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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Molecular Characterization of Firework-Related Urban Aerosols using FT-ICR Mass Spectrometry" *by* Qiaorong Xie et al.

Anonymous Referee #2

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Xi et al. propose a study on the characterization of ambient aerosols using an FT-ICR. 6 samples were analyzed and compared to evaluate the impact of firework on air quality. Overall the data reported in this study are coherent and the structure of the paper is clear. However, additional information should be added as well as some explanation to make this paper more comprehensive.

Page 2, lines 8-9: please reformulate.

Page 2, line 31: Please provide more information regarding the sampling of the aerosol: the size of the particles; i.e., PM1, 2.5, 10? high-volume samplers?

Page 3, line 2-3: I recommend the authors to use a simpler naming system. e.g.,

before-FW-1, after-FW-2, during-FW-1,... it would be much easier to follow the discussion.

Page 4, line 1: The authors should explain why these samples were analyzed only in negative mode.

Page 4, section 2.4: - why did the authors choose an S/N> 6, which is more restricting? Why not using an S/N ratio > 3, which is commonly defined as LoD?

- Is the peak assignment perform before or after blank subtraction? While the authors mentioned that blank filters were collected and analyzed, no information is providing regarding how the blank samples were used for the data analyzing.

- Why did the authors start at m/z 185 rather than m/z 100 as mentioned earlier in the manuscript? A significant amount of potential OA compounds can be missing.

- The authors should not claim any semi-quantitative results as the sensitivity of the ESI is extremely dependent on the functional groups of individual compounds as reported in many studies.

Page 5, lines 26-28: The authors should provide either some references or some supporting information to support their statement.

Page 5, lines 29: How do the authors know the distribution of the ions/compounds as a function of the size provide either reference or supporting information.

Page 6, lines 2-4: While the concentrations of SO42-, Cl- and K+ are significantly different, this is not really the case for WSOC: there is an increase $\sim$ a factor of 2, but what's the daily variability? It is hard to conclude that FW produces a sharp increase. In other words, is the increase statistically different?

Page 6, line 12: How do the authors know the ionization efficiency of the observed compounds? i.e., the concentrations of some ions can be very high but with very poor ionization efficiency. This statement is purely speculative

Page 6, lines 13-14: That's an incorrect assumption/statement. The matrix effect is one aspect. I strongly encourage the authors to check basic studies on ESI and revise their manuscript. Indeed the peak intensity can be impacted by the matrix but also depends on the ionization efficiency of individual compounds which is based on the functional groups present in each compound.

Page 6, line 19: This is actually surprising and not consistent with "normal" product distribution. Indeed in most of the previous studies, most of the identified ions are between 150-250 (i.e., monomers type) and a second mode is present between 300-400 (dimers or high molecular weight compounds), see the previous characterization using ESI-MS (QTOF, Orbitrap, and FT-ICR). The authors should comment on such a curious product distribution. The authors should clearly mention that probably the vast majority of the compounds were lost during the sampling preparation.

What is the reason to remove a major fraction of the organic compounds during the sampling preparation (i.e., page 3, lines 26-27)?

Page 6, line 33 and page 7, lines 1-2: This is overstated, the authors should provide deeper statistical analysis before making such a statement. Are the numbers really statistically different?

Page 7, line 8: Please provide numbers to support such a statement.

Page 7, lines 12-14: I am confused by this sentence. Why did the authors refer to Ms2 studies while they didn't perform such an analysis.

Page 7, line 30: This statement is incorrect. It is not in urban aerosol but in the filter extract, i.e., after removing a major fraction of organic aerosol components.

Page 9, lines 20-27: This section is confusing. please clarify, i.e., within the same paragraph the authors claim that CHON with O>3 are likely organonitrates and a few lines below nitroaromatics. In addition, the authors should keep in mind the difference in terms of ionization efficiency of such compounds: i.e., compounds containing nitro-

functional groups have a very high ionization efficiency (e.g., nitroaromatics), unlike organonitrate compounds.

Why is the CHONS group not discussed in the paper?

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