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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Seasonal Differences in the Composition of Organic Aerosols in Beijing: a Study by Direct Infusion Ultrahigh Resolution Mass Spectrometry" *by* Sarah S. Steimer et al.

Anonymous Referee #2

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General comments:

This paper characterized the elemental composition of polar organic compounds in PM2.5 from Beijing during wintertime and summertime. 918-1586 organic compounds were assigned molecular formulae by direct infusion negative nano-electrospray ionization ultrahigh resolution mass spectrometer. Then the differences of the chemical composition under different pollution conditions, and their potential primary and secondary sources were discussed. The overall strength of this study is acquisition of a detailed dataset of polar organic compounds that spanned summertime and wintertime, low and high pollution conditions. The topic of the paper is well suited for ACP,

and the data itself are interesting. On the whole, the language requires improvement throughout the manuscript. Many sentences are not clearly written, leaving the reader puzzling about their meaning. In addition, the overall weakness is the data interpretation. Much more effort needs to be put into presentation of the results. I have some points where more information is needed or where I disagree.

I use the abstract to illustrate my main concerns of this paper. The authors state in the abstract: . . .. . .There were strong differences in aerosol particle composition between the seasons. . ...which were strongly enhanced in winter, likely due to increased fossil fuel and biomass burning for heating. . .. . .the contribution of sulfur-containing organic compounds strongly enhanced under high pollution conditions. . .. . ..

The highlighted results above are not really exciting. In fact, many researches have reported these differences already. For the advantage of using the ultrahigh resolution mass spectrometer, I suggest the authors to focus on the new findings of this study.

Specific comments:

1. Introduction: The characterization and source identification of organic compounds in PM in Beijing have been extensively studied. I would suggest authors to improve the introduction by summarizing these previous studies and providing some results in line with the major conclusion of this study.

2. Page 2, Line 10-12: "As a central of the project,. . .. . ." It makes no senses for your paper since the information on sampling has been provided in the Section Materials and Method.

3. Page 3: Maybe the meteorological conditions (e.g. temperature, RH, wind speed, wind direction, mixing layer height, etc.) play an important role on the organic components. I would suggest the authors to give a general characteristics of gas and PM pollutants and meteorological conditions during low and high pollution conditions (WH, WL, SH, SL), respectively, since the authors focus on the comparison between the

characteristics of organic groups under different pollution conditions, in the Supplementary Information, for instance?

4. Page 4, Line 16: What does “0.3âĽęH/CâĽğ2.5” mean?

5. Page 4, Line 21: Here x, y and z are the number of carbon, hydrogen, nitrogen atoms. However, in Page 12, Line 7, C, N, H and O are the number of carbon, nitrogen, hydrogen and oxygen. I suggest the authors keep consistent in the nomination to avoid the confusion.

6. Page 5, Lines 17-20: It makes no senses since the air masses have been discussed in your paper.

7. Page 5, Lines 22-25: Here these sentences make no sense for the paper.

8. Page 5: Here DBE was calculated based on the number of C, H, N atoms. I am not sure whether DBE should be calculated with the relative abundance weight since the relative abundance of each molecule in the mass spectrum is different. The same consideration also apply for the other parameters such as H/C, O/C, Xc and so on.

9. Page 6, Line 5: A reference would be helpful.

10. Page 6: I suggest the authors add the number of four different groups identified in different pollution conditions in Figure 1.

11. Pages 6-8: The chemical composition and some ratios (i.e., O/C, H/C) of organic compounds have been characterized by ultrahigh resolution mass spectrometer in some cities such as Beijing and Shanghai, and some typical emission sources (i.e., coal combustion, biomass burning). I suggest the authors compare their result with those reported in literature.

12. Page 7, Line 14: You are right, here a reference would be helpful.

13. Page 7, Line 15: What does “high and low H/C particulate matter” mean?

14. Page 8, Lines 1-2: The SH showed high H/C ratio. The authors suggest that is due to a large proportion of biogenic organic aerosol from plant sources. It might be good here to give more evidences. Is there any assigned formula which could be used as markers for biomass burning or biogenic organic aerosol? For example, nitrophenols, nitrocatechols? They show higher number fraction and/or relative abundance in SH samples?

15. Page 8, Line 9: It might be better to give the ozone concentrations for the WH, WL, SH, SL samples.

16. Page 9: The VK plots show the aromaticity of CHO and CHON is quite different in winter and summer. Please speculate more in depth on the difference.

17. Page 10: Here the authors give some data on polyaromatic compounds. How about the single-ring aromatics? I think they contribute more to the aromatic compounds.

18. Page 12: The authors spend too many words to discuss the aromaticity equivalent (Xc). I suggest the authors focus on the new finding which cannot be deduced from the H/C and O/C ratios.

19. Page 13, Line 21: A reference regarding the heating source would be helpful.

20. Page 16, Line1: The authors state that sulfate concentrations are usually higher in summer than in winter in Beijing. Are you sure? Please give the concentrations of sulfate and nitrate in WH, WL, SH, and SL samples in a Table, for instance, in the Supplementary Information. And in Line 25, you state the lower sulfate concentrations in summer. It is significantly contradictory.

21. Page16: It is a good idea to discuss the relationship between sulfate and nitrate with the number of CHOS and CHON compounds, but I recommend the authors to provide in-depth insights into this discussion. In addition to the secondary formation, Song et al. (EST 2019, 53, 13607-13617; 52, 2575-2585) reported that S-containing compounds account for 36% of the total number of compounds identified, making up

the largest component in coal smoke, and N-containing compounds show high abundance in biomass burning. The primary sources of S- and N-containing compounds should also be considered.

22. Page 16: The authors state that the particles in winter are sampled before they can undergo atmospheric ageing processes, for example reacting with OH radicals and ozone in Page 8, Lines 6-7. It seems inconsistent with the good positive correlation between sulfate and CHOS compounds.

Technical corrections:

1. Page 5, Lines 27-28: What does “Fehler! Verweisquelle konnte nicht gefunden warden” mean? Mistype?

2. Page 5, Line 30: “off” should be “of”.

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