

## COMPUTING UNIT FOR THE QUADRIPOLE MASS SPECTROMETRY AUTOMATIC CONTROL

**Ştefan Popescu**

*National Institute for Research and Development of Isotopic and Molecular Technologies , P.O.  
Box 700, R 3400 ,Fax 420042 , Cluj Napoca ,Romania.*

### ABSTRACTS.

The quadrupole mass spectrometer is one of the most powerful and versatile analytical tools available to the chemists and physicists. Those characteristics of QMG which have most often resulted in its choice over competing instruments are:

Ultrahigh sensitivity, fast scanning capability, no magnets required, linear mass display ,ease of computerization, high reliability, ease of operation, capable of remote operation.

Automatic monitoring of partial pressures in vacuum systems and process control create additional problems for the mass spectrometer. Existing mass spectrometers can be adapted with more or less interface to the operation by a computer .It has been the goal of our developments in the field of quadrupole mass spectrometry to integrate two interface elements into the basic mass spectrometer electronics.

### KEY WORDS.

linear voltage level - pick sample tandem , automatic control and acquisition

### 1.INTRODUCTION.

A big part of the Q.M.S. (Quadripole Mass Spectrometry) applications are in Trace and Hazardous Gas Analysis:

**Air pollution Studies.** The ultrahigh sensitivity and portability of the QMS have made it most desirable for air pollution and exhaust gas analysis studies.

**Industrial Hygiene.** A portable QMS can be used to detect and identify hazardous gases where they are found even though the concentration may be far less than 1 ppm.

**Metabolic Function Respiratory Gas Analysis.** The QMS is ideally suited to the analysis of expired and blood gases because of its small size ,high sensitivity and fast response .

**Residual Gas Analysis and Leak Detection.** The QMS qualities make it invaluable in measurement of residual gases ,contaminants and leaks in vacuum chambers .  
In large environmental chambers the quadripole probe is often operated remotely at a considerable distance.

In advanced technology experiments, a few QMG applications are:

**Molecular and Ion Beam Studies.** In these experiments the QMS probe can be mounted in or close to the beam to measure reaction products, contaminations , or sputtering from surface placed in the ion beam.

**Process Kinetic Studies.** The speed and sensitivity of QMS contribute to permit measurement of kinetic reactions eve where small amounts of samples are involved.

**Irradiated Materials Studies.** The QMS probe can be operated remotely for studying materials irradiated with high fluxes. Here evolved gases and contamination are sensed using high the high sensitivity of the QMS.

The quadrupole mass filter separates ions according to their mass-to-charge ratio ( $m/z$ ) and uses four parallel positioned cylindrical rods on which both HF and DC voltage are applied. HF means a stable High Frequency voltage .

The basic mechanical structure of quadrupol mass spectrometer is:

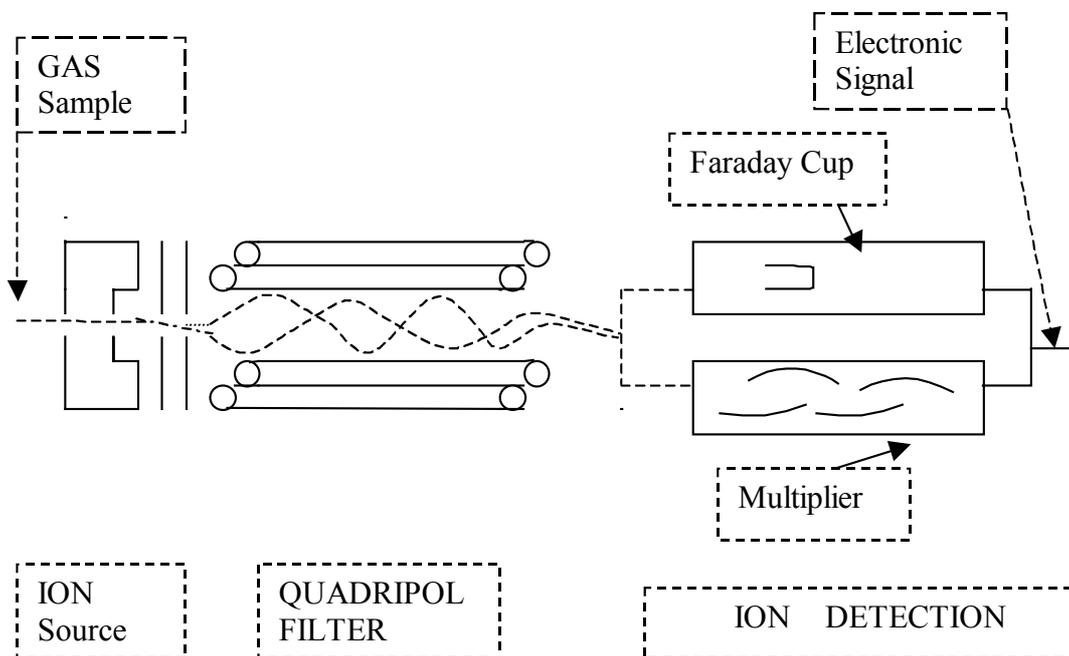


Fig.1. Quadrupole mass filter.

The mass scanning is accomplished by varying the voltage amplitude of DC and RF generator. By choosing a particular RF to DC ratio ,it is possible to select only one specific ion with required  $m/z$  , to pass down the quadrupole filter. All other ions go into unstable oscillating flights pots , strike the quadrupole roads, and are not received by the collector to be measured. The  $m/z$  ratio is expressed in m.a.u. (mass atomic unit)

2. OPERATING PRINCIPLE OF LINIAR MASS SPECTROMETER.

For an automatic processing of the mass signal with one PC, for operations are needed.

2.1.To command the RF and DC generators using a programmable saw-tooth generator.

2.2.To collect the correspondent mass signal accordingly to the supervisor programme.

2.3.To make possible to do the mass scanning at varied scanning speeds, like 1,3 or 10 s /

m.a.u.

2.4.To assure the facility to do programmable cyclic scanning of groups of mass units.

The general functional diagram is:

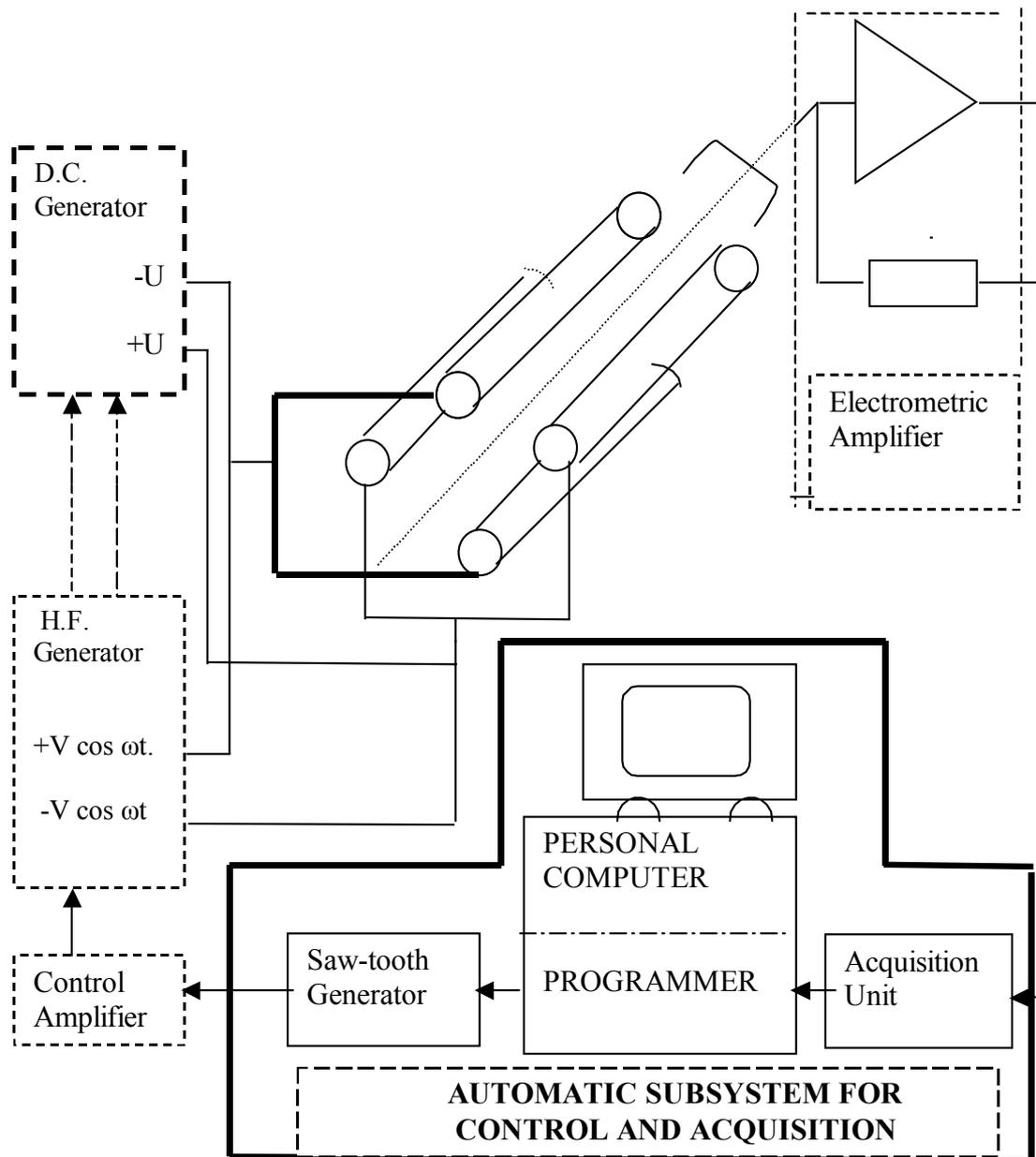


Fig.2.General diagram for the quadripol mass spectrometer system.

### 3.AUTOMATIC SUBSYSTEM FOR CONTROL AND ACQUISITION.

Consequently to the above duties (points 2.1-2.4) of the A.S.C.A., the following structure arises:

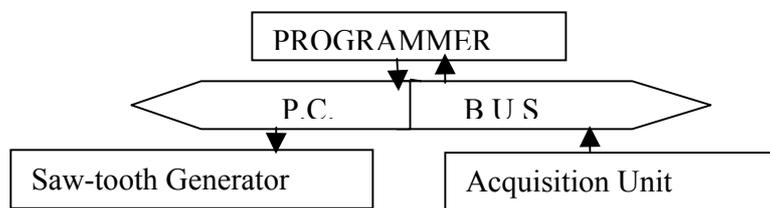


Fig.3.Block diagram of the **Automatic Subsystem for Control and Acquisition.**

.The method of operation of the A.S.C.A. is based on the cooperation between all three functions hardware and software:

3.1.The scanning function is made up by a saw-tooth generator realised on the basis of a numeric to analogue converter. One 12 bits D.A.C. is used , and provide 4096 scanning steps. Therefore , for a range of 1-100 mass atomic units , we have approximately 40 samples per m.a.u. , and for a range of 4-300 m.a.u. we have approximately 13 samples (10 samples being considered quite enough for a good mass pick preservations ).

3.2.The acquisition function is realised on the basis analogue to numerical converter . One 12 bits A.D.C. is used. This means that for a range of 0-10V at electrometric amplifier output , there is a resolution of 10/4094 V, approximately 2,4 mV.

3.3.The ‘tandem’ function , suggest that there is one tandem between a level of scanning voltage and the corresponding mass pick sample .This tandem between mass scanning and pick acquisition is automatic generated and controlled by the software programmer component.

The standard scanning speeds (time/m.u.a.) of the ‘tandem process’ are automatic achieved by program.

### 4.CONCLUSIONS.

The advantages of using one PC to coordinate the internal activity of a quadripolar mass spectrometer are:

4.1. The precision increasing of the **linear voltage level-pick sample tandem** if it is used a better DAC and a better CAD (14,16, 20 bits).

4.2.Oone unlimited combinations numbers of scanning cycles and mass segments.

4.3.The using the same system resources for the automatic mass scanning – mass acquisition process ,and for mathematical processing of mass spectrum , provide a high accuracy of mass pick measurement.

4.4. The likely limitations can easily be improved by updating the AS.C.A.

### 5.BIBLIOGRAPHY.

- [1].SPECTROMASS LTD-Specialist Mass Spectrometers ,February 1989.
- [2].SPECTROSCOPY International November/December 1991, Volume 3,Number 7.
- [3].Mass Spectrometry Reviews-Volume 12/Number 5/6/1993, page 378.
- [4].Journal of The American Society for Mass Spectrometry, JANUARY 1994, Volume 5, Number 1, page 27.
- [5].SPECTROSCOPY EUROPE Vol. 6, No 6, November/December 1994.
- [6]. SPECTROSCOPY EUROPE Vol. 9, No 2, March/April 1994.
- [7].Review of scientific instruments, December 1999 , Volume 70 , Number 12, page 4676.