Intermediate-Volatility Organic Compounds: A Potential Source of Ambient
Oxidized Organic Aerosol

SUPPORTING INFORMATION

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This Supporting Information contains four pages. It includes a brief glossary of AMS-
related terms that are not completely explained in the text, as well as an example of the
calculation of organic aerosol mass at $m/z$ 28.
Glossary of common AMS-related terms

*This glossary is a guide and is not intended to be a comprehensive introduction for readers who are new to the AMS or mass spectrometry. Please visit the AMS publications website (http://cires.colorado.edu/jimenez/ams-papers.html) for a comprehensive list of AMS literature.

HOA – Hydrocarbon-like organic aerosol. Determined by Zhang et al (ES&T 2005) via a custom principle component analysis of ambient samples collected in Pittsburgh. HOA resembles lubricating oil, diesel exhaust, and fresh traffic emissions; m/z 57 (specifically C₄H₉⁺) is a tracer ion for HOA.

HR-ToF – High resolution, time-of-flight. This is used to describe time-of-flight mass spectrometers with better than 1 amu resolution. For example, C₃H₇⁺ and C₂H₃O⁺ (both m/z 43) can be resolved and quantified.

O/C – Molar oxygen-to-carbon ratio. For AMS data, O/C is determined using the elemental analysis method of Aiken et al (see text for references). O/C is an indicator of the overall level of oxidation of organic aerosol.

OM/OC – Ratio of organic mass to organic carbon. Also determined by the method of Aiken et al. Organic mass is the sum of oxygen, carbon, nitrogen, and hydrogen in the organic aerosol.

OOA resembles aged organic aerosols seen in rural areas and humic-like substances such as fulvic acid. $M/z$ 44 (specifically $CO_2^+$) is a tracer ion for OOA. OOA-1 and OOA-2 – Positive matrix factorization (specifically of ambient data collected in Mexico City) reveals that the OOA factor can be resolved into fresh SOA (OOA-2) and more aged and oxidized SOA (OOA-1).

UMR – Unit mass resolution. This is used to describe mass spectrometers (e.g., quadrupole mass spectrometers) that can resolve ions at a nominal mass difference of 1 amu. For example, $m/z$ 43 and 44 form distinct peaks, but $C_3H_7^+$ and $C_2H_5O^+$ (both $m/z$ 43) form a single peak.

**Particle signal at $m/z$ 28**

Figure S1 shows two methods for determining particle signal at $m/z$ 28. The upper panels show data for a high $C_{OA}$ (>40 µg m$^{-3}$), high-NO$_x$ photooxidation of n-heptadecane. These conditions favored the formation of particle mass at $m/z$ 28, and this phenomenon was only observed in this study under these conditions. The lower panels show data from a more typical experiment, the low $C_{OA}$ (<10 µg m$^{-3}$), low-NO$_x$ photooxidation of n-heptadecane.

The left-hand panels show the separation of organic signal at $m/z$ 28, mostly CO$^+$, from N$_2^+$ according to the method of Grieshop et al. (1) Organic signal is clearly evident in the upper left panel as an increase in the total $m/z$ 28 signal after the lights are turned on. No such increase in the $m/z$ 28 signal is evident in the lower left panel. This method is confirmed by particle time of flight data in the right-hand panels. Particle signal at ~2.5 ms is evident in the upper right panel, whereas there is no particle signal in the lower
right panel. The dashed black lines correspond to m/z 28 contributing 10% (=0.2 µg m⁻³) of the maximum observed OA mass for the low C_{OA} case.

Figure S1.

References