
Olga Hogrefe1, Brian P. Frank2, Yele Sun1, Qi Zhang1, Min-Suk Bae1, James J. Schwab1, G. Garland LaI1 and Kenneth L. Demerjian1

1 - Atmospheric Sciences Research Center, U-Albany, State University of New York; 2 – NYS Department of Environmental Conservation

Introduction

• Three intensive urban and rural field campaigns were conducted (EPA/NYSERDA PMTACS-NY Supersite program): Queens College (Summer 2001, Winter 2004) and Whiteface Mountain (Summer 2002);
• 45-50% of PM mass can be attributed to carbon-containing species (2001-2004);
• PM organic carbon characterization was done using an Aerodyne Aerosol Mass Spectrometer (Q-AMS);
• It has been shown that natural hydrocarbons are an important contributor to PM organic fraction in rural and urban environments.

• Objectives of this project:
  - To study physical and chemical properties of laboratory-generated oxygenated organic aerosols of known composition and of ambient importance.
  - To develop characteristic high-resolution mass spectra for compound-specific PM products.
• Information obtained in this study will be further used to quantify the AMS-measured organic mass fraction of PM2.5 made in urban and rural environment during the PMTACS-NY field campaigns.

Measurements of OOC Aerosols

Aerosol Instrumentation

• Aerodyne HR-ToF-AMS,
• TSI Scanning Mobility Particle Sizer (SMPS),
• TSI Condensation Particle Counter (CPC),
• Sunset Labs OCEC monitor,
• R&P Differential TEOM Mass Monitor

Aerodyne High Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-ToF-AMS)

For current experiment:
• HR-ToF-AMS is switching between the two ion optical modes: V and W.
• W-mode data were used for High Resolution mass spectrometric analysis of laboratory-generated OOC aerosols.
• AMS heater temperature ~600°C.
• Data are saved every 5 min.
• Mass spectrum of a solvent blank were recorded and subtracted from a mass spectrum of an OOC of interest prior to the High Resolution analysis.
• A multiple-peak Gaussian curve fit algorithm similar to that of DeCarlo et al. (2006) was used to deconvolute a unit mass peak into separate contributions for specific elemental combinations based on small differences in mass defect.
• Data are collected at a resolution > 1000. Results in figures and table at right are from analysis of high resolution data subsequently combined into single m/z bins.
• Criteria for “major” m/z selection: signal intensity ≥ 3% of total “organic” signal.


Organic Compounds Used for Generation of Organic Aerosols

<table>
<thead>
<tr>
<th>Compound</th>
<th>Formula</th>
<th>Mw</th>
<th>Structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oxalic Acid</td>
<td>C₂H₂O₄</td>
<td>90</td>
<td></td>
</tr>
<tr>
<td>Malonic Acid</td>
<td>C₂H₂O₄</td>
<td>104</td>
<td></td>
</tr>
<tr>
<td>Succinic Acid</td>
<td>C₄H₄O₄</td>
<td>118</td>
<td></td>
</tr>
<tr>
<td>Glutaric Acid</td>
<td>C₄H₆O₄</td>
<td>132</td>
<td></td>
</tr>
<tr>
<td>Adipic Acid</td>
<td>C₄H₆O₄</td>
<td>146</td>
<td></td>
</tr>
<tr>
<td>Glyoxylic Acid</td>
<td>C₂O₃H₂</td>
<td>74</td>
<td></td>
</tr>
<tr>
<td>DL-Malic Acid</td>
<td>C₄H₄O₄</td>
<td>134</td>
<td></td>
</tr>
<tr>
<td>cis-Pinonic Acid</td>
<td>C₆H₈O₃</td>
<td>184</td>
<td></td>
</tr>
<tr>
<td>Phthalic Acid</td>
<td>C₄H₄O₄</td>
<td>166</td>
<td></td>
</tr>
<tr>
<td>Levoglucosan</td>
<td>C₈H₁₀O₄</td>
<td>162</td>
<td></td>
</tr>
<tr>
<td>Palmitic Acid</td>
<td>C₁₆H₃₂O₂</td>
<td>256</td>
<td></td>
</tr>
<tr>
<td>Oleic Acid</td>
<td>C₁₆H₃₂O₂</td>
<td>282</td>
<td></td>
</tr>
</tbody>
</table>

Size Distributions of Selected Generated OOC Aerosols

Summary

• Twelve pure oxygenated organic compounds of known composition and commonly found in ambient air were used to generate polydisperse aerosols in controlled laboratory conditions;
• Optimal parameters for polydisperse aerosol generation and conditioning were found;
• Physical and chemical characterizations of generated aerosols were performed;
• Characteristic mass spectra for each compound were developed using the HR-ToF-AMS;
• Major m/z peaks and their elemental compositions for each OOC were identified;
• Results of the High Resolution mass spectrometric analysis are consistent with expectations based on chemical structure of OOCs (for example, very few oxygenated fragments in palmitic and oleic acids mass spectra, mostly oxygenated fragments in oxalic and glyoxylic acids mass spectra, etc.).

Acknowledgements

This work was supported by the New York State Energy Research and Development Authority (NYSERDA), contract # 8643