

Atmos. Meas. Tech. Discuss., referee comment RC2  
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## Comment on amt-2022-147

Anonymous Referee #1

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Referee comment on "Real-time measurement of phase partitioning of organic compounds using a proton-transfer-reaction time-of-flight mass spectrometer coupled to a CHARON inlet" by Yarong Peng et al., Atmos. Meas. Tech. Discuss.,  
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This paper describes the use of an online CHARON inlet coupled to PTR-MS to measure the gas to particle fractions of a range of semi-volatile organic compounds. It combines experiments using a broad range of standard compounds and then expands this to look at real world data collected in Beijing. The main finding is that fragmentation of large molecules during the ionization process occurs and that this can have important implications when estimating gas-particle partitioning. This is a well-written paper and is well within scope AMT. The authors have provided the community with useful knowledge and some suggestions for how these difficulties could be overcome. I recommend publication after the following comments have been addressed.

Figures: My main issue with this paper is a lack of clarity in the figures. Figure 1b is impossible to read with so many overlapping points. I think Figure 2 is meant to show the fragmentation pattern and how they change (or not in this case) at different temperatures. But the use of a log scale and a bar chart makes this very difficult to see. Also, each mass spectrum should have a labeled x-axis as these are all different.

I also think the use of a log scale in Figure 3c) and d) makes this very hard to interpret. It is difficult to see the relative percentages of the different groups using a log scale, where the pink colour is large but actually the % is relatively small. I would convert this to a linear scale or provide a scaled 100 % plot in addition to the one here.

## Minor comments

Line 241: Why have the nitrophenols been excluded from the analysis?

Figure 1b: There are no blue or purple points at 70 C. Is there a reason for this? The figure legend needs more details. Is this normalized to the CPC counts at 300 nm diameter? Does the "PTR-TOF-MS" signal include the fragment ions?

Line 330: Sucrose has a lower EF and this is attributed to dehydration. However, the light blue point in figure 1C (2,7-dihydroxynaphtalene) also looks to have a lower value but this compounds doesn't fragment.

Figure 2: I would have liked to have seen more discussion of the fragmentation data. What are the red labels on some peaks? They are not the molecular ion so I'm not sure why they are a different colour.

Line 348: I think you need to make clear at the start of this section that you have moved to discussing the field data.

Line 350-352: What does "agree very well mean"? In figure S5 you have R values. Can these be added to figure S4?

Line 355: Figure S5 shows a comparison of specific compounds not total carbon mass.

Line 356: This comparison is interesting – it seems that when the mass is low towards the end of the measurement period, there is a larger discrepancy between the two methods. Do you have any suggestions for why this is?

Line 358: I cannot see a plot of CHARON derived total OA or its comparison to AMS data?

Line 394: Is there any explanation for why the O<sub>4</sub> group is closest or is it just by chance? In Figure 4, adding additional functional groups to the O<sub>4</sub> species makes the agreement worse. Perhaps these are less prone to fragmentation?

Figure 4: I think you should present the data in Figure 4 in a table in addition to the plots. This would be more useful for readers.

Line 430: I agree with your final comment here but I think you need to be clear that currently this isn't possible as you can't predict what the parent molecule was.