# 1 Elucidating determinants of aerosol composition through

2 particle-type-based receptor modeling

# **3 Supplementary Material**

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#### 1 1 Semi-continuous measurements and meteorology

2 Figure S1 illustrates the meteorological conditions observed during the campaign, as well as PM<sub>2.5</sub> mass concentrations and trace gas mixing ratios. The mean temperature (T), relative 3 humidity (RH) and wind speed (WS) of the campaign were 22°C, 64% and 3.1 m s<sup>-1</sup>. The 4 5 wind direction was highly variable throughout each day due to the measurement site's proximity to the Lake Erie, although the surface winds predominantly came from the south-6 7 west, with moderate influences from the north-west and north-east. A comparison with year-8 long meteorological data for the Windsor measurement site showed that wind direction 9 observations for this campaign were close to the yearly average.

Overall, the PM<sub>2.5</sub> mass concentration during the study period was typical for the BAQS-Met 10 region (Jeong et al., 2010), with an average value of 11.5 µg m<sup>-3</sup>. Two high PM episodes 11 were recorded during the study, the first spanning four days from 24-27 June (PM<sub>2.5avg</sub>=20.3 12  $\mu$ g m<sup>-3</sup>), and the second from 9-10 July (PM<sub>2.5avg</sub>=25.8  $\mu$ g m<sup>-3</sup>) (Fig. S1). The first PM 13 episode coincided with air masses following trajectories from the south, and was typified by 14 slightly cooler but more humid and slower moving air from Ohio (T<sub>avg</sub>=23.7°C, 15  $RH_{avg}=72.4\%$ ,  $WS_{avg}=2.9$  m s<sup>-1</sup>). The second PM episode was typified by hotter but less 16 humid and faster moving air from the southwest (T<sub>avg</sub>=27.6°C, RH<sub>avg</sub>=65.5%, WS<sub>avg</sub>=4.6 m s<sup>-1</sup> 17 <sup>1</sup>). While some air masses originated from the less densely populated Canadian Prairie 18 19 provinces, they typically passed over the Windsor/Detroit metropolitan area, bringing a more 20 direct impact of fresher emissions to Harrow. The hourly average mixing ratios for O<sub>3</sub>, NO, 21 NO<sub>2</sub>, NO<sub>v</sub>, SO<sub>2</sub> and CO over the three weeks were 42.0, 0.7, 4.9, 7.4, 3.4 and 196.4 ppbv respectively with hourly maxima of 83.1, 34.3, 25.6, 27.5, 56.0 and 668.4 ppbv respectively. 22

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### 24 2 ATOFMS Particle Types

Forty-six particle types were generated using the ART-2a clustering algorithm, of which the top 33 most populous (with > 500 particles) were classified into seven broad categories based on their mass spectra, time series and size distributions for describing PMF results. The particle size distribution, particle type mass spectra by family, and their respective contributions are shown in Figs. S3 - 9 and Table 1 respectively. The seven families were EC\_OC, EC, OC\_S\_N, OC, AMINE, FIREWORKS and DUST and are described below. Particle type families were named based on their characteristic chemical species although the
 FIREWORKS and DUST families were named as their chemical composition and temporal
 trends were definitive.

### 4 2.1 EC\_OC Particle Type Family

Four particle types contributed to the EC\_OC family and comprised 22% of the total 5 measured particles. These particle types were named EC\_OC as they all contained elemental 6 carbon (EC), as denoted by carbon ion fragments at  $C_{\pm 12n}$  with  $n \le 5$ , along with positive ion 7 8 organic carbon (OC) fragments. The organic ion fragments were noted at  $m/z + 27 [C_2H_3^+]$ 9 and  $m/z + 43 [C_2H_3O^+]$ ; while peaks observed at m/z + 43 could have isobaric interferences 10 from other ions such as  $[C_3H_7^+]$ ,  $[C_2H_5N^+]$ , and  $[CHNO^+]$ , the lack of expected corresponding 11 fragments at other m/zs indicates that m/z + 43 is likely dominated by the oxidized organic 12 fragment  $[C_2H_3O^+]$ . Varying degrees of chemical processing were observed in these particle types as demonstrated by their sulphate content. Both C1 and C4 contained significant 13 14 amounts of sulphate, as represented by the m/z - 97 [HSO<sub>4</sub><sup>-</sup>] ion, with C1 appearing the most aged of all EC\_OC particle types due to its significantly higher sulphate content. These 15 particle types were likely neutralized due to their significant  $[NH_4^+]$  levels. Sulphate peaks 16 17 were only weakly evident in C3 and C8, and appeared to be below detection levels. However 18 the weak overall signal of these particle types precluded their assignment as fresh or 19 unprocessed particles. Thus varying levels of sulphate combined with oxidized organic 20 fragments indicate that these particle types were moderately to highly aged elemental carbon particles. Such aged EC particle types, containing significant oxidized organic and sulphate 21 22 content, have been reported in numerous ambient ATOFMS field campaigns (Dall'Osto et al., 2006, Moffet et al., 2008, Healy et al., 2010). They have been typically reported as aged 23 24 primary EC emissions.

## 25 2.2 EC Particle Type Family

The EC family consisted of only two particle types, C11 and C16, and represented 6% of the measured particles by ATOFMS. These types were named EC due to elemental carbon ion fragments  $C_{\pm 12n}$ , with  $n \le 12$  and 8 in the positive and negative ion spectra respectively. While these two particle types were generally similar in their mass spectra, their size distributions suggested very different histories. The C11 particle type was the smallest amongst all 33, with a geometric mean diameter of 0.32µm. In general, this particle-type

resembled particles generated from source diesel emissions studies (Spencer et al., 2006) due 1 2 to its small diameter and EC ion fragments. While such a small diameter EC particle type typically suggests fossil fuel combustion emissions, it was unusual that a strong peak at m/z3 23  $[Na^+]$  was present without other ions typical of diesel emission (e.g., Ca<sup>+</sup> and PO<sub>3</sub><sup>-</sup>) 4 5 (Spencer et al., 2006, Toner, et al., 2006), This specific particle-type has only been observed in two other ambient studies (Dall'Osto and Harrison, 2006; Moffet et al., 2008), whereby in 6 7 both it could not be conclusively identified. Regardless, the aforementioned characteristics of 8 this particle-type strongly suggest it is associated with diesel fuel combustion emissions. By 9 contrast, the C16 particle type did not contain any detectable sodium, was much larger in 10 geometric mean diameter (0.76µm), and displayed significantly higher sulphate and nitrate 11 peaks than C11. As such, the C16 particle type was likely associated with aged elemental 12 carbon emissions, and may have been an aged version of C11. Hence both particle types were 13 linked with primary elemental carbon emissions of different atmospheric ages.

## 14 2.3 OC\_S\_N Particle Type Family

Making up 27% of the measured particles, the OC\_S\_N family (C2, C5, C6, C7, C10, and 15 16 C14) was named as such due to significant contributions from organic compounds, sulphate 17 and nitrate. All particle types in this family were identified by their high  $[K^+]$  and organics 18 ion counts in the positive spectrum. The organics were suspected to be oxidized as all of the particle type mass spectra displayed peaks at m/z -89 [(COO)<sub>2</sub>H<sup>-</sup>], indicative of highly 19 20 oxidized organic carbon. The sulphate and nitrate content in the particle types was useful for 21 understanding differences in chemical processing in these particle types. For instance, C2, 22 C6, and C7 all contained significant sulphate as well as sulphuric acid  $[H(HSO_4)_2]$ , the latter 23 a marker of particle acidity, with C7 as the most acidic among these particle types. The 24 formation of sulphuric acid in these particles could be the result of heterogeneous production 25 on particle surfaces, uptake of  $SO_{2(g)}$  and subsequent oxidation in the aqueous phase, or homogeneous oxidation of SO<sub>2(g)</sub> in the gas phase and subsequent condensation on particle 26 27 surfaces (Whiteaker and Prather, 2003; Ault et al., 2010). All of these particle types appeared related to biomass burning emissions; this was suspected not only from their very high  $[K^+]$ 28 29 peaks, but also from the presence of organic acid fragments in their mass spectra such as m/z -45 [CHOO<sup>-</sup>], -59 [C<sub>2</sub>H<sub>3</sub>O<sub>2</sub><sup>-</sup>] and -71 [C<sub>3</sub>H<sub>3</sub>O<sub>2</sub><sup>-</sup>], all of which have been associated with the 30 fragmentation of the biomass burning tracer levoglucosan (Silva et al., 1999; Qin and Prather, 31 32 Interestingly, the C7 particle type showed the lowest organic acid and highest 2006).

sulphuric acid peaks, an effect which may be the result of a sulphuric acid coating preventing 1 2 measurement of organic acids present in the core of these particles. Organic nitrate ions present in these particles, such as m/z - 26 [CN<sup>-</sup>] and 42 [CNO<sup>-</sup>], further supported the notion 3 of a biomass burning emissions source (Dall'Osto and Harrison, 2006). Based on these 4 5 characteristic ions, all particle-types from this family (with the exception of C5) resembled particles reported from biomass burning source characterization studies (Silva et al., 1999, 6 7 Healy et al., 2010). While the C5 particle type appeared similar to others in the OC S N 8 family in terms of its [K<sup>+</sup>], organic, sulphate and nitrate content, it did display significant 9 differences to suggest another source-type. First, its OC and EC peaks were much higher, 10 with prominent  $C_{\pm 12n}$ ,  $n \le 5$ . Second, its temporal trend was significantly different than the 11 others, and was nearly identical to C8, a member of the EC\_OC family. Consequently the emissions source-type for C5 was inconclusive. In summary, the OC S N family comprised 12 13 mostly biomass burning particles having undergone a range of chemical processing with the 14 possibility of another source-type having produced C5.

## 15 2.4 OC Particle Type Family

16 While many of the particle types identified in this study contained significant amounts of OC, 17 the OC particle type family particles (C13, C15, C18, C27, and C30), which accounted for 18 12% of the measured was named as such as it appeared to have the highest organic content relative to other species such as EC and secondary inorganics. In fact, the negative ion mass 19 20 spectra for all particle types within this family contained relatively low signal compared to some other particle types (i.e. EC\_OC family), which suggested they experienced little 21 22 chemical processing. Most particle types from this family (C13, C15, C18 and C30) were all very similar to one another, and also appeared similar to several particle types in the OC\_S\_N 23 family due to high  $[K^+]$  and oxidized organic carbon peaks. This combination would typically 24 25 suggest biomass burning emissions, as suspected for most of the OC\_S\_N particle types, yet the lack of expected associated levoglucosan related peaks indicated this could not be the 26 27 case. Moreover, aromatic fragments, such as  $m/z + 51 [C_4H_3^+]$ , 63  $[C_5H_3^+]$ , 77  $[C_6H_5^+]$ , 91  $[C_7H_7^+]$ , 115 and 128 (Liu et al., 2003), alluded that these particles did not arise from 28 29 secondary organic aerosol from biogenic emissions; fragments such as m/z + 63 and 128 suggested the presence of polycyclic aromatic hydrocarbons (PAHs) in these particles (Qin 30 31 and Prather, 2006). Thus these particle-types could not be attributed to a specific source class. The C27 particle type within this family appeared significantly different than the 32

others; significant contributions from high molecular weight fragments were noted in the
positive and negative ion mass spectra, likely from either oligomeric species or PAHs, or a
combination thereof (Gross et al., 2006; Denkenberger et al., 2007; Qin and Prather, 2006).
Thus all of the OC particle types contained significant organic carbon levels and appeared to
have undergone little chemical processing.

### 6 2.5 AMINE Particle Type Family

7 Two particle types, C9 and C20, contained significant contributions from amine compounds 8 and together represented a small fraction of the measured particles (6%). Typified by high 9 mass spectral contributions at m/z + 59 [N(CH<sub>3</sub>)<sub>3</sub><sup>+</sup>], as well as significant contributions of 10 other organic species, these particle types appeared episodically, mostly in one large episode beginning at approximately 22:00 on 4 July, diminishing at approximately 04:00 the next 11 12 morning. The episodic appearance of these particle types can likely be attributed to gaseous phase trimethylamine (TMA) partitioning to acidic particles through cloud/fog processing, as 13 14 reported by (Rehbein et al., 2011); this was supported by a strong temporal association with periods of high relative humidity (>90%), and particle acidity as denoted by a sulphuric acid 15 peak at m/z -195 [H(HSO<sub>4</sub>)<sub>2</sub>]. Laboratory experiments performed by Rehbein et al. 16 17 successfully related the uptake of gaseous amines into the particle phase with particle acidity, 18 with higher acidity leading to increased amine uptake (Rehbein et al., 2011). These 19 experiments showed that TMA, when measured by ATOFMS, fragments primarily to the m/z20 +59 peak, which is the same distinguishing peak in these amine particle types. Given the low 21 wind speeds associated with the episodic appearance of these particles, it is likely that TMA 22 and possibly other amine species partitioned to pre-existing particles rather than aminecontaining particles having been transported to the measurement region. 23

### 24 2.6 FIREWORKS Particle Type Family

Four particle types were related to fireworks emissions, and represented 9% of the measured particles. These large-diameter particle types ( $D_{va} > 0.8\mu m$ ), which represented 9% of the total measured particles, dominated a particle event observed in the early morning of 5 July. The AMINE and FIREWORKS particle types showed very similar temporal trends, however the FIREWORKS types peaked three hours later at approximately 07:00. Such a temporal difference indicates that a different source or atmospheric process is responsible for their presence. Generally, the mass spectra and size distributions were very similar for these

particle types, supporting a common source-type. A fireworks source-type was suggested for 1 2 these particle types due to the significant contributions from potassium chloride and potassium nitrate fragments to their mass spectra (e.g. peaks at  $m/z + 39 [K^+]$ , m/z + 113/1153  $[K_2Cl^+]$ , m/z +125  $[K_2NO_2^+]$ , m/z +140  $[K_2NO_3^+]$  and m/z -163  $[K(NO_3)_2^-]$ ). Also observed 4 5 were significant contributions from alkali metal cations as denoted by peaks at m/z + 23 [Na<sup>+</sup>], +24  $[Mg^+]$ , +40 $[Ca^+]$  and +96  $[Ca_2O^+]$ , and discernable peaks at m/z +138  $[Ba^+]$  and +154 6 7 [BaO<sup>+</sup>]. All of these species have been noted in previous fireworks studies: KNO<sub>3</sub>, a major 8 component of "black powder", the oxidant used to ignite the fireworks (Drewnick et al., 2006; 9 Vecchi et al., 2008), in conjunction with the ATOFMS' very high sensitivity to K (Gross et 10 al., 2000), may both explain the very high K ion signals within these particle types. Alkali 11 and alkaline earth metals such as Na, Mg, Ca and Ba have been associated with the combustion of fireworks (Vecchi et al., 2008; Joly et al., 2010). Due to the presence of these 12 13 metallic species, the most populous particle-type from this family, C12, was nearly identical to ambient pyrotechnic particles measured by ATOFMS in Riverside, California (Liu et al., 14 1997). The significant contributions from [NO<sup>-</sup>] species could either be attributed to 15 16 condensation of nitrate, or nitrate from the combustion of black powder. Thus these particle 17 types appeared to be related to a particular source or fireworks, and were likely transported to 18 the site, given their off peak hour appearance in the very early morning.

## 19 2.7 DUST Particle Type Family

Ten particle types contributed to the DUST family (C17, C21, C22, C24, C25, C26, C29, 20 C31, C32, and C33), all of which exhibited large geometric mean vacuum aerodynamic 21 22 diameters ranging from 0.64 to 1.42 µm; together they totalled 18% of the total measured particles. These particle types were characterized by very high peaks associated with several 23 dust related species, such as m/z + 23 [Na<sup>+</sup>], 27 [Al<sup>+</sup>], +40 [Ca<sup>+</sup>] and +56/57 [CaO/CaOH<sup>+</sup>], 24 25 and were very similar to aluminium and calcium rich dust particles measured in several other ATOFMS field studies (Guazotti et al., 2001; Dall'Osto et al., 2004; Dall'Osto et al., 2006, 26 27 Sullivan et al., 2007). While these particle types appeared spectrally similar to the fireworks particles in terms of their most prominent ions, they showed distinctly different temporal 28 trends, appearing much more frequently. Some particle types within this family were very 29 distinct and could be attributed to specific types of dust. For instance, C22 contained silicates 30 (e.g. m/z - 60 [SiO<sub>2</sub><sup>-</sup>] and -76 [SiO<sub>3</sub><sup>-</sup>]) and phosphates (e.g. m/z - 63 [PO<sub>2</sub><sup>-</sup>] and -79 [PO<sub>3</sub><sup>-</sup>]); 31 both these species were characteristic of aged soil dust particles identified in Atlanta, Georgia 32

(Liu et al., 2003). Also, C29 appeared to be related to sea salt due to significant contributions 1 2 from m/z +23 [Na<sup>+</sup>] and large geometric mean diameter ( $D_{ya} = 1.42 \mu m$ ); the lack of m/z -35 [Cl<sup>-</sup>] indicated that these particles are not pure NaCl. Rather the significant nitrate content 3 4 suggested these particles experienced significant chemical processing: gaseous nitric acid 5 likely reacted with NaCl particles to form HCl, thus displacing the Cl and introducing nitrate into the particles (Zhuang et al., 1999). The significant nitrate content in all of these particle 6 7 types indicated they have all experienced some degree of chemical processing. While it is 8 unexpected to observe marine aerosol as far inland as Harrow, Ontario, chemically processed 9 salt particles suspected to be of marine origin have been reported in nearby inland areas such 10 as Toronto, Ontario and Stockton, New York (Rehbein et al., 2010; Sunder Raman and 11 Hopke, 2007).

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## 13 **3 PMF** analysis of scaled particle-types

An enhanced ATOFMS particle scaling procedure has been developed by Jeong et al., and is presented in a companion manuscript (Jeong et al., 2011). This method was used to scale single particles from this study for the purpose of quantitative PMF analysis of scaled particle number concentrations. The following section briefly describes the scaling procedure.

A scaling factor was applied to each particle, which is given by the ratio of the number ofparticles measured by the APS and FMPS to the ATOFMS:

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For 
$$D_a > 0.52 \mu m$$
,  $S_{d_{a,j}} = \frac{N_j (APS)}{N_j (ATOFMS)}$ 

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22 For 
$$D_a < 0.52 \mu m$$
,  $S_{d_a < 0.52 \mu m} = \frac{N_{0.1-0.52 \mu m}(FMPS)}{N_{d_a < 0.52 \mu m}(ATOFMS)}$ 

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where  $N_{j(APS)}$  and  $N_{j(ATOFMS)}$  are the hourly total particle number concentrations as measured by the APS and ATOFMS measurements in the size bin (j) respectively;  $N_{0.1-0.52um(FMPS)}$  is the hourly total number concentration of particles in the range from 0.1-0.52um (aerodynamic diameter) measured by the FMPS. Further details of these calculations can be found in Jeong et al., 2011. Note that calculations in Jeong et al. were performed using volume concentrations for purposes of later arriving at mass concentration. In this analysis, scaling calculations were made using number concentrations. Calculations using volume concentrations were also explored although were found to provide highly similar results to
 number concentration. The analysis was thus kept in terms of number concentration to enable
 comparison with unscaled PMF analysis results.

The particle-type assignments as determined by cluster analysis (section 2.3 of the manuscript) were used for the scaled particle analysis, and thus the only change to the data was the total hourly number counts for each particle-type. Consequently, the particle scaling resulted in modified particle-type time series for PMF analysis. Both the data and error matrices were prepared using the methods presented in section 2.4 of the manuscript. Furthermore, since solutions for C3=0 (as used in the unscaled analysis) would not converge, a C3 of 0.05 was used.

In general, all solutions ranging from 1 to 12 factors were not robust, and were thus undesirable. A 9 factor solution was chosen for comparison purposes with the unscaled analysis, and the factor profiles and time series are shown in Figs. S11 and S12 respectively. The following paragraphs elaborate on how the solutions were judged in terms of robustness.

15 Fig. S13 shows the effect of increasing the number of factors on the scaled PMF solution. For the 9 factor solution, it can be seen that the data are reconstructed with an  $R^2$  of 0.92, which 16 was less than that found in the unscaled analysis ( $R^2=0.96$ ). The Q/Q<sub>exp</sub> value for this 17 18 solution was 5.63, which was greater than that of the unscaled analysis. Given that the errors 19 were approximately only 10% less on average than those supplied for the unscaled analysis, and the  $Q/Q_{exp}$  value for 9 factors was so much larger, it could be seen that the errors 20 21 generated for the scaled analysis were inadequate for modelling these scaled particle-type 22 time series.

23 The particle-type profiles (Fig. S11) and time series (Fig. S12) for the 9 factor solution from 24 PMF analysis of the scaled data were compared to those from the unscaled data. Many of the 25 particle-types could not be modeled adequately by PMF and consequently were not useful for 26 factor identification. In fact, the OC family of particle types was hardly represented by the 9 27 factor solution, as evidenced by the lack of reproduced particle counts at the beginning of the campaign. It was also difficult to interpret particle-type profiles as they tended to be more 28 29 broadly distributed across particle-type families within the factors than in the unscaled PMF analysis. No new logical conclusions regarding factor composition were ascertained from this 30 31 analysis.

As with the unscaled PMF analysis, the 9 factor solution was subjected to 100 bootstrap runs 1 2 and was initiated from 100 different seed values. Bootstrapping showed that the solution did not appear reproducible, as none of the runs could be "remapped" onto the base case. Using 3 4 100 different random seed values to initiate PMF analysis also showed undesirable results: 5 none of the solutions produced identical  $Q/Q_{exp}$  values (min = 5.51, max = 5.99, median = 5.74) suggesting that each solution was different. The variability in these results indicated 6 7 that the 9 factor solution was unstable. To verify the instability in PMF solutions in these data 8 and errors, 10 random starts or seeds were used from 1 to 12 factors. In each case, the  $Q/Q_{exp}$ 9 values differed significantly, in a similar manner to the 9 factor solution.

10 As stated in the manuscript, this undesirable result was attributable to the large scaling factors 11 required to scale up particles from the smallest size bin ( $D_a < 0.52 \mu m$ ), which experienced the 12 greatest transmission losses. Effectively, scaling caused the times series of each particle type 13 to be dominated by the portion of that particle type within the smallest size bin. Given the 14 lower efficiency of the ATOFMS for these small particles, these time series were often the 15 noisiest. Comparing Figs. S2 and S10 it can be seen that particles with  $D_a < 0.52 \mu m$  were 16 scaled up by about 2 orders of magnitude more than larger particles. Thus, PMF analysis was 17 essentially performed on scaled particle-type time series that were dominated by the 18 convolution between a very large scaling factor and a noisy time trend from the smallest hit 19 particles. Further, the temporality of these smaller particles is inevitably dictated by a 20 different set of atmospheric determinants than those impacting the set of particles measured 21 directly by ATOFMS, rendering comparison between these scaled and unscaled solutions 22 One approach to partially control for this effect would be to remove the unsound. 23 contribution of the small particles from the dataset, although there still remains several orders 24 of magnitude in difference between number concentrations measured by APS for the most 25 and least populous size bins. A more rigorous approach would be to separate each particle-26 type into several size bins for PMF analysis, in order to separate out the variability of smaller 27 particles subjected to large scaling factors from larger particle with lower scaling factors. 28 This approach was considered for this dataset although low hourly counting statistics 29 precluded size segregation of each particle type. Such an approach would be worth exploring 30 using data with higher overall particle counts. In summary, the unscaled PMF solution 31 presented in the manuscript emphasizes the characteristics of particles in the size ranges 32 efficiently detected by the ATOFMS, rather than those of  $D_a < 0.52 \mu m$  which were measured 33 with lower efficiency.



Figure S1: Time series of meteorological measurements (wind direction, wind speed, relative humidity, and temperature) as well as  $PM_{2.5}$  mass concentration (including the two PM episodes) and trace gases (SO<sub>2</sub>, CO, NO/NO<sub>2</sub>/NO<sub>y</sub> and O<sub>3</sub>) collected at the Harrow measurement site from 19 June – 11 July 2007.

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2 Figure S2: Size distribution of particles desorbed and ionized by ATOFMS during BAQS-

- 3 Met.
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4 Figure S4. Average mass spectra of particle types within the EC family.





4 Figure S6: Average mass spectra of particle-types within the OC family.



4 Figure S8: Average mass spectra of particle-types within the FIREWORKS family.



2 Figure S9: Average mass spectra of particle-types within the DUST family.





Figure S10: Size distribution of particles desorbed and ionized by ATOFMS during the
BAQS-Met campaign and then scaled according to the method of Jeong et al. (2011).



3 Figure S11: Time series of the nine factor solution for the scaled particle-types (a) and PMF

4 reconstructed scaled hourly ATOFMS particle counts (b).



Fraction of Factor Profile (Sums to 1)



Figure S12. Factor particle-type profiles of the nine factor solution for the scaled particle-types.

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Figure S13. The impact of increasing the number of factors on the scaled PMF solution in
terms of R<sup>2</sup> and normalized Q value.

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