Elemental analysis of Oxygenated Organic Coating on Black Carbon Particles using a Soot-Particle Aerosol Mass Spectrometer

Mutian Ma¹, Laura-Hélèna Rivellini², YuXi Cui¹, Megan D. Willis³, Rio Wilkie⁴, Jonathan P. D. Abbatt⁴, Manjula R. Canagaratna⁵, Junfeng Wang⁶, Xinlei Ge⁶, Alex K.Y. Lee¹,²

¹ Department of Civil and Environmental Engineering, National University of Singapore, Singapore
² NUS Environmental Research Institute, National University of Singapore, Singapore
³ Lawrence Berkeley National Lab, Chemical Sciences Division, Berkeley, CA, USA
⁴ Department of Chemistry, University of Toronto, Toronto, ON, Canada
⁵ Aerodyne Research, Inc., Billerica, MA, USA
⁶ School of Environmental Science and Engineering, Nanjing University of Information Science and Technology, Nanjing, China

Correspondence to: Alex K. Y. Lee (ceelkya@nus.edu.sg)
Table S1. Summary of elemental ratios and time series correlation of PMF factors based on co-located measurements in Beijing summer (Xie et al., 2019a; Xu et al., 2019), Beijing winter (Wang et al., 2019; Xie et al., 2019b), California Research at the Nexus of Air Quality and Climate Change (CalNex) 2010 campaign (Massoli et al., 2015), Fontana, CA (Chen et al., 2018; Lee et al., 2017), and Tibet (Wang et al., 2017; Xu et al., 2018).

<table>
<thead>
<tr>
<th>Location / Campaign</th>
<th>HR-ToF-AMS Study</th>
<th>PMF factor</th>
<th>H:C</th>
<th>O:C</th>
<th>Study PMF factor</th>
<th>H:C</th>
<th>O:C</th>
<th>R</th>
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<tbody>
<tr>
<td>Beijing summer</td>
<td>Xie et al. (2019a)</td>
<td>LO-OOA</td>
<td>1.34</td>
<td>0.49</td>
<td>Xu et al. (2019)</td>
<td>LO-OOA</td>
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<td>0.28</td>
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<td>Xie et al. (2019b)</td>
<td>LO-OOA</td>
<td>1.61</td>
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<td>Wang et al. (2019)</td>
<td>OOA1</td>
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<td>0.37</td>
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<tr>
<td>Beijing winter</td>
<td>Xie et al. (2019b)</td>
<td>MO-OOA</td>
<td>1.36</td>
<td>0.97</td>
<td>Wang et al. (2019)</td>
<td>OOA2</td>
<td>1.57</td>
<td>1.23</td>
</tr>
<tr>
<td>CalNex</td>
<td>Massoli et al. (2015)</td>
<td>SV-OOA</td>
<td>1.58</td>
<td>0.54</td>
<td>Massoli et al. (2015)</td>
<td>SV-OOA</td>
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<td>0.45</td>
</tr>
<tr>
<td>CalNex</td>
<td>Massoli et al. (2015)</td>
<td>LV-OOA</td>
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<td>1.4</td>
<td>Massoli et al. (2015)</td>
<td>LV-OOA</td>
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<td>1.16</td>
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<td>Fontana, CA</td>
<td>Chen et al. (2018)</td>
<td>VOOA</td>
<td>0.78</td>
<td>1.4</td>
<td>Lee et al. (2017)</td>
<td>OOA2</td>
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<td>0.63</td>
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<tr>
<td>Tibet</td>
<td>Xu et al. (2018)</td>
<td>MO-OOA</td>
<td>1.04</td>
<td>0.96</td>
<td>Wang et al. (2017)</td>
<td>BBOA</td>
<td>1.48</td>
<td>0.51</td>
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* The inter-conversion factors that were determined in this work, were applied for calculating H:C and O:C ratios.
Table S2. Summary of H:C, O:C and OS, determined by the SP-AMS

<table>
<thead>
<tr>
<th>Class</th>
<th>Species</th>
<th>Formula</th>
<th>True value Tungsten vaporizer</th>
<th>Laser vaporizer</th>
</tr>
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<tbody>
<tr>
<td></td>
<td></td>
<td>H:C</td>
<td>O:C</td>
<td>OSc</td>
</tr>
<tr>
<td>Multifunctional</td>
<td>Citric acid</td>
<td>C₆H₈O₇</td>
<td>1.33</td>
<td>1.17</td>
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<tr>
<td>Multifunctional</td>
<td>Glycolic acid</td>
<td>C₂H₄O₃</td>
<td>2.00</td>
<td>1.50</td>
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<tr>
<td>Multifunctional</td>
<td>Malic Acid</td>
<td>C₄H₆O₅</td>
<td>1.50</td>
<td>1.25</td>
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<tr>
<td>Multifunctional</td>
<td>Tartaric acid</td>
<td>C₆H₄O₆</td>
<td>1.50</td>
<td>1.50</td>
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<tr>
<td>Diacids</td>
<td>Adipic Acid</td>
<td>C₆H₁₀O₄</td>
<td>1.67</td>
<td>0.67</td>
</tr>
<tr>
<td>Diacids</td>
<td>Azelaic Acid</td>
<td>C₉H₁₆O₄</td>
<td>1.78</td>
<td>0.44</td>
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<tr>
<td>Diacids</td>
<td>Glutaric acid</td>
<td>C₅H₈O₄</td>
<td>1.60</td>
<td>0.80</td>
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<tr>
<td>Diacids</td>
<td>Malonic acid</td>
<td>C₃H₄O₄</td>
<td>1.33</td>
<td>1.33</td>
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<tr>
<td>Diacids</td>
<td>Oxalic acid</td>
<td>C₂H₂O₄</td>
<td>1.00</td>
<td>2.00</td>
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<tr>
<td>Diacids</td>
<td>Succinic acid</td>
<td>C₄H₆O₄</td>
<td>1.50</td>
<td>1.00</td>
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<tr>
<td>Alcohols</td>
<td>Arabitol</td>
<td>C₅H₁₂O₅</td>
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<td>Alcohols</td>
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<td>C₆H₁₂O₆</td>
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<td>1.00</td>
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<tr>
<td>Alcohols</td>
<td>Levoglucosan</td>
<td>C₅H₁₀O₅</td>
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<td>0.83</td>
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<tr>
<td>Alcohols</td>
<td>Sucrose</td>
<td>C₁₂H₂₂O₁₁</td>
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<td>0.92</td>
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<tr>
<td>Alcohols</td>
<td>Xylitol</td>
<td>C₅H₁₀O₅</td>
<td>2.40</td>
<td>1.00</td>
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Table S3. Summary of H:C, O:C and OS, determined by the SP-AMS 2

<table>
<thead>
<tr>
<th>Species</th>
<th>Class</th>
<th>Formula</th>
<th>True value</th>
<th>Tungsten vaporizer</th>
<th>Laser vaporizer</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>H:C O:C OSc</td>
<td>H:C O:C OSc</td>
<td>H:C O:C OSc</td>
<td>H:C O:C OSc</td>
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<tr>
<td>Cis-Pinonic acid</td>
<td>Multifunctional</td>
<td>C_{10}H_{16}O_{3}</td>
<td>1.60 0.30 -1.00</td>
<td>1.69 0.25 -1.19</td>
<td>0.48 1.30 -0.34</td>
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<tr>
<td>Citric acid</td>
<td>Multifunctional</td>
<td>C_{6}H_{8}O_{7}</td>
<td>1.33 1.17 1.00</td>
<td>1.40 1.00 0.59</td>
<td>0.94 1.39 0.49</td>
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<tr>
<td>Glutamic acid</td>
<td>Multifunctional</td>
<td>C_{3}H_{6}N_{4}O_{3}</td>
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<td>Glycolic acid</td>
<td>Multifunctional</td>
<td>C_{2}H_{4}O_{3}</td>
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<td>Multifunctional</td>
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<td>NA</td>
<td>1.00 1.81 0.19</td>
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<tr>
<td>Malic acid</td>
<td>Multifunctional</td>
<td>C_{4}H_{6}O_{5}</td>
<td>1.50 1.25 1.00</td>
<td>1.56 1.10 0.64</td>
<td>0.60 1.55 -0.35</td>
</tr>
<tr>
<td>Pyruvic acid</td>
<td>Multifunctional</td>
<td>C_{3}H_{4}O_{3}</td>
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<td>1.32 0.74 0.15</td>
<td>1.52 1.94 1.10</td>
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<tr>
<td>Tartaric acid</td>
<td>Multifunctional</td>
<td>C_{4}H_{6}O_{6}</td>
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</tr>
<tr>
<td>Adipic acid</td>
<td>Diacids</td>
<td>C_{6}H_{10}O_{4}</td>
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<td>1.60 0.43 -0.74</td>
<td>0.46 1.87 -0.95</td>
</tr>
<tr>
<td>Azelaic acid</td>
<td>Diacids</td>
<td>C_{9}H_{16}O_{4}</td>
<td>1.78 0.44 -0.89</td>
<td>1.62 0.32 -0.99</td>
<td>0.32 1.94 -1.30</td>
</tr>
<tr>
<td>Glutaric acid</td>
<td>Diacids</td>
<td>C_{5}H_{8}O_{4}</td>
<td>1.6 0.80 0</td>
<td>1.46 0.57 -0.33</td>
<td>0.56 1.80 -0.68</td>
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<tr>
<td>Maleic acid</td>
<td>Diacids</td>
<td>C_{6}H_{10}O_{4}</td>
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<td>1.56 1.10 0.64</td>
<td>0.65 1.34 -0.04</td>
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<tr>
<td>Malonic acid</td>
<td>Diacids</td>
<td>C_{3}H_{4}O_{4}</td>
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<td>1.58 1.09 0.59</td>
<td>1.13 1.83 0.43</td>
</tr>
<tr>
<td>Oxalic acid</td>
<td>Diacids</td>
<td>C_{3}H_{4}O_{4}</td>
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<td>0.92 2.42 3.92</td>
<td>1.68 1.34 2.02</td>
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<tr>
<td>Succinic acid</td>
<td>Diacids</td>
<td>C_{4}H_{8}O_{4}</td>
<td>1.50 1.00 0.50</td>
<td>1.64 0.50 -0.64</td>
<td>0.55 1.89 -0.79</td>
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<td>Polyacids</td>
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<td>1.30 0.65 -0.01</td>
<td>0.56 1.57 -0.45</td>
</tr>
<tr>
<td>1,5-Pentanediol</td>
<td>Alcohol</td>
<td>C_{5}H_{10}O_{2}</td>
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<td>NA</td>
<td>0.44 1.70 -0.82</td>
</tr>
<tr>
<td>Dextrose</td>
<td>Alcohol</td>
<td>C_{6}H_{12}O_{6}</td>
<td>2.00 1.00 0</td>
<td>NA</td>
<td>0.87 1.87 -0.13</td>
</tr>
<tr>
<td>Phenol</td>
<td>Alcohol</td>
<td>C_{6}H_{12}O_{6}</td>
<td>1.00 0.17 -0.67</td>
<td>NA</td>
<td>0.62 1.81 -0.57</td>
</tr>
<tr>
<td>Bis(2-ethylhexyl)Sebacate</td>
<td>Esters</td>
<td>C_{26}H_{50}O_{4}</td>
<td>1.92 0.15 -1.62</td>
<td>NA</td>
<td>0.1 2.23 -2.03</td>
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</table>
Table S4. Summary of H:C, O:C and OSc, determined by the SP-AMS 3

<table>
<thead>
<tr>
<th>Species</th>
<th>Class</th>
<th>Formula</th>
<th>True value</th>
<th>Tungsten vaporizer</th>
<th>Laser vaporizer</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>H:C</td>
<td>O:C</td>
<td>OSc</td>
</tr>
<tr>
<td>Cis-Pinonic Acid</td>
<td>Multifunctional</td>
<td>C_{10}H_{16}O_{3}</td>
<td>1.60</td>
<td>0.30</td>
<td>-1.00</td>
</tr>
<tr>
<td>Citric acid</td>
<td>Multifunctional</td>
<td>C_{6}H_{8}O_{7}</td>
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<td>1.17</td>
<td>1.00</td>
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<td>1.00</td>
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<tr>
<td>Tartaric acid</td>
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<td>C_{4}H_{6}O_{6}</td>
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<td>1.50</td>
<td>1.50</td>
</tr>
<tr>
<td>Azelaic Acid</td>
<td>Diacids</td>
<td>C_{9}H_{16}O_{4}</td>
<td>1.78</td>
<td>0.44</td>
<td>-0.89</td>
</tr>
<tr>
<td>Glutaric acid</td>
<td>Diacids</td>
<td>C_{5}H_{8}O_{4}</td>
<td>1.60</td>
<td>0.80</td>
<td>0</td>
</tr>
<tr>
<td>Malonic acid</td>
<td>Diacids</td>
<td>C_{3}H_{4}O_{4}</td>
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<td>1.33</td>
<td>1.33</td>
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<tr>
<td>Pimelic acid</td>
<td>Diacids</td>
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<td>0.57</td>
<td>-0.57</td>
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<td>0.92</td>
<td>0</td>
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<td>Xylitol</td>
<td>Alcohols</td>
<td>C_{5}H_{12}O_{5}</td>
<td>2.40</td>
<td>1.00</td>
<td>-0.40</td>
</tr>
</tbody>
</table>
Figure S1. Mass spectra of arabitol, measured by the SP-AMS 1 using the tungsten (a) and laser (b) vaporization schemes. (c) Normalized cumulative histogram of mass-to-charge ratios for the oxygenated organic compounds measured by the SP-AMS 1. The blue area indicates that the thermal vaporization scheme tends to provide organic fragments with smaller m/z, whereas the red area indicates that the laser vaporization scheme tends to give organic fragments with larger m/z.
Figure S2. Mass spectra of levoglucosan, measured by the SP-AMS 1 using the tungsten (a) and laser (b) vaporization schemes. (c) Normalized cumulative histogram of mass-to-charge ratios for the oxygenated organic compounds measured by the SP-AMS 1. The blue area indicates that the thermal vaporization scheme tends to provide organic fragments with smaller m/z, whereas the red area indicates that the laser vaporization scheme tends to give organic fragments with larger m/z.
Figure S3. Comparisons between the measured and true values of H:C, O:C, and OSc determined by the two SP-AMS using the laser vaporization scheme. The I-Asp method was used for the elemental analysis. Red circles and blue triangles represent data measured by SP-AMS 1 and 2, respectively. The dashed lines represent 1:1 line.
Figure S4. Comparison of elemental ratios determined by the I-A$_{op}$ method and the I-A method with the interconversion factors applied.
Figure S5. Relative error of H:C (a) and O:C (b) ratios from SP-AMS 1 and 2 calculated with LV and TV methods. TV I-A (red), LV I-A (blue), LV I-A (green) and LV I-A scaling factor (purple) are included in the comparison.
Reference


