Atmos. Meas. Tech. Discuss., 8, C3725–C3727, 2015 www.atmos-meas-tech-discuss.net/8/C3725/2015/
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8, C3725-C3727, 2015

Interactive Comment

Interactive comment on "Characterization of the mass dependent transmission efficiency of a CIMS" by M. Heinritzi et al.

Anonymous Referee #1

Received and published: 4 November 2015

This paper describes the determination of the mass-dependent ion transmission efficiency of a Tofwerk "APi-ToF" with and without a (nitrate) CI source. Overall, the determinations are well done, and nicely described. The mass-dependent ion transmission of a mass spectrometer is no doubt important to understand and all operators of such instrument should do such tests.

However, that does not mean each determination on an instrument should be published as stand alone papers. The main reasons being that the scientific and technical merits of this work do not extend beyond the authors' instrument, much as a calibration factor for one instrument does not apply to another. While there could be value in either reporting a new insight into what the key controls on a response function are, or describing a new method for constraining the dependencies, such new insights or

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methods are not presented here.

I acknowledge that applying some of the methods used herein to a nitrate CI APi-Tof may not have been done before (or perhaps were done, but buried within a paper on a different topic or not even mentioned), i.e., there is something "new" here, but these aspects are barely incremental and do not qualify as significant advances. I also acknowledge that it can be incredibly frustrating for students and PIs because such characterizations are essential to being able to do new science or to understand a new instrument, but by themselves, the results are not broadly useful enough to justify further taxing the pool of over-taxed reviewers. Indeed the authors state this in a way, on page 11375: "Finally, even the smallest changes of the inner geometry of the instrument, e.g. caused by shipping, can affect ion beam alignment and thus cause different transmission characteristics."

That the ion transmission efficiency depends upon optics in the mass spectrometer is well known (as the authors describe), and it is even well known that electric fields in the ionization region affect mass transmission. For example, the PTR community and others have used this fact to ensure either that clusters are broken apart in the ionization region, and therefore have a very low transmission efficiency, or alternatively, are preserved and transmitted (e.g. lodide and nitrate clusters). The stability of cluster ions, or lack thereof, in electric fields will by definition impart a real or apparent mass dependent effect on ion transmission in a way that depends not just on the ion mass but also composition. If different operators of the same type of instrument choose different electric fields (or pressures, etc) either intentionally or not, the effect will be different and thus 1 mass transmission curve is not relevant to data from a different instrument or even the same instrument with different voltage or pressure settings.

Explaining new insights into the fundamentals of what controls mass dependent ion transmission for a given system, or how to generally optimize those to arrive at a desired mass dependent transmission curve would both be a useful contribution, but the current paper does not offer that type of analysis.

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The methods used for determining the transmission efficiency are not novel either. As part of ion molecule reaction rate constant determinations, Huey et al J. Phys Chem 1995 vol 99 No. 14 report doing exactly the same method of reagent ion titration as used in this manuscript to constrain the mass dependent ion transmission of a quadrupole mass filter. That paper is not referenced here. They state

"The mass discrimination was determined by measuring the ratio of the change in the product ion signal to the change in the reactant ion signal for several ion molecule reactions that produce only one product ion...."

Junninen et al AMT 2010 use a DMA and electrospray ion source to constrain the mass dependent ion transmission of a Tofwerk APi-ToF.

Thus, while I have zero criticisms of the methodology, data quality, or conclusions, I think this information is not sufficient for a stand alone paper, and would be better incorporated as part of another paper, or supplemental information for another paper that can always be referred back to by the authors when needed to support the fact that they do these determinations.

Interactive comment on Atmos. Meas. Tech. Discuss., 8, 11369, 2015.

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