

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 #3

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This study reports the analysis of organic aerosol composition in central Beijing during winter and summer months using orbitrap mass spectrometry coupled with a nano-electrospray ionisation source. A main finding is that the number of S-containing organic species increased with inorganic sulfate concentration. This work provides new information on organic aerosol chemistry in northern China with a scope that fits well within ACP. But there are some issues on data analysis and interpretation, which may require major revisions to resolve.

It is important that the authors discuss the limitations with negative ESI MS analysis, such as its low ionization efficiency towards, or inability to detect, certain types of

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compounds. The calculation of aromaticity equivalent X_c is based on assumptions of elements' valences which may not always hold for atmospheric organics. The authors excluded S-containing species in their calculations of X_c , but nevertheless calculated the X_c for N-containing compounds, in which the valence of N can be either 3 or 5. In addition, the O valence in peroxides is 1 rather than 2 and it is known that organic peroxides can account for a significant fraction of the molecules. The authors should discuss how these issues affect their results and conclusions. Additionally, some discussions on the technical aspects a bit vague and need clarification. See below for specific comments.

This study only compares winter and summer compositional differences, thus is an overstatement to have a title of “Seasonal Differences ...”

Page 2, how was sampling from Birmingham UK decided to be representative of a typical European urban background site?

Page 3, What's the sampling duration for the filters?

Page 3, Line 19, is the concentration corresponding to PM mass or OA mass? How was it known?

Page 4: Line 1-2, what's the mass accuracy of the instrument? Line 7 – 9, this sentence is vague. More information is needed to clarify how this was done. Line 11, be specific about the threshold to remove signals and define how noises are determined. Line 12, “blank subtraction” usually means that all ions were subjected to blank subtraction, but this sentence suggests only the ions less than 10 times of the blank level are removed. This is confusing. Line 20 -21, the formula for DBE calculation has limitations due to the assumptions about element valences. This issue should be clearly stated and the implications on the reported results should be discussed. Line 23 – 24, the sentence “If ...” is confusing. Please be specific.

Page 5: The Panagi et al. paper is not yet published and unavailable. It is not

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appropriate to cite it as a source of information used in this paper. Either provide the paper as supplementary or reiterate relevant key points. The meaning of “the residence time of the air masses (or the integrated concentration of theoretical air mass particles)” is not straightforward, needs clarification. Line 22-24 seems unnecessary, consider to remove. There are strange characters shown at Line 27 – 28. Change “off” to “of” on Line 30

Page 7. Line 14. Ref?

Page 8: Line 1-2, waxy biogenic organic aerosol components likely have high H/C, but not all biogenic compounds have high H/C. It is more useful to define the cutoff value of “high H/C” line 14, what’s the basis for claiming that compounds with $H/C < 1$ and $O/C < 0.5$ are aromatic? Citing a previous study here without proper context is not sufficient.

Page 10, specify the “low” and “high” values use in describing elemental ratios and discussing chemical meanings.

Page 12, 1st paragraph, N also has two valences, so what’s the validity of calculating Xc for N-containing compounds using the given formula?

Page 16, line 33, what’s the reasoning behind this sentence – “This suggests ...”? Why does the correlation suggest how the compounds are formed? The authors appear to imply that the N-containing ions detected in this study are representative of “N-containing organics” in aerosol, but this is misleading as negative mode ESI-MS generally biases against reduced nitrogen compounds. Such issues should be articulated throughout the manuscript.

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