nocturnal conditions.

Ref:

Berndt, T., Hoffmann, E. H., Tilgner, A., and Herrmann, H.: Highly oxidized products from the atmospheric reaction of hydroxyl radicals with isoprene, Nat. Commun., 16, 12, 10.1038/s41467-025-57336-1, 2025.

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