

# Development and characterization of an ion trap mass spectrometer for the on-line chemical analysis of atmospheric aerosol particles

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## Abstract

A novel Ion Trap Aerosol Mass Spectrometer (IT-AMS) for atmospheric particles has been developed and characterized. With this instrument the chemical composition of the non-refractory component of aerosol particles can be measured quantitatively. The set-up makes use of the well-characterized inlet and vaporization/ionization system of the Aerodyne Aerosol Mass Spectrometer (AMS). While the AMS uses either a linear quadrupole mass filter (Q-AMS) or a time-of-flight mass spectrometer (ToF-AMS) as the mass analyzer, the IT-AMS utilizes a three-dimensional quadrupole ion trap. The main advantages of an ion trap are the possibility of performing MS<sup>n</sup>-experiments as well as ion/molecule reaction studies. The mass analyzer has been built in-house together with major components of the electronics. The IT-AMS is operated under full PC control and can be used as a field instrument due to its compact size. A detailed description of the set-up is presented. Experiments show that a mass resolving power larger than 1500 can be reached. This value is high enough to separate different organic species at  $m/z$  43. Calibrations with laboratory-generated aerosol particles indicate a linear relationship between signal response and aerosol mass concentration. These studies, together with estimates of the detection limits for particulate sulfate ( $0.65 \mu\text{g}/\text{m}^3$ ) and nitrate ( $0.16 \mu\text{g}/\text{m}^3$ ) demonstrate the suitability of the IT-AMS to measure atmospheric aerosol particles. An inter-comparison between the IT-AMS and a Q-AMS for nitrate in urban air yields good agreement. For laboratory-generated polystyrene latex particles a MS/MS-study using collision-induced dissociation (CID) with a daughter/parent ion yield of more than 60% has been performed. In the future, similar MS/MS-studies can be conducted for atmospheric particles and for the study of secondary aerosol formation in smog chamber experiments.

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## 1. Introduction

The chemical analysis of aerosol particles with on-line mass spectrometric methods is of interest in many scientific fields. The contributions of these methods for understanding atmospheric chemistry and climate have recently been reviewed [1]. However, many open questions remain. Especially the processes that lead to the formation of secondary organic aerosol (SOA) components are widely unknown. This is mainly due to the huge variety and complexity of organic compounds found in the atmosphere [2]. In addition, analysis of these compounds is

complicated by their fragility [3]. Therefore, the development of new sensitive mass spectrometric methods with soft ionization techniques can help to identify such components in atmospheric particles.

Aerosol mass spectrometry has been the topic of several recent review articles [4–6]. Many existing aerosol mass spectrometers either use time-of-flight mass spectrometers or linear quadrupole mass filters. Nevertheless, in several studies an ion trap has been used for the chemical analysis of aerosol particles. Especially the Laser Spectroscopy and Chemical Microtechnology Group at Oak Ridge National Laboratory has pioneered the application of ion trap mass spectrometry for the on-line analysis of aerosol particles [7–12]. Some advantages of ion trap mass spectrometry are: (1) the compactness of the mass analyzer, (2) a high duty-cycle (fraction of the time spent for ion

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accumulation to the total measuring time) can be achieved, (3) a complete mass spectrum can be recorded for individual particles, (4) reactions inside the trap can be studied, (5) a large mass range is accessible and (6) MS<sup>n</sup>-studies can be performed.

Contributions to the field of aerosol ion trap mass spectrometry can be categorized according to the method of particle vaporization and the subsequent ionization processes. Laser desorption/ionization can be used for single particles in the center of an ion trap by firing an intense laser pulse through a hole in one of the electrodes. The trigger for the laser pulse is determined by the particle velocity which is measured by scattered light signals from two continuous lasers in front of the trap. This method has been used, e.g., to study single bacteria [7], polycyclic aromatic hydrocarbons (PAHs) in particles from diesel engine exhaust [8] or uranium and uranium oxides in airborne particles [9]. In these studies an inlet system consisting of a nozzle and two skimmers was used, recent modifications of the instrument operate with an aerodynamic lens [10,11]. Using an aerodynamic lens and an optimized detection system, single particles with diameters as small as ~200 nm can be analyzed with high efficiency by a portable instrument. However, quantitative measurements are limited when using the laser ablation technique.

An instrument that also analyzes single particles by laser ablation is the nanoaerosol mass spectrometer (NAMS) that is used for particles with sizes of ~10 nm [13,14]. Since it is not possible to detect these particles by their scattered light, charged particles are captured in the trap. A high-energy laser pulse (150 mJ) that is focused tightly (fluence ~100 J/cm<sup>2</sup>) creates a plasma, therefore only atomic fragment ions are produced. These ions are ejected from the trap and analyzed in a reflectron/time-of-flight mass spectrometer.

Hoffmann et al. [15] describe an instrument that has mainly been used for the analysis of secondary organic aerosol particles. The particles are vaporized inside a heated tube, ionized at atmospheric pressure by chemical ionization (APCI) and are subsequently analyzed in an ion trap. A similar method has been used by Dalton et al. [16] by combining glow discharge ionization (GDI) with ion trap mass spectrometry.

Harris et al. [12] have very recently reported the application of a modified commercial ion trap for the study of warfare-related species on aerosol particles. The particles are brought into the vacuum by an aerodynamic lens and are thermally vaporized inside the ion source region. Ions are created externally either by electron impact or chemical ionization.

Here we present a novel Ion Trap Aerosol Mass Spectrometer (IT-AMS). The IT-AMS provides on-line measurements of the chemical composition of the non-refractory component of aerosol particles. The three-dimensional quadrupole ion trap mass analyzer has been designed and machined in-house. It is combined with an inlet and evaporation/ionization system taken from the commercial Aerosol Mass Spectrometer (AMS, Aerodyne Research Inc., USA) that contains an aerodynamic lens, a vaporizer and an electron impact (EI) ion source.

In this paper we describe the set-up of the IT-AMS. Results from characterization studies are shown that include a mass calibration measurement, a comparison with a Quadrupole-AMS

(Q-AMS) for urban particulate nitrate and a MS/MS-experiment for laboratory-generated polystyrene latex particles.

## 2. Experimental set-up and theory of operation

The Ion Trap Aerosol Mass Spectrometer is a combination of a three-dimensional quadrupole ion trap mass spectrometer and an aerosol inlet chamber containing an evaporation/ionization system. The latter one has been purchased from Aerodyne (Aerodyne Inc., USA) and is identical to the system used by the commercial Aerosol Mass Spectrometer. The AMS uses either a linear quadrupole mass filter (Q-AMS [17]) or a time-of-flight mass spectrometer (ToF-AMS [18,19]) as the mass analyzer.

Fig. 1 shows a schematic diagram of the IT-AMS. The flow into the instrument is controlled by a critical orifice ( $d \sim 120 \mu\text{m}$ ) that maintains a flow rate of  $\sim 120 \text{ cm}^3/\text{min}$  at ambient pressure and temperature. The aerosol passes through an aerodynamic lens that focuses the particles into a narrow beam [20,21]. At the same time the incoming gas is efficiently removed. The combination of these two effects results in a substantial enrichment of the particulate phase over the gas phase. The size range of particles that are transmitted by the aerodynamic lens with almost 100% efficiency is approximately 60–600 nm. The chopper wheel that is used within the AMS to provide size resolved chemical information about the particles [17] is currently not used for the IT-AMS because it is not possible to obtain size-resolved chemical information when using only one chopper wheel. This is due to the fact that the time needed to analyze ions within the IT-AMS is considerably longer than the difference in particle flight times due to their different sizes. Therefore, at the moment, only the integral chemical composition of all particle sizes is measured. Size resolved mass spectra could be obtained in the future by using two chopper wheels that are operated in a way that only a certain particle size range reaches the ion source and the trap.

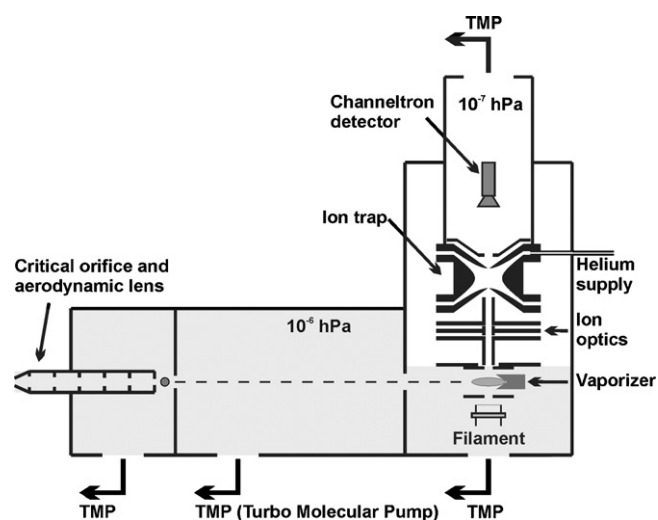


Fig. 1. Schematic diagram of the Aerosol Ion Trap Mass Spectrometer (IT-AMS). The IT-AMS is a combination of a flight chamber taken from the commercial Aerosol Mass Spectrometer (AMS, Aerodyne Research Inc., USA) shown with a gray background and a newly set-up three-dimensional quadrupole ion trap.

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