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**RESEARCH PAPER**

# Structure and Property of Ladder Electrode Linear Ion Trap Mass Analyzer

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**Abstract:** The theoretical simulation and optimization of a new linear ion trap mass analyzer-ladder electrode ion trap mass analyzer (LeLIT) was described. The LeLIT was consisted of two pairs of ladder electrodes and one pair of end-electrodes. Compared with conventional rectilinear ion trap (ReLIT) which is built with plate electrodes, LeLIT can adjust and optimize the electric field distribution to obtain optimal performance. Meanwhile, the structure of LeLIT is more similar to the geometrical structure of hyperbolic electrode than that of ReLIT, but it is much easier for processing compared with hyperbolic electrode. According to the simulation results, the optimization of electric field distribution inside the ion trap could be realized through adjusting its geometric parameters such as height, width and field radius ratio of ladder electrodes, which was expected to further optimize the mass spectrometry performance of ion trap. As indicated by theoretical simulation results, mass resolution of 10150 at the scanning speed of 225 Da $s^{-1}$ was obtained with a LeLIT (dimension of $X_0 \times Y_0$ = 9 mm × 5 mm). LeLIT can significantly improve the mass resolution while maintaining its simple structure. As indicated by the preliminary experiment results, LeLIT has a good analyzing performance as tandem mass spectrometry.

**Key Words:** Linear ion trap; Ladder electrode; Electric field distribution; Mass resolution; Tandem mass spectrum analysis

## 1 Introduction

As one of major analytical technologies in chemistry field, mass spectrometry has been extensively applied to many other fields such as life sciences, environment monitoring, and food safety. In particular, combination of mass spectrometry with some separation techniques such as capillary electrophoresis, chromatography has become an important tool for proteomic and metabolic analysis[1–6].

Mass analyzer serves as the core part of mass spectrometer. As one of the most popular mass spectrometers, ion trap mass analyzer has the features of simple structure, relatively lower vacuum requirement, tandem mass spectrometry analysis, etc. Ion trap mass analyzer is also a preferred option for miniaturization of mass spectrometer. As indicated by previous studies, the performance of linear ion trap (LIT) was mainly determined by the electric field distribution inside ion trapping region. Whereas, electric field distribution is strongly determined by the geometric structure of the ion trap electrodes and their assembly[7–10]. As both three-dimensional ion trap and conventional LITs are composed of hyperbolic electrodes, the difficulty in ion trap processing and assembly inhibited their extensive application in ion trap mass spectrometry. Several kinds of ion traps with simpler electrodes[11–15] have been developed recent years, but the performance of mass spectrometry, especially the mass resolving power, was limited due to some higher order fields of diversified constituents that produced besides the quadrupole electric field. The printed circuit board (PCB) ion trap is available for optimizing the electric field distribution by applying differential voltages on different parts of electrodes[11]. Nevertheless, the distribution of internal electric

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field is mainly optimized by changing the geometric structure of the ion trap. Geometric profile of ion trap includes geometric shape of electrodes and their assembly precision, which may affect the electric field distribution as well as the mass spectrometry performance of ion trap.

Some researchers developed the rectilinear ion trap (ReLIT) combining the simple structure of cylindrical ion trap and linear ion trap[12–15]. Rectilinear ion trap can simplify hyperbolic electrode to obtain the structure of plate electrode, which has significantly simplified the structure of linear ion trap. However, extremely simple structure has also resulted in complicated compositions of electric field components inside the ion trap, whereas both of the ion injection hole and ejection slit may also result in the increase in compositions of high-order electric fields. Later, other researchers further developed asymmetrical arc electrode ion trap[16], semi-circular electrode ion trap[17] and triangular electrode ion trap[18,19]. Among them, the structure of triangular electrode was more similar to hyperbolic electrode structure than that of rectangular ion trap. In addition to the simplification of electrode, it can also minimize the high order field in an attempt to minimize mass resolution distortion resulting from high order fields.

A new type of linear ion trap-ladder electrode linear ion trap (LeLIT) was proposed in this work. In comparison with rectangular plate electrode, the geometrical structure of ladder electrode linear ion trap is more similar to that of triangular or hyperbolic electrode ion traps. It can be imagined that a ladder electrode composed of multiply ladders can eventually obtain approximate hyperbolic electrode as well as better mass analysis performance. In this study, we preliminarily designed a two-step ladder electrode ion trap in order to obtain optimal structure through adjusting electrode width, height and field radius ratio during theoretical simulation. A mass resolution over 10000 at the scanning speed of 225 Da $s^{-1}$ could be obtained theoretically. Compared with rectangular trap, the resolution of ladder electrode linear ion trap was significantly improved under the same conditions. The experimental results showed that ladder electrode linear ion trap could perform reasonable mass analysis and tandem mass spectrometry analysis.

## 2 Theoretical computation

### 2.1 Geometrical model of LeLIT

The cross section of a LeLIT for theoretical simulation is shown in Fig.1. The ladder electrode was divided into two layers: an upper (narrower) layer and a lower layer (broader). The $a_x$ and $a_y$ represent the width of lower layer electrode, and $a_x = a_y = 10$ mm. The $h_{1x}$, $h_{1y}$ represent the height of upper ladder electrodes, and $h_{2x}$ and $h_{2y}$ represent the height of lower ladder electrodes respectively. The $b_x$ and $b_y$ represent the width of narrower ladder electrode. The electric field distribution inside the ion trap region was adjusted by adjusting $b_x$ and $b_y$ during theoretical analog. Each electrode was designed with a funnel shape ion ejection hole. The width of the end of the ion ejection hole oriented towards inside of the ion trap was 0.8 mm. $X_0$ and $Y_0$ refer to the dimension of rectangular region for electric field distribution inside the LeLIT, in which $Y_0 = 5$ mm. Therefore, the field radius ratio could be easily adjusted through the adjustment of $X_0$. To simplify theoretical analog process, and save the analog time, we simplified the parameters of the geometrical structure. As a result, the adjustable geometrical parameters were only limited to $X_0$, and the ladder electrode height was fixed as $h = h_{1x} = h_{1y}$ and the width was fixed as $b = b_x = b_y$, as shown in Fig.1.

### 2.2 Relationship between mass resolution and width, height and field radius ratio of ladder electrodes

During theoretical analog, it is applicable to obtain optimal structure of LeLIT through adjustment of geometrical parameters so as to further investigate the performance of LeLIT mass analyzer. Firstly, we used Simion software[20,21] to obtain the distribution of electric field inside LeLIT with different geometrical parameters, as shown in Table 1.

On this basis, we further used Axsim software to simulate the ion motion inside the LeLIT to define the relationship between the mass resolution and the geometrical parameters. Helium gas with pressure of 0.0080 Pa was used as the collision gas during simulations, whereas the hardball collision model was used as the collision model. Ions with $m/z$ 609, 610 and 611 were used during analog, which were ejected in the method of resonance excitation. A sine-wave radio frequency (RF) voltage was applied to the ion trap, in which the RF frequency was 768 kHz, and one third of RF frequency was used as the frequency of AC ion ejection signal, namely 768 kHz/3 = 256 kHz. It is applicable to improve ion ejection efficiency through the regulation of AC voltage and the fine adjustment of AC frequency during analog. Basic analog conditions corresponding to all analog results were identical. To ensure optimal mass resolution, the amplitude of resonance excited signals imposed on the LeLIT with different geometrical parameters have been optimized to some extent.

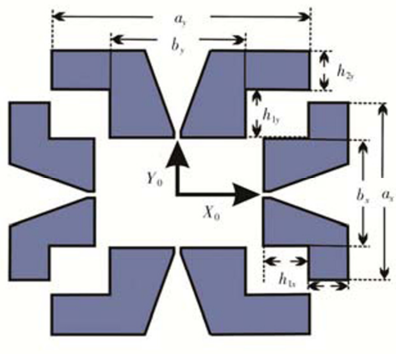


Fig.1 Cross section diagram for geometrical structure of ladder electrode linear ion trap (LeLIT)