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Atmospheric Measurement Techniques Discussions

Interactive comment on "MS/MS studies for the selective detection of isomeric biogenic VOCs using a Townsend Discharge Triple Quadrupole Tandem MS and a PTR-Linear Ion Trap MS" *by* M. Müller et al.

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General comments:

This is an interesting and well written article that will certainly be of value to the practitioners of PTR-MS and newcomers in the field. The usefulness and limitations of the newly developed techniques of QqQ-MS and PTR-LIT to perform collision-induced dissociation experiments on protonated molecules with the aim of differentiating isomers are very well documented. The experimental study appears to be very carefully

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conducted, and detailed information is provided on the various types of experiments. Unfortunately, the results are a little disappointing in that the techniques do not allow yet for the selective detection of individual monoterpenes and sesquiterpenes, despite considerable efforts and progress. This result does not surprise me; interestingly, the chemical reactivities of isomeric monoterpenes such as alpha-pinene, beta-pinene and 3-carene towards oxidants like the OH radical and ozone are also very similar. The results obtained for the isoprene oxidation products such as MVK and MACR appear to be more convincing and promising. I take this opportunity to encourage the authors to apply their techniques in the future to the differentiation of other gas-phase oxidation products of isoprene in laboratory oxidation experiments. There are still exciting and novel gas-phase species other than MVK and MACR that need to be more thoroughly investigated or to be uncovered. A few minor revisions mainly with regard to terms relating to mass spectrometry are suggested as detailed below.

Specific comments:

Most comments relate to standard definitions of terms relating to mass spectrometry, which can be found in the following publication: "Standard definitions of terms relating to mass spectrometry (IUPAC Recommendations 2006)" by Murray et al. (http://old.iupac.org/reports/provisional/abstract06/murray_prs.pdf)

Page 1838 – line 6: a correction is suggested here: ". . .. protonated molecules." Ions are already protonated.

Page 1838 – lines 20-24: I suggest to refer early on in the introduction to the recent comprehensive review article on the current status of secondary organic aerosol from the oxidation of BVOCs: Hallquist et al., The formation, properties and impact of secondary organic aerosol: current and emerging issues, Atmos. Chem. Phys., 9, 5155-5236, 2009.

Page 1838 – line 12: As already pointed out by another reviewer (P. Palmer), I also do not consider the CID regime applied in QqQ-MS as high-energy but rather as low-

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energy, because the energy deposited in the ions is in the eV range and lower than 25 eV. The latter energy can only be achieved with laboratory frame energies in the keV range, which is not the case here.

Page 1840 – line 16: I suggest to write “the mass analyzer, . . .”; the abbreviation “MS” is commonly used to denote “mass spectrometry”.

Page 1841 – line 2: see comment made above about “high-energy”.

Page 1843 – line 3 (and other places elsewhere): correction suggested here: “ . . . fragment ions with the highest abundances (or signal intensities) at . . .”

Page 1843 – line 6: the abbreviation “m” is used throughout the work instead of “m/z” which is the term recommended by IUPAC. As a practitioner of MS, I find this practice somewhat strange and like to recommend that the authors adopt the IUPAC term “m/z (in italic)”.

Page 1843 – line 12: the abbreviations “E/N” and “Td” need to be defined.

Page 1843 – line 24: I suggest to adopt the term “protonated molecule” instead of “quasimolecular ion”; according to the recent IUPAC recommendations the term “quasi-molecular ion” is deprecated.

Page 1847 – line 24: “parent ion” is another term deprecated by IUPAC. The recommended term is: “precursor ion”.

Technical (typographical) corrections:

Page 1841 – line 5: . . . , and it can . . .

Page 1841 – line 13: . . . (+)-3-carene and . . .

Page 1841 – line 19: . . . at a constant flow rate . . .

Page 1844 – line 11: . . . shown . . .

Page 1846 – line 7: . . . a monocyclic structure . . .

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Page 1849 – line 27: . . . other isomeric compounds . . .

Table 4: Highest fragment ion signals . . .

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