

Interactive comment on “Development and characterization of a High-Temperature Proton-Transfer-Reaction Mass Spectrometer (HT-PTR-MS)” by T. Mikoviny et al.

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The authors would like to thank the referee for her/his careful reading and helpful remarks.

P. 191, line 3: I find it very useful that the authors give the reagent ion counts along with O_2^+ counts. Please also provide typical water dimmer counts at m/z 37.

We have included the requested information in the manuscript.

“Typical reagent ion count rates in the new HT-PTR-MS were 7×10^6 cps of H_3O^+ ions

(O_2^+ : 5×10^4 cps; $H_3O^+(H_2O)$: 8×10^5 cps) in the high E/N-mode and 4.5×10^6 cps of $H_3O^+(H_2O)$ ions (H_3O^+ : 3×10^5 cps; O_2^+ : 1×10^4 cps; $H_3O^+(H_2O)_2$: 3×10^5 cps) in the low E/N-mode.”

P. 191, line 9: The authors stated that ‘the quadrupole mass spectrometer was optimized for the detection of high m/z-signals’. It would be useful to get a very short description of this procedure.

We have added a short description of the optimization procedure.

“In addition, the quadrupole mass spectrometer was optimized for the detection of high m/z-signals by increasing the reference potential for the mass spectrometer lenses (V1 in the Pfeiffer IS 420 supply) from ~ 50 V to ~ 70 V. This resulted in a ~ 25 % higher detection efficiency for ion signals with m/z > 100, but in a ~ 10 % lower detection efficiency for the primary ion signals.”

P. 192, line 8: The authors mention in the paper that high temperature (200°C) is the reason for higher fragmentation. In this case it is useful to look more carefully at fragments. Hexanal fragment at m/z 83 is accounted for but how about decanal fragment? If parent ion m/z 157 expels water then it might be useful to look at m/z 139. Please comment.

Unpublished data from our laboratory indicate that decanal is the most stable of all n-aldehydes (C₃-C₁₀). The m/z 139 fragment was negligibly small in the low E/N mode.

P. 193, line 1-12: Perhaps this paragraph is the weakest part of the paper as it discusses a relatively high background signals for low m/z peaks. Please give an idea of where this background is coming from. Maybe from the new materials that were used for the drift-tube construction? Also describe the way your background was measured.

We now give the experimental details of the background measurement in section 2.2. A

short paragraph on potential sources of the instrumental background has been added.

“2.2 Set-up for instrument calibration and background characterization”

“The instrumental background was measured by delivering humidified zero air to the instrument.”

“We consider material outgassing to be the main source of the observed background. Preliminary results from our laboratory indicate that PEEK shows enhanced outgassing at temperatures above 100° C.”

P. 193, line 7: ‘These are, however, not the target analytes of a HT-PTR-MS instrument.’ This sentence is somewhat confusing as later on the results are given for m/z 18, 62, 79.

The reviewer’s remark is correct. Although the HT-PTR-MS was primarily built for measuring high m/z analytes, we have so far explored its use mostly with low m/z compounds. The two sentences have been removed.

Removed: “These are, however, not the target analytes of a HT-PTR-MS instrument. Semi- or non-volatile species have higher molecular weights.”

P. 194, line 16: Ammonia measurement is very interesting. Do you see any problem with huge intensity at neighbouring m/z 19 peak?

This is not a problem if the QMS is properly tuned. In addition, ammonia measurements should be carried out using O_2^+ (m/z 32) as primary ions because of a significantly lower instrumental background (for details see Norman et al., 2007).

P. 202, fig.4: Mention in the caption that m/z 85 is the fragment. Clarify in the text why you pick m/z 85 fragment as levoglucosan marker and not the parent ion.

We have made the requested change and have added a short paragraph on levoglucosan detection.

“Levogluconan was found to fragment upon protonation in both the high and the low E/N-mode. The dominant fragment ion signal was observed at m/z 85. Other major fragment ion signals were observed at m/z 69 and m/z 97. At even lower E/N-values (~ 50 Td) than those routinely used in this study, we observed a characteristic m/z 145 ion signal which corresponds to dehydrated protonated levogluconan.”

Figure caption: “levogluconan (m/z 85; fragment - see text)”

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