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THE POLLUTANTS DETECTION BY QUADRUPOLE ION TRAP MASS SPECTROMETRY

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Abstract

A quadrupole ion trap mass spectrometer was calculated, designed and machined, with a view to descovering a new way of operating more appropriate to the pollutants analysing. The apparatus is now in testing stage.

Introduction

The quadrupole ion trap (QIT) mass spectrometer is a sensitive and versatil analytical system, able of identifying both large and small molecules and determining their molecular structure.

It is an excellent tool for chemical analysis composed from three hyperbolic electrodes, consisting of a ring and two endcaps.

The ions produced in the ion trap mass spectrometer are trapped and sequentially ejected from the ion trap to a conventional electron multiplier detector.

If a gas species is introduced in the trapping volume the mass resolution of the instrument is greatly improved by contracting the ion trajectories to the center of the trap and reducing the kinetic energy of the ions. In this way the ion of a given mass from a packet, and the ion packed is ejected more quickly and efficiently then a diffuse cloud of ions may be ejected, and the mass resolution will be improved. The mass range of the quadrupole ion trap is considerably higher than that obtained on a quadrupole instrument and lower than that achievable on a time-of flight mass spectrometer.

With the ion trap techniques is possible to perform multiple stage of mass spectrometry greatly increasing the amount of structural information obtainable for a given molecule.

The motion of ions in a quadrupole field can be described mathematically by the solution of the Mathieu equation.

The basic working principle of the quadrupole ion trap

The potential in any point of the inner space of the ion trap can be expressed as:

$$\phi = \frac{\phi_0}{r_0^2}\left(\lambda x^2 + \sigma y^2 + \gamma z^2\right)$$

where ϕ_0 is the applied electric potential, λ, σ and γ are weighting constants for the x, y, z coordinates respectively, and r_0 is a constant defining the quality of ion trap of the device [1].

It is essential that the Laplace condition be satisfied. In this case the field in x, y and z direction is linear and mathematically

$$\lambda + \sigma + \gamma = 0$$

To satisfy the Laplace condition the weighting constants must have the following values: $\lambda = \sigma = 1$ and $\gamma = -2$.

The expression for the potential at any point in a quadrupole ion trap is:

$$\phi_{x,y,z} = \frac{\phi_0}{r_0^2}\left(x^2 + y^2 - z^2\right)$$

or in cylindrical coordinates

$$\phi_{r,z} = \frac{\phi_0}{r_0^2}\left(r^2 - 2z^2\right)$$

ϕ_0 is either an r.f. potential $V\cos\Omega t$ or a combination of a d.c potential, U, of the form

$$\phi_0 = U + V\cos\Omega t$$

where Ω is the angular frequency (in rad s^{-1}).

The force acting on an ion is expressed as:

$$m\frac{d^2x}{dt^2} = \frac{-2e}{r_0^2}\left(U + V\cos t\right)x$$

The equations of motion of an ion in the three dimensional quadrupole field are:

$$\frac{d^2z}{dt^2} - \frac{4e}{mr_0^2}\left(U - V\cos\Omega t\right)z = 0$$

$$\frac{d^2r}{dt^2} + \frac{2e}{mr_0^2}\left(U - V\cos\Omega t\right)r = 0$$

With the substitution:

$$a_z = -2a_r = -\frac{16eU}{m\Omega^2 r_0^2}$$

$$q_z = -2q_r = -\frac{8eV}{m\Omega^2 r_0^2}$$

$$\xi = \frac{\Omega t}{2}$$

the Mathieu equation is obtained. Considering the potential apllied on the ring electrode (ϕ_0) and the potential applied on the end-cap electrodes of an ion trap the following expression is obtained: $r_0^2 = 2z_0^2$

This equation has governed the physical shape of the ion trap [2].

The testing of the QIT

We calculated, designed and realized a quadrupole ion trap with the following parameters: r_0 = 10 mm, z_0 = 12 mm, f = a MHz, V = (0÷2)kV.

In fig. 1 the schematic presentation of the apparatus is done.

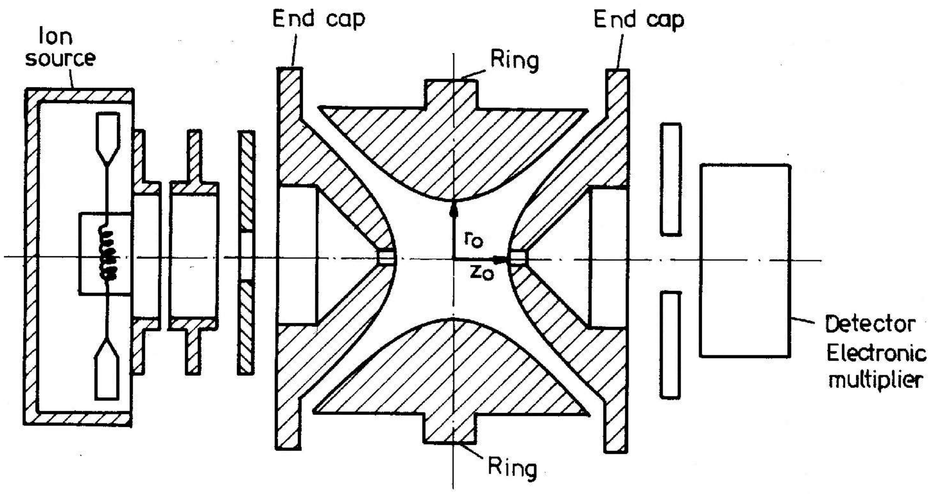

Fig. 1

The ions produced into an ion source, electron bombardament type, are extracted and directed to the ion trap. The ion trap confines the ions and also work as a mass spectrometer in that the mass/charge ratio of the confined ion species can be measured.

The confining capacity of the qudrupole ion trap (QIT) arise from the formation of a trapping potential well when appropiate potential are applied to the electrodes of the ion trap [1].

Ejection of ions from the potential well is achieved by applying an appropriate r.f. potential to one of the ion trap electrode.

The ion species that leave the QIT impinge upon an external detector creating some electric signals dispersed in time which constitute a mass spectrum.

Negative and positive ions can be analysed.

To test the QIT, an experimental installation was achieved, composed from a vacuum stand to produce a high vacuum level of (10^{-6}-10^{-7}) mbar and a mechanical system with electric feedtroughs atmosphere-vacuum, to supply the electronic components of the ion trap.

The folowing electronic elements necessaries to supply the QIT were produced in our laboratory:

- ion source supplying device
- gate puls generator
- radio frequency generator
- low frequency generator
- high voltage supply for ion detector
- electrometric amplifier

The ion source supplying device produces the current for filament warming and the electrode polarization voltages, which assures electron and ion beam generation.

The gate puls generator produces the voltage puls applied to the gate electrode of the ion source to permit extraction of the ion packet from the ion source and its injection in the ion trap.

The radiofrequency voltage applied to the ring electrode of the ion trap (1MHz, 2kV) necessary to produce the inner electric field, that rotates the ions, is supplied by radiofrequency generator.

The low frequency generator produces the 50 kHz voltage, with 0÷10V amplitude, applied to the endcap electrodes, for ion packet extraction.

The electrometric amplifier is a current-voltage convertor based an the electrometric operation amplifier. It bring the output channel of the secondary electron multiplier from the 0-1 μA domain in the 0÷10V domain of the analog-digital measurement current.

The control and measurement device assures the relations between the electronic elements and the computer by:

- generating logic control signals
- generating analogic signals for language control
- measuring the output voltage of the electrometer amplifier
- receiving commands from the computer
- transmitting to the computer the obtained results

The experimental installation was put in function and the first results were obtained.

The experiment are in course.

Conclusions

A quadrupole ion trap mass spectrometer was designed and machined in our laboratory to study new improved methods of spectral exploration typical of different categories of pollutants analysis.

At the moment the apparatus is under way of testing.

REFERENCES

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2. R.E. March, R.J. Hughes, Qudrupole Storage Mass Spectrometry, Chemical Analysis vol 102, John Wiley and Sons, New-York,(1989).