Development of a Thermal Desorption Chemical Ionization Ion Trap Mass Spectrometer for the Chemical Characterization of Ultrafine Aerosol

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Rapid online measurements of the chemical composition of ultrafine aerosol particles (< 100 nm diameter) are a key component to investigate health effects of particulate matter, atmospheric heterogeneous chemistry, and atmospheric particle nucleation and growth. Recently, a triple quadrupole thermal desorption chemical ionization mass spectrometer (TDCIMS) was successfully employed to measure chemical compounds of atmospheric aerosol in the 6-20 nm diameter range (Smith et al., 2004).

Here, we report advances in the development of a new TDCIMS instrument using a quadrupole ion trap mass spectrometer and a modified inlet design. The main improvements of this new instrument are its reduced size and weight, faster and more efficient passage of particles through the instrument, and the analytical versatility of an ion trap mass spectrometer.

The basic principles of the TDCIMS technique (Voisin et al., 2003) will be briefly described: Ambient aerosol particles entering the instrument are charged, a size-segregated subsample of the aerosol is selected with a differential mobility analyzer (DMA), and the monodisperse aerosol is collected on an electrostatic precipitator. In order to improve instrument sensitivity, the charged particles cross the flow of a clean sheath gas that prevents contamination of the collector from the ambient gas. Finally, the collected sample is thermally desorbed in the ion source region of the mass spectrometer and analyzed for characteristic ions.

The new instrument configuration has been designed for fast and efficient transport of ultrafine particles from the particle inlet to the electrostatic precipitator. Reduced volumes of the sampling lines and the electrostatic precipitator minimize sample mixing to allow for conditional sampling procedures. In addition, radial DMAs with simple outlet geometries are applied to reduce loss of particles in the DMA exit regions. Overall, the compact design of an ion trap mass spectrometer facilitates transportation and application of the instrument in field studies.

Ion trap mass spectrometry is a versatile technique to analyze ions generated from the thermal desorption of aerosol particles. In a first step, ions are trapped in a superposition of oscillating and static electric fields. In a second step, the stored ions are ejected from the trap according to their mass-to-charge ratio by changing the electric field. Depending on the studied ions, storage and ejection times allow fast scanning of mass spectra. In typical laboratory experiments, we record 1 to 10 spectra per second. Thus, changes in the ion composition during thermal desorption with a temperature ramp can easily be followed.

During storage, ions can be manipulated in various ways. In order to reduce background interferences, unwanted ions are ejected from the ion trap through multiple-frequency resonance ejection. In preliminary laboratory experiments, we applied a filtered noise field (FNF) in order to increase the signal-to-background ratio. On this basis, multidimensional MS analysis of individual compounds by resonant excitation of isolated ions will be further investigated. This approach shows promise to characterize organic molecules in ultrafine aerosol particles through mass spectral analysis of parent and daughter molecules in multiple fragmentation steps.

First experimental results of the new thermal desorption chemical ionization ion trap mass spectrometer will be presented and discussed.

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