Atmos. Chem. Phys. Discuss., 12, C739–C740, 2012
www.atmos-chem-phys-discuss.net/12/C739/2012/

Atmospheric Chemistry and Physics Discussions

Interactive comment on "High molecular weight SOA formation during limonene ozonolysis: insights from ultrahigh-resolution FT-ICR mass spectrometry characterization" *by* S. Kundu et al.

Anonymous Referee #1

Received and published: 20 March 2012

General comments: This is a good application of FT-MS and demonstrates the use of the technique to atmospheric chemistry. The paper does not delve into much new chemical insight or into the optimization of the FT-ICR-MS method used; it comes off as much more concerned with massaging the data, but does not get into the specifics of the method, either. All in all, it is good work, but the focus prevents it from illuminating the implications of the compounds observed. Specific comments: You do not mention what temperatures at which you store and transport your samples, or the time between collection and analysis. You do mention that it is "freezing" and "cold", but that is unspecific, and does not address biological activity or the opportunity for volatilization of compounds. You do not seal your filters in a gas-tight manner, either, which provides

Full Screen / Esc
Printer-friendly Version
Interactive Discussion
Discussion Paper

the opportunity for gases ambient to your freezer to condense on the filter, including water. You do not address method artifacts from the exposure of your samples to water during storage and especially in preparation (hydrolysis or hydration of species, for example). Also, do you include an acidic spike to aid in ESI? You do not discuss any methods to assess the extent to which your preparation affects your measured sample composition; what were your findings if you did this? About your filters: what are the dimensions of the filter? Do you do any cleaning prior to using the filter (i.e. baking)? Do you extract the entire filter or a portion of it? What was the mass loading of aerosol on each filter? You extract them in 5 mL – do you reduce the volume at all to concentrate your samples for analysis? What grade solvent did you use and what was the source? Did you assess recovery of different classes of compounds from the filter by your extraction method? You mention repeatedly results involving the detection of hydroperoxides, gem-diols and hemiacetals. Are you certain that these are reasonable products to be detecting in their native form (i.e. not further reacted to a more stable structure)? How are you certain? About space charge effects and future work you may do, you may wish to read Gorshkov et al., J. Am. Soc. Mass Spectrom. 2010, 21, 1846. Technical corrections: In section 2.2: You discuss putting the ESI probe in position “B”. This piece of information is not helpful, as you do not explain the significance of position “B”. You mention the normalized collision energy level being “100%” – this is not a helpful quantity. Provide the real values or at least a range of values. You use the phrase “MS/MS mass spectra” – refer to them as “tandem mass spectra”. Do check your spelling and grammar; there were several problems found.

Interactive comment on Atmos. Chem. Phys. Discuss., 12, 2167, 2012.