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Short communication

Performance of a low voltage ion trap

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ABSTRACT

Reduced power operation of a mass analyzer with minimum loss of spectral resolution and mass range is desirable in portable instruments. Miniaturizing quadrupole-based ion traps can be especially worthwhile since the RF amplitude necessary for mass analysis scales with the square of the analyzer dimensions. The performance of a miniature, stainless steel, rectilinear ion trap (RIT) with dimensions of 1.66 mm × 1.43 mm (x_0 and y_0 respectively) is characterized by sampling externally generated ions and performing mass analysis without benefit of differential pumping to simulate conditions in a miniature system. This system is capable of detecting analyte ions of up to m/z 1250 at operating voltages of 610 $V_{0\text{-p}}$ (drive frequency of 1.105 MHz), and with spectral resolution on the order of 2 Th (FWHM) across the entire mass range. The ability to acquire structural information through tandem MS is also demonstrated.

1. Introduction

Demand for in situ detection of specific compounds at the parts-per-billion (ppb) and parts-per-million (ppm) levels is one of the factors driving the development of portable mass spectrometers [1–5]. The ability to successfully miniaturize and/or simplify the geometry of instrument components, particularly the electronics, vacuum system, and mass analyzer [6,7] is the key to this development. Quadrupole ion trap mass analyzers are well suited for use in portable instruments due to their ability to operate at elevated pressures (10^{-2} to 10^{-3} Torr), relaxing the vacuum system requirements, and the ability to use a single mass analyzer for tandem MS experiments. Additionally, ion traps, especially those with electrodes of simple geometry such as the cylindrical ion trap [8] (CIT) and the rectilinear ion trap [7] (RIT), are more easily scaled to mini [9–11] and micro [12–15] dimensions than other mass analyzer types.

RITs are simplified linear ion trap mass analyzers consisting of planar electrodes, viz. two end caps, and pairs of Y-electrodes and X-electrodes, respectively. At the usual size scale the optimized, dimensions are 5 mm × 4 mm nominally (one-half the distance between opposing X and Y-electrodes) [7]. This device has been well characterized and utilized as the mass analyzer in portable instruments for in-field applications [16–19]. Since the operating voltage scales as the square of the dimensions of the trapping electrodes, and power scales to the square of the RF amplitude, greatly reduced power requirements needed for portable instruments can be achieved by size reduction [10].

RIT mass analyzers have previously been fabricated with nearly the same geometry as used in this work and they have given peak widths of approximately 1.5–2 Th (FWHM) [20,21]. However, these earlier experiments did not employ small total MS systems, and notably they did not suffer from the limited pumping capabilities characteristic of handheld MS systems. In this work a miniaturized, steel, RIT was characterized in a single stage manifold, without ion optics or specialized buffer gas, and under pressure conditions comparable to those of a portable mass spectrometer utilizing a discontinuous atmospheric pressure interface (DAPI) to sample externally generated ions [22–24]. The performance of a miniaturized, steel, RIT analyzer (1.66 mm × 1.43 mm for X_0 and Y_0 respectively; 1/3rd the scale of the usual RIT dimensions) operated at pressures expected for a portable instrument is characterized and evaluated in this study.

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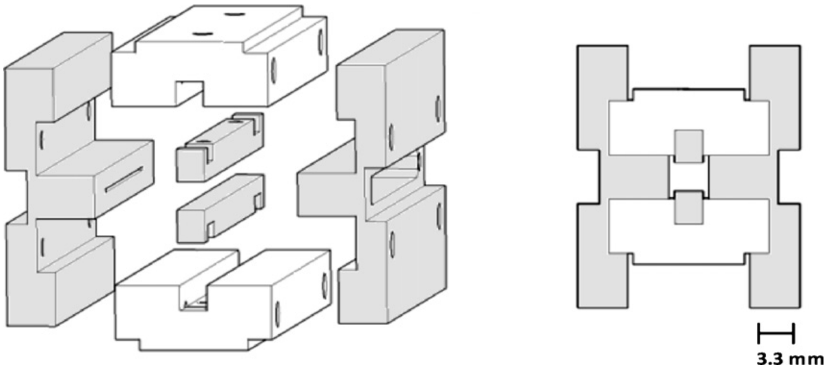

Fig. 1. Computer aided design (CAD) model of the miniature RIT trapping electrodes and ceramic spacers. The ceramic spacers (white) ensure proper alignment of the trapping electrodes (gray) and act as insulators.

2. Materials and methods

Machining of the electrodes (304 stainless steel) was executed using computer numerical control (CNC) followed by hand polishing of the inner electrode surfaces to a mirror finish. Precision cut Macor ceramic established the inter-electrode distances and formed the insulating spacers between adjacent electrodes (Fig. 1). Analyzer assembly was completed by hand. Upon final assembly the average gap spacing (distance between adjacent X and Y-electrodes) was 0.590 mm, and the trapping dimensions (distance between opposing X and Y-electrode pairs) were 1.66 mm and 1.43 mm respectively. These measurements were made using an optical microscope (SmartScope MVP 300, Optical Gauging Products, Inc.) and are accurate to ±1 μm. The length of the ion trap (*z*-dimension) and the dimensions of the ion ejection slits in the X-electrodes were measured to be 40 mm and 0.33 mm × 25 mm, respectively, as measured with a micrometer (Mitutoyo, CD-6 BS). As in all linear ion traps, the *z*-dimension of this device is critical to the ion trapping volume but does not impact the generation of a quadrupolar field in the *x*–*y* plane. A confining force is however, established in the *z*-dimension by applying a DC potential to the end cap electrodes.

Mass calibration and experimental determination of the upper limit of the *m*/*z* range was determined using polyethylene glycol (PEG) in methanol/water (1:1 by vol.) at concentrations ranging from 10 μM to 100 μM. The PEG mix was prepared from seven oligomers with average molecular weights ranging from approximately 100 to 600 (Sigma–Aldrich, Inc.) all used without further purification or modification. PEG was selected for its ability to produce singly charged, sodiated adducts in the presence of sodium salts. Ions generated by nano-ESI were pulsed into the vacuum manifold using a discontinuous atmospheric pressure interface (DAPI) [22–24]. This ion introduction interface is comprised of a controllable, short duration valve (ASCO Scientific, Florham Park, NJ) with a conductive rubber capillary as the seating material (Simolex Rubber Corp., Plymouth, MI). When the DAPI valve is open, gas phase neutrals and the ions generated in the ambient environment are passed to the low pressure (base pressure $\sim 10^{-4}$ to 10^{-6} Torr) vacuum manifold that contains the mass analyzer. Once the DAPI valve is closed, the introduced ions are trapped while neutral gas phase molecules are pumped away. This decreases the operating pressure of the ion trap, and allows the electron multiplier (Photonics, Magnum 5903) to be turned on. In the scan function implemented for these experiments (Fig. 2), the DAPI valve was opened to the atmosphere for 50 ms and then closed for the duration of the pump down and mass scan period, which was approximately 2000 ms. The stainless steel ion introduction capillary was aligned co-axially with the aperture in the ion trap front end cap and positioned such that there was a 1 mm gap between the two components. This allowed gating of the ions into the trap using the front end cap voltage and it avoided perturbation of the quadrupolar field by inserting the capillary directly between the X and Y electrodes.

A laboratory built system that utilized LCQ Duo (Thermo Fisher Scientific, San Jose, CA) electronics and LCQ Duo Tune 1.0 software/Ion Trap Control Language interface was used for electronic

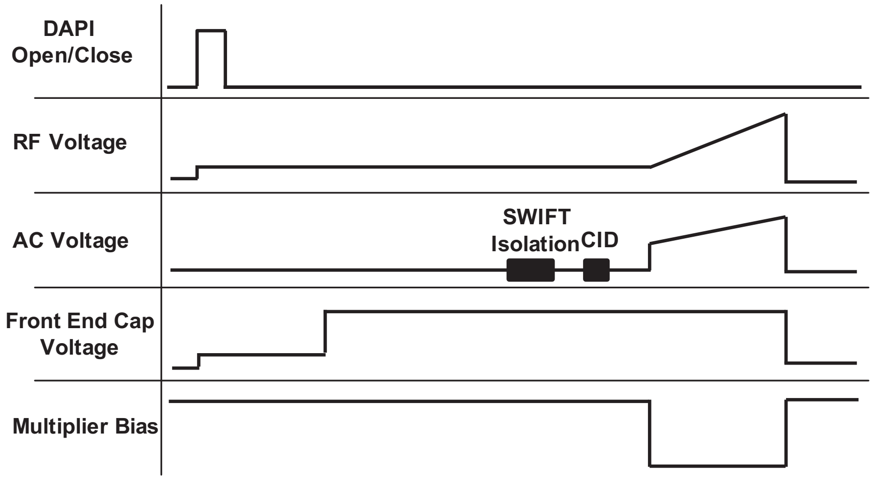

Fig. 2. Scan function used to operate the miniaturized RIT. During experiments in which no ion isolation or activation was conducted amplitudes and time segments for SWIFT and CID were set to zero.