Supplement of Atmos. Chem. Phys., 16, 2631–2640, 2016 http://www.atmos-chem-phys.net/16/2631/2016/doi:10.5194/acp-16-2631-2016-supplement © Author(s) 2016. CC Attribution 3.0 License.





## Supplement of

The real part of the refractive indices and effective densities for chemically segregated ambient aerosols in Guangzhou measured by a single-particle aerosol mass spectrometer

Guohua Zhang et al.

Correspondence to: Xinhui Bi (bixh@gig.ac.cn)

The copyright of individual parts of the supplement might differ from the CC-BY 3.0 licence.

## 1 The meteorological conditions over the study

Temporal profiles (in 1 hour resolution) of local meteorological parameters, including solar radiation, temperature (Temp), relative humidity (RH), wind direction (WD) and wind speed (WS), and air quality parameters (i.e., NO<sub>x</sub>, SO<sub>2</sub>, O<sub>3</sub>, PM<sub>1</sub>) are shown in Fig. S1. These parameters were provided by Guangdong Environmental Monitoring Center (<a href="http://www.gdemc.gov.cn/">http://www.gdemc.gov.cn/</a>). Ambient Temp, RH, and WS over the study varied between 10.8–31 °C, 20.7–89.8%, and 0.2–3.9 m/s, with average values of 21.2 °C, 59.9%, and 1.1 m/s, respectively. The concentration peaks for NO<sub>x</sub>, SO<sub>2</sub>, and PM<sub>1</sub> were often observed during the nighttime, due to the accumulation of pollutants under unfavorable meteorological conditions with lower WS and lower boundary layer depth.

## 2 The mass spectral patterns for the single particle types

The mass spectral characteristics are displayed in Fig. S4, and a brief description is provided as follows.

OC group: Mass spectra for OC particles mainly contain the OC markers, and also some other OC peaks such as  $50[C_4H_2]^+$ ,  $51[C_4H_3]^+$ ,  $55[C_4H_7]^+$  and  $63[C_5H_3]^+$ . Besides, a large peak at m/z 39 is also observed in mass spectra of OC, which might be explained by coagulation between OC and  $39[K]^+$  or condensation of organic species onto biomass seed [*Moffet et al.*, 2008]. Particle mass spectra in HMOC type show the presence of m/z 50, 51, 63, 77, 91, 115, and 128 [*Silva and Prather*, 2000; *Sodeman et* 

- 37 al., 2005]. By including the ion peak from sulfate/nitrate, OC particles were subdivised
- into OC-S, OC-SN, and HMOC.
- 39 EC group: Mass spectra of LC-EC type are dominated by the distinct carbon ion
- clusters ranged from m/z -120 to m/z 180, with minor ion intensities from other species.
- SC-EC type is associated with short carbon clusters ions peaks  $(C_n^{+/-}, n < 6)$ , generally
- 42 internally mixed with intense sulfate ion peak. Differently, NaK-EC type shows the
- carbon ion clusters mainly in the negative mass spectra, combined with dominant peaks
- from  $23[Na]^+$  and  $39[K]^+$  in the positive ones.
- 45 ECOC group: ECOC particles have typical carbon ion clusters (12[C]<sup>+/-</sup>,
- 46  $24[C_2]^{+/-}$ , ...,  $12n[C_n]^{+/-}$ ) with  $36[C_3]^+$  as dominant fragments, together with OC
- 47 markers (e.g.,  $27[C_2H_3]^+$ ,  $29[C_2H_5]^+$ ,  $37[C_3H]^+$ , and  $43[C_2H_3O]^+$ ). K-rich particles
- 48 contain potassium  $(39[K]^+)$ , sulfate  $(-97[HSO_4]^-)$ , nitrate  $(-46[NO_2]^-$  and  $-62[NO_3]^-)$ ,
- 49 and carbonaceous species (e.g.,  $12[C]^+$ ,  $27[C_2H_3]^+$ ,  $29[C_2H_5]^+$ ,  $36[C_3]^+$ ,  $37[C_3H]^+$ ,
- 43[C<sub>2</sub>H<sub>3</sub>O]<sup>+</sup>, -26[CN]<sup>-</sup>, -42[CNO]<sup>-</sup>) as major components, similar to those reported in
- other studies [Moffet et al., 2008; Silva et al., 1999]. The association of sulfate and/or
- 52 nitrate separated the ECOC particles into ECOC-S, ECOC-SN, K-S, K-SN, and K-N
- 53 [*Zhang et al.*, 2015].
- Metal rich group: Peaks corresponding to 23[Na]<sup>+</sup>, 39[K]<sup>+</sup>, 46[Na<sub>2</sub>]<sup>+</sup>,
- 81/83[Na<sub>2</sub>Cl]<sup>+</sup>, nitrate and chloride (-35[Cl]<sup>-</sup> and -37[Cl]<sup>-</sup>) are present in mass spectra
- of Na-rich, indicating transport and evolution of sea salt particles [Gaston et al., 2011;
- 57 Gaston et al., 2013]. Na-K type is characterized by dominant peaks from 39[K]<sup>+</sup>,

relatively less intense peak from 23[Na]<sup>+</sup>, nitrate and silicate (-76[SiO<sub>3</sub>]<sup>-</sup>). They are probably from dust and/or industry sources [*Moffet et al.*, 2008]. Fe-rich type is identified by strong peaks from iron at m/z 54, 56 and 57, according to their isotopic components. Similarly, Pb-rich type is identified by strong peaks m/z 206-208, and Curich is characterized by the presence of isotopic peaks at m/z 63 and 65. Fe-Cu-Pb represents the internally mixed Fe, Cu, Pb in the individual particles.

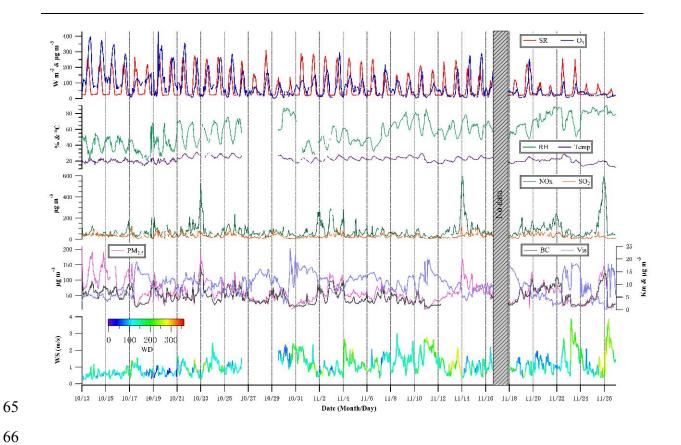


Fig. S1. Temporal profiles (in 1 h resolution) of  $PM_1$ , visibility, and black carbon (BC), gaseous pollutants ( $SO_2$ ,  $NO_x$ , and  $O_3$ ) and meteorological parameters, during the  $13^{th}$  October– $26^{th}$  November 2012 in Guangzhou.

68

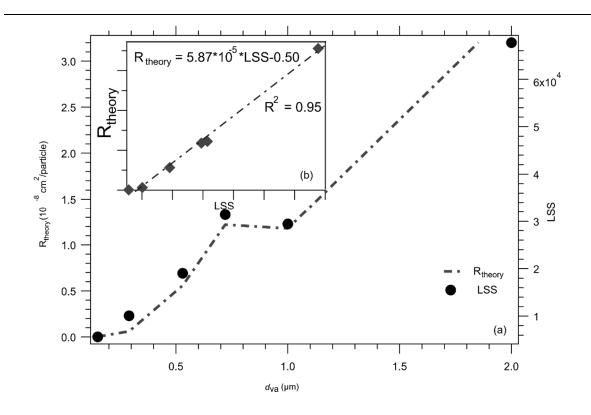


Fig. S2. (a) Upper limit of light scattering signals and theoretical PSCS for PSL as a function of size (0.15, 0.3, 0.5, 0.72, 1, and 2  $\mu$ m) and (b) their relationship. For PSL, n = 1.59 and  $\rho_{eff} = \rho_p = 1.054$  g cm<sup>-3</sup>.

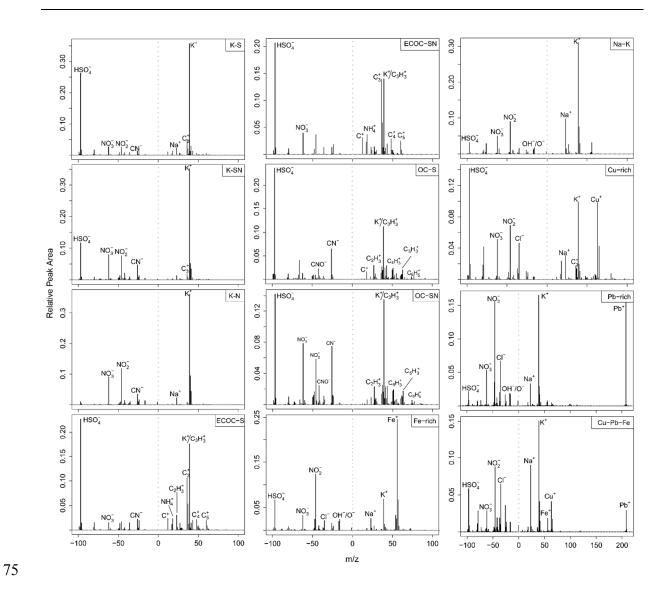


Fig. S3. Mass spectra for the observed single particle types in the atmosphere of Guangzhouduring fall of 2012.

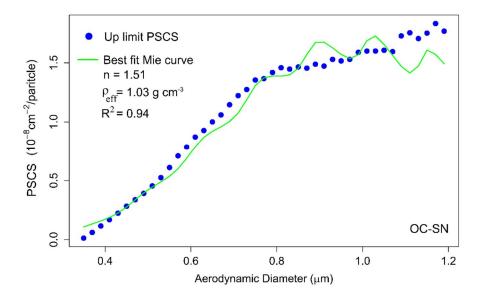
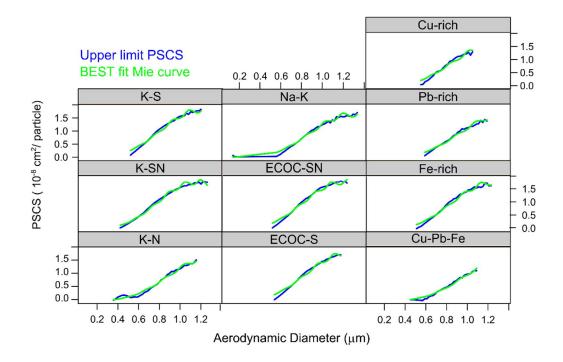


Fig. S4. Measured and best fit theoretical PSCS for OC-SN particle type.



83

81

Fig. S5. Measured and best fit theoretical PSCS for various particle types observed

in the present study.

## REFERENCES

- Gaston, C. J., H. Furutani, S. A. Guazzotti, K. R. Coffee, T. S. Bates, P. K. Quinn, L. I.
- Aluwihare, B. G. Mitchell, and K. A. Prather (2011), Unique ocean-derived particles
- serve as a proxy for changes in ocean chemistry, *J. Geophys. Res.-Atmos.*, 116(D18310),
- 89 1-13, doi:10.1029/2010jd015289.
- Gaston, C. J., P. K. Quinn, T. S. Bates, J. B. Gilman, D. M. Bon, W. C. Kuster, and K. A.
- Prather (2013), The impact of shipping, agricultural, and urban emissions on single
- particle chemistry observed aboard the R/V Atlantis during CalNex, J. Geophys. Res.-
- 93 Atmos., 118(10), 5003-5017, doi:10.1002/Jgrd.50427.
- Moffet, R. C., B. de Foy, L. T. Molina, M. J. Molina, and K. A. Prather (2008), Measurement
- of ambient aerosols in northern Mexico City by single particle mass spectrometry,
- 96 Atmos. Chem. Phys., 8(16), 4499-4516.
- 97 Silva, P. J., D. Y. Liu, C. A. Noble, and K. A. Prather (1999), Size and chemical
- characterization of individual particles resulting from biomass burning of local Southern
- 99 California species, *Environ. Sci. Technol.*, 33(18), 3068-3076.
- Silva, P. J., and K. A. Prather (2000), Interpretation of mass spectra from organic compounds
- in aerosol time-of-flight mass spectrometry, *Anal. Chem.*, 72(15), 3553-3562.
- Sodeman, D. A., S. M. Toner, and K. A. Prather (2005), Determination of single particle
- mass spectral signatures from light-duty vehicle emissions, *Environ. Sci. Technol.*,
- *39*(12), 4569-4580.
- Song, X. H., P. K. Hopke, D. P. Fergenson, and K. A. Prather (1999), Classification of single
- particles analyzed by ATOFMS using an artificial neural network, ART-2A, *Anal.*
- 107 *Chem.*, 71(4), 860-865.
- 108 Zhang, G. H., B. X. Han, X. H. Bi, S. H. Dai, W. Huang, D. H. Chen, X. M. Wang, G. Y.
- Sheng, J. M. Fu, and Z. Zhou (2015), Characteristics of individual particles in the
- atmosphere of Guangzhou by single particle mass spectrometry, *Atmos. Res.*, 153(0),
- 286-295, doi:10.1016/j.atmosres.2014.08.016.