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Comment

Interactive comment on “Application of high resolution Chemical Ionization Mass Spectrometry (CI-ToFMS) to study SOA composition: focus on formation of oxygenated species via aqueous phase processing” by D. Aljawhary et al.

Anonymous Referee #1

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General comments:

This manuscript describes the use of a high resolution chemical ionization mass spectrometer to monitor SOA composition during aqueous phase oxidation. By using different reagent ions, the authors were able to monitor a larger fraction of the organic compounds than would have been possible using only one reagent ion. The results from each reagent ion were then compared, both with each other and with an AMS, an instrument commonly used to study SOA properties. The use of multiple reagent

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ions highlights the need of complementary methods to obtain a more complete picture of the chemical sample, whether gas or particulate phase. No single reagent ion can detect all species of interest, and each additional measurement yields another piece of the puzzle.

The aqueous phase processing that the CIMS was applied to is also an important area to study, as understanding SOA formation and evolution requires knowledge of both gas and condensed phase oxidation. The authors could stress more that the technique applied in this paper is not limited to only aqueous phase processing.

The scientific quality is very high, and the results are presented clearly. The manuscript is well-suited for publication in AMT, and I only have some minor suggestions for revisions that can be found below.

Specific comments:

I suggest removing "focus on" from the title, and possibly moving the "application to" in it's place.

The introduction is a bit lengthy, and could be more focused on the issues discussed in this paper. For example, the ability to detect single molecules is high-lighted in the introduction, but actual molecular results seem to be awaiting a subsequent publication. Meanwhile, many of the most intriguing results in this paper arise from the use of several different reagent ions, but hardly any background is given on the importance of choosing the "correct" reagent ion when doing CIMS. I would in general like to see some more discussion on the different reagent ions. Are the authors able to recommend one reagent ion over the others, in situations where switching is not an option? Or is it important to always use several to detect "all" compounds? And what fraction of the SOA is believed to be detected with the reagent ions used here? Maybe all compounds still weren't measured, and other reagent ions should be considered?

Section 2.2: It sounds like the oxidation takes place for 4h, and the sampling occurs

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later. Only in Fig.3 does it become clear that the solution is actually sampled throughout the oxidation process. This should be noted already in this section for clarity.

Page 6168, lines 14-15: Were the three reagents switched continuously, or were experiments made with different samples? The only reference to how the switching was done in practice seems to be in the caption of Fig. 4 that states "One reagent ion was used at a time.", but this is not very helpful. The switching should be explained in the methods section, especially as the simplicity of the switching is high-lighted in the conclusions.

Technical corrections: Several small spelling corrections are needed, some of which I have noted below. I recommend a thorough read through the paper before submitting the final version to remove mistakes with singular/plural, missing articles, etc.

6151, 1-8: Several Canagaratna references are not needed here. The last two can be removed.

6151, 9: First "ESI" can be removed.

6154, 18: "spectrometer"

6157, 16-17: "Protonated water clusters and iodide water clusters reagent ions experiments..." is confusing and should be reformulated.

6158, 4: "ions"

6158, 5-6: I have never seen such exact resolution numbers quoted, and doubt that these were this exact even between two consecutive spectra. Regardless, the authors should rather state that the resolution was 4100-4300 or "just above 4000" for all experiments instead.

6158, 14: Fix parenthesis in citation.

6161, 12: "analogue". Also, it is not clear in which way it is analogous.

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6161, 24-26: "To illustrate, it was observed (not shown) in the sensitivity test (Sect. 3.1) the presence of ions for $(\text{H}_2\text{O})_n\text{H}^+$ and in $\text{CH}_3\text{C}(\text{O})\text{O}^-$ reagent ions, which was not expected based on Reactions (R1) and (R2)." This sentence is very confusing and should be reformulated.

6167, 1: "compared to"

Fig. 8: AMS symbol is "water"?

Fig. 9: The average OSc point seems to be missing. Also, I think the light vs dark dots are explained differently in the text and in the figure.

Interactive comment on Atmos. Meas. Tech. Discuss., 6, 6147, 2013.

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