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Interactive comment on "On the similarities and differences between the products of oxidation of hydrocarbons under simulated atmospheric conditions and cool-flames" *by* Roland Benoit et al.

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With "On the similarities and differences between the products of oxidation of hydrocarbons under simulated atmospheric conditions and cool-flames", Benoit et al. compare the molecular composition of limonene subjected to low temperature combustion conditions to literature data for limonene subjected to ozonolysis. The authors use the datasets to examine differences and similarities due to the reaction pathways and explore potential reaction mechanisms responsible for the observed composition. The dataset and interpretations are both very good quality, and the manuscript is techni-

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cally sound. The justification for the study and its importance to understanding atmospheric chemistry are not well developed, however, and the manuscript requires revisions so readers can understand the importance of the work. These and other comments are discussed below. General Comments: At the end of the introduction (lines 67-75), the authors describe the study's aim as to compare the molecular composition of laboratory "cool flame" combustion of limonene to that of limonene subjected to atmospherically-relevant conditions. While this section describes the study aim/objective, what is needed is a justification/purpose for the study. How will comparing these two datasets provide valuable new information for our understanding of atmospheric organics (or human health, pollution, climate, etc.)? Just how these comparisons will benefit atmospheric chemists needs to be clearly stated so the study can be placed in proper context. Additionally, in the conclusions section (lines 391-407), the authors note that the composition of autoxidation processes are similar to those of ozonolysis and photooxidation, but they never make an argument for why the reader should care about these results. How this work enhances our understanding of atmospheric organic composition or processes in the atmosphere is never explained. The authors need to revise the Introduction and Conclusions sections to very clearly state the justification for and implications of the study. Additional Comments: - In section 2, "a.u." are used as units in multiple location. I am not familiar with these units. Please clarify. Line 89, please spell out FIA HESI/APCI for the reader who is unfamiliar with these acronyms. Line 112, Cite Kendrick (1963). Line 169, "Chemical formula with relative intensity was less than 1 ppm were not considered." To what does 1 ppm refer? Please explain how this relative intensity is calculated (relative to what? the highest magnitude peak? the total spectral magnitude?). In the Figure 2 caption, the circle symbols are not color coded as they are in the figure. Please fix or describe the color coding with words. Line 204, why were the auto oxidation experiments restricted to 2 s residence times? Can the short residence times relative to the ozonolysis and photo oxidation experiments explain the differences in composition? Figure 3 caption – the "aliphatics hydrocarbon," "aromatic hydrocarbon," and "unsaturated hydrocarbon"

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compound classes classified exactly? Intuitively, the unsaturated hydrocarbon classification would refer to compounds having at least one double bond and would extend to higher H/C ratios. Aromatic hydrocarbons would be likely to show lower H/C ratios than merely unsaturated hydrocarbons. Please clarify how these classifications are calculated and use classification names that represent the probably compound structural characteristics. Figure 8 – the novelty and importance of these figures is overstated by the authors. Molecular formula exact mass datasets have been mathematically compared to identify reaction precursors and products in several previous studies (e.g., Gomez-Saez et al., 2016; Abdulla et al., 2020, and others). The same information can be visualized using Kendrick Mass defect analysis (using the expected difference(s) in elemental composition between precursor and product in place of CH2), vK diagrams, or other visualization techniques. The comparisons made in this instance are robust and valuable. The visualization and comparison are not as novel as stated by the authors.

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