Responses to reviewer's comments

We thank the reviewer for their detailed, helpful, and overall supportive comments. We have revised the manuscript to account for each comment. Responses to the individual comments are provided below. Reviewer comments are in bold. Author responses are in plain text. Modifications to the manuscript are in italics. Line numbers in the response correspond to those in the revised manuscript text file. All changes made in the revised manuscript have been highlighted in red font.

1. **Introduction: Actually, there have been quite a few studies using similar high-resolution mass spectrometry to investigate the molecular characteristics and formation mechanisms of NOCs. These should be clearly stated in the background section so as to more accurately highlight the novelty of this study.**

We thank the reviewer for this valuable comment. We agree that the original Introduction did not sufficiently link the current study to previous molecular-level investigations of atmospheric NOCs conducted using HPLC-Orbitrap MS. In the revised manuscript, we have added a brief discussion of recent studies employing high-resolution mass spectrometry to characterize NOCs and related compounds in atmospheric aerosols, including investigations of nitroaromatic compounds and molecular-level composition of organic aerosols (e.g., Li et al., 2020; Wang et al., 2022).

At the same time, we have clarified the novelty of the present study. While previous studies have characterized the molecular composition and formation of NOCs in a variety of environments, comparable molecular-level investigations remain scarce in Southeast Asia, particularly in Myanmar. Furthermore, systematic investigations into the characteristics and formation pathways of atmospheric NOCs in Myanmar remain limited.

Revisions are in lines 117-123 of main text, "*Previous ultra-high-performance liquid chromatography coupled with orbitrap mass spectrometry (UHPLC-Orbitrap MS) studies have successfully characterized the molecular composition of* *atmospheric NOCs and nitroaromatic compounds in urban environments such as Beijing (Li et al., 2020; Wang et al., 2022). However, comparable molecular-level investigations remain largely unavailable in Southeast Asia, particularly in Myanmar, a region strongly influenced by severe air pollution and frequent biomass burning (Zhang et al., 2022; Nway et al., 2020)*".

2. Methods section: The uncertainties of the measurement methods should be specified, particularly for the water-soluble organic nitrogen that is directly relevant to the analysis in this study.

We thank the reviewer for this helpful suggestion. Following the reviewer's recommendation, we have added a detailed description of the quality assurance and quality control (QA/QC) procedures and measurement uncertainties associated with the determination of water-soluble inorganic ions and WSTN in Section 2.2.1. Specifically, process blanks, replicate analyses, spike recovery tests, and field blank assessments were conducted to evaluate analytical precision and accuracy. The relative differences between duplicate measurements were generally less than 5%, the spike recoveries for WSTN ranged from 90% to 110%, and the concentrations of target species in field blanks were less than 5% of those measured in ambient samples, indicating negligible impacts on the reported concentrations.

Considering that WSON was calculated as the difference between WSTN and WSIN, the overall uncertainty of WSON is expected to be within the combined analytical uncertainties of these measurements and does not affect the major conclusions of this study.

Modified in lines 161-171, *"Quality assurance and quality control (QA/QC) procedures were implemented throughout the analyses. For the determination of water-soluble inorganic ions, one procedural blank was analyzed for every 20 samples. In addition, duplicate analyses were performed for 10% of the samples during instrumental measurements, and the relative difference between duplicate measurements was generally less than 5%. For WSTN determination, one duplicate* *sample was analyzed for every 10 samples, with relative differences between duplicate measurements also below 5%. Spike recovery tests were conducted to evaluate analytical accuracy, and the recoveries generally ranged from 90% to 110%. Furthermore, the concentrations of target species in field blank samples were less than 5% of those measured in ambient samples, indicating negligible effects on the quantified concentrations."*

3. The justification for the model setup should be more sufficient. For example, "Testing showed the model required around 9 hours of spin-up (starting from midday local time) before concentrations settled." How was the threshold for determining when concentrations "settled" defined?

The reviewer is correct that "settled" alone is a vague statement and that a quantitative description is preferred. The text around spin-up in Section 2.3 has therefore been updated to lines 295-298 in main text:

"Testing showed the model required around 9 hours of spin-up (starting from midday local time) before mass concentrations of all components, including radicals, were within 5 % of their concentration 24 hours later, and therefore results were taken over the 24 hours of simulation from 9-33 hours through the simulation."

4. "These results are consistent with the findings of Sun et al. (2025), who reported that..." The comparison of the results should utilize atmospheric observation data from similar regions to reflect the differences between coastal and urban areas. Currently, selecting only one paper for comparison is not representative.

We thank the reviewer for this valuable suggestion. We agree that comparison with a single observational study may not be sufficiently representative. We would like to clarify that Sun et al. (2025) is a review article that synthesized molecular composition data from a wide range of atmospheric environments, including urban regions (e.g., Beijing, Shanghai, Guangzhou, and Stuttgart), forested regions (e.g., Hyytiälä and the Amazon), and remote environments such as the Arctic. The citation was intended to demonstrate that the predominance of CHO compounds, followed by CHON and/or CHOS compounds, has been observed across diverse atmospheric settings.

To further strengthen the comparison, we have additionally included a wintertime observational study from Beijing based on UHPLC-Orbitrap MS, which likewise reported CHO, CHON, and CHOS compounds as the three dominant molecular classes (Wang et al., 2022). These additional comparisons provide stronger support that the molecular composition pattern observed in this study is not unique to our sampling location but has been widely reported in both urban and non-urban atmospheric environments.

The relevant content is in lines 337-346. *"Similar molecular composition patterns have been reported in a wide range of atmospheric environments. Sun et al. (2025) summarized observations from urban, forest, and remote regions worldwide and showed that CHO compounds generally dominate atmospheric organic matter, followed by CHON and/or CHOS compounds. Consistent with this review, a wintertime study in Beijing using UHPLC-Orbitrap MS also identified CHO, CHON, and CHOS as the three most abundant molecular classes (Wang et al., 2022). These results suggest that the predominance of these compound classes is a common feature of atmospheric organic matter, although their relative contributions may vary depending on local emission sources and atmospheric processing."*

5. How large is the uncertainty of the semi-quantitative analysis based on high-resolution mass spectrometry? Is there any corresponding methodological paper as a basis? These details should be clearly described in the main text. Furthermore, after the semi-quantification, does the total mass variation of these organic molecules align with the variation of the total organics? Has any further validation been conducted?

We thank the reviewer for this important comment. We acknowledge that it is difficult to rigorously quantify the uncertainty associated with semi-quantitative concentrations derived from high-resolution mass spectrometry peak intensities. The primary limitation arises from compound-dependent ionization efficiencies and response factors in ESI sources, which can vary substantially among different molecular species. Because authentic standards are unavailable for the vast majority of detected compounds, absolute quantification and a comprehensive uncertainty assessment are currently not feasible. Therefore, *the semi-quantitative approach adopted in this study is intended primarily to compare relative abundance patterns and temporal variations among compound classes rather than to provide absolute concentrations.* We have clarified these limitations in the revised manuscript (in lines 206-208).

To evaluate the reliability of the semi-quantitative results, we compared the summed semi-quantified concentrations of detected organic compounds with independently measured WSOC concentrations. A strong positive correlation was observed ($r = 0.88$), indicating that the temporal variation of the semi-quantified organic compounds is consistent with that of WSOC. This agreement provides independent support for the applicability of the semi-quantitative approach used in this study.

6. Why is the identification criterion for nitrophenols O/N ≥ 3 instead of O/N ≥ 2?

We thank the reviewer for this comment. The criterion of O/N ≥ 3 was adopted because nitrophenols contain at least one nitro group ($-NO_2$) and one hydroxyl group (-OH). Therefore, the minimum theoretical O/N ratio for a nitrophenol molecule is 3 (three oxygen atoms and one nitrogen atom). In contrast, an O/N threshold of 2 could also include other nitrogen-containing compounds that possess a nitro group but lack the hydroxyl functionality. Therefore, O/N ≥ 3 was used as a more conservative criterion for the identification of nitrophenol-like compounds.

7. The interpretation of the box model results requires more substantial data analysis. For example, “The box modelling results have shown that the Raoult effect driven by changes in aerosol water content, which are driven by changes in

RH, exerts a physical influence over $C_8H_9NO_4$/$C_6H_5NO_4$, since $C_8H_9NO_4$ is more sensitive to the effect." However, no specific data analysis is presented to support this.

We thank the reviewer for this comment. We agree that the mechanistic basis and data analysis for box model interpretation was not sufficiently explained in the original manuscript. Therefore, more detail around the mechanisms at play in the box model and their application to interpretation of box model results is now provided in the revised Methods and Results section. During this revision we realized that attributing thermodynamic partitioning changes only to the Raoult effect was misleading as a solubility effect is also at play, therefore, 'Raoult effect' has been replaced by 'partitioning thermodynamics' throughout the paper. The methods section now reads:

"The model treats gas-particle partitioning dynamically with thermodynamics driven by the Kelvin term, component mole fraction (Raoult's law), particle-phase solubility and pure component vapor pressures, as described in O'Meara et al. (2021)." in lines 221-224.

and

"The different particle-phase solubilities were not directly measured, but were represented through activity coefficients following previous studies of structurally similar aromatic nitro-compounds (Lee et al., 2000). The $C_6H_5NO_4$ molecule contains hydroxyl and nitro functional groups that enhance polarity and hydrogen-bonding interactions with aerosol water, and was therefore assumed to behave relatively close to ideal solution conditions. In contrast, $C_8H_9NO_4$ contains additional non-polar organic functionality, which is expected to increase non-ideal interactions and reduce effective aqueous-phase solubility." in lines 267-275.

And

"The combination of different volatilities and solubilities of $C_6H_5NO_4$ and $C_8H_9NO_4$ in a thermodynamic simulation of gas-particle partitioning presents the

potential for different sensitivities to varying particle-phase water content, which is quantitatively investigated in the results." in lines 279-282.

Furthermore, further quantitative analysis is provided in Section 3.3.2 to support the interpretation of box model results:

"Several factors are at play in the simulated results of Fig. 7, the increase in gas-phase OH concentration from winter to summer (photochemistry effect), the increasing influx rate of benzene from a minimum in Yangon summer to a moderate value in Yangon winter and a maximum for both seasons for Mandalay, the changing partitioning thermodynamics for $C_8H_9NO_4$ *and* $C_6H_5NO_4$ *due to the changing absorptive molar concentration of particles and changing water mole fraction that affects solubility as explained in Section 2.3."* in lines 518-524.

And

"Considering first just the Mandalay results (Fig. 7a), for which the influx rates of $C_6H_5NO_4$ *and* $C_8H_9NO_4$ *precursors were constant across all RH, modelled* $C_8H_9NO_4/C_6H_5NO_4$ *changes from 0.69 to 0.54 as RH changes from 80 to 60 %, whilst observations report a change from 0.59 to 0.48. Because both 80 and 60 % were during the winter period, the modelled change is not due to changing actinic flux, similarly although the decrease in gas-phase water content from 80 to 60 % RH leads to a slight decrease in OH concentration, the change in consumption of the parent VOCs is negligible, therefore photochemistry does not explain the change in ratio. The only remaining explanation for the ratio changes available to the model is changes to the particle phase due to changed partitioning thermodynamics. The decrease in particle-phase concentration of* $C_8H_9NO_4$ *from 80 to 60 % RH is 30 %, whilst the decrease is 10 % for* $C_6H_5NO_4$*. Therefore, the greater sensitivity of* $C_8H_9NO_4$ *to changing partitioning thermodynamics, which results from changes to both absorptive particle concentration and particle-phase solubility, results in changed* $C_8H_9NO_4/C_6H_5NO_4$*. Variations in sensitivity are dependent on the product of component activity coefficient and vapour pressure, which gives an effective volatility or* c^*_{eff}*. For* $C_8H_9NO_4$*,* c^*_{eff} *changes from 2400 to 1800 µg* m^{-3} *between 80 and 60 % RH, whilst for* $C_6H_5NO_4$ c^*_{eff} *changes from 82 to 64 µg* m^{-3}*. These effective volatilities*

can be divided by the component molar masses to give units of mol m^{-3} *and combined with the total absorptive molar concentration (*$c_{n,abs}$*) of the particle phase in an equation for equilibrium gas-particle partitioning (Pankow 1994) to demonstrate the different thermodynamic sensitivity of the two components:*

$$\xi_i = \left(1 + \frac{c^*_{n,i,eff}}{c_{n,abs}}\right)^{-1} \quad , \qquad (3)$$

where ξ *is the equilibrium condensing fraction of component* i *and* n *is the molar concentration. Using the simulated* $c_{n,abs}$ *of* 3.59×10^{-6} *and* 7.28×10^{-6} *mol* m^{-3} *for the 60 and 80 % RH scenarios, respectively, gives a factor change in* ξ *(*$\xi_{i,80\%RH}/\xi_{i,60\%RH}$*) of 1.33 for* $C_8H_9NO_4$ *and 1.04 for* $C_6H_5NO_4$*."*

"Whilst partitioning thermodynamics continues to act to decrease condensation of $C_8H_9NO_4$ *and* $C_6H_5NO_4$ *as RH decreases from 60 % in Mandalay winter to 40 % in Mandalay summer, the particle-phase loading of both* $C_8H_9NO_4$ *and* $C_6H_5NO_4$ *actually increases, driven by the increased OH concentration that results from enhanced photochemistry.* $C_6H_5NO_4$ *appears to be particularly sensitive to changing atmospheric oxidizing capacity, as its relative increase is greater than that of* $C_8H_9NO_4$*, with fractional increases of 140 and 70 % respectively. Analysis of simulated rates of production and destruction at midday shows a production enhancement of factor 2.33 for* $C_6H_5NO_4$ *going from 60 to 40 % RH, whilst the factor for* $C_8H_9NO_4$ *is 1.62 and for both components the rate of chemical destruction is relatively minor so that dilution dominates losses.* (in lines 529-566)

Furthermore, we appreciate better support for box model interpretation is a general comment regarding all aspects of interpretation, therefore, we also improve the data analysis around Yangon results, which now reads:

The Yangon results are all for 70 % RH, and therefore have similar partitioning thermodynamics. For Yangon results, two factors are therefore at play, changing influx rates (Section 2.3 and Fig. S7) and changing photochemistry. Moving from Yangon summer to winter, photochemical changes act to increase $C_8H_9NO_4/C_6H_5NO_4$*, as seen and explained above for Mandalay results between 40 and 60 %. The photochemistry effect for Yangon is isolated from the influx rate effect by the* *hypothetical result in Fig. 7b, and indeed predicts increased* $C_8H_9NO_4/C_6H_5NO_4$ *from Yangon summer. However, both measurements and non-hypothetical simulation (for the latter changed photochemistry and changed precursor influx rates are at play) results show a slight decrease in* $C_8H_9NO_4/C_6H_5NO_4$*. Taking the hypothetical and non-hypothetical simulation results for Yangon winter together shows that the opposing effects of changes in photochemistry and precursor influx rates on* $C_8H_9NO_4/C_6H_5NO_4$ *broadly compensate one another for the non-hypothetical Yangon winter simulation."* (in lines 567-579)