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Atmospheric Measurement Techniques Discussions

Interactive comment on "Characterisation of the transfer of cluster ions through an Atmospheric Pressure interface Time-of-Flight mass spectrometer with hexapole ion guides" *by* Markus Leiminger et al.

Anonymous Referee #2

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This manuscript presents a new type of atmospheric pressure interface TOF mass spectrometer, the ioniAPi-TOF. The main difference to the earlier APi-TOF design is the change from quadrupole ion guides to hexapole ion guides. This is suggested to allow softer transmission of ions through the instrument, which may be possible, but is not convincingly shown in the manuscript, as detailed below. However, as so much of the current frontier research on both gas phase molecules and clusters have relied on solely the APi-TOF, it is a welcome addition to have a new instrument available for comparison. Overall the instrument is described in sufficient detail and I recommend

publication in AMT, following consideration of my comments and concerns below. In particular, the conclusion that the ioniAPi-TOF is able to transmit clusters bound by 17 kcal/mol needs to be more strongly shown.

Major comment:

The measurements of hydronium ions are used to deduce that the transmission of the ioniAPi is much less fragmenting than the APi-TOF. I see several issues with the interpretation of these results.

1. My main concern relates to the fact that no response at all is seen in the hydronium ion distribution before a dV of 4V. The authors seem to assume that this means that no cluster fragmentation is taking place at all. To me this rather seems to be a clear indication that this region of the ioniAPi is not the region where cluster fragmentation is mainly taking place (before the dV is increased high enough). If there is considerable fragmentation taking place somewhere after this region, with collisions able to break clusters of, say, 25kcal/mol, then it is not surprising that the dV in the probed region needs to go very high before starting to have an effect on the cluster distribution. The authors need to be more convincing with this data in order to be able to claim that this instrument is much less fragmenting than similar instruments.

2. As clusters are fragmenting, they will cause an increase in smaller water clusters. This is e.g. seen in the increase of the monomer and dimer clusters. There is no discussion about the potential influence of this on the trimer and tetramer when determining the dV50.

3. In Lopez-Hilfiker et al (2016), dV50 was defined as the voltage where the initial signal decreased to 50%. Here the voltage seems to be determined by the decrease halfway to the arbitrary maximum of the voltage scan.

4. The expansion from atmospheric pressure into the APi will cause significant cooling, and most likely formation of larger water clusters. This should be acknowledged and

considered potential impacts on the results.

Minor comments.

Line 16: ”As we will show” is not commonly used in an abstract summarizing the work.

Line 32: “Owing” would read better as “having”.

Line 74: Please clarify what “interactions with the reagent ion” means here.

Line 74: It is not customary to refer to the instrument being described here as a CI-APi-TOF. That term is typically used only for the atmospheric pressure “Eisele-type” CI inlet, while the one used here is generally called a ToF-CIMS.

Lines 87-100: The entire discussion around Eq. 1 is quite hard to follow, in part due to the complexity of multipole physics in general. I suggest the authors describe a bit more concretely what the function of V* is, and how it will affect the ions. Also, clarify the argumentation why the (r/r0)ˆ4 dependence causes a “larger field free region”, as the simple interpretation of the equation is that the 4th power dependence of a hexapole would lead to a higher impact on the radial energy compared to the 2nd power dependence of a quadrupole.

Figure 3 is referenced before figure 2.

Lines 243-244: This HTOF lacking an APi needs some clarification, as sampling without any atmospheric pressure interface should not be possible here.

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