

Interactive comment on “The Secondary Formation of Organosulfates under the Interactions between Biogenic Emissions and Anthropogenic Pollutants in Summer of Beijing” by Yujue Wang et al.

Anonymous Referee #3

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This manuscript describes measurements of organosulfates and related compounds in Beijing during May-June 2016. Emphasis is placed on understanding the factors that influence organosulfate and nitrooxyorganosulfate formation, particularly during three pollution episodes. The manuscript concludes that sulfate, liquid water content, and acidity are important factors in their formation.

The measurements appear to be carefully conducted and well-described. However, there are some shortcomings in the presentation of the data that should be addressed prior to publication.

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Major comments:

1) The discussion of the trends in organosulfates and co-located measurements in section 3.3 is limited to qualitative descriptions. Correlation analysis (like that conducted between observed organosulfates, Table S2) should be extended to include co-located measurements of sulfate, nitrate, ammonium, liquid water content, aerosol acidity [H⁺], VOC precursors, oxidants, etc. to provide quantitative support for the associations (or lack thereof) that are discussed in this section.

2) Correlation analysis should also be conducted and presented to support the discussion in section 3.5.

3) The phrase “representative organosulfates” is used in several instances (line 22, 218, 411) although the authors do not indicate what these species represent. Rather than using this vague language, the authors should more explicit in describing why the selected compounds were quantified and semi-quantified.

4) The discussion in the paragraph beginning at line 209 implies that the only difference between the three air pollution episodes was their inorganic ion content (which affected aerosol acidity and liquid water content). Do back trajectories, VOC concentrations, and other co-located measurements support this? If not, how could variations in other atmospheric conditions explain the organosulfate observations?

5) The overall concentration of organosulfates observed in Beijing seems to be very low (~150 ng/m³). In encourage the authors to discuss this observation and include it in their comparison to prior studies.

6) A table comparing key species and total organosulfate concentrations across this and prior studies would be a useful addition to the supplement to support the comparison of data.

7) In two places (line 117 and 173) the authors indicate that the organic carbon concentration was held constant across samples analyzed by Orbitrap, in order to decrease

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ion suppression. The authors should provide a reference to support this statement and/or evidence to support that ion suppression did not occur.

8) The SPE method described at line 118 indicates that select compounds are removed by the SPE process. However, there is no mention until line 207-215 what effect the SPE has on organosulfates. I suggest making a note at line 120 indicating that further discussion of the impact of this clean-up procedure on organosulfates is discussed in section 3.1.

9) Line 150 – please explain how semi-quantification is achieved for a surrogate standard that appears to be comprised of a mixture of compounds (e.g., “alpha-pinene OS”).

10) The discussion at lines 198-202 implicates long-chain alkanes and diesel/biodiesel emissions as the source of several organosulfates. Can the authors please comment on the (un)certainly of these assignments and the possibility that they may derive from monoterpenes (given the similarities in the molecular formulas to the monoterpene-derived organosulfates mentioned later in the same paragraph)?

11) Line 225-227, please include the city, state, and country for each of the measurement sites discussed. Centreville and summertime Alabama are presented as though they are different locations, when they are one in the same.

12) I encourage the authors to consider their use of significant figures in reporting their data. Many organosulfate concentrations are listed to four significant figures, while their contributions to organic carbon have only one. The former seems to be too many (considering measurement uncertainties and use of surrogate standards) and the latter seems to be not enough.

13) In Table S2, please label which compounds are “isoprene OS” that are mentioned at line 238.

14) In several places, the wording should be adjusted so as to better reflect that many

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species were semi-quantified and absolute concentrations remain unknown. At line 244: “The concentration of quantified isoprene OS. . .” At line 271 “. . .were the second most abundant signals among the observed species. . .”

15) In Figure 1, please write out the dates “24 May night” and “30 May night” rather than “0524N” and “0530N”.

16) In the figure 2 caption, please point the reader to the specific section where the information about the missing water-soluble OS can be found (3.1)

17) In the Figure 2 caption, please explain that these plots only include the select species quantified or semi-quantified by LCMS.

18) There is a lot going on in Figure 4. Can this be simplified? Or perhaps broken into multiple graphs that do not have so much overlap? Also, because there is so much going on, adding the key findings / takeaway messages from the graphs to the caption would help the reader.

19) Figure S1 – delete 2016 from the date on the x-axis (as this takes up unnecessary room). It would be helpful to designate what is daytime and nighttime in this figures as is done in many of the other figures.

20) Table S1 would benefit from organization by m/z so that the table can be easily navigated by other researchers who are likely to look up the data in this way.

Technical/editorial comments

21) Line 20: “the majority”

22) Line 22: “mass spectrometry was employed”

23) Define LWC at line 27

24) Define SIA species at line 28

25) “0.02%” of OA at line 46 seems too small, is this reasonable?

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- 26) Line 109: “flow rates were”
- 27) Line 164: Mg₂⁺ (rather than Ma₂⁺)
- 28) Line 172: do not need to say “percent” in either instance, since it is earlier in the sentence.
- 29) Line 283: “favorable for OS formation”
- 30) Hettiyadura et al. (2015) propose a mechanism for the formation of the isoprene organosulfate with m/z 211 that is consistent with the hypothesis presented by Surratt et al. (2008).
- 31) Line 343: “times larger than daytime”
- 32) Line 349: “levels at night. . .”
- 33) Line 351: “was in excess and no longer the limiting factor in NOS formation.
- 34) Line 380: “NOSs form via”
- 35) Line 382: “formation of isoprene OSs or NOSs, epoxides first form. . .”
- 36) Line 393: “increase further with MVK+MACR.”
- 37) Line 419: “OS concentrations”
- 38) Line 430: “NO₂ levels at night. . .”

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