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:

Altieri, K. E., Fawcett, S. E., Peters, A. J., Sigman, D. M., and Hastings, M. G.: Marine biogenic source of atmospheric organic nitrogen in the subtropical North Atlantic, P.

Natl. Acad. Sci. USA, 113, 925-930, https://doi.org/10.1073/pnas.1516847113, 2016.

Chen, J., Li, C., Ristovski, Z., Milic, A., Gu, Y., Islam, M. S., Wang, S., Hao, J., Zhang, H., He, C., Guo, H., Fu, H., Miljevic, B., Morawska, L., Thai, P., Lam, Y. F., Pereira, G., Ding, A., Huang, X., and Dumka, U. C.: A review of biomass burning: Emissions and impacts on air quality, health and climate in China, Sci. Total Environ., 579, 1000-1034, https://doi.org/10.1016/j.scitotenv.2016.11.025, 2017.

Ditto, J. C., Machesky, J., and Gentner, D. R.: Analysis of reduced and oxidized nitrogen-containing organic compounds at a coastal site in summer and winter, Atmos. Chem. Phys., 22, 3045-3065, https://doi.org/10.5194/acp-22-3045-2022, 2022.

Duan, J., Huang, R. J., Li, Y., Chen, Q., Zheng, Y., Chen, Y., Lin, C., Ni, H., Wang, M., Ovadnevaite, J., Ceburnis, D., Chen, C., Worsnop, D. R., Hoffmann, T., O'Dowd, C., and Cao, J.: Summertime and wintertime atmospheric processes of secondary aerosol in Beijing, Atmos. Chem. Phys., 20, 3793-3807, https://doi.org/10.5194/acp-20-3793-2020, 2020.

Guo, H., Xu, L., Bougiatioti, A., Cerully, K. M., Capps, S. L., Hite Jr, J. R., Carlton, A. G., Lee, S. H., Bergin, M. H., Ng, N. L., Nenes, A., and Weber, R. J.: Fine-particle water and pH in the southeastern United States, Atmos. Chem. Phys., 15, 5211-5228,

https://doi.org/10.5194/acp-15-5211-2015, 2015.

Jiang, H., Li, J., Tang, J., Zhao, S., Chen, Y., Tian, C., Zhang, X., Jiang, B., Liao, Y., and Zhang, G.: Factors Influencing the Molecular Compositions and Distributions of Atmospheric Nitrogen-Containing Compounds, J. Geophys. Res.-Atmos., 127, e2021JD036284, https://doi.org/10.1029/2021JD036284, 2022.

Kondo, Y., Miyazaki, Y., Takegawa, N., Miyakawa, T., Weber, R. J., Jimenez, J. L., Zhang, Q., and Worsnop, D. R.: Oxygenated and water-soluble organic aerosols in Tokyo, J. Geophys. Res.-Atmos., 112, https://doi.org/10.1029/2006JD007056, 2007.

Li, Y., Chen, M., Wang, Y., Huang, T., Wang, G., Li, Z., Li, J., Meng, J., and Hou, Z.: Seasonal characteristics and provenance of organic aerosols in the urban atmosphere of Liaocheng in the North China Plain: Significant effect of biomass burning, Particuology, 75, 185-198, https://doi.org/10.1016/j.partic.2022.07.012, 2023.

Lin, P., Rincon, A. G., Kalberer, M., and Yu, J. Z.: Elemental Composition of HULIS in the Pearl River Delta Region, China: Results Inferred from Positive and Negative Electrospray High Resolution Mass Spectrometric Data, Environ. Sci. Technol., 46, 7454-7462, https://doi.org/10.1021/es300285d, 2012.

Liu, T., Xu, Y., Sun, Q.-B., Xiao, H.-W., Zhu, R.-G., Li, C.-X., Li, Z.-Y., Zhang, K.-Q.,

Sun, C.-X., and Xiao, H.-Y.: Characteristics, Origins, and Atmospheric Processes of Amines in Fine Aerosol Particles in Winter in China, J. Geophys. Res.-Atmos., 128, e2023JD038974, https://doi.org/10.1029/2023JD038974, 2023.

Luo, Y., Zeng, Y., Xu, H., Li, D., Zhang, T., Lei, Y., Huang, S., and Shen, Z.: Connecting oxidative potential with organic carbon molecule composition and source-specific apportionment in PM2.5 in Xi'an, China, Atmos. Environ., 306, 119808, https://doi.org/10.1016/j.atmosenv.2023.119808, 2023.

Samy, S. and Hays, M. D.: Quantitative LC–MS for water-soluble heterocyclic amines in fine aerosols ($PM_{2.5}$) at Duke Forest, USA, Atmos. Environ., 72, 77-80, https://doi.org/10.1016/j.atmosenv.2013.02.032, 2013.

Song, J., Li, M., Zou, C., Cao, T., Fan, X., Jiang, B., Yu, Z., Jia, W., and Peng, P. a.: Molecular Characterization of Nitrogen-Containing Compounds in Humic-like Substances Emitted from Biomass Burning and Coal Combustion, Environ. Sci. Technol., 56, 119-130, https://doi.org/10.1021/acs.est.1c04451, 2022.

Wang, Q., Shao, M., Zhang, Y., Wei, Y., Hu, M., and Guo, S.: Source apportionment of fine organic aerosols in Beijing, Atmos. Chem. Phys., 9, 8573-8585, https://doi.org/10.5194/acp-9-8573-2009, 2009.

Wang, X., Hayeck, N., Brüggemann, M., Yao, L., Chen, H., Zhang, C., Emmelin, C., Chen, J., George, C., and Wang, L.: Chemical Characteristics of Organic Aerosols in Shanghai: A Study by Ultrahigh-Performance Liquid Chromatography Coupled With Orbitrap Mass Spectrometry, J. Geophys. Res.-Atmos., 122, 11,703-711,722, https://doi.org/10.1002/2017JD026930, 2017.

Wang, X., Shen, Z., Liu, F., Lu, D., Tao, J., Lei, Y., Zhang, Q., Zeng, Y., Xu, H., Wu, Y., Zhang, R., and Cao, J.: Saccharides in summer and winter $PM_{2.5}$ over Xi'an, Northwestern China: Sources, and yearly variations of biomass burning contribution to $PM_{2.5}$, Atmos. Res., 214, 410-417, https://doi.org/10.1016/j.atmosres.2018.08.024, 2018.

Wang, Y., Hu, M., Hu, W., Zheng, J., Niu, H., Fang, X., Xu, N., Wu, Z., Guo, S., Wu, Y., Chen, W., Lu, S., Shao, M., Xie, S., Luo, B., and Zhang, Y.: Secondary Formation of Aerosols Under Typical High-Humidity Conditions in Wintertime Sichuan Basin, China: A Contrast to the North China Plain, J. Geophys. Res.-Atmos., 126, e2021JD034560, https://doi.org/10.1029/2021JD034560, 2021.

Xu, Y., Dong, X. N., He, C., Wu, D. S., Xiao, H. W., and Xiao, H. Y.: Mist cannon trucks can exacerbate the formation of water-soluble organic aerosol and $PM_{2.5}$ pollution in

the road environment, Atmos. Chem. Phys., 23, 6775-6788, https://doi.org/10.5194/acp-23-6775-2023, 2023.

Xu, Y., Miyazaki, Y., Tachibana, E., Sato, K., Ramasamy, S., Mochizuki, T., Sadanaga, Y., Nakashima, Y., Sakamoto, Y., Matsuda, K., and Kajii, Y.: Aerosol Liquid Water Promotes the Formation of Water-Soluble Organic Nitrogen in Submicrometer Aerosols in a Suburban Forest, Environ. Sci. Technol., 54, 1406-1414, https://dx.doi.org/10.1021/acs.est.9b05849, 2020.

Zeng, Y., Ning, Y., Shen, Z., Zhang, L., Zhang, T., Lei, Y., Zhang, Q., Li, G., Xu, H., Ho, S. S. H., and Cao, J.: 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, J. Geophys. Res.-Atmos., 126, e2021JD034791, https://doi.org/10.1029/2021JD034791, 2021.

Zeng, Y., Shen, Z., Takahama, S., Zhang, L., Zhang, T., Lei, Y., Zhang, Q., Xu, H., Ning, Y., Huang, Y., Cao, J., and Rudolf, H.: Molecular Absorption and Evolution Mechanisms of PM2.5 Brown Carbon Revealed by Electrospray Ionization Fourier Transform–Ion Cyclotron Resonance Mass Spectrometry During a Severe Winter Pollution Episode in Xi'an, China, Geophys. Res. Lett., 47, e2020GL087977,

https://doi.org/10.1029/2020GL087977, 2020.

Zhang, B., Shen, Z., He, K., Sun, J., Huang, S., Xu, H., Li, J., Ho, S. S. H., and Cao, J.-j.: Insight into the Primary and Secondary Particle-Bound Methoxyphenols and Nitroaromatic Compound Emissions from Solid Fuel Combustion and the Updated Source Tracers, Environ. Sci. Technol., 57, 14280-14288, 10.1021/acs.est.3c04370, 2023.

Zhang, T., Shen, Z., Huang, S., Lei, Y., Zeng, Y., Sun, J., Zhang, Q., Ho, S. S. H., Xu, H., and Cao, J.: 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, Sci. Total Environ., 853, 158600, https://doi.org/10.1016/j.scitotenv.2022.158600, 2022.