Loading-Dependent Elemental Composition of α-pinene SOA Particles

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Supplementary Material For: Loading-Dependent Elemental Composition of α-Pinene SOA Particles

by

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Literature Cited


Table S1. SOA particle mass loadings and the measured O/C and H/C atomic ratios used in the basis-set fitting (i.e., entries of Table 2).

Figure S1. Correlation plots between unit-mass-resolution signal intensity and high-resolution oxygen-to-carbon atomic ratio. Except for the bottom-left panel, vertical axes show the percent contribution of the signal intensity of the indicated m/z value to the total organic signal. For the bottom-left panel, the vertical axis shows the ratio of the signal intensity at m/z 44 to that at m/z 43.

Figure S2. Measured oxygen-to-carbon atomic ratio vs. the 44/org signal for SOA particles produced from the dark ozonolysis of α-pinene. The linear regression through the data is shown in the solid line. The data points and the regression of Aiken et al. (2008) for ambient ground and aircraft measurements during the MILAGRO campaign are also shown. Equations for the linear fits and correlation coefficients are given in the figure.

Figure S3. Example of the deconvolution of a high-resolution mass spectrum for fragments at m/z 43. Peaks representing high-resolution model fits of C_2H_3O^- and C_3H_7^+ are shown in the figure (DeCarlo et al., 2006). Panel i shows the residual between the recorded data and model fits for panel ii (gold), panel iii (grey), and panel iv (red). Panel ii, which was recorded with the AMS chopper open, shows the mass spectrum of the particles and the background. Panel iii, which was recorded with the AMS chopper closed, shows the mass spectrum of the background. Panel iv, which shows the difference of panel iii from panel ii, represents the mass spectrum of the particles. In each panel, the open circles show the recorded signal (Hz). The
solid lines show the model fits in gold, grey, or red for individual peaks and in black for the sum of the model fits. The solid green bars indicate the peak intensity of each fit.

**Figure S4.** Contribution of the signal intensity at $m/z$ 60 to the total organic signal intensity (i.e., 60/org) for increasing SOA particle mass loading for the dark ozonolysis of $\alpha$-pinene. The average 60/org across all loading is 0.23%. Increased signal at $m/z$ 60 is interpreted as a marker of biomass burning particles when observed in the mass spectra of atmospheric particles (Schneider et al., 2006; Docherty et al., 2008). Figure S4, however, shows that some of the signal intensity at $m/z$ 60 can also be attributed to SOA particles.
<table>
<thead>
<tr>
<th>SOA loading (μg/m³)</th>
<th>O/C</th>
<th>H/C</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>0.45</td>
<td>1.38</td>
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<tr>
<td>1.3</td>
<td>0.43</td>
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<tr>
<td>6.6</td>
<td>0.36</td>
<td>1.40</td>
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<tr>
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<tr>
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<tr>
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<td>1.51</td>
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<tr>
<td>138.0</td>
<td>0.29</td>
<td>1.51</td>
</tr>
</tbody>
</table>

Table S1
Figure S1
This Work:
- Laboratory Data
- Fit to Data: $O/C = 0.0227 \times (44/\text{org}) + 0.169$
  $R^2 = 0.87$

Aiken et al. 2008:
- Mexico City Airplane
- Mexico City Ground
- Fit to Data: $O/C = 0.0382 \times (44/\text{org}) + 0.0794$
  $R^2 = 0.84$
Figure S3
Figure S4