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RESEARCH PAPER

Rapid Mass Analysis of Reserpine and Arginine by Ion Trap Mass Spectrometer

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Abstract: A fast mass analysis method using digital ion trap technology was reported. The mass analysis was realized by scanning the frequency of digital RF voltage and dipole ion resonance voltage during ion injection period without the conventional ion cooling, ion resonance ejection or ion cleaning process. It can decrease about three fourth of traditional analysis time using ion trap mass spectrometry. The ion signal was optimized through the modification of frequency scanning rate, ion gate voltage and other experimental parameters. For example, an optimal mass spectroscopy of reserpine (*m*/*z* 609) and arginine (*m*/*z* 174) were obtained when the ion gate voltage was 9 V and the digital RF frequency was scanned from 1 MHz to 400 kHz at rate of 2385 Th s^{-1}. The results indicated that the obtained mass spectra were in very good agreement with conventional analytical method using ion trap mass analyzer.

Key Words: Ion trap mass spectrometer; Digital ion trap; Mass scanning; Fast mass analysis

1 Introduction

Mass spectrometer is one of the most important analytical instruments and widely applied to micro or even trace analysis in chemistry, life sciences, food safety, environmental detection, national defense, aviation and aerospace field,pharmaceutics, etc[1–5]. Ion trap mass spectrometer can store ions and perform tandem mass spectrometric analysis besides its characters of rapid and high sensitive analysis, so it can provide abundant information about molecule composition and structure[6–8]. Besides, even more analytical information can be obtained by a complex mass spectrometer system prepared by combining the ion trap with other mass analyzer such as time-of-flight mass analyzer, quadrupole mass analyzer, and orbit trap mass analyzer, etc[9].

It is well known that the principle of both quadrupole ion trap (QIT) and quadrupolemass spectrometer (QMS) are based on quadrupole field theory that the ions with different mass-to-charge (*m*/*z*) ratios can be separated by quadrupolar electric field. On other hand, there is a big difference between their mass analysis processes[10–12]. In QMS as shown in Fig.1a, the electric field distribution inside the mass analysis region is varying through continuously scanning the voltages on each rod electrodes, and an ion with certain *m*/*z* could have stable motion trajectory, by which the ion could pass the rod-set system and reach the ion detector corresponding to a special quadrupolar field distribution, while other *m*/*z* ions do not have stable motion trajectory and collide with electrodes. Theoretically, a very few mechanical error of rod geometry would induce some small amount of higher order electric field components, which could significantly destroy the QMS mass resolution[13,14], so very high mechanical accuracy within several micron is strictly required for getting reasonable mass resolution. For example, 1000 mass resolution would need a 3-μm mechanical accuracy or better one.

As shown in Fig.1b, the ion trap mass analysis is realized

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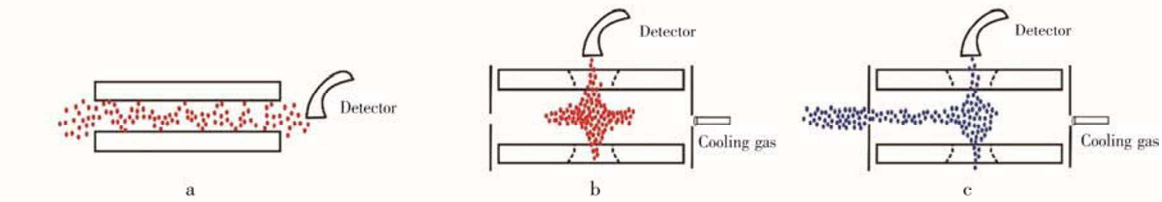

Fig.1 Schematic diagram of mass analysis process with quadrupole ion trap and quadrupole mass spectrometer
(a), quadrupole mass spectrometer; (b), ion trap mass analyzerusing the conventional method; (c), ion trap mass analyzerusing new method

via ion resonance excitation. Theoretically, an ion with unique *m*/*z* would have its own secular frequency, and have stable motion trajectory inside the ion trapping region before it is resonance excited. In the experiment, the ion with certain *m*/*z* can be resonance excited to higher kinetic energy by applying an AC voltage to the ion trap electrodes if the AC frequency is equal to the ion secular frequency. All the *m*/*z* ions can be continuously resonance excited, ejected out and detected when the AC frequency is continuously scanned. Although the secular frequency of ion motion in ion trap is dependent on the electric field distribution, the ion resonance excitation and ejection is independent of the electric field distribution. It means that the higher order field has less effect on the mass resolving capability of ion trap. Therefore, with the same mass resolution, lower mechanical accuracy of geometrically machining and assembly is required for QIT compared with QMS. For example, with 20 micron tolerance, QIT would have higher than 1000 mass resolution while QMS only have about 100[15].

In general, the mass analysis with QIT includes four stages: ion injection, ion cooling, ion resonance ejection and ion cleaning[16–18]. Each stage needs tens of ms and one analysis cycle needs about 100 ms. In the past decades, the simplification and miniaturization of ion trap electrodes were the main subject in mass spectrometry field, for instance, linear ion trap[9], cylindrical ion trap[19], rectangle ion trap[20], PCB ion trap[15] and triangle ion trap[21] were developed successively. However, little attention was paid to the method of rapid mass analysis, which caused great gap for rapid, high throughput and on line analysis.

Herein, a method of rapid mass analysis using digital ion trap technology was introduced. The mass analysis was simply realized by scanning the digital RF frequency and dipole ion resonance voltage in ion injection process without performing other stages. The mass analysis process was greatly simplified, and the analysis time was reduced. The method is a high efficient and rapid analysis technique by QIT.

2 Experimental methods

2.1 Instrument

All experiments were performed on a homemade electrospray-ceramic rectangular ion trap mass spectrometer system. As can be seen from Fig.2, the vacuum system included three-stage differential pumping regions. The first region was pumped to 0.5 Torr by a mechanical pump (8 L s^{-1}), and the second and the third regions were pumped with turbomolecular pump (600 L s^{-1}) backed up by mechanical pump (8 L s^{-1}) independently. Typically, the vacuum in the third region with ion trap mass analyzer was 1 × 10^{-5} Torr and the vacuum decreased to 1 × 10^{-4} Torr during experiment. Helium was used as cooling gas in experiments. Briefly, ions produced from electrospray (ESI) source passed through sampling plate, sampling skimmer, quadrupole ion guide, ion optical lenses and finally were analyzed by the ceramic rectangular ion trap.

In these experiments, ion trap was powered by digital ion trap mode system[18,22,23] which composed of digital square wave detecting system, resonance excitation module, RF square wave amplification system, digital collection system

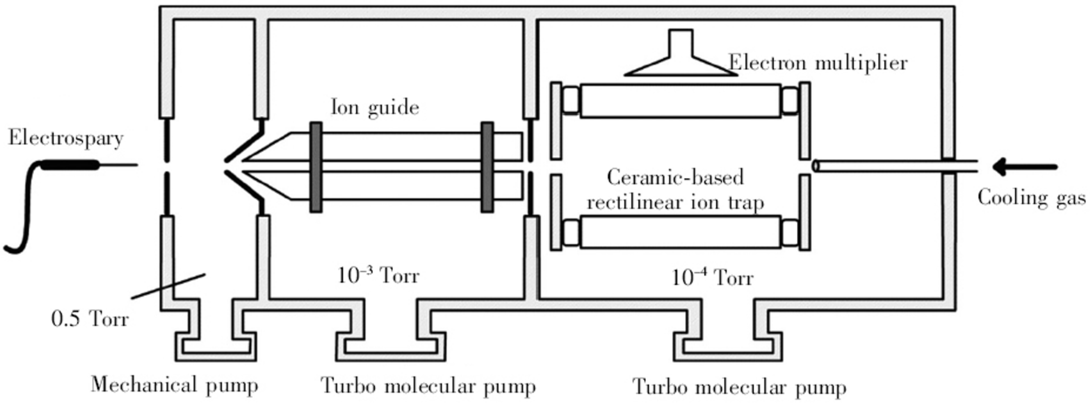

Fig.2 Schematic diagram of ion trap mass spectrometer system