General.

We would like to appreciate the editor and reviewers for providing the valuable comments and a better perspective on our work to improve the manuscript. In particular, we are very grateful to the editor and reviewers for giving us the opportunity to make revision. We have revised our manuscript by fully taking the reviewers' comments into account. Responses to specific comments raised by the reviewers are described below. All the changes made and appeared in the revised text are shown in red. All detailed answers to comments are displayed in blue.

Comments of Referee #1 and our responses to them

Comments:

This study focused on the measurement and characterization of nitrogen-containing organic compounds in $PM_{2.5}$ collected in Urumqi over a one-year period. As mentioned in the manuscript, Urumqi is the largest inland city farthest from the ocean in the world. However, I have found that work on organic aerosols is rarely reported here. Thus, the manuscript can contribute a significant amount of valuable field data and will appeal to the readership in the field of atmospheric chemistry. Moreover, the authors present an interesting result indicating significant differences in the composition of aerosol nitrogen-containing organic compounds released from the combustion of fresh and old biomass materials. Biomass burning is usually a general concept in many previous studies, for which further refinement or classification is necessary. Thus, the topic is very meaningful. Overall, I recommend this paper for publication after addressing the following minor *comments.*

Response: We appreciate your professional review for our article. We have revised the manuscript to address the comments. Our responses to the specific comments and changes made in the manuscript are given below.

Specific comments:

1) *Lines 34–40: The expression is too concise, which may make it difficult for readers to understand why "It further confirmed different impacts of the combustion of fresh- and old-age biomass materials on NOC compositions". Please clarify it.*

Response: This section has been revised to enhance reader comprehension. See below for details (Lines 37–43).

Lines 37–43: …For CHN compounds, alkyl nitriles and aromatic species showed higher abundance in the warm and cold periods, respectively. Alkyl nitriles can from fresh biomass material combustion associated with the dehydration of amides (the main CHON compounds in the warm period). In contrast, aromatic species were tightly related to old-age biomass burning. These findings further suggested different impacts of the combustion of fresh- and old-age biomass materials on NOC compositions in different seasons…

2) *Some references about NOC should be cited in line 63-94. The Roles of N, S, and O in molecular absorption features of brown carbon in PM2.5 in a typical semi-arid megacity in northwestern China. Journal of Geophysical Research-Atmospheres, 2021, 126. Connecting oxidative potential with organic carbon molecule composition and source-specific apportionment in PM2.5 in Xi'an, China. Atmospheric Environment, 2023, 306, 119808.*

Response: We appreciate the introduction of these excellent and interesting references. All references you mentioned above have been added in the revised manuscript (Lines 66-67).

Lines 66-67: …(Samy and Hays, 2013; Jiang et al., 2022; Lin et al., 2012; Xu et al., 2023; Luo et al., 2023; Zeng et al., 2021)…

3) *Line 80: please delete "on"*

Response: The revision has been made in the revised manuscript (Line 82).

4) *Lines 266–269: This content involves the uncertainty of pH prediction. Thus, I suggest the author move this discussion to section 2.3. Compound categorization and predictions of ALW, pH, and hydroxyl radical. Furthermore, please clarify how pH is*

predicted.

Response: We thank you for these insightful comments. Based on your suggestion, we have modified this section as shown below (Lines 277–279).

Lines 277–279: …Moreover, the calculated mean pH value was 6.86 ± 1.71 (**Table S1**) during the warm period, which implies that the fine aerosol particles in the warm period in Urumqi was neutral or slightly alkaline.

Furthermore, we have clarified how pH is predicted in Section 2.3 Compound categorization and predictions of ALW, pH, and hydroxyl radical. The added descriptions in the revised manuscript are shown below (Lines 202–209).

Lines 202–209: …The model output results based on our data set showed that 94% and 90% of NO_3^- were in the aerosol phase in the cold and warm periods, respectively. Hence, the predictions of pH and ALW were conducted without considering gaseous nitric acid (Guo et al., 2015; Wang et al., 2021). 78% and 21% of NH_4^+ were in the aerosol phase in the cold and warm periods, respectively. Moreover, it is important to note that gaseous NH_3 measurements were not conducted and ammonia partitioning was not considered in this study. Thus, a bias correction of 1 pH unit was applied to calculate the aerosol pH values (Guo et al., 2015; Wang et al., 2021).

5) *Lines 214–216: … urban aerosols… Please clarify the research site.*

Response: The revisions have been made in the revised manuscript (Lines 225–226).

6) *Lines 228 and 231: ...94−1.13 for CHO and 1.27−1.47 for CHON...0.42–0.43 for CHO and 0.27–0.45 for CHON...*

Response: The revisions have been made in the revised manuscript (Lines 239–243).

7) *In section 3.2 Some references about sources profile should be cited to discussed the sources and formation mechanisms of NOC*

Source profiles of molecular structure and light absorption of PM2.5 brown carbon from residential coal combustion emission in Northwestern China. Environmental Pollution, 2022, 299, 118866.

Optical properties, molecular characterizations, and oxidative potentials of different polarity levels of water-soluble organic matters in winter PM2.5 in six China's megacities. Science of The Total Environment, 2022, 853, 158600.

Insight into the Primary and Secondary Particle-Bound Methoxyphenols and Nitroaromatic Compound Emissions from Solid Fuel Combustion and the Updated Source Tracers. Environmental Science & Technology, 2023,57, 14280−14288.

Response: We greatly appreciate your suggestions. All references you mentioned above have been added in the revised manuscript.

Lines 66–67: …(Samy and Hays, 2013; Jiang et al., 2022; Lin et al., 2012; Xu et al., 2023; Luo et al., 2023; Zeng et al., 2021; Zhang et al., 2022; Zeng et al., 2020)…

Lines 91–92: …(Jiang et al., 2022; Wang et al., 2017; Ditto et al., 2022; Altieri et al., 2016; Xu et al., 2020; Liu et al., 2023; Zhang et al., 2022; Zeng et al., 2020)…

Lines 317–318: …(Duan et al., 2020; Kondo et al., 2007; Zhang et al., 2023)...

Lines 310-311: …(Li et al., 2023; Wang et al., 2017; Chen et al., 2017; Wang et al., 2009; Wang et al., 2018; Zhang et al., 2022).

8) *Lines 287–288: CHON compounds can be derived from the reactions between CHO species and reactive nitrogen species.*

Response: The revision has been made in the revised manuscript (Lines 297–298).

9) *Line 310: What are the main types of old-age plant tissues? Please clarify it.*

Response: We have clarified the main types of old-age plant tissues as described below (Lines 319–322).

Lines 319–322: …It should be noted that the materials used for biomass burning in the cold period in rural China are typically old-age plant tissues, such as dead branches of pine trees, dead branches of shrubs, corn straw, and rice straw (**Figure S3**), …

10) *Line 316: Please also provide the OSc range of CHO compounds in ESI+.*

Response: We thank you for the insightful comment. The OS_C ranges of CHO compounds in ESI+ have been added in the revised manuscript (Lines 328–329).

11) *Lines 318–319: I suggest the authors provide percentage data for BBOA and SV-OOA.*

Response: The percentage data for BBOA and SV-OOA have been added in the revised manuscript (Lines 330–332).

12) *Lines 387–388 and 395: ...C7H5O5N, and C8H9O3N (confirmed by their authentic standards), together contributed...C7H7O3N (methyl-nitrophenol), and C7H7O4N (methyl-nitrocatechol)...*

Response: The revision has been made in the revised manuscript (Lines 398–400 and 407–408).

13) *Line 456: Please change Simoneit et al. (Simoneit et al., 2003) to Simoneit et al. (2003).*

Response: The revision has been made in the revised manuscript (Line 480).

14) *Lines 424–427: Aromatic compounds can also originate from fossil fuel combustion in the winter period, please consider this possibility.*

Response: The added descriptions in the revised manuscript are shown below (Lines 454–466).

Lines 454–466: …A study about molecular characterization (ESI+ mode) of humic-like substances emitted from the combustion of old-age biomass materials (i.e., dry corn straw, rice straw, and pine branches) and coals showed that OA from old-age biomass burning typically contained much more CHN_2 compounds (55–64%) than that from coal (20–37%), while OA from coal-smoke showed more CHN_1 compounds (78–84%) compared to that from old-age biomass materials (15–22%) (Song et al., 2022). In this study, the signal intensity of CHN_1 compounds in the cold period was about 40% higher than that in the warm period, while that of CHN_2 compounds showed a 160% increase from the warm period to the cold period. Thus, although the contribution of fossil fuel (e.g., coal) combustion to NOCs in the cold period cannot be ignored, our results at least suggested that the biomass burning-derived CHN compounds showed a more significant increase compared to coal combustion-derived compounds from the warm period to the cold period in Urumqi.

At last, we deeply appreciate the time and effort you've spent in reviewing our manuscript.

Reference:

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Comments of Reviewer #2 and our responses to them

Comments:

This manuscript presents results from a detailed study of the chemical composition of aerosol particles collected at regular intervals over a year in Urumqi. The samples are characterized by soft ionization with UPLC-ESI-QToFMS and a focus is placed on the nitrogen containing molecular formulas identified in the mass spectra. The authors find differences in the composition of the CHON and CHN compounds between the colder and warmer periods and they attribute the majority of this difference to the variation in the fuels burned in the warmer period (wildfires) vs colder (combustion for heat). Overall, this is a very detailed and well carried out study that is clearly written. I have minor concerns about some of the data analysis and once these are addressed, I recommend acceptance of the manuscript.

Response: We appreciate the reviewer's valuable comments on our work. Our responses to the specific comments and changes made in the manuscript are given below.

Specific Comments:

1) *Thank you for providing the data for the figures. For the peak identification, how many of the measured peaks could not be identified? Was there a mass dependence to this (i.e., were there high mass peaks that were measured that could not be identified?).*

Response: We greatly thank you for your professional review of our article. These are very critical issues. In this study, the number of molecules that were excluded accounted for no more than 2% of the total number of molecules. Moreover, the signal intensity of these excluded peaks also accounted for no more than 2% of the total signal intensity.

In ESI+, the identified peaks were classified into several major compound categories based on their elemental compositions, including CHO, CHON, and CHN. The CH compounds were excluded because of their small number (0.43% of the total number of compounds in ESI+) and low signal intensity (0.33 ± 0.28% of the total signal intensity in ESI+) being identified in this study. In ESI−, the identified peaks were classified into CHO, CHON, CHOS, and CHONS. S-containing compounds were not discussed in this work because of our focus on N-containing compounds.

For the compounds with high mass peaks (> 700 Da), their signal intensities accounted for 1.12% and 1.37% of total signal intensities in ESI+ and ESI−, respectively. Thus, these compounds were also excluded in discussion, as indicated by many previous studies (Wang et al., 2021; Yuan et al., 2023; Xie et al., 2020). In general, the main conclusions of this study are unaffected by the exclusion of these compounds.

More descriptions have been added in **Sect S1**, which was shown below (Pages S4-S5).

Pages S4-S5: …The CH compounds were excluded because of their small number (0.43% of the total number of compounds in ESI+) and low signal intensity (0.33 ± 0.28% of the total signal intensity in ESI+) being identified in this study. For the compounds with high mass peaks (> 700 Da), their signal intensities accounted for 1.12% and 1.37% of total signal intensities in ESI+ and ESI−, respectively. Thus, these compounds were also excluded in discussion, as indicated by many previous studies (Wang et al., 2021; Yuan et al., 2023; Xie et al., 2020) …

2) *The sentence starting on line 55 is confusing and I recommend revising it: "Moreover, the modified forms of some nitrogen-containing organic compounds (NOCs) and volatile organic compounds (VOCs) by ozone (O3), hydroxyl radical (•OH), and nitrogen oxide (NOx) can lead to an increase in the health hazards of OA, among which nitrated amino acids and nitrated polycyclic aromatic hydrocarbons are two representative hazards (Franze et al., 2005; Bandowe and Meusel, 2017)." What does "modified forms" mean? The second half of the sentence (starting ...along with nitrated amino acids...) is also incomplete and may be better as its own sentence.*

Response: We apologize for the confusion caused by our expression and thank you for your suggestions. The expression "modified forms" refers to the products or intermediate products of the interactions of ozone (O_3), hydroxyl radical (•OH), and nitrogen oxide (NO_x) with some nitrogen-containing organic compounds (NOCs) and volatile organic compounds (VOCs). The revision has been made in the revised manuscript (Lines 55–60).

Lines 55–60: …Moreover, the further oxidation or nitrification of some nitrogen-containing organic compounds (NOCs) and volatile organic compounds (VOCs) by ozone (O_3), hydroxyl radical (•OH), and nitrogen oxide (NO_x) can lead to an increase in the health hazards of OA (Franze et al., 2005; Bandowe and Meusel, 2017). Nitrated amino acids and nitrated PAHs are two representative hazard NOCs (Franze et al., 2005;

Bandowe and Meusel, 2017).

3) On line 238, the possibility for CHO compounds to be precursors for CHON compounds is raised. Please clarify if this is referring to possible reactions in the gas-phase, in the particle-phase, or both?

Response: The CHON compounds can be tightly associated with secondary formation processes involving the reactions of reactive nitrogen with gas-phase and particle-phase CHO compounds (Bandowe and Meusel, 2017; Zarzana et al., 2012; Laskin et al., 2014). For example, laboratory experiments have suggested that the oxidation of isoprene and α-/β-pinene in the presence of NO_x can form large amounts of CHON compounds (Surratt et al., 2010; Rollins et al., 2012; Nguyen et al., 2015). The reduced nitrogen species (e.g., NH_3 and NH_4^+) have been demonstrated to contribute to the formation of NOCs in particle-phase (Zarzana et al., 2012; Laskin et al., 2014). Xu et al. (2023) characterized the variations of molecular compositions in urban road $PM_{2.5}$, suggesting that organic nitrates increased largely through the interactions of atmospheric oxidants, CHO compounds, and aerosol liquid water in both gas-phase and particle-phase. In general, CHO compounds can be important precursors for the formation of NOCs (via reactions in the gas- and/or particle-phases).

More discussions are presented at Lines 71–89. Based on your suggestion, the revision was made in the Lines 250–252.

Lines 250–252: …This indicated that CHO compounds may be important precursors for the formation of NOCs (via reactions in the gas- and/or particle-phases) or that they have similar origins.

4) In Table S4: how were the identifications made that are in the footnote (a, b, c, d)? For this and other tables, how is "relatively high signal" defined?

Response: These compounds were identified or inferred based on their MS/MS fragments or the molecular formulae of the products obtained from **Figure 5.** More descriptions were added in the page S11.

Page S11: These compounds were identified or inferred based on their MS/MS fragments or the molecular formulae of the products obtained from Figure 5.

We apologize for the confusion caused by our expression. The correct expression is that "Characteristics of the observed CHON compounds with relatively high signal intensity compared to other CHON compounds in ESI+ mode in the warm period (Page S11). The titles of other tables (**Table S6** and **Table S7**) were also updated (Pages S13-S14).

5) *The mass error calculations here look to be a little incorrect (ppm values). I agree with the assignments and the errors I calculate are within the boundaries from the paper (5 ppm), but these values should be double checked.*

Response: The mass errors in **Table S5** were the results directly output by the data processing software. In general, mass error calculations for mass spectrometry (Brenton and Godfrey, 2010) can be expressed as follows:

$$\Delta m_i = \frac{(m_i - m_a)}{m_a} \times 10^6 \; in \; ppm \; (parts \; per \; million)$$

where m_i is the measurement value, m_a is the calculated mass value.

To check the accuracy of the mass errors obtained from the software, we added the theoretical masses of the ions detected by the instrument to **Table S5** (Page S12) and calculated the mass error for each compound according to the above equation. We found that the calculated results were consistent with the output values, indicating that the mass errors obtained from the instrument are reliable.

Once again, we deeply appreciate the time and effort you've spent in reviewing our manuscript.

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