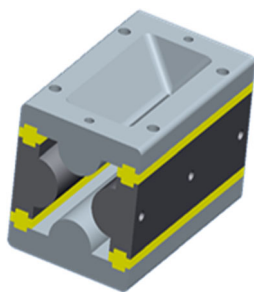


Design and Performance Evaluation of a Linear Ion Trap Mass Analyzer Featuring Half Round Rod Electrodes

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Abstract. A novel linear ion trap mass analyzer featuring half round rod electrodes (HreLIT) has been built. It is mainly composed of two pairs of stainless steel electrodes which have a cross-section of half round rod and a pair of end electrodes. The HreLIT has a simple structure and so it could be assembled by hand with relatively high mechanical accuracy. The external dimension of HreLIT is 50 mm×29.5 mm×28 mm (length×width×height) and its internal volume is about 3.8 cm³. A home-made HreLIT mass spectrometer with three-stage vacuum system was built and the performance of HreLIT was characterized using reserpine solution and PPG standard solution. When the scan rate was 254 u/s, mass peak with FWHM of 0.14 u was achieved for ions with m/z 609, which corresponds to a mass resolution of 4350. The

HreLIT was also operated at a low q value of 0.28 to extend its mass range. The experiment result showed a mass range of over 2800 u and the amplitude of radio frequency (rf) signal was only 1560 V (0-p). Three-stage tandem mass spectrometry was successfully performed in the HreLIT, and the collision-induced dissociation (CID) efficiencies of MS² (CID of ions with m/z 609) and MS³ (CID of ions with m/z 448) were 78% and 59%, respectively.

Keywords: Linear ion trap, Radial ejection, Mass analyzer, Round rod electrode, Mass Resolution

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Introduction

It is well known that linear ion trap has greater ion capacity and higher trapping efficiency for externally injected ions than a traditional 3-dimensional ion trap [1–3]. Therefore, it could accumulate many more ions before space charging effect occurs. These advantages lead to a significant improvement of analytical performance such as sensitivity and dynamic range. Owing to its good performance and capability of tandem mass spectrometry, the linear ion trap mass spectrometer has been commercialized and used in many fields [4–7].

There are mainly two types of linear ion traps, the radial-ejection linear ion trap [8] (ReLIT) and axial-ejection linear ion trap [9, 10] (AeLIT). During mass analysis, ions would be ejected in the radial direction in the ReLIT, while in the axial direction in the AeLIT. The AeLIT has the same instrument

setup as quadrupole mass filter. If driven by a radio frequency (rf) power supply with resolving DC voltages, the AeLIT could be operated as quadrupole mass filter without any hardware change, which is a unique advantage among the ion trap mass analyzers. The ReLIT could only be operated as ion trap, but it has relatively higher ion ejection efficiency than AeLIT during mass analysis. It is reported that the ReLIT would produce an ion ejection efficiency of about 88% if two ion detectors were used to detect ions [8], and the ion ejection efficiency of a regular AeLIT is about 23% [10].

The conventional ReLIT is mainly produced by three axial sections of electrodes, and each section is composed of two pairs of hyperbolic-shaped electrodes [8]. Although high mass resolution and great ion capacity are achieved in the ReLIT, it still has some disadvantages, such as structural complexity, difficulty of manufacture and assembly, relatively high cost, and difficulty of miniaturization. These disadvantages give adequate reasons for developing different types of ReLIT with simplified geometry.

Ouyang and co-workers developed rectilinear ion trap (RIT) [11, 12], which is mainly composed of two pairs of rectangular electrodes with planar-shaped surface instead of the

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hyperbolic-shaped electrodes as used in a conventional ReLIT. The RIT was used to build electron impacted ion (EI) source-based and electrospray ionization (ESI) source-based mass spectrometer. The reported highest mass resolution of RIT was 2700, which was achieved for the mass peak m/z 1922 in an ESI-based RIT mass spectrometer [11]. Furthermore, the RIT made great contribution to miniaturization of ion trap mass spectrometer [13–17]. Handheld RIT mass spectrometers with discontinuous atmospheric pressure interface and various types of ionization sources, such as desorption electrospray ionization source (DESI) and low temperature plasma ionization source (LTP), were developed [13, 18, 19]. Li et al. developed another type of planar-shaped electrode ReLIT, the ion trap array mass analyzer (ITA) [20]. The ITA was mainly built with two parallel printed circuit board (PCB) plates, and each plate was fabricated to several rectangular electrodes. An ITA contains multiple mass analysis channels, and each channel could work as a regular rectilinear ion trap. EI-based and ESI-based ITA mass spectrometers were built, and high-throughput mass analysis was performed in an ESI-based ITA mass spectrometer [20–23]. The reported highest mass resolution of 1000 was achieved for the mass peak m/z 391 [20]. Xiao et al. built a triangular-electrode linear ion trap (TeLIT) with two pairs of triangular-shaped electrodes and two end electrodes. The TeLIT showed a mass resolution of 1500 at mass peak m/z 609 [24].

All the simplified ReLITs mentioned above were built for ease of fabrication, low cost, and miniaturization, etc. However, the process of simplifying the geometry of ReLIT would lead to a relatively big loss of analytical performance, including mass resolution and sensitivity. Fortunately, these simplified ReLIT mass spectrometers could satisfy the needs of some particular fields such as fast screening and environmental protection, etc. [25, 26]. To extend the application areas of simplified ReLIT, it is better to find some new methods to simplify the ReLIT while minimize the loss of analytical performance.

In practical, simplified geometry, quadrupole mass filter and AeLIT built with round rods has been widely used in commercialized quadrupole mass spectrometers. The round rods are much simpler to manufacture and can be mounted with high precision. With an optimum ratio of rod radius (r) to the filed radius (r_0), the quadrupole mass filter could have an analytical performance very close to a conventional one built with hyperbolic rods [27–31]. However, the structure and optimizing result could not be directly used in simplified ReLIT. First, the ReLIT should have slots in one pair of its electrodes, which would change the internal electric fields. Second, for the benefit of ion storage and cooling, the ReLIT should have a relatively closed structure to maintain a higher pressure inside the ReLIT. Douglas and Kononkov made a simulation of linear ion trap with round rods [32], and their research focused on the effect of the ratio of r and r_0 on mass resolution. The simulation result showed that a mass resolution of 5250 could be obtained in an optimized linear ion trap with round rod electrodes. The simulation result could be applied to both ReLIT and AeLIT. However, the slots on the ReLIT were not considered during

the simulation. So the simulation results, especially the performance of ReLIT with round rods, would require experimental verification.

In the present work, a novel linear ion trap mass analyzer featuring half round rod electrodes (HreLIT) was built. Its structure is described and its analytical performance is characterized experimentally.

Experimental

Design and Structure of HreLIT

As shown in Figures 1 and 2, the prototype of HreLIT was mainly built with two pairs (x and y) of electrodes and a pair of end electrodes. The x and y electrodes could be considered to be composed of two parts: a rectangular part and a half round rod part, and the two parts were manufactured together in one electrode using stainless steel. The x electrode is 46 mm in length and 29.5 mm in width, and the radius of the half round rod is 5.0 mm. A 28 mm×0.6 mm (length×width) slot was centrally located on the x electrode and ions would be ejected from the slot during mass analysis. The y electrode is 46 mm in length and 15.5 mm in width, and the radius of the half round rod is 5.0 mm. The gap between the x and y electrodes is 2.0 mm. The cross-shaped strip between x and y electrodes is manufactured with polyetheretherketone (PEEK), which would have the function of insulation, positioning, and making the structure more gas tight. With this structure, the whole HreLIT could be assembled by hand and its total mechanical error is measured to less than 20 μm , which mainly indicates the parallelism error of both x and y electrodes.

The field radius (r_0), which refers to the distance of y electrode to the geometrical center of the HreLIT, is 4.0 mm in dimension. Slot on x electrode would affect the internal electric fields distribution usually by decreasing quadrupole filed component and adding harmful high-order fields. The “stretched” structure had been commonly used in 3-dimensional ion trap and ReLIT to solve this problem [3, 8, 12]. In this work, the x electrode was moved out from center 0.75 mm beyond its normal position, so the distance between x electrode and geometrical center (x_0) was 4.75 mm.

The internal field distribution was calculated using software named PAN33, which was developed based on the potential array of SIMION. The non-stretched HreLIT without slots on x electrodes was also simulated. The simulation was made in two dimensions (x and y) and the calculation result is shown in Table 1. It was found that there was more quadrupole field component in the stretched HreLIT than in the non-stretched structure.

The two end electrodes were placed in the axial direction, which would form a DC trapping potential along the axial direction of HreLIT during mass analysis. The end electrodes were made of stainless steel plates with 2.5 mm aperture on the center of the plates. The distance between end electrodes and x (y) electrodes was 2.0 mm.

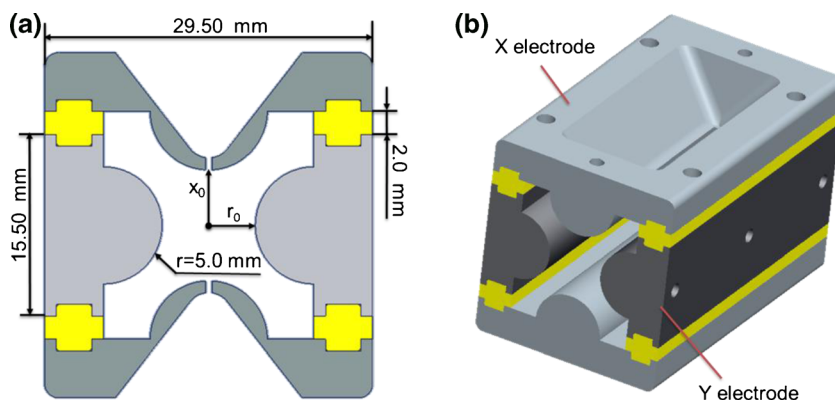


Figure 1. Structure of HreLIT: (a) cross-section of HreLIT; (b) assembly of HreLIT

Instrument Setup

The HreLIT was tested on a home-built ESI-based mass spectrometer with three-stage vacuum chamber, which was fabricated from aluminum. A rotary vane pump (Penta 35; Pfeiffer Vacuum, Asstar, Germany) with a pumping speed of $34 \text{ m}^3/\text{h}$ was used to drive the first stage of vacuum system. Two turbomolecular pumps (Hipace 300; Pfeiffer Vacuum) with pumping speed of 260 L/s were connected to the second and third stage of the vacuum chamber, respectively. The first stage of vacuum was measured using a Pirani gauge (TPR 280; Pfeiffer Vacuum) and the third stage of vacuum was measured using a Pirani/cold cathode gauge (PKR 251; Pfeiffer Vacuum).

A heated stainless steel capillary was assembled on the first stage of the vacuum chamber for ion transferring. The ion transfer capillary had an internal diameter of 0.508 mm and was 150 mm in length. Its temperature could be steadily controlled and adjusted from 50°C to 250°C during work. A stainless steel skimmer with an aperture of 1.5 mm was placed behind the ion transfer capillary. A hexapole ion guide was placed in the second stage of vacuum chamber to transfer ions. The hexapole ion guide was 200 mm in length and was built with stainless steel round rods. The rod radius and field radius of the hexapole ion guide were 2.5 mm and 4.5 mm , respectively. Two balanced rf signals with 180° phase shift were

applied to alternate rods of the hexapole. The frequency and amplitude of the rf signal were 1.0 MHz and 150 V (0-p, short for zero to peak), respectively. A prototype of HreLIT was assembled in the third stage of the vacuum system, and an electron multiplier (Detech 2312; Detector Technology, Inc., Palmer, MA, USA) was placed near the slot of one of the x electrodes to detect ejected ions during operation. Helium was used as buffer gas and was admitted into the HreLIT. The pressure of the third vacuum chamber was measured outside the HreLIT. Without helium buffer gas, the pressure was about $2.3 \times 10^{-5} \text{ Torr}$, and after helium was admitted into the HreLIT, the pressure was about $3.0 \times 10^{-5} \text{ Torr}$.

The HreLIT was operated using the technique of mass selective instability scan and resonance ejection. As shown in Figure 3, the home-made power supply system was composed of a rf resonator, an AC signal generator, and two identical transformer coils (T1 and T2). The rf resonator was tuned at a resonant frequency of 1.01 MHz and two balanced rf signals with 180° out of phase were produced. The two transformer coils were used to couple AC signal to rf signal. Only the primary coil of T1 was driven by an AC signal generator, and the two outputs of T1 were connected to x electrodes. At the same time, the two outputs of T2 were connected to y electrodes. The primary coil of T2 was grounded, so the function of T2 was to keep balance of the two rf signals after coupling the

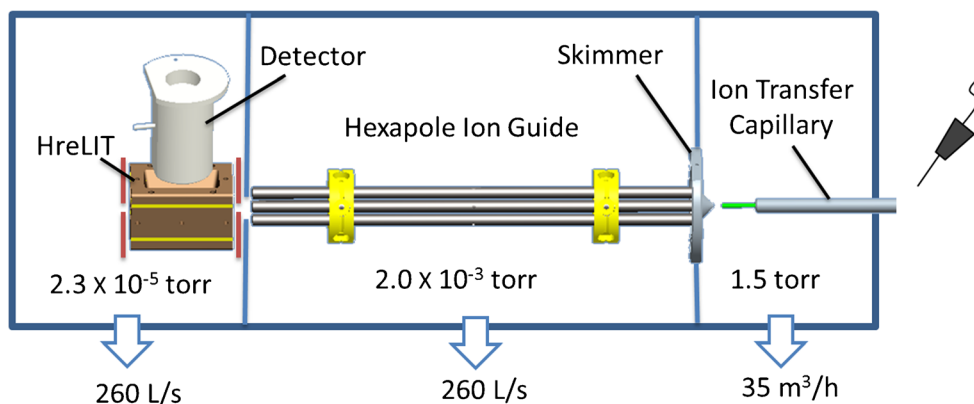


Figure 2. Instrument setup of the HreLIT mass spectrometer

Table 1. Electric Field Distribution of HreLIT

	A ₂	A ₄	A ₆	A ₈	A ₁₀
Non-stretched (without slots)	96.93%	0	1.65%	0	1.5%
Non-stretched (with slots)	90.79%	0.74%	2.68%	1.75%	4.04%
Stretched 0.75 mm (with slots)	96.67%	0.56%	0.92%	0.43%	1.42%

AC signal. The amplitude of AC signal could be adjusted from 0 to 15 V (p-p, short for peak-to-peak), and its frequency could be adjusted from 1 to 500 kHz. An electronic control board was developed base on ARM and FPGA and it could provide various functions, such as amplitude modulating of rf signal, time diagram control, programming DC amplifying, and data acquisition. A storage waveform inverse Fourier transform (SWIFT) could be generated by the control board as well, which would be used for mass selected ion isolation.

Results and Discussions

Two samples were used to experimentally characterize the performance of HreLIT. Reserpine in methanol/water solution (1:1 v/v, with 0.5% acetic acid; 1×10^{-5} MOL/L) was used to test the mass resolution and capability of tandem mass spectrometry of HreLIT. The mass range was tested using polypropylene glycol (PPG) standard solution (1×10^{-6} MOL/L).

The DC voltages applied on the ion optics were optimized and then fixed during operation. The voltages applied on ion transfer capillary and skimmer were 30 and 8.1 V, respectively. A DC offset of 6.3 V was applied on hexapole ion guide. The DC float for the rf signal was 0 V during all operation. The high voltage applied on the electron multiplier was -1200 V during ion detection. In all experiments, the ion transfer capillary was

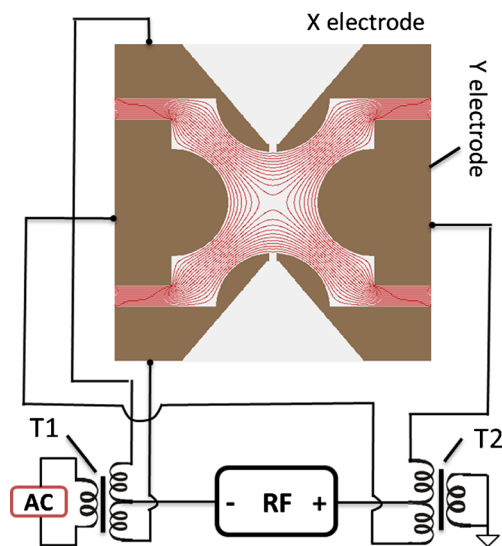


Figure 3. Rf power supply connection and internal field contour distribution of HreLIT

heated to 200°C . The ESI source was operated at a high voltage of 5000 V and the flow rate of sample solution was $0.5 \mu\text{L}/\text{min}$.

Mass Resolution

Ions were first injected into the HreLIT and accumulated for 1 ms during ionization period, and the rf voltage was fixed on 150 V (0-p). The DC voltage applied on the front end electrode of HreLIT was optimized, and the highest intensity was achieved when the DC voltage was adjusted to 5.9 V. These stored ions were then cooled for 30 ms through collision with helium buffer gas. The DC voltage on the front end electrode of HreLIT was pulled up to 40 V to prohibit ion entrance. In the scan period, the rf voltage was ramped from 130 to 1160 V (0-p).

The frequency of AC waveform is an important parameter, which determines the q value at which ions are ejected [33]. The influence of q value to mass resolution was studied experimentally, and it was found that the highest mass resolution was achieved with q value in the range between 0.78 and 0.83. In subsequent experiments, an AC waveform with frequency of 332.5 kHz was applied, which corresponds to q value of about 0.78. We chose this q value because it could provide both good mass resolution and relatively wide mass range. The AC waveform was not phase-locked with the rf signal, but the initial phase of the AC waveform could be adjusted by software in our control system. Different initial phase of AC waveforms was tried in the experiments, and little effect on mass resolution or peak intensity was found. The DC voltage applied on the back end electrode of HreLIT was fixed to 40 V in all periods.

It has been established that the scan rate has a great impact on mass resolution of ion trap [8, 12, 20, 24, 33, 34]. Actually, in the operation mode of mass-selective instability with resonance excitation, mass resolution of ion trap is proportional to the interaction time of the ions with the auxiliary excitation field [33]. Slow scan rate leads to more interaction time and, therefore, higher mass resolution. The relationship of scan rate and mass resolution of HreLIT was studied experimentally. During the experiment, another important parameter, the amplitude of AC waveform, was optimized and the highest resolution was achieved when it ramps from 0.5 V to 1.0 V (p-p). Amplitude out of this range leads to an increase in peak width and, therefore, a decrease in mass resolution. This amplitude range could satisfy different scan rates in the range of 254–3200 u/s. As shown in Figure 4, when 254 u/s, mass peak with FWHM of 0.14 u was achieved for the ions with m/z 609, which corresponds to a mass resolution of 4350. However, slow scan rate would lead to a loss of sensitivity. With an increase of interaction time of the ions with auxiliary excitation, some ions would be lost before being ejected to the ion detector. It was estimated that some ions were dissociated by collision with background gas and others were lost by colliding the electrodes of ion trap. The relationship between scan rate and peak intensity was studied experimentally, and the result showed that the intensity decreased to 42.1% when the scan

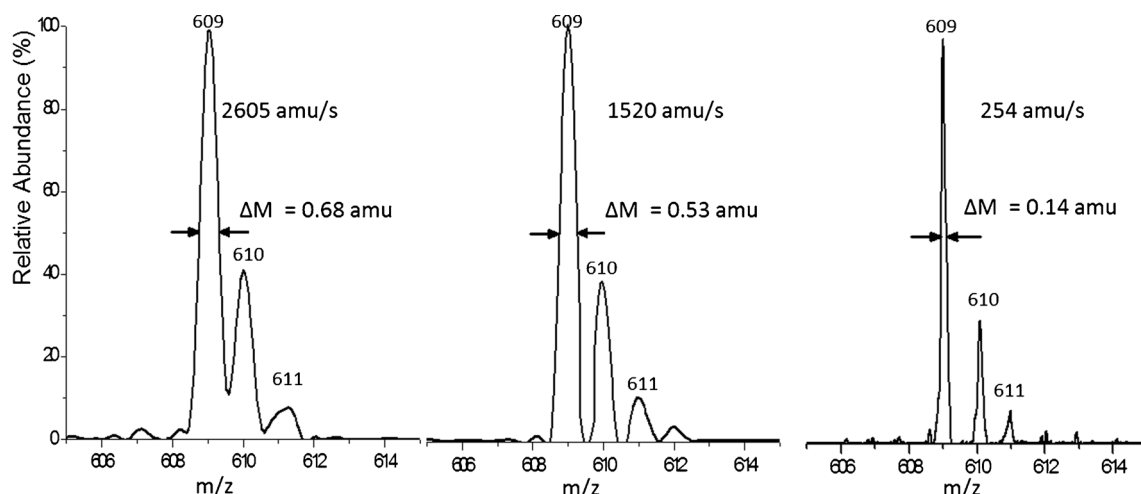


Figure 4. Mass resolution of HreLIT at different scan rate: (a) scan rate of 2605 u/s; (b) scan rate of 1520 u/s; (c) scan rate of 254 u/s

rate varied from 2605 to 254 u/s, which would be an acceptable ion intensity loss in practical applications.

The DC voltage applied on the two end electrodes would affect the axial distribution of ion clouds in the HreLIT. In the scan period, the voltages on two end electrodes were adjusted to 20, 40, 60, and 80 V, respectively, and no obvious change on mass resolution was observed. The experiment results indicated that the HreLIT had a relatively high mechanical accuracy to maintain the same electric fields distribution along the axial direction. However, when the voltages on two end electrodes were pulled up to 200 V during mass analysis, space charging

effect occurred because ions were compressed to the center of the HreLIT, and an obvious decrease of mass resolution was observed.

Tandem Mass Spectrometry

Three-stage tandem mass spectrometry (MS^3) was successfully performed in the HreLIT and the experiment results were shown in Figure 5. Ions with m/z 609 were first isolated by a combination of an AC waveform and a SWIFT waveform. In the isolation period, the amplitude of rf signal was fixed at

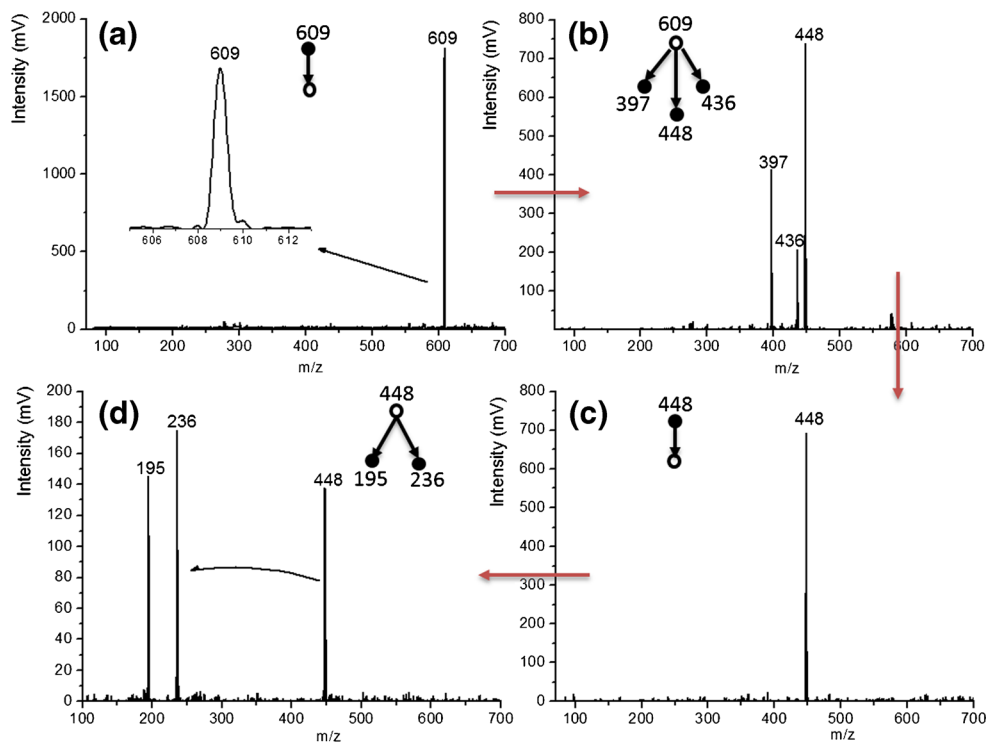


Figure 5. Three-stage tandem mass spectrometry in HreLIT: (a) isolation of ions with $m/z=609$ u; (b) CID of ions with $m/z=609$ u; (c) isolation of ions with $m/z=448$ u. (d) CID of ions with $m/z=448$ u

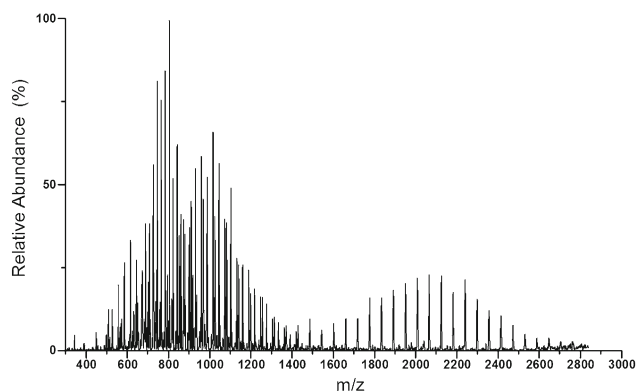


Figure 6. Mass spectrum of PPG

390 V (0-p), and an AC waveform with frequency of 110.6 kHz and amplitude of 1.0 V (p-p) was first applied for 20 ms to ejection ions with m/z 610. Then a SWIFT waveform was applied for 30 ms to eliminate all other ions except those with m/z 609. The SWIFT waveform had a frequency range of 50–550 kHz and an amplitude of 8 V (p-p), and the frequency notch was 108–115 kHz. The number of points in the SWIFT waveform was 2^{14} , and the frequency spacing was about 400 Hz. These calculated points were converted using a digital-to-analog converter working at an output rate of 2.5 MHz. The experiment result was shown in Figure 5, and it indicated that over 95% of ions with m/z 610 were ejected, whereas the intensity loss of ions with m/z 609 was less than 15%.

After a 10 ms cooling period, CID of ions with m/z 609 was performed. In the CID period (for MS^2), the amplitude of rf signal was maintained at 390 V (0-p), which corresponds to q value of about 0.31 for ions with m/z 609. An AC waveform with frequency of 111.2 kHz and amplitude of 0.56 V (p-p) was applied for 30 ms to activate ions. Through collision with buffer gas, ions with m/z 609 were dissociated and product ions with m/z 448, 436, and 397 were produced. The CID efficiency (intensity ratio of product ions to parent ions) was calculated to be about 78%. A 10-ms cooling period was followed by a CID period, and the amplitude of rf signal was adjusted to 260 V (0-p). Ions with m/z 448 were then isolated using SWIFT waveform with frequency notch of 95–105 kHz and amplitude of 8 V (p-p). In the CID period (for MS^3), the amplitude of rf signal was fixed at 260 V (0-p), which corresponds to a q value of about 0.28 for ions with m/z 448. An AC waveform with frequency of 100.0 kHz and amplitude of 0.38 V (p-p) was applied for 30 ms to activate the parent ions. About 80% of parent ions were dissociated and product ions with m/z 238 and 195 were produced. The CID efficiency (here refers to intensity ratio of product ions to dissociated parent ions) of MS^3 was about 59%.

Mass Range Extension

The maximum amplitude of rf power supply used in the experiment was about 1600 V (0-p), which limits the

mass range of the HreLIT to about 1000 u. The electronics of rf power supply would be optimized to get a higher amplitude. Mass range of HreLIT could also be extended by operating at a low q value, and so it could be used to analyze larger molecules. Ions produced in PPG standard solution were injected into the HreLIT for 3 ms, and the amplitude of rf signal was 162 V (0-p). Then ions were cooled for 30 ms before mass analysis. In the scan period, the amplitude of rf signal was ramped from 130 to 1560 V (0-p). The ejection q value was carefully selected to get maximum mass range while maintaining an acceptable mass resolution at the same time. In the experiment, an AC waveform with a frequency of 100.0 kHz was coupled to rf signal and then applied on the x electrodes, which made ions ejected at a q value of about 0.28. The amplitude of AC waveform was ramped from 1.5 to 2.0 V (p-p). The experiment result was shown in Figure 6, which indicated that a mass range of over 2800 u was achieved in the HreLIT. The mass resolution varied among the mass range in low q operation mode. In the mass range of 300–800 u, the peak width (FWHM) was less than 1.0 u; in the mass range of 800–1600, the peak-width (FWHM) was less than 2.5 u; and in the mass range of 1600–2600 u, the peak width was around 4.0 u.

Conclusions

A prototype of HreLIT was built, and its performance was characterized experimentally. The HreLIT had a much simpler structure than a conventional hyperbolic-shaped electrode linear ion trap, and so it has several advantages, such as ease of fabrication and assembly, low cost, and ease of miniaturization. Despite structural simplification, good performance was achieved from the HreLIT. The experiments showed a mass resolution of 4350 and a mass range of over 2800 u. The highest mass resolution achieved from simplified ReLIT was reported. Furthermore, three-stage tandem mass spectrometry was successfully performed in HreLIT. The prototype of HreLIT has a normal size, and its geometrical parameters r and r_0 are 5.0 and 4.0 mm, respectively. The HreLIT could be miniaturized and used to build a portable ion trap mass spectrometer with good analytical performance. In our laboratory, miniaturized rf power supply with low power consumption is under development. Nevertheless, a lot of geometry and electric field optimization work could be done, including optimizing r/r_0 and stretched distance, and even higher mass resolution would be expected.

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