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Atmospheric
Chemistry
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Discussions

Interactive comment on "Secondary organic aerosol formation from the photooxidation of isoprene, 1,3-butadiene, and 2,3-dimethyl-1,3-butadiene under high NO_x conditions" *by* K. Sato et al.

Anonymous Referee #1

Received and published: 9 March 2011

General comments:

This is an interesting and timely study aiming to improve our understanding of SOA formation from isoprene and related dienes in the presence of NOx, which is relevant to ambient fine aerosol in the urban environment. A well-designed series of smog chamber experiments is performed, and the results appear to be carefully interpreted. The authors suggest that oligoesters containing nitrooxypolyol residues could be a possible source for 2-methyltetrols found in ambient samples collected under high-NOx conditions. This could very well be the case; however, another likely source that

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is not considered in this study are organosulfates containing nitrooxypolyol residues. The latter organosulfates have been detected in ambient fine aerosol but it remains to be seen whether oligoesters containing nitrooxypolyol residues are also present. A short note on this issue would be appropriate.

Specific comments:

Some of the comments made below concern 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 4314 – line 17 (and page 4332 – line 17): The verb “discovered” is too strong in my opinion; I would write “characterized”.

Page 4315 – line 8-11: The authors write: “The products formed from isoprene oxidation (i.e., 2-methyltetrols, C5-alkenetriols, and 2-methylglyceric acid) have been observed in ambient fine particles” and cite a number of suitable references. It is noted that the first study in which 2-methylglyceric acid [although under the wrong name of 2,3-dihydroxymethacrylic acid, which was corrected in a subsequent study (Edney et al., 2005)] was characterized in ambient fine aerosol from K-puszta, Hungary, is not mentioned. I suggest to include this reference:

Claeys, M., Wang, W., Ion, A. C., Kourtchev, I., Gelencsér, A., and Maenhaut, W.: Formation of secondary organic aerosols from isoprene and its gas-phase oxidation products through reaction with hydrogen peroxide, Atmos. Environ., 38, 4093–4098, 2004.

Page 4316 – line 9: Another group of SOA tracers that are worth mentioning in this context are organosulfates containing a nitrooxypolyol residue. These compounds are formed from isoprene in the presence of NOx and sulfuric acid (also present in the polluted urban environment), and have been detected in ambient fine aerosol with the

LC/(-)ESI-MS technique. References:

Gómez-González, Y., Surratt, J. D., Cuyckens, F., Szmigielski, R., Vermeylen, R., Jaoui, M., Lewandowski, M., Offenberg, J. H., Kleindienst, T. E., Edney, E. O., Blockhuys, F., Van Alsenoy, C., Maenhaut, W., and Claeys, M.: Characterization of organosulfates from the photooxidation of isoprene and unsaturated fatty acids in ambient aerosol using liquid chromatography/(-)electrospray ionization mass spectrometry, J. Mass Spectrom., 43, 371–382, 2008.

Surratt, J. D., Lewandowski, M., Offenberg, J. H., Jaoui, M., Kleindienst, T. E., Edney, E. O., and Seinfeld, J. H.: Effect of acidity on secondary organic aerosol formation from isoprene, Environ. Sci. Technol., 41, 5363–5369, 2007.

Surratt, J. D., Gómez-González, Y., Chan, A.W. H., Vermeylen, R., Shahgholi, M., Kleindienst, T. E., Edney, E. O., Offenberg, J. H., Lewandowski, M., Jaoui, M., Maenhaut, W., Claeys, M., Flagan, R. C., and Seinfeld, J. H.: Organosulfate formation in biogenic secondary organic aerosol, J. Phys. Chem, A., 112, 8345–8378, 2008.

Page 4319 – line 13: ESI is used as ionization technique; I do not understand why a corona current is used. A corona current is generally used in the Atmospheric Pressure Chemical Ionization (APCI) but not in the ESI technique.

Page 4320 – line 8: Molecular weight (MW) has no dimensions but molecular mass has (Da): thus correct would be ". . ... having a molecular weight of 68 . . ..." or ". . .. . . having a molecular mass of 68 Da . . ..."

Page 4320 – line 8: The term "protonated ions" is a wrong term; the correct term is "protonated molecules". If an ion would be protonated, we would have a doubly-charged ion.

Page 4320 – line 12: ". . . were detected as protonated molecules at . . .."

Page 4324 – line 11: The term "quasimolecular ion" is deprecated according to the IUPAC guidelines. I would write: "Generally, analyte molecules are deprotonated to

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form [M –H]- ions during the negative-mode ESI process", and further on in the next sentence: ". . .. . . to be deprotonated molecules".

Page 4332 – lines 10 and 12: I suggest to be more specific here and replace "unsaturated aldehyde" by "methacrolein".

Fig. 4: Replace in the x-axis "Mass to chage ratio (amu)" simply by "m/z (in italic)". According to the IUPAC guidelines, the three-character symbol m/z (in italic) is used to denote the dimensionless quantity formed by dividing the mass of an ion in unified atomic mass units by its charge number (regardless of sign).

Technical corrections:

Page 4317 – line 17: the abbreviation "GC-FID" should not be used to refer to the instrument but to the technique; I would write: ". . .. . . and gas chromatography with flame ionization detection (GC-FID; . . ...)"

Page 4318 – line 16: . . ... two GC-FID instruments, ...

Page 4320 – lines 2-4: I suggest to write: ". . .. . . by high-pressure liquid chromatography/accurate mass (3 ppm) time-of-flight mass spectrometry (LC/TOFMS; Agilent, Model 6210). A 10-μL aliquot of analytical sample was injected into the LC/TOFMS instrument." I suggest to use a slash (instead of a hyphen) to denote a hyphenated technique; also the abbreviation "MS" denotes "mass spectrometry" and not the instrument.

Page 4322 – line 6: LC/TOF mass spectrum

Page 4322 – line 7: . . ... was conducted by LC/TOFMS (Fig. 4).

Page 4322 – line 8: The results obtained in the experiment with . . ...

Page 4326 – line 16: 2-Methylglyceric acid contains both a hydroxyl and a carboxyl group.

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Page 4329 – line 2: . . .. by LC/TOFMS analysis . . ..

Page 4329 – line 24: . . .. by LC/TOFMS analysis.

Page 4331 – line 3: . . . by LC/TOFMS analysis in . . ...

Table 2: replace “LC-TOF” by “LC/TOFMS”

Fig. 4 - legend: Flow-injection LC/TOF mass . . ...

Fig. 5 - legend: Typical LC/TOFMS base peak . . ..

Fig. 10 – legend: . . .. and (b) LC/TOFMS during . . ...

Fig. 11 – legend: . . ..., and (c) LC/TOFMS . . ...

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 4313, 2011.

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