Rapid Chemical Description of Organic Aerosols with a Direct Inlet Probe Coupled to Trapped Ion Mobility Time-of-Flight Mass Spectrometry

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Introduction and Motivation

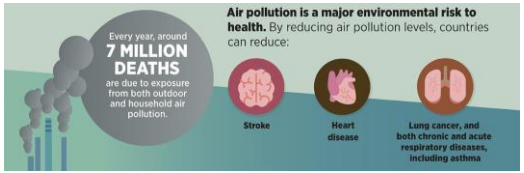


Fig. 1 Potentially global health risk due to particle matter exposure. [1]

Anthropogenic air pollution exposes the environment to organic contaminants with severe health and climate impacts. The tremendous molecular complexity of organic aerosols motivates the development of novel analytical approaches.
Chemical description most often involves tedious extraction procedures. Complementary approaches are direct thermal desorption techniques. In this study, **a direct inlet probe (DIP)** ion source coupled to **trapped ion mobility spectrometry time-of-flight mass spectrometry (TIMS-TOF)** and **Fourier-transform ion cyclotron resonance mass spectrometry (FT-ICR MS)** is presented as a rapid and robust sample introduction technique for aerosol samples.

Material and Method

Combustion aerosols from diesel engine and logwood stove (biomass, lignite) were investigated in this study. The particulate matter was sampled directly from the quartz fiber filters with a cleaned glass capillary. Subsequently, the sample introduction into the ionization source was conducted with the DIP and **atmospheric pressure photoionization (APPI)** without a dopant. All experiments were performed on a commercial Bruker timsTOF instrument. To verify the elemental composition an ultra-high resolution FT-ICR-MS (12T, Bruker solariX XR) was used with the same filters.

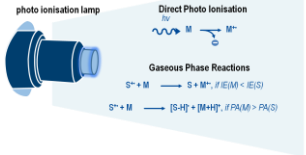


Fig. 2 Ionization reactions in an APPI source.

Results and Discussion I

As a fast technique, the DIP source is used as the first separation with an **analysis time of roughly five minutes.** The source enables a separation according to the temperature. In the first phase mainly vaporization of smaller molecules occurs. (Fig. 4b) The second phase is totally different, as a result of the degradation of larger molecules, many small *m/z*-values can be found in the lower mass range. The complexity increases and also higher *m/z*-values can be analyzed.

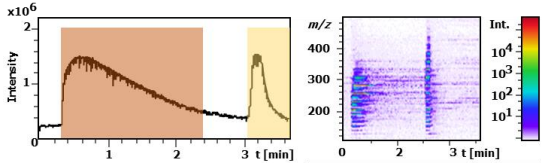


Fig. 4 a) Time-profile of the total ion current (TIC) b) Survey of the signals from diesel engine exhaust. In brown, the thermal desorption phase (250 °C) and in yellow the pyrolysis phase (450 °C) is highlighted.

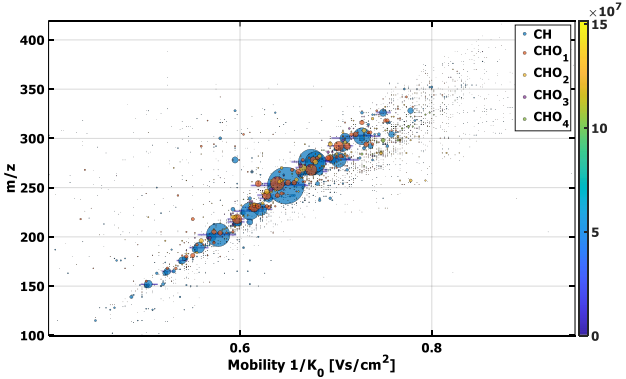
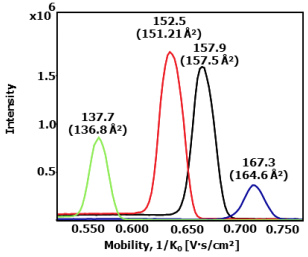


Fig. 5 Two dimensional representation of the m/z versus reduced mobility for the desorption phase of a wood combustion aerosol analyzed by DIP-APPI-TIMS-TOF. Apex peak position are given with the respective compound classes color-coded.

Results and Discussion II



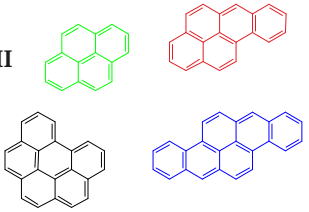


Fig. 5 IMS-profile of *m/z* 202.077 (green) 252.0935 (red) 276.0938 (black) and 302.1094 (blue) with the resulting collision cross section estimated with internal calibration function and calculated values in brackets.[2,3] **Tentative structures are given above.**

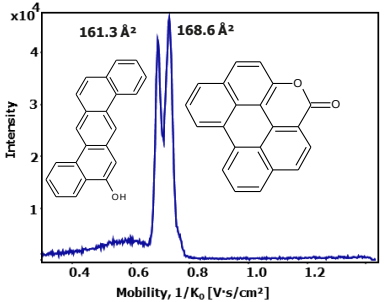


Fig. 6 IMS-profile of *m/z* 294.1041 ($C_{22}H_{14}O$, DBE 16) and 294.0678 ($C_{21}H_{10}O_2$, DBE 17). The isobaric interference, accounting for the CH versus O mass split of ~36 mDa, can be separated by the TIMS.

Conclusion

Direct inlet probe coupled to trapped ion mobility time-of-flight mass spectrometry as well as ultra-high resolution Fourier-transform mass spectrometry both equipped with atmospheric pressure photo ionization can be deployed for the **direct molecular-level description of organic aerosols.**

Acknowledgement

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