

Interactive comment on “Measurement of alkyl and multifunctional organic nitrates by Proton Transfer Reaction Mass Spectrometry” by Marius Duncianu et al.

Anonymous Referee #2

Received and published: 2 January 2017

The paper “Measurement of alkyl and multifunctional organic nitrates by Proton Transfer Reaction Mass Spectrometry” by Duncianu et al., investigates the organic nitrates in the gas phase using an optimized PTR-ToF-MS instrument at tens of ppt detection limit range. The paper is well written with high scientific quality data and deserves publication after considering the revisions.

Comments: 1. The authors mentioned the synthesis of few organic nitrates performed during these investigations. However, the purity of the synthesized compounds is verified only by FTIR as the authors stated in line 370. Please consider to add in Supporting information section the IR gas phase spectra of the synthesized compounds. Additionally, please consider that FTIR analysis is a less appropriate method for checking

Printer-friendly version

Discussion paper



purity of the new compounds when the impurities may have similar functional groups as the synthesized compound. Did you perform NMR analysis of the synthesized compounds? If you compared the synthesized compounds with existing IR reference spectra please specify the reference of the database used. Additionally, please add information of the infrared gas phase cross section values for the organic nitrates obtained in this study as you mentioned to calculate them (line 339-351).

2. There is stated in the Abstract and Introduction sections that was performed optimization of the PTR-ToF-MS instrument for the measurements of organic nitrates in the atmosphere but the studies presented in the manuscript are exclusively recorded in a simulation chamber using dry air conditions. My concern related to the measurements into the atmosphere is mainly due to the interference species (gas and particles) and humidity. Did you perform any test for humidity effect? May you comment how these interference could affect the results (decomposition, clustering, partition, hydrolysis, etc.)?

3. As there is a FTIR instrument available for insitu measurements in the chamber, it will be worth comparing FTIR vs PTR-MS concentration-time dependency for each class of organic nitrates at the most effective PTR-MS conditions during the organic nitrate accommodation into the chamber. These comparisons may add important information for quantitative analysis of organic nitrates using PTR-MS. Such test may also check for possible response delay in the PTR measurements due to the nitrates deposition on the sampling line for example.

4. In the Conclusion section, authors conclude that NO^+ adduct ionization mode is "suitable for measurement of organic nitrates during lab studies but also in ambient air". There are tests performed in the ambient air?

Specific and technical:

Line 34: Please use subscript for NO_y and NO_x in entire manuscript.

[Printer-friendly version](#)[Discussion paper](#)

Line 51 Please add a reference for the formation of carbonyl-nitrates by NO₃-oxidation of alkenes.

Line 174: The AC and DC electrical field better symbolize with capital letters and explain the ac and dc meaning.

Line 183: Provide more details for the sampling line (diameter, etc). Heating up to 40° C prevents adsorption for all investigated species? Have you performed a sampling efficiency study for different compounds (monofunctional organic nitrates, hydroxyl nitrates, dinitrates, carbonyl nitrates, etc)? Please comment on this sampling efficiency.

Line 188: The PTR-MS inlet system has been optimized for various temperatures to study possible decomposition processes of the organic nitrates? If yes, there is a need for some more comments.

Line 312: please express the meaning of LISA abbreviation.

Line 338: add “.” after “al” in “Doussin et al, 1997”

Line 343: please revise the units for IBIs. There is “cm molecule-1”

Line 347: Beaver et al., 2012 and Bates et al., 2014 do not provide IBIs values for the PANs and hydroxynitrates. Please revise.

Line 361: “H₂O < 0,5 ppm” use dot instead comma

Line 362: “CO < 0,1 ppm” use dot instead comma

Line 742: there is a text which should be erased.

Line 752: “C₅H₇-C(O)OONO₂” is in fact “C₄H₇-C(O)OONO₂”

Reference: - Please be consistent with journal title and use abbreviated or full name but not mixed. - Please be consistent with using capital letter or not for the words forming the title of the articles. - Please move “Shepson” from end of reference list to the right place.

[Printer-friendly version](#)[Discussion paper](#)

Interactive comment on Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2016-318, 2016.

AMTD

Interactive
comment

Printer-friendly version

Discussion paper

