Response to comments of anonymous referees # 1

It is interesting to determine the chemical composition and interactions during SOA formation in mixed VOC systems (photooxidation of α-pinene, isoprene, o-cresol and their binary and ternary mixtures in the presence of NOx and ammonium sulphate seed particles) by using non-targeted LC-Orbitrap MS. The method is innovative. But more detailed information about the methods can be provided.

We kindly thank the reviewer for their time and effort in providing comments for our manuscript. Please see our responses below (shown in blue).

Introduction:

What are the pros and cons of using non-targeted LC-Orbitrap MS analysis for data interpretation can be addressed?

We appreciate the opportunity to expand on the benefits and challenges. We will introduce the advantages of using non-targeted LC-Orbitrap MS analysis for data interpretation in section 1.3, from line 101, which has been changed to *"……application. Non-targeted analysis extracts the chemical information of all detected compounds in a sample dataset, providing tentative identification of unknown compounds via library screening, while allowing the rapid chemical characterisation of complex mixtures through the chemical classification of detected compounds in a given sample Place et al. (2021) and Pereira et. al 2021. Mezcua et al. (2011) reported that 210 pesticides were successfully been detected and identified in 78 positive samples of fruit and vegetable samples by using automatic non-targeted screening method in LC-TOF analysis. High-resolution accurate mass spectrometry (HRAM-MS)-based non-targeted screening analysis were applied in chemical characterized of tobacco smoke, and successfully identified a total of known 331 compounds and 50 novel compounds as being present in the sample (Arndt et al., 2019). "*

The challenges associated with its use will be introduced in section 1.3, from line 108; the section has been rephrased to *"……low concentration species. However, non-targeted screening methods are not infallible and rigorous testing of autonomous platforms must be performed to understand potential limitations of these tools. Moreover, it is challenging to make semiquantitative or quantitative measurements of unknown compounds in complex matrices. It is worth to noting that quantitative measurements of unknow compounds is a general limitations of ESI operation and not directly attributed to non-targted screen method, but arguably become more important. It is difficult to perform quantitative measurement of unknow compounds due to the analytical standards for SOA products are limited and only a few molecules out of the thousands detected compounds might be known. Therefore, it is also challenge to determine sample extraction recoveries during sample extraction procedures. The approach of using the normalized abundance of compounds in the sample does not consider different compound ESI efficiencies, which can be influenced by the molecular structure among other parameters (Priego-Capote and Luque De Castro, 2004) . For example, Cech and Enke (2000) found out that ESI response increased for peptides with more extensive non polar region. Cech and Enke (2001) further examined and concluded that analytes with more polar portion*

has lower ESI response than the more nonpolar analytes. Differences in ESI efficiencies of individual compounds may impact normalized abundance of chemical groupings, particularly when comparing sample compositions which differ appreciably.

Method:

There are lots of anthropogenic VOC precursors, why o-cresol was chosen as an anthropogenic precursor in this study?

The work in this paper is a subset of a more comprehensive chamber study of SOA formation from mixed precursors and here focuses on the chemical composition of the SOA formed using LC-Orbitrap MS. A comprehensive and detailed description about the experimental design of the project is presented in Voliotis et al. (2022), which describes the choice of VOC precursors, and their "representativeness" in section 2.1.

We choose *o*-cresol as a moderate SOA yield anthropogenic precursor with comparable reactivity towards the available oxidants (OH radicals) as the two biogenic VOC in a mixtures (a-pinene and isoprene), such that they each may contribute comparably to the distribution of oxidation products.

Humidity and temperature are important factors for SOA formation, they are controlled by the humidifier and by controlling the air conditioning during the experiment. These parameters should be added in the manuscript.

We included this in section 2.3:

From line 259-261: "*Photochemistry was initiated by irradiating the VOC at a moderate VOC / NO_x ratio using the lamps as described above. The temperature and relative humidity conditions were controlled at 50 % ± 5 % and 24 ± 2°C, respectively during the experiment. The concentration of NO_x and O_3, particles number concentration and mass concentration were monitored during the experiment using the online instruments .*"

Why was the mass concentration of seed particle doubled in single isoprene experiment?

The seed particles were inadvertently added into the chamber with increased mass concentration for the single isoprene system. Whilst this could have resulted in a greater partitioning of oxidation products leading to more SOA particle mass forming, the particle mass and resulting yield in the single precursor isoprene system was negligible (SOA particle mass concentration ~0 µg /m^3), consistent with other studies using neutral seeds.

How many repeated experiments performed in each experiment type?

Three replicate experiments were conducted for all systems except the single precursor isoprene systems. This information has been added in the section 2.4.2, Line 315: "*To provide*

confidence in the components in each system detected by the non-targeted method, only those compounds found in all three replicate experiments (two in the single precursor isoprene and binary o-cresol/isoprene systems) and not found in any background "clean" experiments were attributed to a particular single precursor or mixed system."

Before filter sampling, any denuder was used to remove VOCs, NOx and oxidants?

No denuder was used to remove VOCs, NO_x and oxidants before filter sampling owing to the challenge associated with gaseous denuding at the high sampling flow rate. Chamber air was flushed out at around 3 m^3 min^{-1} onto the filter, taking some 5 minutes for sample collection. Du et al. (2021) had combined the online (FIGAREO-CIMS) and offline mass spectrometric (LC-Orbitrap MS) techniques to characterize the chemical composition of secondary organic aerosol (SOA) generated from the photooxidation of α-pinene in the MAC. The study of Du et al. (2021) reported that the distribution of particle-phase products is highly consistent between the FIGAERO-CIMS and LC-Orbitrap MS negative ionisation mode for the α-pinene SOA products, suggesting near negligible (or at least comparable) gas phase absorption artefact introduced during filter collection in both techniques.

Results and discussion:

Online data from gas chromatography mass spectrometer (GCMS), condensation particles counter, differential mobility particle sizer (DMPS) and aerosol mass spectrometer (AMS) are very useful for data interpretation. But the results were not reported in this study.

As mentioned above, this is part of a more comprehensive study of SOA formation in mixtures. The full instrument description is given in in Voliotis et al. (2022), and the DMPS, GCMS and AMS, along with the online FIGAREO-CIMS, data are presented therein, and in several companion papers (Du et al., 2021; Shao et al., 2022)
The online GCMS data show the decay of precursors at each system in Figure 1(d)-(f). We could not extract more information about the chemical composition of gas-phase products from the online GCMS in our experiments, but the products are reported in Du et al., (2022a,b). The AMS data were utilised to show the evolution of SOA mass of each precursor system and presented in Figure 1(a), but high resolution data are compared in detail with FIGAREO-CIMS data and offline LC-Orbitrap MS data in Shao et al. (2022, in prep).

Lots of data were presented in this study, (e.g. number of detected SOA compounds, molecular composition, compositional analysis). The novel part of this study is about the unique-to-mixture products due to the interactions between VOC products. This section can be extended and provide more mechanistic understanding of their formation.

We thank to the reviewer for this suggestion. To provide more mechanistic understanding of their formation required structure identification and quantification of the unique-to-mixture compounds, which require standards. Mechanistic inferences are provided in the combined use of FIGAREO-CIMS data and offline LC-Orbitrap MS in Du et al. (2022a,b) and further work to elaborate on the potential mechanisms is recommended in line with these studies.

We include this at the end Conclusion section: "*This study did not examine the molecular structure of the unique compounds/potential tracers in the mixture precursors systems. The future studies suggest focus on identifying the molecular structure of unique-to-mixture components will help better understand the detailed mechanisms of interactions involved in ambient SOA formation from mixture VOC oxidations.*"

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Voliotis, A., Du, M., Wang, Y., Shao, Y., Alfarra, M. R., Bannan, T. J., Hu, D., Pereira, K. L., Hamilton, J. F., Hallquist, M., Mentel, T. F., and McFiggans, G.: Chamber investigation of the

formation and transformation of secondary organic aerosol in mixtures of biogenic and anthropogenic volatile organic compounds, Atmos. Chem. Phys. Discuss., 2022, 1-49, 10.5194/acp-2021-1080, 2022.

Response to comments of anonymous referees # 2

General Comments:

This work by Shao et al. is a follow up to the work by McFiggans et al. in Nature 2019 on the impacts of mixed VOC systems on SOA formation. They performed a series of batch mode chamber experiments with single and mixed precursors of biogenic and anthropogenic origin in the presence of NO_x and aerosol seed. Offline analysis of the SOA composition was performed primarily with LC-MS to elucidate which species dominate and dictate the SOA formation in mixtures and identify any cross products. This work is novel and of value to the community, although I find it to be overly verbose and rambling and suggest editing to make it more concise and flow better if possible. This is appropriate for ACP after addressing the other suggestions below.

Specific Comments:

Line 134: I think this is well established and suggest re-wording "might be the reason" to something more definitive

Line 134 revised from "which *might be the reason*" to "*which is the reason…".*

Line 207: What is the residence time in the chamber?

The MAC is operated as a batch reactor and is not operated in "flow through" mode. The air is held continuously after introduction, as described in Shao et al. (2022), so essentially has an infinite residence time (though component lifetimes clearly would be limited by the losses to, and interactions with, the Teflon walls). The experimental duration is typically 6 hours, though experiments up to 24 hours are possible.

Section 2.4.1: Is it possible for chemical transformations to occur during the 2 hr ambient temperature rest, sonication, or drying? Would this be observable? Can you comment on how this may impact results?

It is difficult to determine the quality of the aerosol extraction procedure using non-targeted analysis due to the difficulty of unknown compound identification. The analytical standards for SOA products are limited and only a few molecules out of the thousands detected compounds might be known. Therefore, it is also difficult to determine sample extraction recoveries during sample extraction procedures, since various compounds will have different recovery efficiencies that can be influenced by the molecular structure (Priego-Capote and Luque De Castro, 2004).However, we note that the sample extraction procedure performed in this study is common practice for the analysis of OA, with the majority of studies using either water or methanol as the extraction solvent, followed by sonication and evaporation(Gao et al., 2006; Hamilton et al., 2008; Kourtchev et al., 2016) It should be noted that we used methanol as extraction solvent since sonication using water can result in the formation of hydroxyl radicals (Miljevic et al., 2014). Moreover, a procedure-controlled sample using a blank filter subject to the same extraction procedure, was performed and analysed using LC-Orbitrap MS analysis. Any artefacts introduced into the samples during sample preparation were excluded from the sample data (see Pereira et. a. 2022 for further information).. However, This does not

provide insights into potential chemical transformations in the OA samples. Investigating potential chemical transformations during the preparation of the OA samples using non-targeted screening would be incredibly challenging. A control sample (*i.e.* a portion of the same OA sample to allow comparison) would still need to undergo some form of extraction into solvent to allow LC-MS analysis. Further, evaporation and resuspension of the sample into a smaller volume (i.e. sample concentration) will almost certainly be required to allow detection of the trace-level compounds present in OA. However, individual compounds within OA could be targeted to investigate possible chemical transformations, spiking a known quantity of a chemically labelled authentic standard (e.g. deuterated) into the OA sample before solvent extraction. This would allow any chemical transformations to be observed and the extraction recovery of the spiked compound to be determined. We recommend in Pereira et. al. 2022 investigating the recovery efficiencies of authentically identified compounds in future work to quantify any potential losses and provide insights into the quality of the extraction procedure. The work presented here was performed prior to the publication of Pereira et. al. 2022 and subsequently does not include this in investigation.

Line 304: Where would the sodium and potassium come from?

Sodium and potassium could come from several sources during sampling preparation and analysis, such as the mobile phase additives, solvent impurities and so on. The main source is leaching from glassware used to prepare the solvents (Kruve and Kaupmees, 2017). The sentence in the line 302- 304 rephrased to

"*The method provides molecular formulae assignment of detected compounds using the following elemental restrictions: unlimited carbon, hydrogen and oxygen atoms, up to 5 nitrogen and sulphur atoms, and in positive ionisation mode, 2 sodium and 1 potassium atom are also allowed (sodium and potassium are typically introduced into the samples via glassware)*."

Figure 2: Are these common molecular *structures* or molecular *composition*?

These are common discrete molecules. We compared the molecule list between different precursor systems and identified the common molecules which were only considered to be the same detected molecular species if they had a retention time within 0.1 minutes.

The captions in Figure 2 rephased to " *Number of common discrete molecules and unique compounds in single and binary precursors mixed experiments detected by negative ionization mode LC-Orbitrap MS. Product are considered identical in the mixed and single precursor systems if the molecules has the same empirical formula and a retention time difference <0.1min.*"

Also, the caption in Figure 3 rephased to "*Number of common discrete molecules and unique compounds in single and binary precursors mixed experiments detected by positive ionization mode LC-Orbitrap MS. Product are considered identical in the mixed and single precursor*

systems if the molecules has the same empirical formula and a retention time difference <0.1min."

Figure 4: Why does essentially all the signal contain nitrogen for cresol and any mixtures with cresol? This is discussed ~line 520 but not the reasoning for why N-containing species are highly dominant.

Nitrogen containing compounds, such as those containing amide groups or nitro groups, efficiencently ionize using electrospray ionization (Oss et al., 2010). As the MCM v3.3.1 and our study shown, *o*-cresol photo oxidation produces a number of different kinds of nitro-aromatic compounds, such as methyl-nitrocatechol and methyl-nitrophenol. These compounds have high negative mode sensitivity using electrospray ionisation, contributing to substantial signal in the systems that contain *o*-cresol.

This is mentioned in line 526-528, line 576-577, line 783-784, line 851-852, and line 954-956 in the manuscript. Reference (https://doi.org/10.1021/ac902856t) will add in line 528 to further support the explanation.

Line 467: Suggest using HOM definition from Bianchi et al (https://pubs.acs.org/doi/10.1021/acs.chemrev.8b00395): highly oxygenated organic molecules

The definition of HOM in line 467 had been rephased to "highly *oxygenated organic molecules*"

Lines 466-472: This section on HOM is not well fleshed out and doesn't seem to flow with the discussion. Suggest removing or re-writing. Please add a reference for this sentence, or remove: "Autoxidation may therefore contribute to CHO products with carbon numbers 16 – 20 in α-pinene oxidation"

We rephased the sentences from line 466 to 472 as shown below:

"*Autoxidation of RO_2 radicals in the gas-phase occurs rapidly via inter/intramolecular hydrogen abstraction leading to forming R radicals with subsequent O_2 addition (Mentel et al., 2015; Jokinen et al., 2014). The new RO_2 radicals can undergo further autoxidation reaction, or react with RO_2 to generate dimer accretion products (Zhao et al., 2018; Berndt et al., 2018), leading to so-called highly oxygenated organic molecules (HOM) with very-low volatilities (Bianchi et al., 2019). Autoxidation may therefore contribute to CHO products with carbon numbers 16 – 20 in α-pinene oxidation (Berndt, 2021; Ehn et al., 2014)*"

Line 477: Please state how much SOA was formed. It is confusing that this line (and above) states ~0 µg/m3 was formed but the section goes on to discuss the compounds measured in the particle phase

The SOA particle mass was 0.1 µg/m^3 in single precursor isoprene system. The sentence in line 477 rephrased to "*As also seen in Fig.1(a), negligible SOA particle mass was generated in the single precursor isoprene system (0.1*µg */m^3, close to our chamber background*". We measured the SOA particle mass by using the online HR-TOF-AMS, which detected negligible mass in the chamber, at the same order as the background chamber levels. This does not mean that there were no particulate components derived from isoprene present, just that the total mass was

practically indistinguishable from the background mass using our online instrumentation. The compound measurements we report were obtained from offline LC-orbitrap MS analysis, with its ability to detect compounds with trace sensitivity much lower than the limit of detection of the AMS. The compounds could be detected by LC-Orbitrap MS, and use automate non – targeted screening method to assign the molecular formulae as long as the masses error < 3 ppm, signal-to-noise ratio > 3, and the isotopic intensity tolerance was within ± 30 % of the measured and theoretical isotopic abundance.

Lines 493-494: This doesn't reflect the current state of knowledge and is an insufficient explanation/discussion. Several recent studies have shown that small particles are detected in SOA as a result of decomposition, typically via thermal processes, during analysis. While this work doesn't utilize heating techniques, it does involve substantial sample prep (see comment on section 2.4.1).

As stated in the response for the comment on section 2.4.1, it is difficult to determine the likelihood of potential chemical transformation in the OA sample during the aerosol extraction procedure. An extra sentence will be added at line 495:

"*The possibility that small detected molecules were formed in the filter sample extraction process cannot be ruled out. For example, degradation of organic compounds can be induced by ultrasonic extraction of particulate matter from filters (Miljevic et al., 2014; Mutzel et al., 2013),"*

Lines 496-498: I'm confused why the experiment would be designed in a way that is well documented to not make SOA when the stated point of this work is to make SOA and measure the particle phase composition? Please explain the reasoning for this experimental design and how this advances our understanding of multi-component SOA formation.

Our experimental program aims to establish a framework to understand interactions in systems of mixed anthropogenic and biogenic VOCs. Therefore, we choose precursors considering the potential diversity in VOC sources contributing to the ambient atmosphere, building on the previous insight from McFiggans et al.(2019) which used a binary mixture of biogenic low yield (isoprene) and high yield (α-pinene) precursors. The aim is to further investigate the interaction in systems of mixed low, moderate or high yield VOCs, with both anthropogenic or biogenic species able to compete for the available OH.

There is a clear indication of suppression of the yield of α-pinene in its mixture with isoprene, but as with the *o*-cresol / isoprene mixture, there is a possible indication of enhancement, though this is too small to be unambiguous. In the ternary system, it is unclear if there is a suppression or enhancement effect with regard to measured total SOA particle mass, but chemical interactions are evident from the unique-to mixture components. All these results about SOA yield across different precursors systems, details of experimental design, and the complexity of the systems introduced substantial challenges to their interpretation were comprehensively elucidated in the companion paper Voliotis et al. (2022).

We still could measure and analyse the SOA particulate product from isoprene, which is well documented to make little SOA particle mass under neutral seed conditions, by use of the LC-Orbitrap MS technique and its unprecedented high-resolution accurate mass (HRAM) allowing unambiguous identification of molecular formulae. .

Line 501: Can you be sure these species are created from isoprene + OH and not impurities in your isoprene source or chamber contamination?

The isoprene gas precursor was introduced into the chamber by injecting liquid isoprene (Sigma-Aldrich, purity >=99%) through a rubber seal into a glass bulb that temperature was kept at approximately 100℃, and flush to the chamber by using nitrogen as carrier gas. The glass bulb was warm and flushed with N_2 during the "pre-experiment" protocol before the conducted experiment ensuring contamination in the glass bulb was flushed out and maintain cleanness. Thus, we are confident that these species are not contamination or impurities in the isoprene source.

Our chamber had conducted off-gasing and actinometry experiments regularly to determine the chamber background contamination. Filter samples also been collected after each off-gasing and actinometry experiment, that followed the same sample extraction procedure and LC-Orbitrap MS analysed method. None of the reported compounds were found in these background experiments and any contamination from chamber introduced into the experimental samples can therefore be excluded.

Line 679: Here you mention the possibility of fragmentation of larger species resulting in the smaller species measured in the particle phase. Please include references (e.g. https://pubs.acs.org/doi/abs/10.1021/acs.est.5b04769).

The reference (Lopez-Hilfiker et al., 2016) will be added into the text of manuscript.

Line 765: It isn't clear to me that accretion reactions have occurred during SOA formation rather than alterations during sample prep and analysis. Additionally, if they did occur during the experiment, can you be sure that accretion products would still form under atmospherically relevant precursor and SOA concentrations?

The intensity weighted average values of nC clearly show accretion products to be present in the single precursor isoprene system, the binary α -pinene-containing systems and the ternary system in positive ionization mode. It is indeed difficult to guarantee that the OA chemical transformation did not happen during sample preparation. Therefore, the sentence in line 765 has been rephrased to

"*It is apparent in the positive mode that accretion reactions occurred, and its products play an essential role in the single precursor isoprene system, the binary α -pinene-containing systems and the ternary system. It cannot be discounted that chemical transformation may occur during filter sample preparation, which might impact on the intensity weighted average values of various chemical properties*."

Some of the accretion products, such as $C_{21}H_{33}NO_4$ in binary α-pinene/o-cresol system, $C_9H_{11}NO$, and $C_8H_8O_{10}$ in binary isoprene/*o*-cresol system were found uniquely in the mixed precursors system with non-negligible normalized signal abundance, enabling their use as tracers in the ambient environment.

Technical:

Throughout manuscript: NOx should have a subscript “x” and be NO_x

Changed

Throughout manuscript: change instances of “ml” to “mL”

Changed

Throughout manuscript: change instances of “ug” to “µg”

Changed

Line 222: particles counter à particle counter (plural to singular)

Changed

Reference:

Arndt, D., Wachsmuth, C., Buchholz, C., and Bentley, M.: A complex matrix characterization approach, applied to cigarette smoke, that integrates multiple analytical methods and compound identification strategies for non-targeted liquid chromatography with high-resolution mass spectrometry, Rapid Communications in Mass Spectrometry, 34, 10.1002/rcm.8571, 2019.

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