Comment on amt-2021-420
Anonymous Referee #2

Referee comment on "Combined application of Online FIGAERO-CIMS and Offline LC-Orbitrap MS to Characterize the Chemical Composition of SOA in Smog Chamber Studies" by Mao Du et al., Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2021-420-RC2, 2022

The manuscript titled "Combined application of Online FIGAERO-CIMS and Offline LC-Orbitrap MS to Characterize the Chemical Composition of SOA in Smog Chamber Studies" by Du and Co-authors characterizes the chemical composition of SOA using a combination of two state-of-the-art mass spectrometry techniques: FIGAERO-CIMS (online), and LC-Orbitrap (offline). The chemical system analyzed is the photooxidation of α-pinene using an atmospheric chamber. The authors use hierarchical clustering of the time series of gas-phase and particle-phase oxidation products to get an insight into the phase partitioning of individual molecular compositions and to inform the targeted analysis for the LC orbitrap.

The distribution of particle-phase products is found broadly similar between the FIGAERO-CIMS and LC-Orbitrap MS negative ionization mode.

The hierarchical clustering analysis allowed the identification of cluster properties in terms of average carbon number, oxygen number, oxidation states, for example, enabling interpretation in terms of possible termination pathways of peroxy radicals in the α-pinene photooxidation reactions.

Saturation concentrations of compounds (C*) were carried out using the FIGAERO CIMS and LC orbitrap independently. The substantial differences resulting from the two approaches indicate that further work is required to investigate C*.

The article is well written and presents an interesting and substantial amount of work that is very relevant, of high interest for the scientific community, and well in line with the journal scope.

I recommend publication after the following minor revisions.

Line 147: “… three filters … filters).” The format needs to be fixed, too many parentheses.

Line 161: “The … 80C”. “relativity” should be “relative” and it should be in the past tense, not future.

Line 183: “the filters … contaminants”. It would be good to add a sentence about how (or
if?) this process was quantified as well some more information about the loading of the filters.

Line 202: “characterized for 30 mins” this is unclear. I recommend changing/expanding the sentence to better explain what that entails.

Line 210: “The gas-phase data ... chamber background”. This is unclear. Please change/extend the sentence to explain what the authors mean. The first measurements were used to correct gas-phase data for the background?

Line 453: “5.5 hours into the photochemistry experiment.” Please add why 5.5 hours was chosen.

Line 529-532: “Figure 4a .. photoxidation”. The sentence is unclear. “increasing over time” seems to be referred to the gas phase. Please rephrase to make sure the reader does not get confused.

Figure S3: the x-axis labels are not legible because are too crowded. Please modify the graph to make them legible (have only a subset?) or remove them if they are not necessary to understand the graph.

Line 734: “instrumental sensitivity needs more effort” this sentence is unclear. Do the authors mean that the sensitivity needs to improve?

Figure 5: I recommend adding “Gas-phase” somewhere on the plot

Figure 6: I recommend adding “Particle phase” and “FIGAERO CIMS” somewhere on the plot