AERONOMICA ACTA

A - N° 154 - 1975

A programmable control unit for a balloon borne quadrupole mass spectrometer

by

E. ARIJS and D. NEVEJANS

FOREWORD .

The paper "A programmable control unit for a balloon borne quadrupole mass spectrometer" will be published in the Review of Scientific Instruments.

AVANT-PROPOS

Le texte "A programmable control unit for a balloon borne quadrupole mass spectrometer" sera publié dans Review of Scientific Instruments.

VOORWOORD

De tekst "A programmable control unit for a balloon borne quadrupole mass spectrometer" zal gepubliceerd worden in Review of Scientific Instruments.

VORWORT

Die Arbeit "A programmable control unit for a balloon borne quadrupole mass spectrometer" wird in Review of Scientific Instruments heraugegeben werden.

A PROGRAMMABLE CONTROL UNIT FOR A BALLOON BORNE QUADRUPOLE MASS SPECTROMETER

by

E. ARIJS and D. NEVEJANS

Abstract

For the measurement of the ionic composition of the atmosphere a reprogrammable control unit for a quadrupole mass filter has been constructed. This unit, the heart of which consists of two programmable read only memories, allows the choice of 16 different measuring jobs by 6 telecontrol channels.

The underlying principles as well as the performance of the unit are described.

Résumé

Une unité de contrôle programmable pour un filtre de masse quadrupolaire a été construite pour la mesure de la composition ionique de l'atmosphère. Cette unité, contenant deux mémoires du type "read only", permet le choix de 16 programmes de mesure par 6 canaux de télécommande.

On décrit les principes de fonctionnement ainsi que les performances du système.

Samenvatting

Voor het meten van de ionaire samenstelling van de atmosfeer werd een programmeerbare controle eenheid voor een quadrupool massa filter geconstrueerd. Deze eenheid die gebaseerd is op het gebruik van 2 programmeerbare "read only memories" laat toe de keuze te maken uit 16 verschillende meetprogrammas door middel van 6 telecommando kanalen.

De principes en de resultaten bekomen met deze eenheid worden in deze tekst beschreven.

Zusammenfassung

Eine programmierbare Kontroleinheit für ein quadrupolarer Mass Filter wurde für die Messung der atmosphärischen Ionenkomposition gebaut. Diese Einheit besteht aus zwei "read only memories" und erlaubt 16 verschiedenen Messungen durch 6 Fernsteuerungs-kanalen.

Die Prinzipe sowie die Ergebnisse dieser Einheit werden beschrieben.

1. INTRODUCTION

The ionic composition of the atmosphere has always been one of the major interests of the aeronomist. Thus far however identification of the atmospheric ions has only been made at altitudes greater than 64 km (1-3). For lower altitudes only global ion densities are available (4-6).

In order to determine the ion composition of the stratosphere at about 40 km altitude a balloon borne mass spectrometer has been built at our institute. This instrument basically consists of a quadrupole mass filter, built in a liquid helium cooled cryopump. On top of this a molecular leak (7-8) has been mounted, through which the atmospheric ions emerge into the mass filter. The ion detector is a spiraltron electron multiplier, the signals of which are treated by pulse counting techniques.

Since most of the global ion-density measurements indicate an ion density of the order of 10^3 cm^{-3}, a very low pulse counting rate can be expected if the ions are filtered according to their mass to charge ratio. Therefore a procedure has been choosen, which consists of measuring the ion counting rate in mass domains, rather than at definite mass peaks. This measuring procedure, which will be discussed to a larger extent in the next section, requires a special quadrupole control unit. It is the aim of this paper to describe the technical details of this control unit.

As will become clear from the text, the underlying principles of the unit can be applied to many other balloon borne experiments, in which by a limited number of telecontrol channels several parameters have to be changed.

2. OUTLINE OF THE MEASURING PROCEDURE

As has been shown by Paul and coworkers (9) the equations of motion within the quadrupole field are Mathieu differential equations, which can be solved in terms of the ion mass (m), the DC (U) and RF voltage (V.cosωt), applied on the filter rods and the field

radius (r_0). By putting :

$$a = \frac{8eU}{m\omega^2 r_0^2} \qquad (2.1)$$

$$q = \frac{4eV}{m\omega^2 r_0^2} \qquad (2.2)$$

and solving the equations of motion, the well know stability diagram of figure 1 is obtained.

Under normal laboratory operation the ration U/V is choosen such as to make the scanning line, the slope of which is determined by U/V, intersect the top of the stability region and to obtain a high resolution. By choosing however the working line such as line 2 in figure 1 the quadrupole becomes a band pass mass filter and all ions lying in a mass domain between m_1 and m_2 are passed. The limiting masses m_1 and m_2 are then given by :

$$m_1 = \frac{4eV}{q_2 r_0^2 \omega^2} \qquad (2.3)$$

$$m_2 = \frac{4eV}{q_1 r_0^2 \omega^2} \qquad (2.4)$$

Theoretically the mass domain, which is transmitted by the quadrupole is completely defined by two parameters U and V, once the working frequency ω and the geometry are choosen. It must be mentionned however that the foregoing treatment is oversimplified. In reality many more factors, such as the radial velocity of the ions, the fringing fields, and the finite length of the filter must be taken into account.

The quadrupole mass filter used in our arrangement is the Finningan model 750. Its characteristics are summarized in the following table :
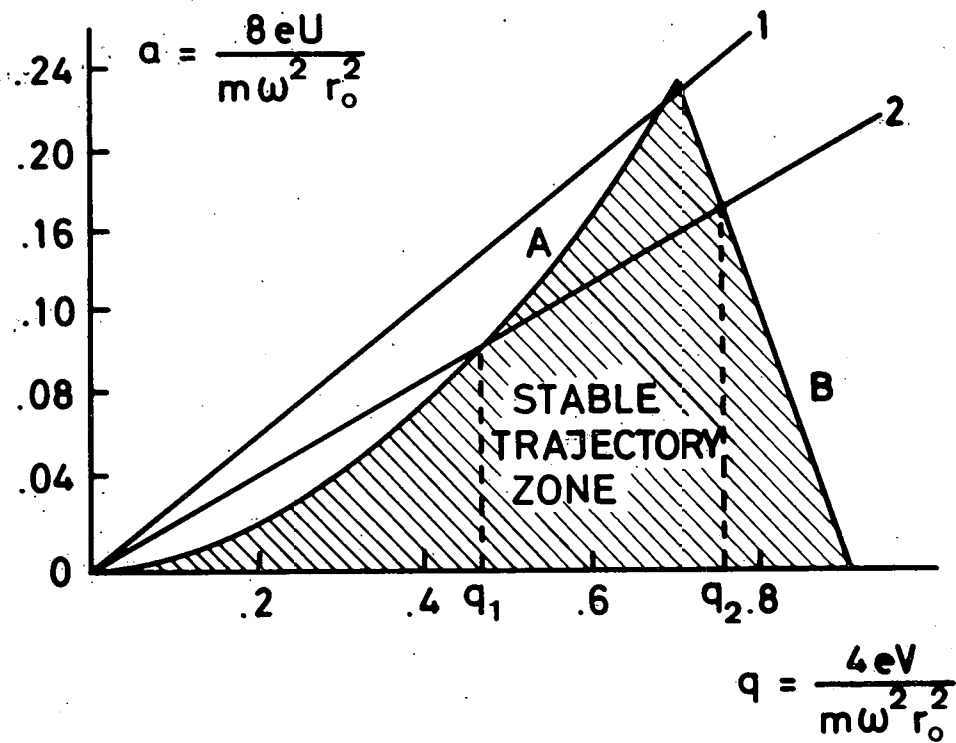
$$a = \frac{8\,eU}{m\,\omega^2\,r_o^2}$$

$$q = \frac{4\,eV}{m\,\omega^2\,r_o^2}$$

STABLE TRAJECTORY ZONE

Fig. 1.- Stability diagram of the Mathieu differential equations.

Rod radius	:	.25 inch
Field length	:	4.5 inch
Radiofrequency	:	2.14 MHz
Maximum injection angle	:	60^0 (at reduced resolution)
Ion injection energy	:	0 - 150 eV
Peak R.F. voltage (ampl.)	:	300 volts
Mass range	:	0 - 110 amu

The last two parameters are determined by the quadrupole voltage supply, which is built in such a way that the DC and RF voltages U and $V\cos\omega t$ are determined by applying proportional control voltages U_c and V_c. A more detailed description of this unit, which has been especially built for this experiment, would be beyond the scope of this paper.

Thus by using the proper control voltages U_c and V_c a mass domain can be filtered by the quadrupole.

In order now to determine the ionic composition of the stratosphere the ion counting rate will be measured in several mass domains. As a first step the regions 5-30 amu, 30-55 amu, 55-80 amu and 80-105 amu will be investigated. Subsequently this domains will be split up in smaller mass domains, each 5 amu large and depending upon the counting rates in these regions a scanning with a higher resolution will be made in several mass domains.

To realize ion counting in a mass domain, the electronics must receive three information factors, namely U_c and V_c (which are proportional to U and V and thus determine the mass domain) and the measuring time t. (In reality however U_c/V_c is transmitted instead of U_c).

For scanning a mass domain however, two additional parameters are necessary, namely ΔV_c and N. In the latter case counting will be realized in N mass domains during a time t, each domain characterized by the following DC and RF voltages :

$$U = \frac{U_c}{\alpha} \left[1 + j \frac{\Delta V_c}{V_c} \right] \qquad (2.5)$$

$$V = \frac{V_c}{\beta} \left[1 + j \frac{\Delta V_c}{V_c} \right] \qquad (2.6)$$

where $j = 0, 1, 2, ..., N-1$ and α and β are the proportionality factors of $U_c = \alpha U$ and $V_c = \beta V$.

In view of the fact that only a limited number (eight) of telecontrol channels were available and that 2 were already used for general purposes (power on-off and squib activation) a unit has been devised which controls the mass domain measurements as well as the scannings by only six telecontrol channels (4 address lines and 2 interrupt lines).

3. GENERAL DESCRIPTION OF THE UNIT

A block diagram of the controller's architecture is shown in figure 2. Essentially the controller consists of a central unit, called the "Master Controller and Memory" (MCM) and several subunits, called "slaves", the number of which can be seven at maximum. In fact these slaves are counters, registers, and digital to analog converters controlling the mass domain and measuring time setting of the mass spectrometer, as will be explained later.

The slaves communicate with MCM through a one directional serial data bus (T-bus), along which MCM transfers binary data stocked in its memory area of 256 words. This memory area is divided in stacks filled with parameters, each parameter dedicated to a particular slave. Every time one wants to switch over to a new mass domain measurement an interrupt circuit is activated by telecontrol, which forces MCM to search in its memory for a new parameter stack needed by the slaves.

In absence of intervention T-bus remains dead, unless a task (measurement) is fully accomplished. In that case one of the slaves responds with an end-of-task signal, starting

4 REFERENCE ADDRESS LINES

MEMORY REFERENCE REGISTER (8 BITS)

MEMORY ADDRESS REGISTER (8 BITS)

PROMS (256 WORDS OF 16 BITS)

TRANSFER REGISTER (16 BITS)

CONTROL LOGIC

INTER-RUPT LOGIC

INTERRUPT LINES

CLOCK SIGNALS

MASTER CONTROLLER AND MEMORY

T-BUS

12 BITS SHIFT REGISTER

MEASURING TIME COUNTER

SLAVE 5

12 BITS SHIFT REGISTER

NUMBER OF STEPS COUNTER

SLAVE 4

T-BUS

12 BITS SHIFT REGISTER

MULTIPLYING DIGITAL TO ANALOG CONVERTER

SLAVE 3

12 BITS SHIFT REGISTER

AC VOLTAGE REGISTER

SLAVE 1

12 BITS SHIFT REGISTER

STEP VOLTAGE REGISTER

SLAVE 2

SERIAL ADDER

DIGITAL TO ANALOG CONVERTER

T-BUS
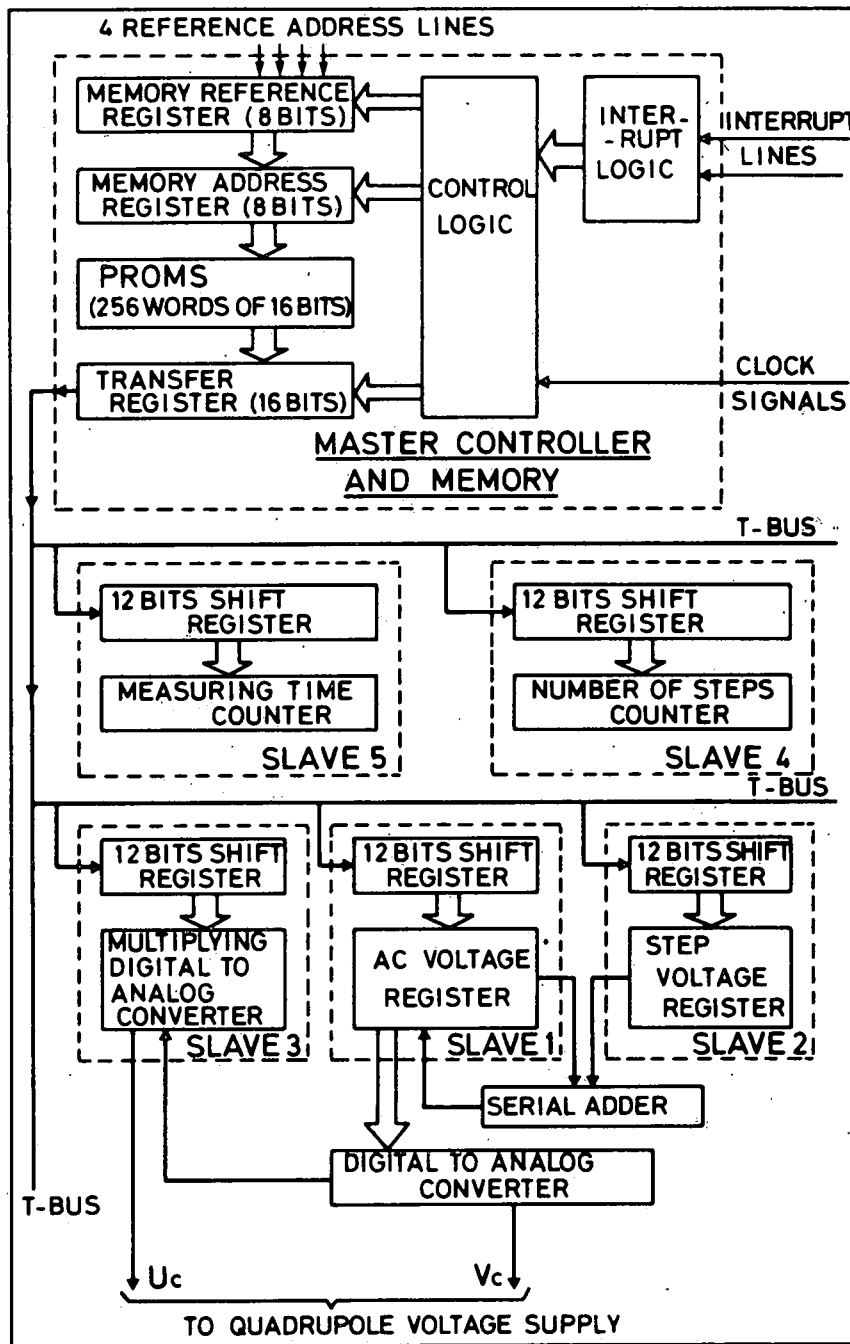
Uc

Vc

TO QUADRUPOLE VOLTAGE SUPPLY

Fig. 2.- General block diagram of the control unit.

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MCM's automatic search mode. This means that MCM takes the parameters needed for the next measurement from the stack, immediately following the last one in use. In other words, in this mode MCM sequentially runs the measurements programmed in its memory.

Another interesting feature of MCM is that when it works in the automatic search mode, it is able to jump after task completion to a stack located anywhere in its memory. In this way looping of programmed tasks is made possible.

4. MASTER CONTROLLER AND MEMORY

As explained in section 3 the Master Controller and Memory is the heart of the reprogrammable controller. In the first place MCM stores all the binary information needed by the rest of the system. Its memory consists of two electrically programmable read only memories (PROMS) of 2048 bits. These circuits (National Semiconductor MM 4203 Q) have non volatile memory and are programmed by charge storage in floating silicon gates. Erasure of information is accomplished by irradiation with U.V. light, which results in discharging the gates to their initial uncharged condition.

The PROMS are organized as 256 words of 16 bits. Words 0 to 15 are reference words (see figure 3, format a), which allow access to words 16 upto 255 through only 4 telecontrol address lines. The latter part of memory is divided in stacks of data words, configured conformal to format b of figure 3. The lower 12 bits of each word represent a parameter value and bits 16, 15 and 14 form the address of the slave which should accept that particular parameter. Furthermore the last data word of a stack has an end-of-stack (EOS) bit equal to 1, telling the MCM logic that it is the last word to be transmitted along T-bus.

Two ways of interrupting the system exist : "absolute priority interrupt", which interrupts on the next 1 second pulse and "search after task interrupt", which waits with interrupting until the actual task is finished. In both cases MCM reacts on the interrupt command by entering the reference word address of 4 bits, transferred by telecontrol, into its memory reference register. The output of the PROMS now holds the selected reference

a) BIT 16 → `0 0 0 0 1 X X X R_8 R_7 ... R_2 R_1` ← BIT 1

SLAVE ADDRESS

FUNCTION CODE 01 → REFERENCE WORD

REFERRED ADDRESS

b) `✳ ✳ ✳ 0 D_12 D_11 ... D_2 D_1` / `1`

SLAVE ADDRESSES 001 TO 111

END-OF-STACK BIT = 1 MEAN LAST WORD OF A STACK

12 BIT DATA PORTION

c) `0 0 0 0 0 X X X J_8 J_7 ... J_2 J_1`

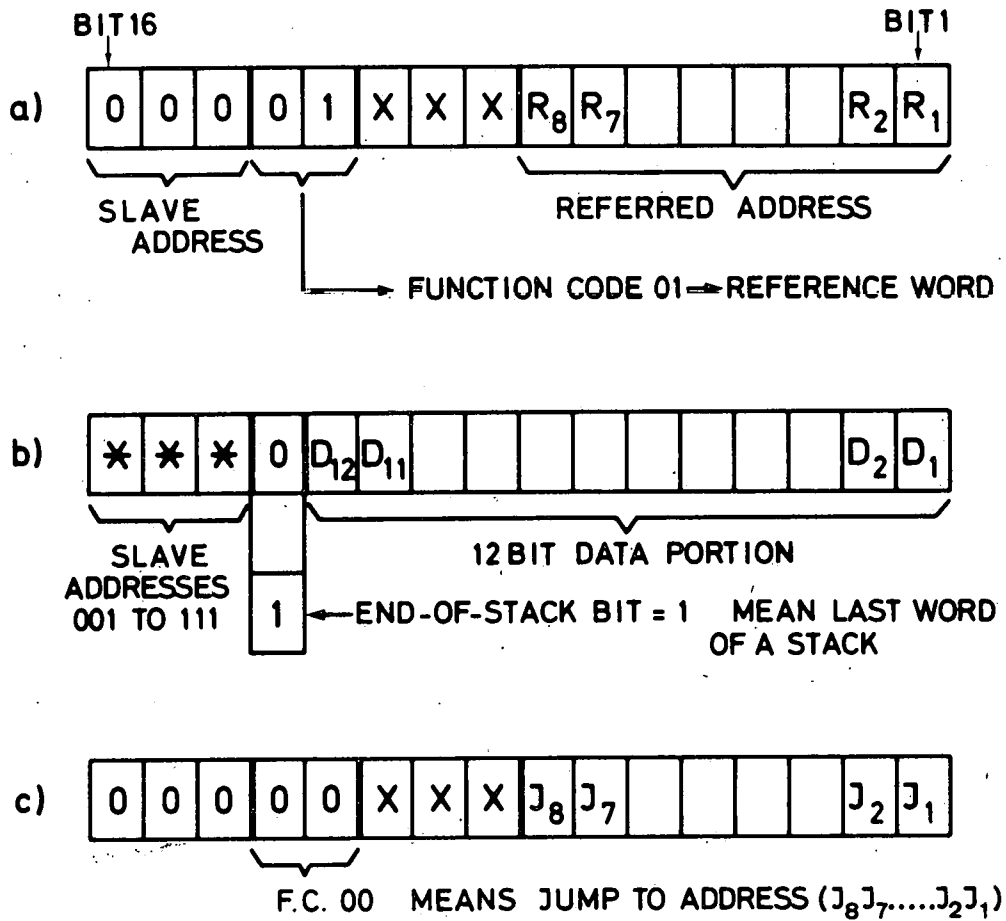F.C. 00 MEANS JUMP TO ADDRESS $(J_8 J_7 ..... J_2 J_1)$

Fig. 3.- Formats of the different memory words : a/ reference words, b/ data words, c/ jump.

word. It is then moved along T-bus to the memory reference register (slave 0) which retains only the 8 bit address portion of it and shifts it into the memory address register. Now all words from this address upto the word with the EOS bit set to 1, are pushed on T-bus by MCM's transfer register, shown in figure 4. Finally MCM stops with its memory address register content equal to the address of the first word of the succeeding stack.

When not receiving any interrupt command MCM waits in a stand-by mode until an EOS signal occurs. As soon as this pulse appears MCM responds by putting the next stack on T-bus.

Jumping or looping in memory works almost in the same way as interrupting. If the first word MCM starts transmitting along T-bus corresponds to format c of figure 3, it is moved towards the memory reference register (slave address 0), which retains only the 8 address bits J8 to J1. From this point on MCM follows the same procedure as in the case of interrupt : the address is loaded into the memory address register and so on.

5. SLAVE UNITS

In the foregoing sections it has been described how the Master Controller and Memory reacts on the intervention of telecontrol. We will now explain how the subunits or slaves are accepting data from MCM.

All slaves are connected to T-bus and to 3 slave address lines, carrying the slave address portion of the actual addressed memory location. Every time MCM pushes a word on T-bus, this address helps the slave to decide if the word was destinated to it. If so, the slave address decoder enables input to a 12 bit shift register, retaining only the lower 12 bits of the accepted word (figure 5).

The bits received in this way become available to other circuits. Two slaves are driving two 12 bit digital to analog converters, which control the RF and DC voltages on the
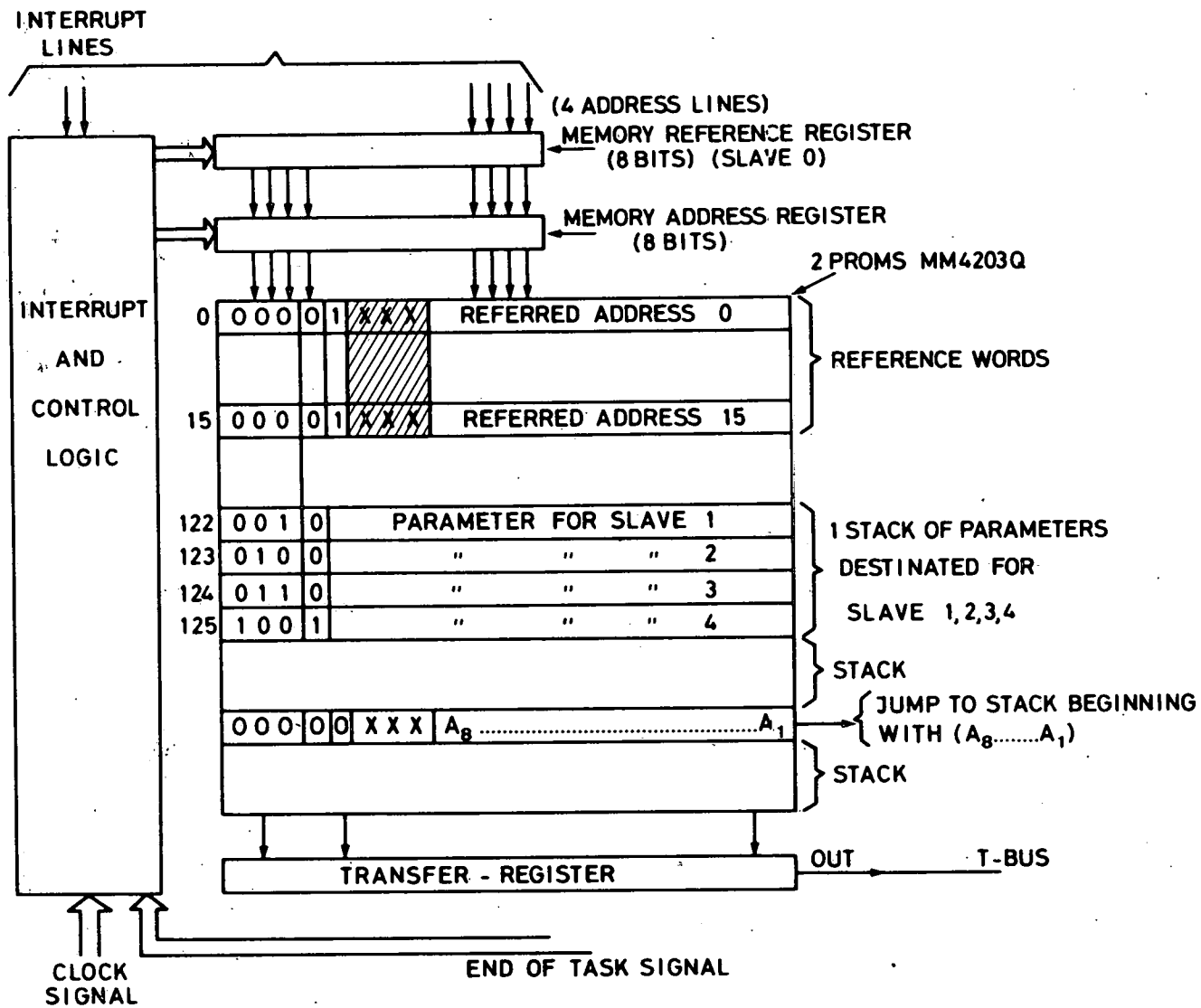
Fig. 4.- Interaction scheme of the memory and the different registers of the Master Controller and Memory.
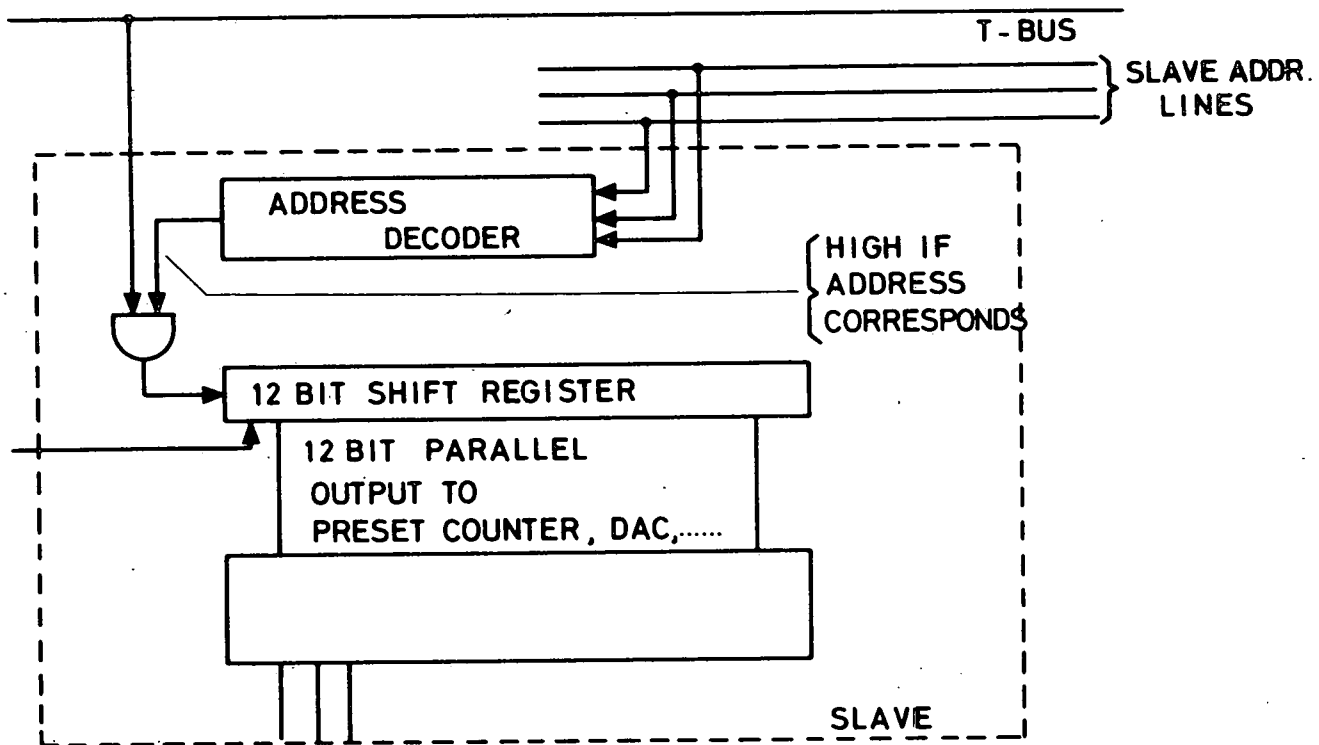
Fig. 5.- Schematic representation of the interaction between MCM and the slaves.

quadrupole rods. Another one produces a gating signal for the ion counter and thus determines how many seconds a counting in a certain mass domain will last.

In fact with a total of three slaves a system can be built capable of measuring the number of ions counted in a predetermined mass domain during a predetermined time. Two other slaves however have been added, offering the possibility to perform measurements in small succeeding domains by adding a fixed amount to the AC voltage and keeping the DC/RF voltage ratio constant. The two parameters concerned with this feature are the RF step size ΔV_c and the number of steps N.

6. PERFORMANCE OF THE SYSTEM

To test the performance of the system, the experimental set up as pictured in figure 6 has been used. Actually this arrangement is the balloon borne mass spectrometer package itself, with some slight modification, such as :

i.   Installation of an electron impact ion source above the molecular leak
ii.   Replacement of the batteries by a set of laboratory power supplies
iii. Pumping by an external Vacion pump (50 liters/sec), instead of the cryopuming system
iv.   Simulation of the telecontrol channels by a switch box, which allowed us to simulate all the telecontrol commands, which can be given in flight conditions
•v.   Replacement of the ion counting system by an electrometer and a strip chart recorder.

In a first test the PROMS of MCM have been programmed as indicated in figure 7. The first 16 words of the PROMS refer to 16 different reference jobs, each of them consisting of 5 tasks (stacks) and a jump. As can be seen from figure 7 the last tasks of one reference job differ from the first task only by their value of U_c/V_c. Actually task 1 of reference job 13, which is completely shown in figure 7, consists of measuring succeedingly 1 second in small mass intervals, each of them characterized by formulas (2.5) and (2.6) with $N = 240$, $V_c = 940$ mV, $\Delta V_c = 4.88$ mV and $U_c/V_c = 0.1803$. The proportionality factors between
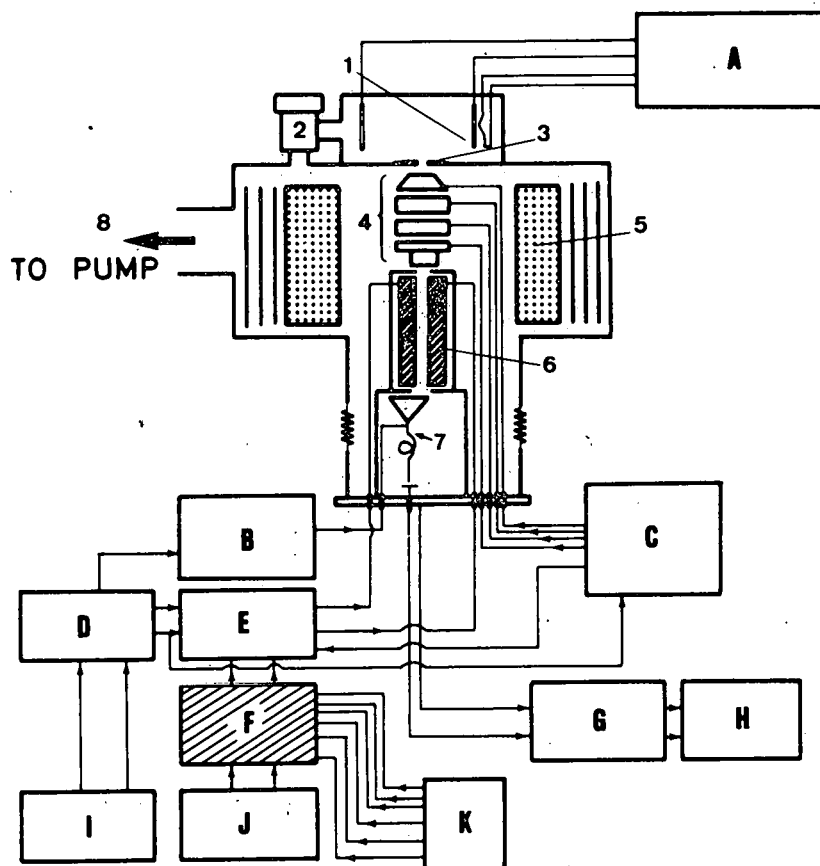
Fig. 6.- *Experimental set-up used during the tests* 1 : Electron impact ion
source, 2 : By-pass valve, 3 : Molecular leak, 4 : Ion lens,
5 : Cryopump, 6 : Quadrupole mass filter, 7 : Channeltron electron
multiplier, 8 : to Vacion pump (50 l/s), A : Ion source control unit,
B : High voltage supply (2.700 V), C : Ion lens control unit, produces
also some voltages for the quadrupole voltage supply, D : Booster,
E : Quadrupole voltage control unit, F : Programmable control unit,
G : Electrometer (Keithley model 417A), H : Strip Chart recorder
(Texas Instr.), I and J : Power supplies (Hewlett-Packard) delivering
28 and 20 V respectively (each replacing one set of batteries),
K : Switch box simulating the telecontrol channels.

16 REFERENCE ADDRESSES

Addr																	
0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0	0	
1	0	0	0	0	1	0	0	0	0	0	0	1	1	1	1	0	
13	0	0	0	0	1	0	0	0	1	1	0	0	0	1	1	1	REFERS TO 199
14	0	0	0	0	1	0	0	0	1	1	0	1	0	1	0	1	
15	0	0	0	0	1	0	0	0	1	1	1	0	0	0	1	1	
199	0	0	1	0	1	0	0	0	0	0	0	1	1	0	0	0	
200	0	1	1	0	1	1	1	0	0	1	1	0	1	1	0	0	TASK 1
201	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	
202	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	
203	1	0	1	1	0	0	0	0	1	1	1	1	0	0	0	0	
204	0	0	1	0	1	0	0	0	0	0	0	1	1	0	0	0	TASK 2
205	0	1	1	1	1	1	1	0	1	0	0	0	0	0	0	0	
206	0	0	1	0	1	0	0	0	0	0	0	1	1	0	0	0	TASK 3
207	0	1	1	1	1	1	1	0	1	0	0	1	0	1	0	0	
208	0	0	1	0	1	0	0	0	0	0	0	1	1	0	0	0	TASK 4
209	0	1	1	1	1	1	1	0	1	0	1	0	1	0	0	0	
210	0	0	1	0	1	0	0	0	0	0	0	1	1	0	0	0	TASK 5
211	0	1	1	1	1	1	1	0	1	0	1	1	1	1	0	0	
212	0	0	0	0	0	0	0	0	1	1	0	0	0	1	1	1	JUMP TO 199

241 TO 256 NOT USED

0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Fig. 7.- Content of the read only memories as programmed for a first test experiment.

- 16 -

U_c and U and V_c and V have been measured separately and are given by :

$$U = 27.4\ U_c \quad \text{and} \quad V = 29.8\ V_c$$

The measurement of task 1 in job 13 thus corresponds to a scanning from mass 11.3 to mass 25.3 amu, with a resolution defined by U/V = 0.166 (the step size ΔV_c is so small here that we can really speak of a scanning). As a matter of fact the resolution in terms of U/V can be varied from 0.108 to 0.180 in steps of approximately 9.10^{-4} through the 80 different tasks of the 16 reference job. Each job can be separately accessed by an interrupt.

Some typical spectra obtained in this way are shown in figure 8. The masses 12, 14, 15, 16, 17 and 18, which originate mainly from hydrocarbons and water vapor, are clearly recognized. The corresponding resolutions of figure 8 are given in table 1.

The value $(U/V)_{calc}$ has been computed by means of the memory content of the PROMS and the $(U/V)_{meas}$ values have been obtained by measuring the control voltages at the output of the control unit. As can be seen the agreement is excellent, taking into account the possible measuring errors.

TABLE 1.- Calculated and measured resolutions for the different measurements
of fig. 7 and fig. 8.

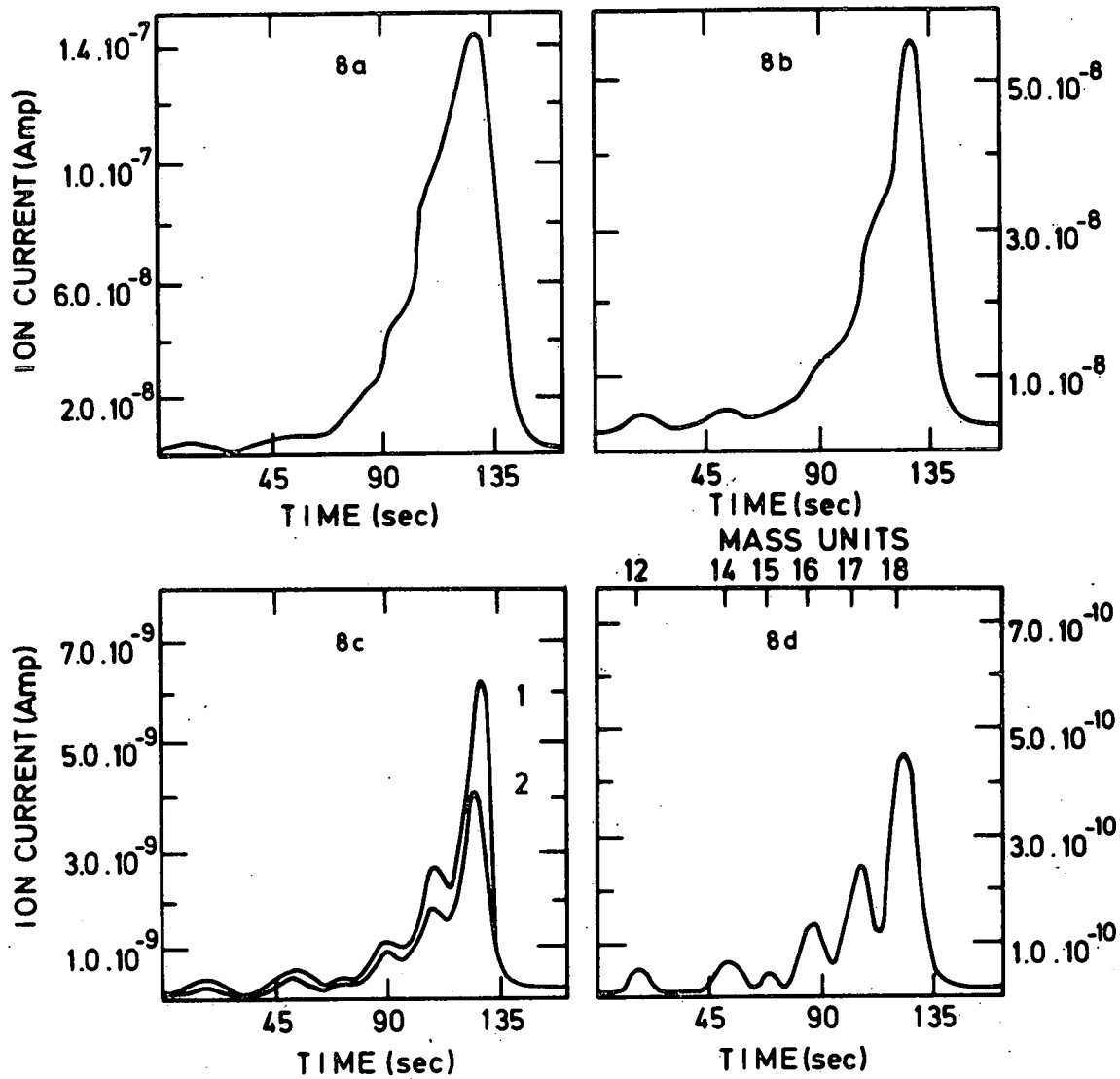| Ref. Job	Task Nr.	Fig.	$(U/V)_{calc}$	$(U/V)_{meas}$
11	1	8a	0.1568	0.1550
12	1	8b	0.1613	0.1605
13	1	8c(1)	0.1657	0.1649
13	2	8c(2)	0.1665	—
14	1	8d	0.1702	0.1693

Fig. 8.- Mass spectra obtained with PROMS as indicated in figure 7.

Furthermore it is noticed that the separation between the different mass peaks becomes more clear when U/V is increased, which is in agreement with the quadrupole theory. It might be surprising that at values of U/V > 0.167 the transmittance of the mass filter is not yet reduced to zero. The accuracy of the U/V values however, depends entirely on the accuracy with which the proportionality factors a and β have been obtained. Since the measurement of these factors is extremely difficult a slight fault can easily be introduced here.

The fact that no better mass resolution could be obtained, than the one in figure 8d is due to high frequency spikes which have been observed at the output of the mass filter control unit. For our purposes however, the obtained resolution is quite satisfactory.

As a second test the PROMS have been reprogrammed as is partly tabulated in table 2. Instead of the control voltages, the actual DC and RF voltages are tabulated, taking into account the measured proportionality factors.

The control voltages have been calculated by setting forward the corresponding mass domain and by approximating the curves A and B of figure 1 by (10)

$$a = \frac{q^2}{2} - \frac{.7}{128} q^4 \qquad (6.1)$$

and

$$a = 1 - q - \frac{q^2}{8} + \frac{q^3}{64} - \frac{1}{1536} q^4 \cdot \cdot$$

Again 16 reference jobs have been programmed, of which only 5 are shown in the table. The other jobs are those described in section 2.

The mass spectra recorded with the new programmed PROMS are shown in figures 9 and 10. Figure 10 represents the ion current measured in succeeding small intervals, which can be calculated by applying formulae (2.3) and (2.4). In this case q_1 and q_2 are
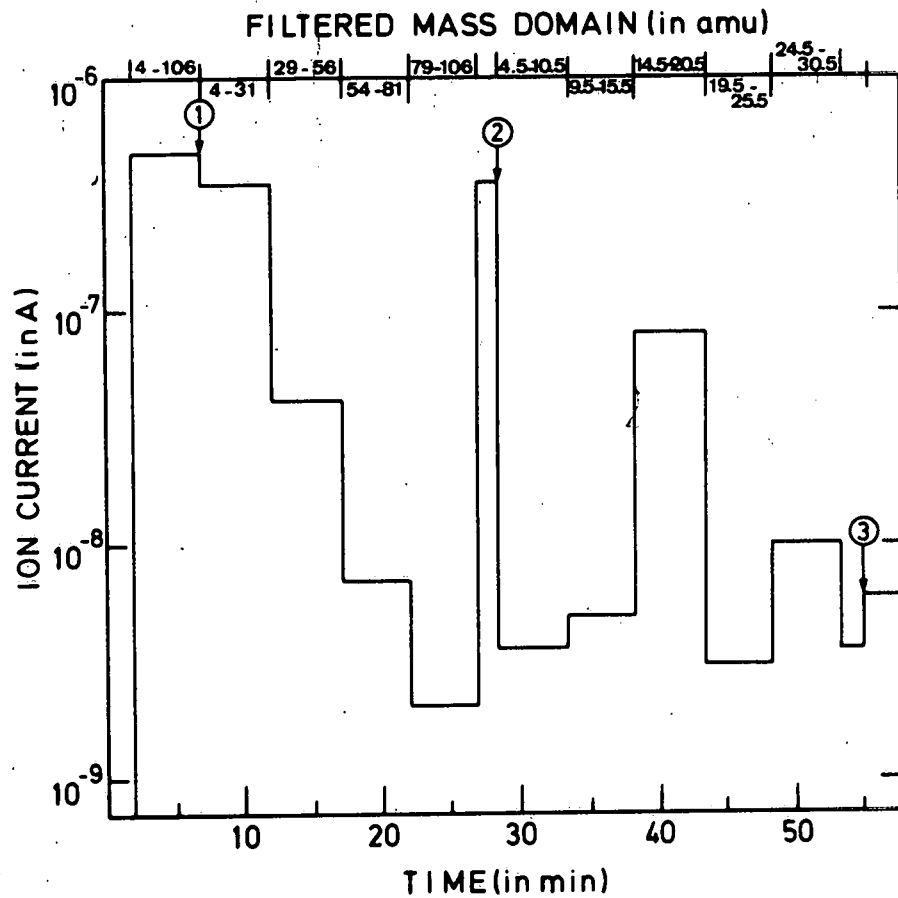
Fig. 9.- Mass spectra as obtained with the reference jobs 0, 1, 2 and 3 of table 2.
The meaning of the encircled numbers is
1 : absolute priority interrupt to ref. job nr 1
2 : absolute priority interrupt to ref. job nr 2
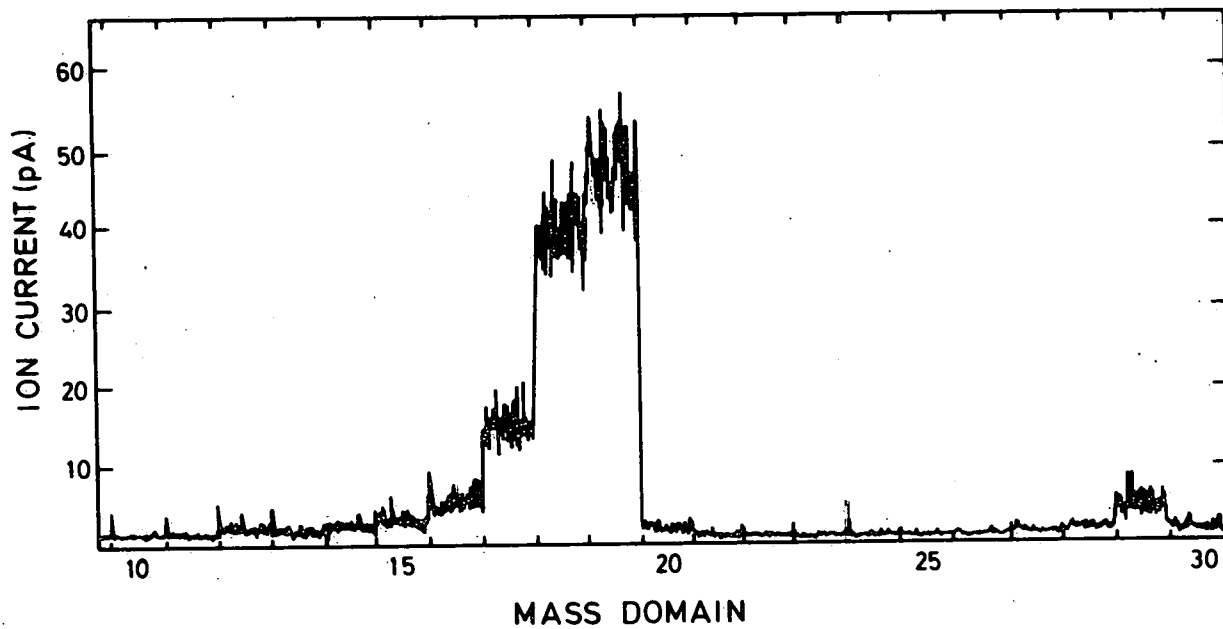3: absolute priority interrupt to ref. job nr 3.

Fig. 10.- Mass spectrum obtained with ref. job nr 6 of table 2.

TABLE 2.- Contents of the PROMS for a second test, the corresponding mass spectra of which
are shown in fig. 9 and 10.

Ref. job	Task	V (volts)	U/V	ΔV (volts)	Time (sec)	Nr of steps	Mass domain
0	1	10	.180	1	120	1	0 - 0
	2	12.5852	$8.44 \ 10^{-3}$	1	300	1	4 - 106
1	1	12.189	.02794	1	300	1	4 - 31
	2	79.2417	.09889	1	300	1	29 - 56
	3	142.728	.12192	1	300	1	54 - 81
	4	205.475	.13333	1	300	1	79 - 106
2	1	12.5684	.08408	1	300	1	4.5 - 10.5
	2	25.4018	.11383	1	300	1	9.5 - 15.5
	3	38.0031	.12788	1	300	1	14.5 - 20.5
	4	50.5239	.13607	1	300	1	19.5 - 25.5
	5	63.0073	.14143	1	300	1	24.5 - 30.5
3	1	75.4706	.14521	1	300	1	29.5 - 35.5
	2	87.9207	.14801	1	300	1	34.5 - 40.5
	3	100.364	.15018	1	300	1	39.5 - 45.5
	4	112.801	.15191	1	300	1	44.5 - 50.5
	5	125.235	.15331	1	300	1	49.5 - 55.5
. .	. .	... ...	.. ..	. .	. .	. .	.. . .
6	1	0.00	.166	2.48	6	100	0 - 100
.	.	...	..	.	.	.	.. . ..

intersecting points of the curves A and B of figure 1, the equations of which are given by formulae (6.1) and (6.2), and the straight line

$$a = 2\, U_j/V_j \cdot q$$

where U_j and V_j are given by

$$U_j = U/V \cdot (V + j\Delta V)$$

$$V_j = V + j\Delta V$$

j being the number of the mass domain as indicated in figure 10. Again the mass peaks of water (mass 18) and its sattelites can be clearly recognized.

From the foregoing tests it can be concluded that the designed control unit is quite suitable for the measurements described in section 1 and 2.

The complete unit can be mounted on two printed circuit boards of 10 x 13,5 cm. Furthermore is must be noticed that, since all the electronics, except the PROMS, are executed in COSMOS components, the power consumption is very low, which makes it very attractive for balloon borne measurements.

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