General.

We would like to appreciate the editor for providing the valuable comments on our work. We have revised our manuscript by fully taking the editor's comments into account. Responses to specific comments raised by the editor 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 the Editor and our responses to them

Comments:

Thank you for your careful consideration of the referee comments. After careful consideration of your response document and revised manuscript, I am happy to accept your manuscript for publication following attention to a few minor corrections. Line numbers refer to the track changes version of the manuscript.

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) *Line 30: "poor-O" change to "O-poor" or "oxygen-poor"*

Response: All relevant content has been revised in the manuscript.

2) *Line 39: "Alkyl nitriles can from fresh" there is a word missing.*

Response: The revision has been made in the revised manuscript (Line 39).

Line 39: …Alkyl nitriles can be derived from fresh biomass…

3) *Line 53: Remove "however"*

Response: The revision has been made in the revised manuscript (Line 54).

4) *Line 59: "nitrogen oxide" --> "nitrogen oxides"*

Response: The revision has been made in the revised manuscript (Line 59).

5) *Line 68: This is up to the authors, but I would recommend removing the Luo et al reference as it has more of a focus on oxidative potential. This reference was added during revision.*

Response: We greatly appreciate your suggestion. The reference you mentioned has

been removed from the revised manuscript (Lines 67–68).

6) *Lines 153-154: Ozone and NOx have substantial diel variability. Please clarify how the representative values are determined.*

Response: As the $PM_{2.5}$ samples in this study were collected daily, we obtained the daily concentrations of ozone and NO_x by averaging the hourly concentration data of ozone and NO_x from the adjacent environmental monitoring station. We have modified this section below (Lines 150–154).

Lines 150–154: During the sampling campaigns, the meteorological data (e.g., temperature and relative humidity) and the concentrations of O_3 and NO_x were recorded hourly from the adjacent environmental monitoring station. These hourly data were then averaged to obtain daily values to match the sampling time of $PM_{2.5}$.

7) *Sect. 2.2: Please add volumes used in the extraction processes.*

Response: We greatly appreciate your suggestions. The volumes used in the extraction processes have been added in the revised manuscript (Line 159 and Line 181).

8) *Line 165: Please define UPLC-ESI-QToFMS*

Response: The revision has been made in the revised manuscript (Lines 164–166).

Lines 164–166: …using an ultra-performance liquid chromatography quadrupole time-of-flight mass spectrometry equipped with an electrospray ionization (ESI) source (UPLC-ESI-QToFMS, Waters Acquity Xevo G2-XS)...

9) *Line 350: "with poor oxygen" --> "that are oxygen poor"*

Response: The revision has been made in the revised manuscript (Line 368).

10) *Figure 1: Some compounds containing sulfur are included in the figure, but are not mentioned anywhere or included in the tables. I am ok with restricting the discussion to only nitrogen and CHO compounds, but in that case the sulfur containing ions should be removed from the figure. In the text (methods section perhaps), it should be clearly stated that S containing ions aren't discussed. It would be good to state the absolute number of formulas that contain S so that the reader can get a sense of how such an exclusion relates to the breadth of the dataset.*

Response: We thank you for the insightful comment. The sulfur-containing ions have been removed from the **Figure 1**. The absolute number of formulas that contain S has been added in **Table S2**. Furthermore, additional statements have been added in **section 2.3**.

Lines 191–195: …primarily including CHO, CHON, and CHN groups in the ESI+ mode and CHO, CHON, CHOS and CHONS groups in the ESI– mode (Wang et al., 2017). CHOS and CHONS compounds were also detected in the ESI– mode, with

numbers of 398 and 112, respectively (**Table S2**). As this study focused mainly on NOCs, sulfur-containing species were not discussed…

11) *SI page S6 text "The identified compounds….Tong et al 2016)" or some similar version should be moved to the main text so that the reader understands how attribution to BBOA, etc. is being done. I leave it to the authors' discretion as to the best location of this text within the main manuscript.*

Response: We greatly appreciate your kind suggestion. Revisions have been made in the revised manuscript.

Lines 199–217: The identified compounds can be further classified into four subgroups based on the number of carbon atoms and OS_C value (Kroll et al., 2011; Xu et al., 2023). Briefly, semi-volatile oxidized organic aerosol (SV-OOA) and low-volatility oxidized organic aerosol (LV-OOA) were associated with multi-step oxidation reactions, with OS_C values between –1 and +1 and molecular formulas less than 13 carbon atoms. BBOA has OS_C values ranging from –0.5 to –1.5 and more than seven carbon atmos. Compounds with OS_C values less than –1 and carbon atoms above 20 may be related to hydrocarbon-like organic aerosol (HOA). Additionally, the modified aromaticity index (AI_{mod}) was also calculated to indicate the aromaticity of organic compounds (details in **Sect. S2**) (Koch and Dittmar, 2006). The van Krevelen diagrams and AI_{mod} values have been proposed to further classify organic matter categories (Xu et al., 2023; Su et al., 2021), according to which the identified five subgroups included saturated-like molecules (Sa, $H/C \geq 2.0$), unsaturated aliphatic-like molecules (UA, $1.5 \leq H/C < 2.0$),

highly unsaturated-like molecules (HU, $AI_{mod} \leq 0.5$ and $H/C < 1.5$), highly aromatic-like molecules (HA, $0.5 < AI_{mod} \leq 0.66$), and (E) polycyclic aromatic-like molecules (PA, $AI_{mod} > 0.66$). Furthermore, it has been suggested that the above subgroups can be subdivided into O-poor and O-rich compounds depending on their O/C ratio (**Table S8**) (Merder et al., 2020; Zhong et al., 2023).

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

Reference:

Koch, B. P. and Dittmar, T.: From mass to structure: an aromaticity index for high-resolution mass data of natural organic matter, Rapid Commun. Mass Spectrom., 20, 926-932, https://doi.org/10.1002/rcm.2386, 2006.

Merder, J., Freund, J. A., Feudel, U., Hansen, C. T., Hawkes, J. A., Jacob, B., Klaproth, K., Niggemann, J., Noriega-Ortega, B. E., Osterholz, H., Rossel, P. E., Seidel, M., Singer, G., Stubbins, A., Waska, H., and Dittmar, T.: ICBM-OCEAN: Processing Ultrahigh-Resolution Mass Spectrometry Data of Complex Molecular Mixtures, Anal. Chem., 92, 6832-6838, https://dx.doi.org/10.1021/acs.analchem.9b05659, 2020.

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Y., Wang, Z., Liu, C.-Q., Jiang, G., and Fu, P.: High Molecular Diversity of Organic Nitrogen in Urban Snow in North China, Environ. Sci. Technol., 55, 4344-4356, https://dx.doi.org/10.1021/acs.est.0c06851, 2021.

Wang, Y., Hu, M., Lin, P., Guo, Q., Wu, Z., Li, M., Zeng, L., Song, Y., Zeng, L., Wu, Y., Guo, S., Huang, X., and He, L.: Molecular Characterization of Nitrogen-Containing Organic Compounds in Humic-like Substances Emitted from Straw Residue Burning, Environ. Sci. Technol., 51, 5951-5961, https://doi.org/10.1021/acs.est.7b00248, 2017.

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