

This study by Harb et al. examines the gas-phase oxidation of phellandrene isomers by NO₃ radicals. They conducted gas-phase measurements via FTIR, a combination of PTR/NO⁺ TOF-MS and NO₃-CI-TOF-MS, and particle measurements via offline Orbitrap, ACSM and SMPS. Overall, their work reports the SOA yields for these reactions, along with qualitative particle phase composition measurements (orbitrap). From their online measurements of the gas-phase components they propose in-depth oxidation mechanisms.

Overall comment:

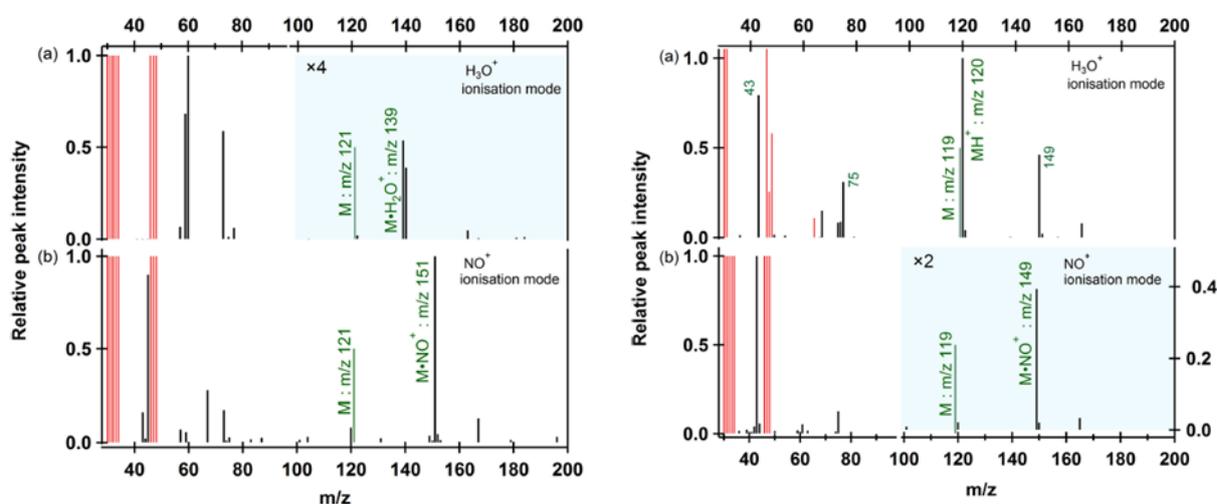
With the manuscript in its current form, I do not recommend this work for publication. This is primarily due to the over-use of the gas-phase data to create detailed mechanisms, when no speciated structural information or quantitation was obtained. Setting the lack of structural information aside, beyond the obvious limitation of the method used (PTR/NO⁺ TOF-MS) that isomers cannot be resolved, at best this method offers complex detection of these multifunctional species with high LODs. In general, traditional PTR/NO⁺ methods are not appropriate for the detection of multi-functional (especially organic nitrate) compounds due to fragmentation, unless a pre-separation method is used to quantitatively interpret the complex product ion distributions. I read the predecessor paper (Duncianu et al., 2017), and while the authors were able to demonstrate the formation of molecular ion adducts - the spectra of these synthesized standards were still complex (3 - 5 ions formed per compound), and generally dominated by fragmentation. I do not think it is appropriate to apply this method to a complex system like the oxidation of phellandrenes without supporting, speciated, methods for product identification and quantitation - especially if the aim is to create a detailed oxidation mechanism.

We thank the reviewer for his comments. However, we would like to clarify some points raised in his comments.

The mechanism proposed based on PTR-MS measurements aims to propose possible formation pathways for the detected products and molecular formulas, including different isomers, as multiple chemical structures are possible for the same m/z. We never claimed to provide any quantification or to identify the major pathways in the mechanism and we fully agree on the fact that this mechanism may not be complete as it is only based on PTR-MS measurements and some products may not have been detected. Many papers in the literature use the same approach (e.g. Fayad et al., 2021; Fouqueau et al., 2022, 2020) and propose mechanisms based on mass spectrometry techniques without isomer resolution. From the reviewer comment, we understand that the way the mechanism was presented was not clear, and to clarify it, the title of the Figure 5 has been modified by replacing “*Proposed mechanism for the oxidation of α -phellandrene by NO₃ radical. First-generation products are colored in blue, and second-generation ones are colored in red.*” by “*Mechanism proposed to explain the formation of first-generation products (colored in blue) and second-generation products (colored in red) detected by PTR-ToF-MS for the reaction of α -phellandrene+NO₃.*” Additionally, the text has been modified accordingly (L23-24, L410-413, L604-605). The title of figure S2 was also updated.

Concerning the method used to identify the products by PTR-MS, we do not agree on the fact that it is not suitable for the detection of organic nitrates. “In general”, PTR-MS is not suitable for the detection of organic nitrates. But here, we operated the instrument with a much lower electric field in the drift tube ($E/N \approx 40$ Td) than normally used ($E/N \approx 130$ Td) to limit fragmentation. In the previous paper from Duncianu et al., 2017 which present the optimization of this method, the mass spectra of alkyl, hydroxy- and carbonyl nitrate standards were measured using both NO⁺ and H₃O⁺ ionization modes, with low E/N (see for example the mass spectra of nitrooxypropanol

(left) and nitroxy-acetone (right) in the figure below). We agree that several peaks are observed but for nitroxy-acetone, the peak at m/z 120 ($M+1$) is the most intense one and for both compounds, the adduct formation is the most intense peak in NO^+ mode.



To our knowledge, all ionization methods, even the "soft" methods, including the conventional PTR-MS with H_3O^+ , lead to some fragmentation. In the figure below (from Kilpinen et al., 2012), is shown an example of fragmentation patterns for different VOCs. Many of them undergo fragmentation and exhibit much more than 3-4 peaks. In spite of this, mass spectrometry methods are powerful techniques to measure VOCs and are widely used by the atmospheric community (e.g. Kim et al., 2010; Li et al., 2020; Maji et al., 2020), in particular in ambient air where mixtures are much more complex than in simulation chambers.

Table 1. Fragmentation pattern in the PTR-MS.

Compound	Ion masses (relative abundance)
Acetone	59 (100)
Propanal	59 (100), 31 (18)
Hexanal	55 (100), 83 (74), 101 (4), 53 (2)
(E)-2-Hexenal	57 (100), 99 (23), 81 (21), 43 (6)
Heptanal	55 (100), 97 (57), 69 (9), 115 (4), 53 (2)
Octanal	69 (100), 41 (47), 111 (26), 55 (11), 71 (7), 129 (6), 67 (2)
(E)-2-Octenal	109 (100), 57 (53), 127 (33), 67 (28), 59 (4), 83 (2)
Nonanal	69 (100), 83 (33), 55 (32), 57 (24), 143 (9), 125 (7), 71 (6), 67 (4)
Decanal	83 (100), 55 (92), 69 (22), 97 (20), 157 (13), 81 (8), 139 (2), 53 (2)
Undecanal	55 (100), 43 (66), 97 (51), 83 (38), 69 (34), 171 (19), 111 (8), 81 (3), 53 (2)
Sulcatone	109 (100), 127 (25), 69 (3), 67 (1)
Geranyl acetone ^a	177 (100), 109 (31), 113 (30), 121 (26), 69 (21), 81 (21), 195 (19), 137 (15), 139 (15), 99 (10), 107 (9), 85 (8), 127 (7), 83 (4)
Benzaldehyde	107 (100), 79 (11)
Benzylalcohol	91 (100), 79 (25)
Limonene ^b	81 (100), 137 (27), 95 (10), 93 (1), 107 (1), 121 (1)

But the most important point is that we used this dual-mode approach using both NO^+ and H_3O^+ ionization modes to identify the products. The simultaneous detection of a product in both ionization modes strengthens the confidence in the assigned molecular formulas and minimizes the risk of attributing fragments to incorrect parent molecules.

Specific comments:

1. In section 2.4 the gas- and particle-phase concentrations of organic nitrates (ONs) are discussed. Was FTIR used for both the gas- and particle-phase measurement? The authors mention collecting particles followed by extraction, but the detection method is not clear. Below they also mention online pON from the ACSM. Also, in line 223-224 referring to these as "molecular concentrations" is mis-leading since this is a bulk measurement.

We thank the reviewer for this comment. FTIR was used for both gas and particulate phase measurements: in-situ long-path FTIR was used for gas-phase measurements (see description in lines 149-160) and off-line FTIR was used for the aerosol phase. Indeed, as explained in the section 2.1 of the manuscript (lines 179-183), off-line FTIR was used to measure the total organic nitrates (ONs) in the particulate phase after having performed extraction in CCl₄. For more clarity, we added a reminder in line 235 on the detection method. The ACSM was also used to determine the total particulate ONs concentration, as mentioned in line 240.

We understand that the term "molecular concentrations" could be misleading in this context, as it might be interpreted as referring to individual molecular-level measurements (e.g., a direct molecular count). To improve clarity and better reflect the nature of the measurements conducted using FTIR, we propose replacing "molecular concentrations" with "measured concentrations," which is more appropriate in this context. This modification has been made in the manuscript (L233). We thank the reviewer for this relevant comment.

2. In section 2.5, the authors mention that the phellandrene oxidation mechanism is not included in the MCM and so they used the limonene mechanism as a proxy. Considering the authors claim that small changes in structure can create large differences in SOA yield/chemistry (e.g., large difference in measured SOA yield between alpha- and beta-phellandrene reported here) the authors need to provide more justification that the use of the limonene mechanism is valid here. For example, does the temporal profile of the decay of precursor and growth of first-generation oxidation products' align? Are the rate constants comparable? Furthermore, has the limonene + NO₃ mechanism currently included in the MCM been validated?

We maintain that small changes in the VOC structure may significantly affect its reactivity, and this was confirmed by numerous studies in the literature but also by the rate constants for limonene and phellandrenes, which are significantly different. Therefore, we agree that the limonene oxidation scheme cannot be used to describe/explain in detail the formation of individual products or SOA from phellandrene oxidation. However, this was not our objective. **We used the numerical simulations only to estimate the NO₃, HO₂ and total RO₂ concentrations so we can then calculate the rates of the RO₂+RO₂, RO₂+NO₃ and RO₂+HO₂ reactions. To do so, we have of course replaced the rate constant of limonene by the one of α- or β-phellandrene, as it was indicated in the manuscript in section 2.5, L276-277.** As NO₃ and N₂O₅ concentrations were below the detection limits, we used the phellandrene decay rate (and the rate constant phellandrene + NO₃ which is known) to constrain the N₂O₅ injection rate and consequently the NO₃ and N₂O₅ concentrations. With this method, we also assume that RO₂ concentrations are well simulated as RO₂ formation rate is directly correlated with the VOC oxidation rate and slight changes in RO₂ chemistry won't significantly affect their total concentration.

Finally, to calculate the rate of the reactions RO₂+RO₂, RO₂+NO₃ and RO₂+HO₂, we used the generic rate constants provided by the MCM for peroxy radicals: $k(\text{RO}_2+\text{NO}_3) = 2.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; $k(\text{RO}_2+\text{HO}_2) = 2.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$; For RO₂ self-reaction, the rate constant differs with the type of RO₂ (primary, secondary, tertiary). For limonene and phellandrenes, NO₃-oxidation is expected to form mainly the most-substituted tertiary alkyl radical, leading to tertiary

peroxy radicals. Therefore, we used, as proposed by MCM, the generic rate constants for tertiary peroxy radicals: $k(\text{RO}_2 + \text{RO}_2) = 9.2 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$;

The use of generic rate constants generates uncertainty on the results, but this is the best that can be done given the lack of experimental data for RO_2 radicals. Also, the objective here is not to determine precisely the reaction rates, but rather to estimate the order of magnitudes.

All this information has been added in the manuscript in section 2.5 (L279-289).

3. In Table 1, the "Date" column can be eliminated and replaced with "experiment 1" etc. This format should be carried out to other figures/discussion (e.g., Figure 2, legend).

Following the reviewer's comment, the "Date" column was removed and replaced with "Experiment [number]." This format has been applied consistently to other figures and throughout the discussion.

4. Section 3.3, line 355 - 357: The off-set at the origin (Figure 3) between measured ON and reacted MT, doesn't this indicate a high background? I'm not sure I understand the statement this the "non-zero slope at the origin suggests these are primary products."

The offset at the origin is very small and not significant. To demonstrate this, the uncertainty on the ordinate at the origin has been calculated as $2 \times \sigma$ (2 x standard deviation) for the two plots. For α -phellandrene, the ordinate at the origin is 1 ± 2 ; for β -phellandrene, it is 2 ± 2 . It can be concluded that the ordinate at the origin is not significantly different from zero. This information has been added in Figure 3.

In Figure 3, the X-axis represents the amount of reacted MT, while the Y-axis represents the concentration of ONs formed. The slope at the origin is not zero indicating that ONs are produced immediately and proportionally as MT is consumed, consistent with the behavior of first-generation products. If ONs were secondary products, their formation would depend on intermediates or additional reaction steps. In such a scenario, the slope near the origin would approach zero, as no ONs would form until intermediates accumulated. The observed linear relationship, starting with a measurable slope at the origin, supports the conclusion that ONs are primary products. The sentence has been rephrased in the manuscript to make it more clear (L376-379): *"Moreover, the slope at the origin is not zero indicating that ONs are produced immediately and proportionally as monoterpene is consumed, which is consistent with the behavior of first-generation products. The fact that the slope remains constant during the experiments also indicates if primary ONs are consumed, they will evolve towards the formation of secondary ONs."*

5. Discussion, lines 395 - 410: Throughout the discussion the authors mention that in their experiments the RO_2 fate was dominated by $\text{RO}_2 + \text{RO}_2$ reactions (> 95 %). However, they say that the generation of the closed shell products from the $\text{RO}_2 + \text{RO}_2$ reaction (either self or cross) to form a hydroxy and carbonyl product pair (Russell Mechanism) was negligible. This disagrees with past measurements which have shown branching ratios of averaging around 50/50 between closed shell products and alkoxy radicals, while variable depending on structure the molecular channel is not negligible for these types of RO_2 structures (see review by Orlando and Tyndall, 2012). For other systems that also form first generation tertiary RO_2 radicals, the closed shell hydroxy nitrate still form through cross reactions in non-negligible quantities (e.g., Clafin and Ziemann, 2018). In this work, the lack of measurement of the hydroxy nitrate, in tandem with the lack of speciated/specific measurements and the complex spectra generated from the method utilized, more so point to the measurement itself not being appropriate to detect these compounds.

The measurement method used in this study (PTR-MS with two ionization modes: H_3O^+ and NO^+) was previously employed in other studies conducted by our group under similar experimental conditions (Fouqueau et al., 2020, 2022) on three monoterpenes (terpinolene, α -terpinene, and γ -terpinene) reacting with NO_3 . These studies demonstrated that hydroxynitrates can indeed be detected, but their formation depends on the specific structure of the monoterpene. Hydroxynitrates ($M=215 \text{ g}\cdot\text{mol}^{-1}$) were detected for γ -terpinene and terpinolene in both ionization modes, whereas this was not the case for α -terpinene. We attributed this to the fact that, for α -terpinene, the most stable peroxy radicals formed are tertiary, which do not readily undergo this reaction pathway. Therefore, we do not believe that the non-detection of hydroxynitrates in this study is linked to the measurement method used. Furthermore, for phellandrenes, the major peroxy radicals formed are also expected to be tertiary, which further supports this interpretation. In fact, from all the terpenes we studied (γ -terpinene, α -terpinene, terpinolene, α -phellandrene, β -phellandrene), we conclude that the hydroxynitrates formation is not observed when the terpene has conjugated double bonds. This can be explained by the fact that the electronic delocalization will favor the most substituted (tertiary) radicals. All this information has been added in the manuscript L432-434: *“The hydroxynitrate was however observed for other monoterpenes having similar chemical structures, such as γ -terpinene and terpinolene (Fouqueau et al., 2022, 2020), whereas this was not the case for α -terpinene (Fouqueau et al., 2020). When comparing the studied terpenes (γ -terpinene, α -terpinene, terpinolene, α -phellandrene and β -phellandrene), it becomes evident that the hydroxynitrate formation is not observed in terpenes with conjugated double bonds. This can be explained by the fact that electronic delocalization favors the formation of the most substituted (tertiary) peroxy radicals, which do not readily undergo this reaction.”*

In addition, the reviewer indicates that our study is not in agreement with the one from Claflin and Ziemann, as hydroxynitrates were “shown” to be formed. First, this study was performed for β -pinene and as discussed earlier, chemistry can differ. But more importantly, **no gas-phase products (including hydroxynitrates) have been detected in the study of Claflin et al.**, and **only assumptions** were made for their formation, based on the detection of products in the aerosol phase. In our opinion, our method, **based on double experimental identification of the products with PTR-MS** (in both NO^+ and H_3O^+ modes) is more reliable than the one proposed by Claflin and Ziemann **which proposes a mechanism for gas-phase chemistry without direct detection of gas-phase products. It is therefore “surprising” to see that the reviewer trusts more the results from this study which proposes a mechanism for gas-phase chemistry without direct detection of gas-phase products, rather than ours which is based on a double identification of the products with PTR-MS** (in both NO^+ and H_3O^+ modes).

6. Figure 5. Throughout the mechanism, the authors have the alkoxy radicals reacting with O_2 to form carbonyls. Justification should be given that this reaction could compete with decomposition under these conditions. The reaction of alkoxy radicals with O_2 is typically negligible compared to decomposition or isomerization at room temperature (see Ziemann and Atkinson, 2012 and the references therein, also Vereecken and Peeters, 2009 and 2010). (besoin d'aide pour répondre à cette question)

Maybe there is a misunderstanding of the mechanism proposed in Figure 5 and we should clarify it. The mechanism is not the full mechanism, and we don't claim that other reaction pathways than those indicated in Figure 5, do not occur. Also, we do not provide any branching ratio between the various alkoxy reaction pathways. This mechanism proposes explanation for the formation of the detected products. So, it cannot be deduced that isomerization of alkoxy radicals

is negligible, but only that products from isomerization were not detected. The title of the Figure 5 has been changed accordingly.

We agree that reactions of alkoxy radicals with O₂ are usually considered to be slower than decomposition and isomerization pathways. But these are general rules based on a very limited number of experimental data (mainly for OH chemistry), and we cannot exclude the reaction with O₂ from the mechanism. For other chemical systems, reaction with O₂ was shown to be significant (e.g. Picquet-Varrault et al., 2000). As indicated in the paper from Ziemann et Atkinson, 2012 suggested by the reviewer, “*the data-base from absolute rate methods concerning the reactions of alkoxy radicals is sparse, and at this time the relative importance of the various alkoxy radical reactions can be obtained from the use of estimation methods.*” The lack of experimental data remains in 2025. So, we consider that we should not exclude any of the possible reaction pathways of the alkoxy radicals.

7. Line 465: The definitive assignment here of carbonyl, hydroxyl, or hydroperoxide compounds is not appropriate from the methods used. For example, the molecular formula of a "carbonyl" could also correspond to an epoxide (or others) as proposed by the authors previously in the paper.

We fully agree with the reviewer that the method used in this study (TOF-CIMS) does not allow for distinguishing between isomers with the same molecular formula, such as carbonyls and epoxides. The assignment of compound classes (e.g., C₁₀H₁₅NO_x and C₁₀H₁₇NO_x) in our manuscript was not intended to be definitive but rather a hypothesis based on a combination of our observations and previous work in the literature on HOM formation (e.g. Dam et al., 2022; Shen et al., 2021; Guo et al., 2022).

To avoid definitive assumptions, we have revised the manuscript to clarify that, for example, we added that C₁₀H₁₅NO_x could correspond to a carbonyl or epoxide (e.g. L492 and Table2- column names). As noted by Bianchi et al. (2019), "The elemental composition of epoxide products is identical to that of ketone products formed from OH loss of COOH groups, making it difficult to assess the relative importance of the two reaction routes solely based on mass."

We have replaced definitive terms with conditional language, such as "which may correspond-L492", throughout the manuscript to reflect this uncertainty.

We thank the reviewer for highlighting this important point, and we have incorporated the suggested adjustments to ensure greater accuracy and clarity in the manuscript. The text has been changed in consequence: “*The radical chain termination of C₁₀H₁₆NO_{2n+1}• and C₁₀H₁₆NO_{2n}• can occur through unimolecular termination channels, such as OH loss following H-abstraction from a carbon with a –OOH group attached, or through bimolecular reactions such as RO₂ + RO₂. These termination reactions lead to the formation of closed-shell products such as carbonyl-nitrates, hydroxynitrates and hydroperoxynitrates. It is important to note that compounds with the same molecular formula, such as hydroxynitrates formed from C₁₀H₁₆NO_x• and hydroperoxynitrates formed from C₁₀H₁₆NO_{x-1}•, cannot be distinguished based on mass spectra analysis using TOF-CIMS. Among the C₁₀-HOM monomers, C₁₀H₁₅NO₈ and C₁₀H₁₇NO₈ were identified as having the highest signal intensities. Notably, the signal of C₁₀H₁₅NO₈ was found to be higher than that of C₁₀H₁₇NO₈. This has also been observed in the chemical systems involving β-pinene + NO₃ (Dam et al., 2022; Shen et al., 2021) and limonene + NO₃ (Guo et al., 2022). Finally, we also identified a family of C₉-HOMs (C₉H₁₄N₂O₉₋₁₀), which were detected with more intense signals for β-phellandrene than for α-phellandrene. These products can be formed by the cleavage of an exocyclic or endocyclic C-C bond followed by autoxidation. For β-phellandrene, a first-generation C₉H₁₄N₂O₉ compound and a second-generation C₉H₁₄N₂O₁₀ compound were detected but we are not able to propose detailed formation mechanisms at this stage.*”

8. Lines 488 - 492: Without measured sensitivities for these ions (which also likely consist of multiple compounds, with varying sensitivities), the detection of one molecular formula being "higher" than the other should not be used to conclude that one type of product is formed more than another, or make conclusions about specific reaction channels. Also, definitively stating that these are carbonyl / hydroxy / hydroperoxy nitrates without supplemental measurement to confirm structure or the presence of these functional groups is inappropriate.

We agree that calibration of the NO_3^- ToF-CIMS is necessary to determine its sensitivity to an organic molecule. However, to date, there is no direct calibration method capable of evaluating all possible organic compounds. Due to the lack of HOM standards, calibration is most often performed using sulfuric acid or, in some cases, other molecules, with the assumption that HOMs and the compounds used for calibration cluster with the reagent ion at similar, collision-limited rates.

Comparisons based on relative abundances are a practice already established in the literature, as demonstrated by studies such as Dam et al. (2022), Shen et al. (2021), and Guo et al. (2022). But, we fully agree with the reviewer that as no calibration was performed for each individual products, we cannot conclude on their quantification. To adopt a more cautious approach, we replaced "most abundant" with "detected with the highest intensities" in the manuscript. We made the assumption that if the compounds have similar sensitivity, comparisons based on their intensities can be considered valid.

9. Line 530 - 545: The qualitative detection of particle phase compounds containing > 3 nitrogen containing (I assume ON) groups, is very interesting. Further exploring the formation of these compounds (multi-phase or particle-phase reactions?) would be very nice.

We share the reviewer's opinion on the importance of exploring the formation of particle-phase compounds containing more than three nitrogen (presumably organic nitrate) groups. As mentioned in lines 550-553, we attempted to identify these compounds in the gas phase using TOF-CIMS but were unable to detect them. Online detection of the particle-phase composition using advanced mass spectrometry techniques, with online particle-phase extraction and ionization adapted to these compounds, could provide valuable insights into their real-time formation and profiles, alongside the "parental" compounds, to help elucidate their formation mechanism. This is an interesting point that must be explored in future works.

10. Lines 536 - 539: Is this a valid assumption (same sensitivity for each compound)? What is the error? The authors need to provide some justification for the use of this, can they show the same sensitivity using proxy compounds? Otherwise the quantitative nature of this discussion should be eliminated.

We have made modifications (section 3.5) to clarify that what we are comparing is a relative intensity and not an abundance. However, for the comparison between α - and β -phellandrenes, we believe it can be kept, even if we do not have sensitivity, since we are comparing the same products under the same operational conditions of the TOF-CIMS and the experiment.

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