

Electronic Supplementary Material

Time-Resolved Molecular Characterization of Limonene/Ozone Aerosol using High-Resolution Electrospray Ionization Mass Spectrometry

Adam P. Bateman,^a Sergey A. Nizkorodov,^{a*} Julia Laskin,^b and Alexander Laskin^c

^a *Department of Chemistry, University of California, Irvine, Irvine, California 92617, USA. E-mail: nizkorod@uci.edu; Fax: +1-949-824-8571; Tel: +1-949-824-1262*

^b *Chemical and Materials Sciences Division, Pacific Northwest National Laboratory, Richland, Washington 99352, USA*

^c *Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington 99352, USA*

Fig. S1, sample SMPS data taken during SOA preparation.

Fig. S2, sample mass spectra of limonene/O₃ SOA.

Fig. S3, a two-dimensional version of Van Krevelen diagram shown in Fig. 1.

Fig. S4, structures of selected first-generation products of limonene ozonolysis.

Fig. S5, particle-size resolved Van Krevelen diagram.

Table S1, summary of peaks excluded and assigned during peak analysis.

A table of all assigned peaks in the positive ion mode mass spectrum of limonene/O₃ SOA in separate file.

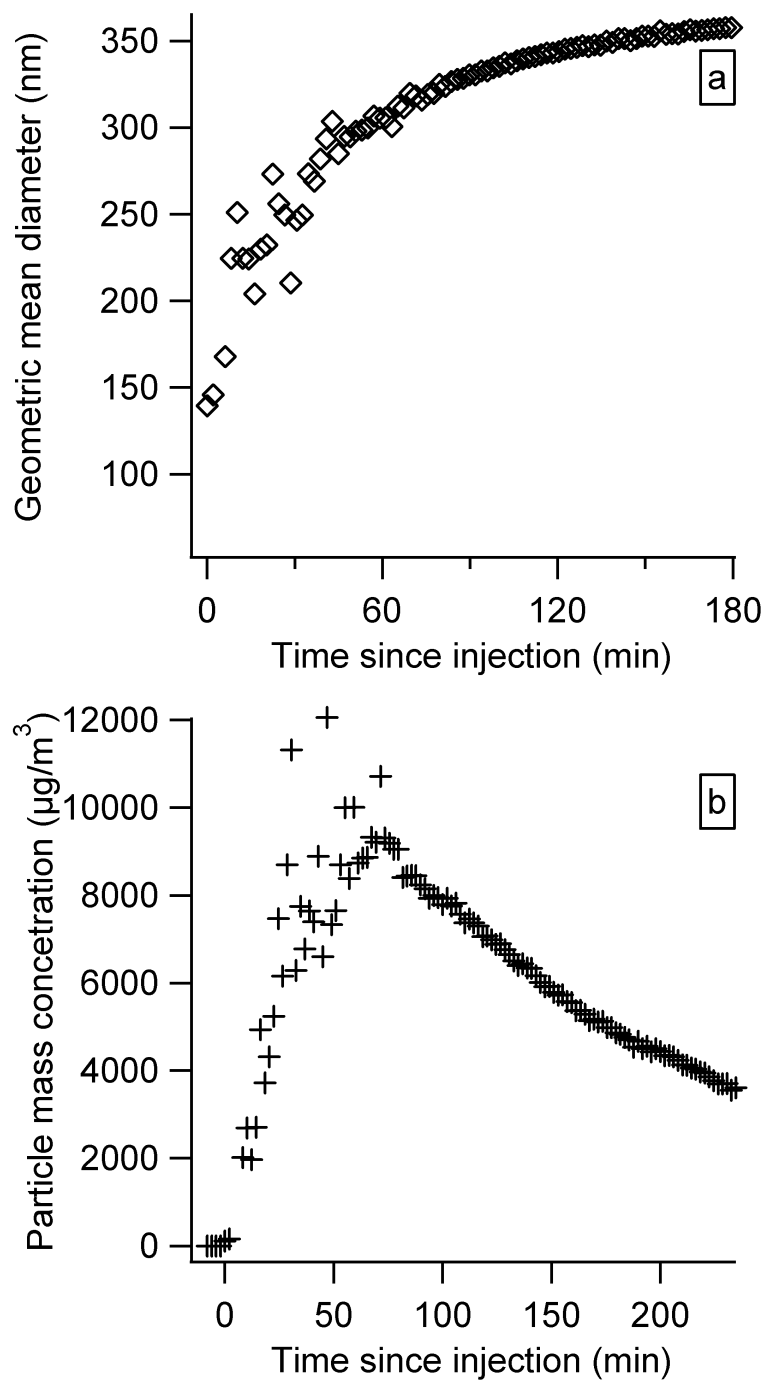


Figure S1. Representative data from SPMS measurements during reaction of limonene and ozone in the dark. The particle geometric mean diameter (a) and total particle mass concentration (b) are plotted versus time from injection of limonene into reaction chamber. The noise in the data is due to the lack of active mixing in the chamber.

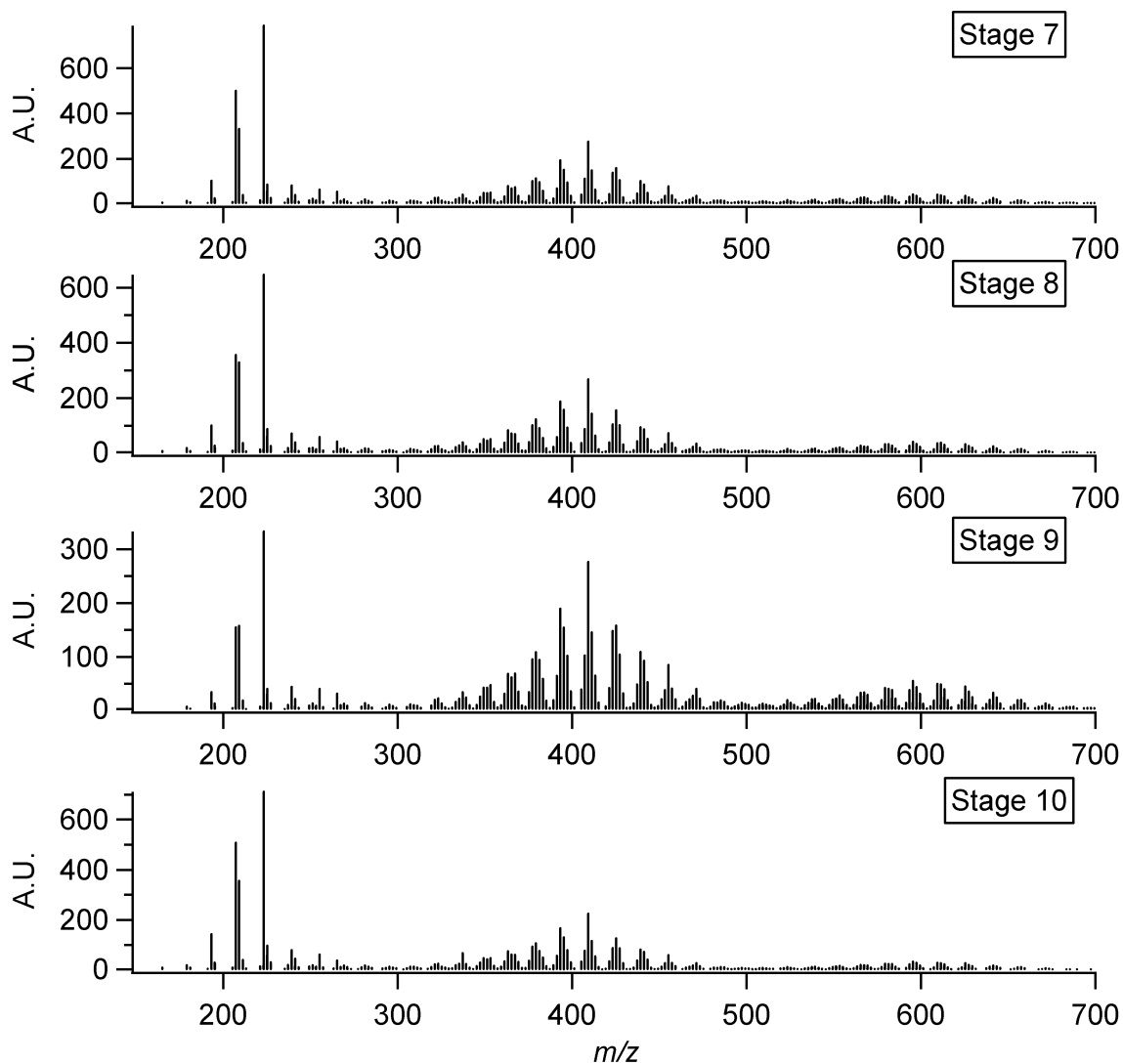


Figure S2. Representative positive ion mode ESI mass spectra from the dark reaction of limonene and ozone 10 min after injection of limonene as collected using MOUDI. The average sizes of the particles decrease from stage 7 to stage 10 but the shapes of the mass spectra remain approximately the same.

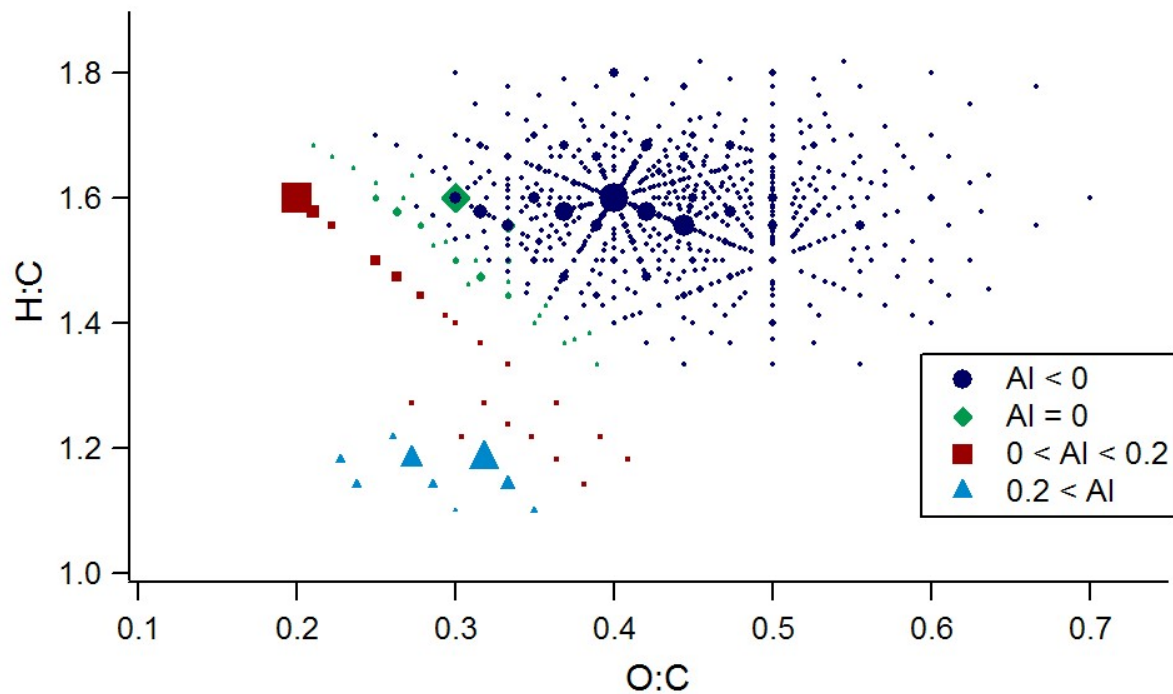
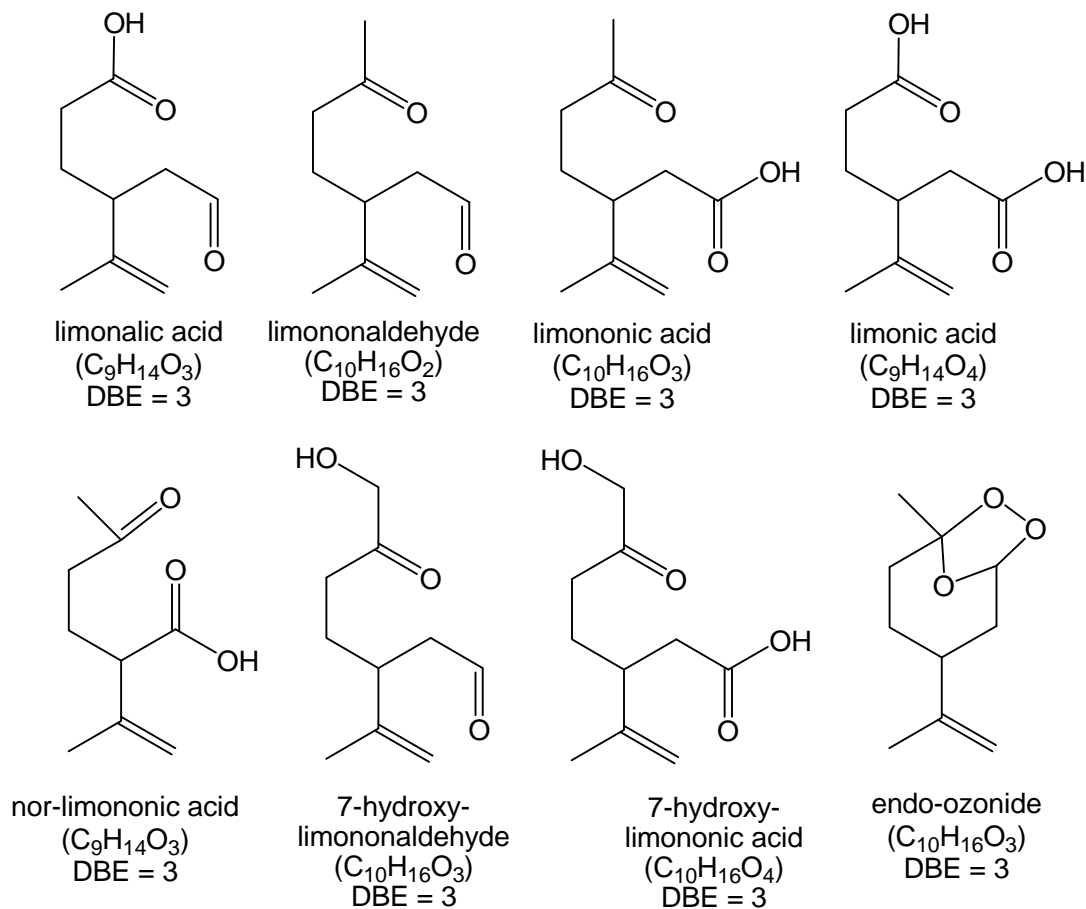


Figure S3. Representative van Krevelen diagram for dark reaction of limonene and ozone. The particles were collected using a drum impactor, extracted into acetonitrile, and immediately analyzed via ESI-MS. This sample corresponds to the first 4 minutes of reaction between ozone and limonene. This is a two-dimensional version of Fig.1 in the manuscript, but in addition we have color coded the points by their values of AI (aromaticity index), and the point size corresponds to peak abundance.

Selected examples of the first generation products resulting from reaction of ozone and the endocyclic double bond of limonene. Most of these products have DBE = 3.



Selected examples of monomeric products with DBE ≠ 3. Such products can arise from chemistry involving isomerizations and/or decompositions of RO radicals formed the decomposition of Criegee intermediates.

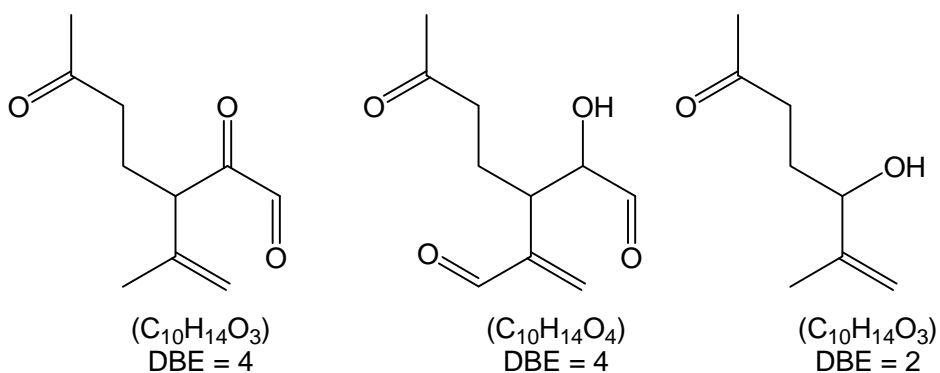


Figure S4. Selected first generation products from limonene ozonolysis along with their molecular formulas, names, and DBE values.

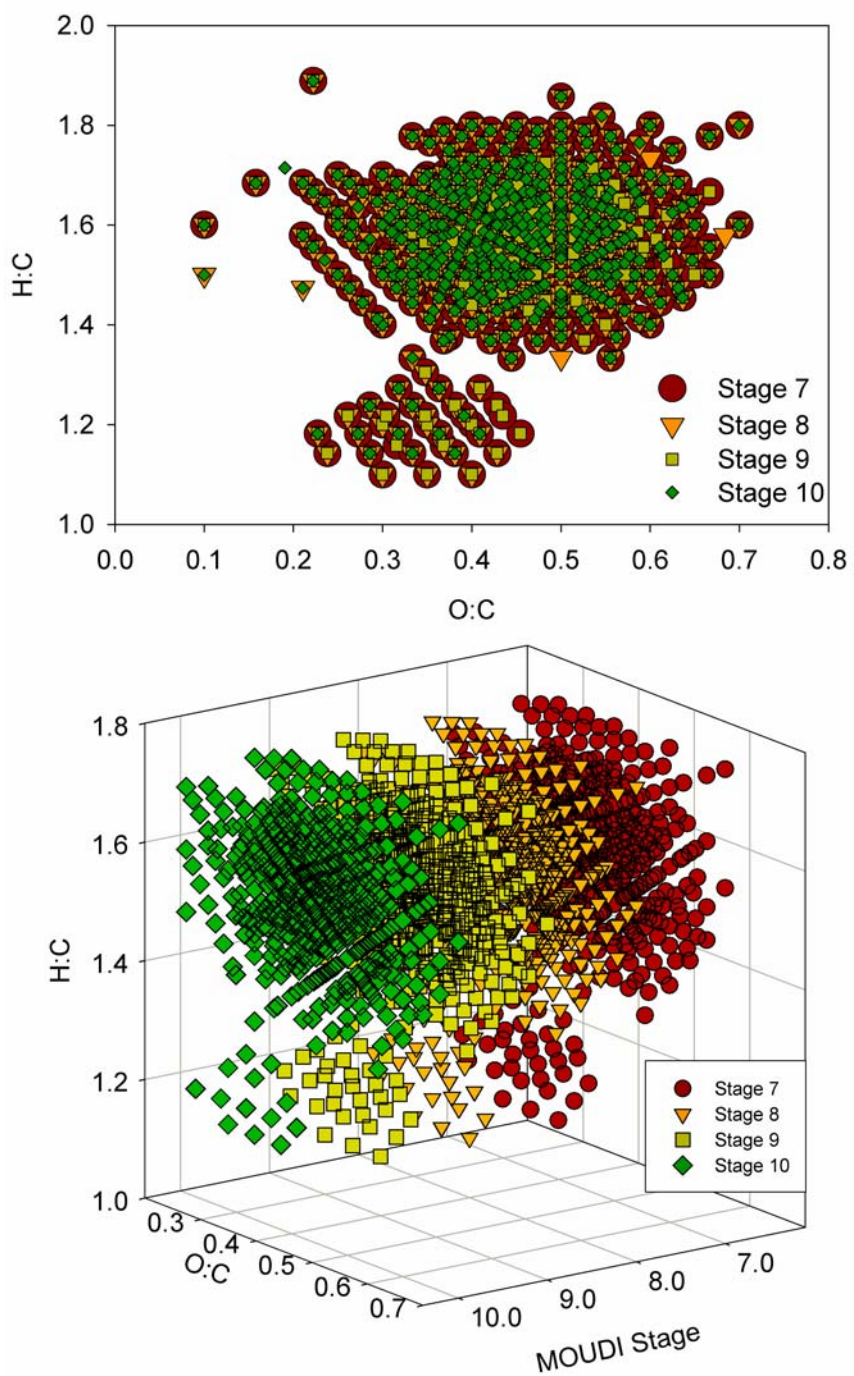


Figure S5 Van Krevelen plots generated from ESI mass spectra from MOUDI stages 7 -10. This sample corresponds to the first 10 minutes of reaction between ozone and limonene.

Table S1. An example providing a sense for the number of peaks excluded during data analysis and included in the final data sets. These numbers refer to mass spectra recorded using drum impactor. Also included is the percent of the total ion for each grouping.

	Number of Peaks	% of Ion Current
Total peaks above S/N = 3	4272	100
Peaks with even nominal m/z	1572	22
Low Intensity peaks (< 1% of the highest)	1411	2
Peaks present in solvent blanks	129	6
Peaks present in filter blanks	78	2
Unassigned peaks	234	5
Assigned peaks	844	63