Molecular characterization of organic aerosol from European and Chinese cities: an ultrahigh resolution mass spectrometry study

Kai Wang[1], Rujin Huang[2], Christopher Kampf[3], Yafang Cheng[3], Ulrich Pöschl[3], Thorsten Hoffmann[1]

[1]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg University, Mainz, 55128, Germany
[2]Institute of Earth Environment, Chinese Academy of Sciences, Xi'an, 710061, China
[3]Multiphase Chemistry Department, Max Plank Institute for Chemistry, Mainz, 55128, Germany

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Presenting author email: kaiwang1@uni-mainz.de

Organic aerosol constitutes a substantial fraction (20-90%) of submicrometer aerosol mass, playing an important role in air quality and human health[1]. However, only about 10-30% of OA has been chemically specified so far[2]. A better understanding of the chemical composition, properties and reactivity of OA are therefore important for assessing the effects of aerosol. Since the thousands of compounds in OA covers a very large chemical space with respect to molecular mass, functional group distribution and polarity at a trace level concentration[3,4], characterization of OA is a challenging analytical task.

Over the past few years, ultrahigh resolution mass spectrometry (UHRMS) coupled with electrospray ionization (ESI) has been applied to characterize the complex organic mixtures in OA at the molecular level. Due to the high mass resolving power and high mass accuracy, the UHRMS techniques can detect thousands of individual organic aerosol components and provide their accurate chemical compositions for each analysis.

In this study, urban ambient aerosol with particle diameter < 2.5 μm ($PM_{2.5}$) was collected in Mainz, Germany and Beijing, China, respectively. Solvent mixture of acetonitrile and water was applied to exact the organic compounds from the filter samples. The extracts were analyzed by Orbitrap (ESI-UHRMS) coupled with ultra-high-performance liquid chromatography (UHPLC) in both negative and the positive modes. The chemical composition difference between the two city OA have been discussed in detail.

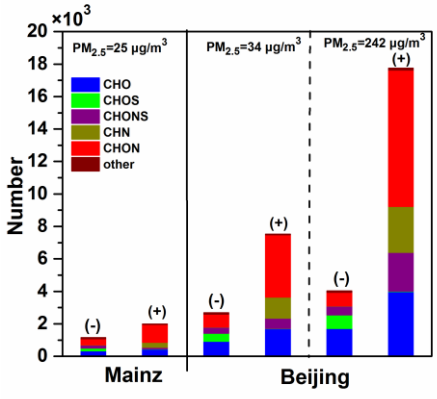

Figure 1. The number of organic compounds in Mainz and Beijing organic aerosols. Each subgroup is marked by the different colore. (-) stands for negative mode, while (+) stands for positive mode.

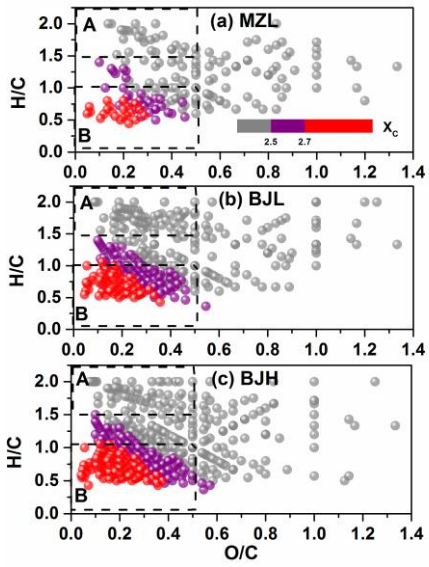

Figure 2. The van Krevelen diagram of CHO compounds detected in ESI-. (a) OA from Mainz. (b) OA from Beijing with low $PM_{2.5}$ concentrations. (c) OA from Beijing with high $PM_{2.5}$ concentrations. Areas 'A' and 'B' refer to aliphatic compounds and oxidised aromatic hydrocarbons in organic aerosol, respectively. The colour bar denotes the aromaticity equivalent (gray ball with XC < 2.50, purple ball with 2.50 ≤ XC < 2.714 and red ball with XC ≥ 2.714).

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Kroll, J. H.; Donahue, N. M.; Jimenez, J. L.; Kessler, S. H.; Canagaratna, M. R.; Wilson, K. R.; Altieri, K. E.; Mazzoleni, L. R.; Wozniak, A. S.; Bluhm, H.; Mysak, E. R.; Smith, J. D.; Kolb, C. E.; Worsnop, D. R. (2011) *Nat. Chem. 3*(2), 133-139.

Hoffmann, T.; Huang, R. J.; Kalberer, M. (2011) *Anal. Chem. 83*(12), 4649-64.

Lin, P.; Rincon, A. G.; Kalberer, M.; Yu, J. Z. (2012) *Environ. Sci. Technol. 46*(14), 7454-7462.

Noziere, B.; Kalberer, M.; Claeys, M.; Allan, J.; D'Anna, B.; Decesari, S.; Finessi, E.; Glasius, M.; Grgic, I.; Hamilton, J. F.; Hoffmann, T.; Iinuma, Y.; Jaoui, M.; Kahnt, A.; Kampf, C. J.; Kourtchev, I.; Maenhaut, W.; Marsden, N.; Saarikoski, S.; Schnelle-Kreis, J.; Surratt, J. D.; Szidat, S.; Szmigielski, R.; Wisthaler, A. (2015) *Chem. Rev. 115*(10), 3919-83.