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WITH THE FAST DATA ACQUISITION SYSTEM OF A TIME-OF-FLIGHT MASS SPECTROMETER

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SYNOPSIS OF A COMPUTER PROGRAM DESIGNED TO INTERFACE A  
PERSONAL COMPUTER WITH THE FAST DATA ACQUISITION SYSTEM  
OF A TIME-OF-FLIGHT MASS SPECTROMETER

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## INTRODUCTION

This report is extracted from three other publications which contain more detailed descriptions of the instrumentation [1,2] and the complete program [3,4] for interfacing a personal computer with the fast digital data acquisition system of a time-of-flight mass spectrometer. It summarizes the essential features used in high-repetition rate spectrometry to capture complete mass spectra every 20-35 microsec -- providing the time resolution needed for the study of various transient events. The goal was to record in a very manageable system the large amounts of data produced by the spectrometer in short time intervals and to have the immediate operator option of presenting the recorded spectral data in several different formats. An important part of the goal was to have the system do this with a high degree of automation, which included the tasks of mass labeling the spectra and logging the pertinent instrumental parameters.

In implementing the above, the design objectives of the program included the following:

- 1) A means for labeling a mass axis for spectrum displays.
- 2) A means for calibrating the system so that the mass labeling of the different species is correct.
- 3) A display of all the spectra (per event) resolved over time (three-dimensional display).
- 4) A means for displaying every single spectrum two dimensionally.
- 5) A display of the average of all spectra acquired per experimental event (in a two-dimensional display).

The program to control the system was written in FORTRAN 77 interfaced with PASCAL, graphics, and I/O software.

## EXPERIMENTAL SETUP

### A) Mass Spectrometer

The time-of-flight mass spectrometer has been described

previously [1]. The vapors to be analyzed are obtained either by vaporizing a sample of solid material with a pulsed or a continuous laser beam or by leaking vapor at a constant rate from a reservoir. With a constant-leak reservoir containing a known gas and known leak rate, the spectrometer is calibrated for both mass labeling and sensitivity.

Utilizing the basic principle of time-of-flight mass spectrometry, the flight time of an ion is expressed by the following relationship:

$$t_f = k_1 (m/z)^{1/2} + k_2$$

where

- $t_f$  = time of flight,
- $k_1$  = constant that depends on the potential difference by which the ion has been accelerated and the length of the flight path,
- $k_2$  = constant that depends on the time delays within the system.

These constants are determined in the computer program from a least-squares statistical calibration using a known gas.

#### B) Data Acquisition Instrumentation

This is a somewhat updated version of an earlier one [2]. As can be seen in figure 1, the amplified signal is fed into the Transiac [5] CAMAC (Computer Automated Measurement and Control) system. The Transiac 2101 Transient Recorder system consists of a Model 2001S Transient Recorder, a Model 4100 Averaging Memory Module, and a Model 6101 CAMAC interface for the IBM-XT computer. The function of the 2001S is to digitize the incoming signals and hold them in its memory. The 4100 is a summing device which is operational in the averaging mode.

The system can work in two modes: transient mode and averaging mode. In the transient mode, the 2001S memory is set either to 16 or 32 kilobytes (the maximum memory size of the 4100 is 8 kilobytes). The 2001S then transfers data from its memory to the computer via the 6001 CAMAC interface. The transient mode is used to obtain time-resolved spectra of the vapor pulse by storing individual spectra (or segments thereof) sequentially in the available memory. In the averaging mode, the memory in the 2001S is set only long enough to cover the desired segment of a single spectrum (8 kilobytes or less). Thus, as the 2001S digitizes the data, spectra are additively accumulated in the 4100 memory. The system can be programmed for 1 to 65536 sweeps (spectra), and then the 2001S will continue to digitize and send data to the 4100 until the set number of sweeps has been completed. Since the 4100 acts as a summing device, the data sent to the computer is divided (via the program) by the number of sweeps to obtain an average spectrum. As mentioned before, the averaging mode is normally used to calibrate the system (i.e., from a steady-state gas source).

In order to obtain the optimum time-sampling of vapor pulses, the data acquisition system requires another module to control the start and duration of the recording interval, i.e., the desired spectral mass range to be recorded in the 2101 system.

This complementary module is the Timing & Delay Generator Model SP-1186-2 (built by Cal-Av Labs, Campbell, CA 95008); it contains a crystal-controlled clock to control all the timing functions and is plugged into the CAMAC crate next to the Transiac modules. This module is not programmable (although it can be modified in the future to be programmable), instead its operation is controlled by means of four thumbwheel switches on the front panel.

Three parameters set by the switches in the T & D Generator are needed, subsequently, to analyze the data and they are automatically read by the computer via the CAMAC bus:

- (1) Period: this is the period of one mass spectrometer cycle (20 to 99  $\mu$ s). The period determines the repetition rate of the mass spectrometer.
- (2) Record Delay: time lag between the start of the spectrometer period and the time selected to start recording each spectrum (0 to 99  $\mu$ s), i.e., the lowest m/z value.
- (3) Record Width: time duration (also, 0 to 99  $\mu$ s) of the actual data recording that starts after the Record Delay. 100 MHz clock pulses are sent to the external clock input of the 2001S during only this interval, thereby establishing the preselected mass range to be recorded during each TOFMS period.

Of course, the sum of the Record Delay plus the Record Width cannot be greater than the repetition rate (spectrometer period), otherwise the transient recorder would overlap the next spectrometer period.

The fourth thumb-wheel switch provides for the transient mode an adjustable delay between the laser pulse and triggering of the transient recorder; this optimizes the recording of spectra to coincide with the arrival of the vapor pulse at the TOFMS.

The T & D Generator can be used for the transient mode and the averaging mode. In the transient mode, the system is triggered by a laser shot, while in the averaging mode the system is triggered by a computer request to start recording. Thus, the Timing & Delay generator allows a maximum possible amount of useful data recorded for the limited amount of memory available in the Transient Recorder.

#### C) Computer

The computer is an IBM-XT with a monochrome monitor and a Hercules graphics card that produces a resolution of 720 by 348 points on the screen. The computer also has an AST card, a GPIB card to interface with the plotter, and an Intel 8087 math coprocessor to speed up calculations. The memory has been fully expanded to 640 kilobytes.

## PROGRAM

The program LMSDA (Laser Mass Spectrometer Data Acquisition) consists of a main program, SPEC, divided into blocks that perform different operations and call several subroutines when necessary. All codes are written in FORTRAN except for the subroutines CODE and KEYS, which are written in PASCAL. Other subroutines are obtained from commercial software (i.e., Multihalo, Microsoft, National Instruments and Transiac); which are generally provided as object files and thus are not modifiable. A brief explanation of the main program and the subroutines is given below, and the program flow chart is presented in Fig. 2.

### A) Main Program

The blocks in the main program can be reached by the operator by means of menus which assign function keys to the different blocks. These blocks are the following:

- (1) Instrument set up (labels 200 to 300)
  - The desired record length and sampling interval are programmed into the 2101 Transient Recorder System.
  - The desired number of sweeps (1 to 65536) is programmed into the 4100 module (for a record length greater than 8 kilobytes, the number of sweeps is set to 1).
  - Radiometer Calibration Factor is set. This number is utilized to calculate the laser beam energy incident on the target material.
  - The forms of data acquisition and display are chosen: either the vapors are produced by a laser beam or by a constant-leak source, and the graphics may be either 2- or 3-dimensional.
  - The number of points (memory addresses) to be displayed is set.
  
- (2) Data acquisition and manipulation (labels 300 to 400)
  - It allows data acquisition from the mass spectrometer and the subsequent transfer of data to the memory of the computer. Mass spectrometer data are stored in a 33000 component, 1-dimensional array. Also, various experimental parameters from other related equipment are read by a 15-channel scanning digital voltmeter and sent to the computer (through the CAMAC).
  - Once all the data has been transferred to the computer, the number of spectra is determined, and an average spectrum is computed from them and stored in a 3000 component, 1-dimensional array; this is subsequently used for mass labeling.
  - The peaks of the spectra are found and labeled. Time-to-mass conversion is performed here. Thus, It is necessary to know precisely how many points of memory correspond to one spectrometer period, and this is where the repetition rate, record delay and record width

information comes into play.

(3) Graphics display

The graphics display can be either 2- or 3-dimensional:

(a) Three-dimensional graphics (labels 400 to 500).

Features of this display are the capability to expand certain sections of the graph, to send the data to a plotter, and to print all the measurements in the printer. Also, a printer hard copy is available. In Figs. 3 and 4, a plotter drawing and a printer hard copy are shown. In addition, plots of area under each recorded mass peak versus time can be obtained. Fig. 5 shows individual masses at  $m/z = 12, 24, 36$  ( $C_1, C_2, C_3$ ) versus time from a single laser shot. The individual mass expansion FORTRAN code is located between labels 1000 and 1200, because it was added to the main program after the 2-D graphics and other program blocks were written.

(b) Two-dimensional graphics (labels 500 to 600).

The two-dimensional representation has the same available features as the three-dimensional representation, but the two-dimensional graphs can be scrolled by displaying individual spectra sequentially. A two-dimensional printer copy of a single spectrum is shown in Fig. 6.

(c) Three-dimensional average (labels 600 to 700).

This display has the same available features as the two-dimensional display, and it shows the averaged spectrum resulting from averaging all of the spectra in the three-dimensional display. Fig. 7 is the averaged spectrum of the three-dimensional display shown in Figs. 3 and 4.

(4) Digital Voltmeter (DVM) (labels 700 to 800).

Whenever this block is called, channels 1 through 15 of the digital voltmeter are scanned (continually) and the readings are displayed on the screen. Fig. 8 shows a typical output.

(5) Calibration (labels 900 to 997).

In order to calibrate data, a two-dimensional averaged spectrum is displayed on the screen. A cursor is used to find the peaks of the masses, and, for each peak, the mass value is entered into the computer. The program then utilizes least-square statistical methods to find the values of  $k_1$  and  $k_2$  for the relation  $t_f = k_1(m/z)^{1/2} + k_2$ . Fig. 9 shows a calibration example. In this case, a check after calibration is being done. The peak mass value shown on the screen is 127.11, which rounded off to its nearest integer is 127 (the  $m/z$  value of the  $SF_5$  fragment from  $SF_6$ ).

(6) Storing data.

The spectrometer output and all relevant measurements can be stored in a diskette for later use.

## B) Subroutines

- (1) **CAMV3**  
This is a subroutine provided by Transiac Corporation; it allows the transfer of data between the CAMAC system and the computer.
- (2) **CONVERT**  
As the name indicates, this subroutine converts a real number into a string of character variables. This procedure is necessary in order to print real numbers on the screen, because HALO will not accept real numbers as text variables for printing on the display.
- (3) **DATAIN, DATAOUT**  
DATAOUT stores all relevant data into a file in a diskette, and DATAIN retrieves the data from a file into the program. Thus, particular experiments can be recorded for later review.
- (4) **DATTIM**  
Provided by Microsoft and modified slightly, SPEC calls DATTIM to obtain the time and date from the AST card.
- (5) **HALO subroutines**  
These are from Multihalo Cybernetics, Inc., and they are called from the main program to draw points and lines on the screen. Therefore, all graphics are drawn using these subroutines.
- (6) **HEADING**  
It is in charge of printing the title, laser shot number, date and time of the experiment on the screen graphics.
- (7) **INTCON**  
Similar to CONVERT, this subroutine converts an integer to a character representation of the integer.
- (8) **KEYS, CODE and DOSQXX**  
The first two subroutines are written in PASCAL, and the last one was provided by Microsoft Corporation. KEYS calls DOSQXX to detect function key operations on the IBM PC-XT, mainly to read entered numbers in the menu selection. CODE calls DOSQXX in order to control the placement of the numbers on the graphic display.
- (9) **LAXIS**  
Converts a real number (time, in microseconds) in scientific notation to its character representation including the exponent. This is necessary in order to print the spectrometer period on the screen when using



HALO (i.e., for the graphics mode; see the time-axis of the 3-D graph).

(10) MFIB

This is a subroutine provided by National Instruments that facilitates the interfacing of FORTRAN with the GPIB card. Thus, GPIB functions can be called from the FORTRAN code of SPEC.

(11) PLOT

It sends commands -- in HP-IL language -- to the plotter to draw the three-dimensional graph. This operation is complicated because the data must be sent through the GPIB card, which only accepts ASCII representations of variables, so every variable -- characters, integers, real numbers -- must be converted into its ASCII representation before it can be sent sequentially to the plotter.

(12) SPDA

This sends to the printer the measurements read by the digital voltmeter (DVM).

#### REFERENCES

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2. Lincoln, K.A. and Bechtel, R.D., "A Fast Data Acquisition System for the Study of Transient Events by High-Repetition Rate Time-of-Flight Mass Spectrometry," Int'l. J. Mass Spectrom. and Ion Proc. (in publication).
3. Bechtel, R.D., "Laser Mass Spectrometer Data Acquisition," Thesis written for the B.S. Degree in Electrical Engineering, Santa Clara University, Santa Clara, California, June 1986.
4. Mateos, M.A. and Yang, C.Y., "Improvement of a Mass Spectrometer System to Produce Computerized Output from Laser-Vaporized Materials," Final Report submitted by the School of Engineering, Santa Clara University to NASA Ames Research Center, June 30, 1987.
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### DATA ACQUISITION INSTRUMENTATION FOR TIME-OF-FLIGHT MASS SPECTROMETER

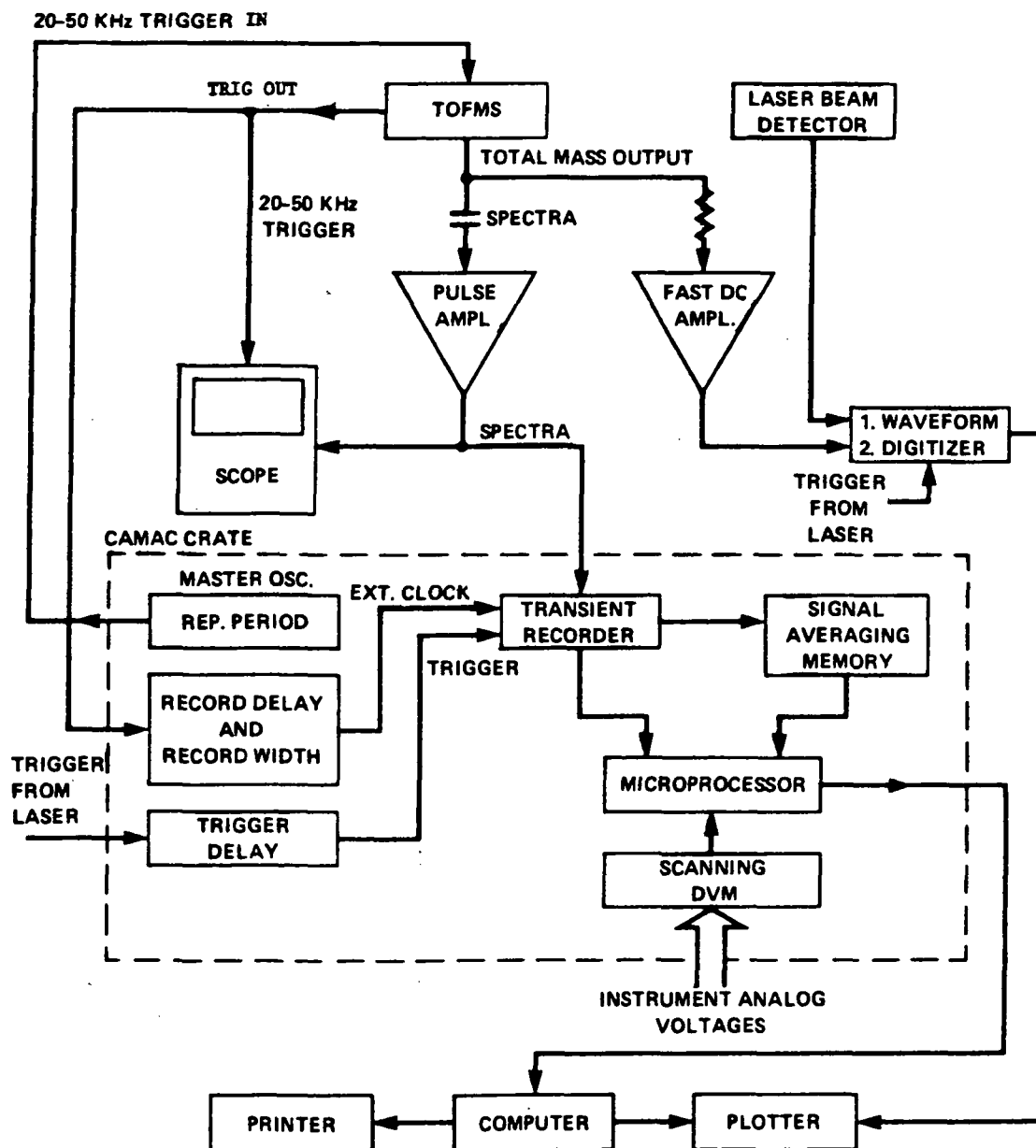


Fig. 1. Instrumentation system flow chart

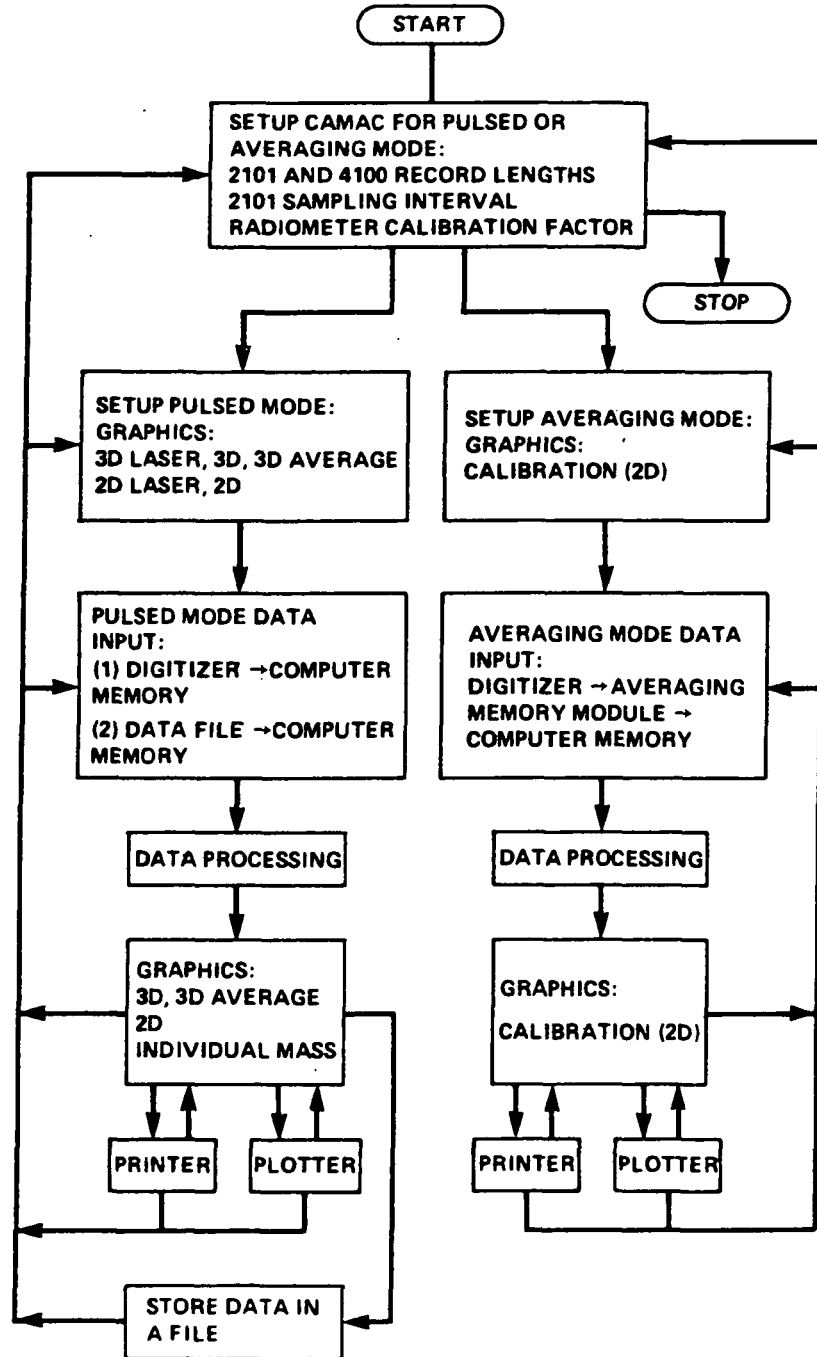


Fig. 2. Computer program flow chart

## LASER MASS SPECTROMETER PARAMETERS

CH.03	LASER PS	-6.371 KV	CH.01	RADIOMETER	-1.051
CH.04	PRESSURE			( $\times 2.000$ )	2.101 JOULES
CH.05	ELECTRON ENERGY	-70.435 eV	CH.07	TRAP CURRENT	1.028 $\mu$ A
CH.08	MCP VOLTS=	1.539 KV	CH.09	ION CURRENT	-.021 $\mu$ A
CH.10	DUTY CYCLE	.155	CH.11	ION DEFLECTOR	.000 KV
CH.12	FREQUENCY	31.250 kHz			

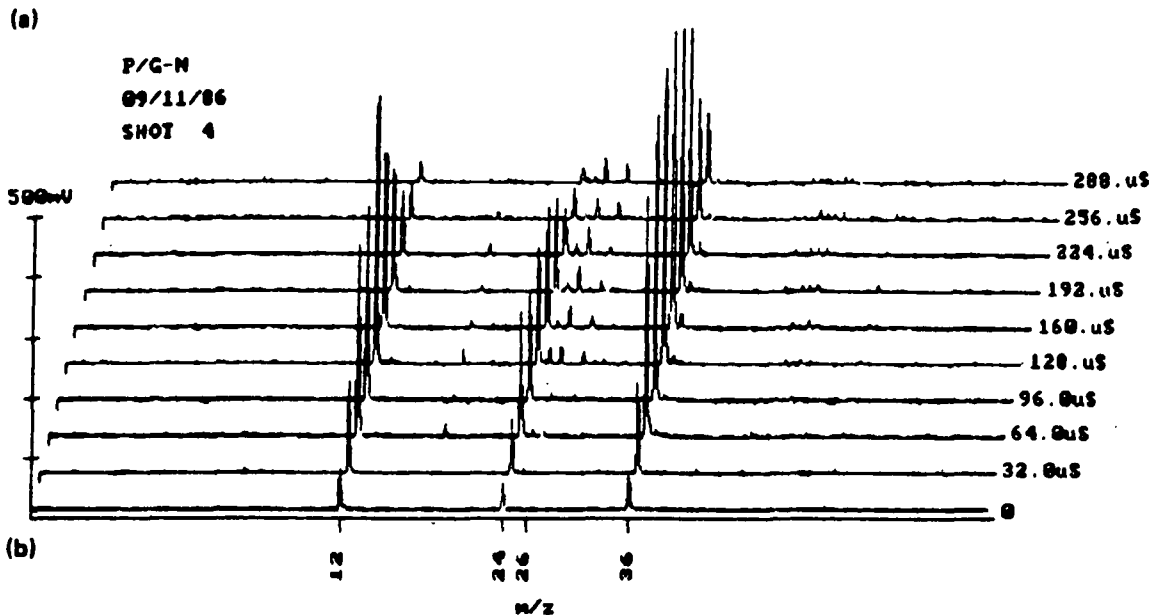


Fig. 3. Immediate computer outputs. (a) Printout of instrument parameters. (b) Screen printout of 3-D video display.

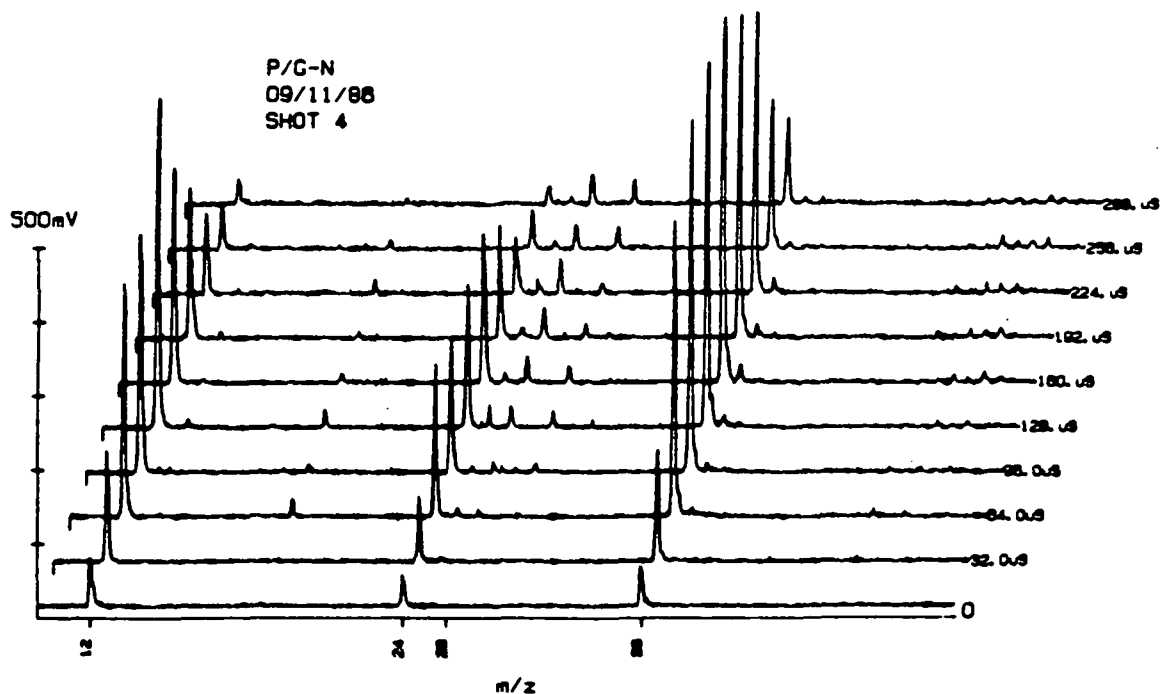


Fig. 4. Plot of 3-D spectra within a selected mass range.

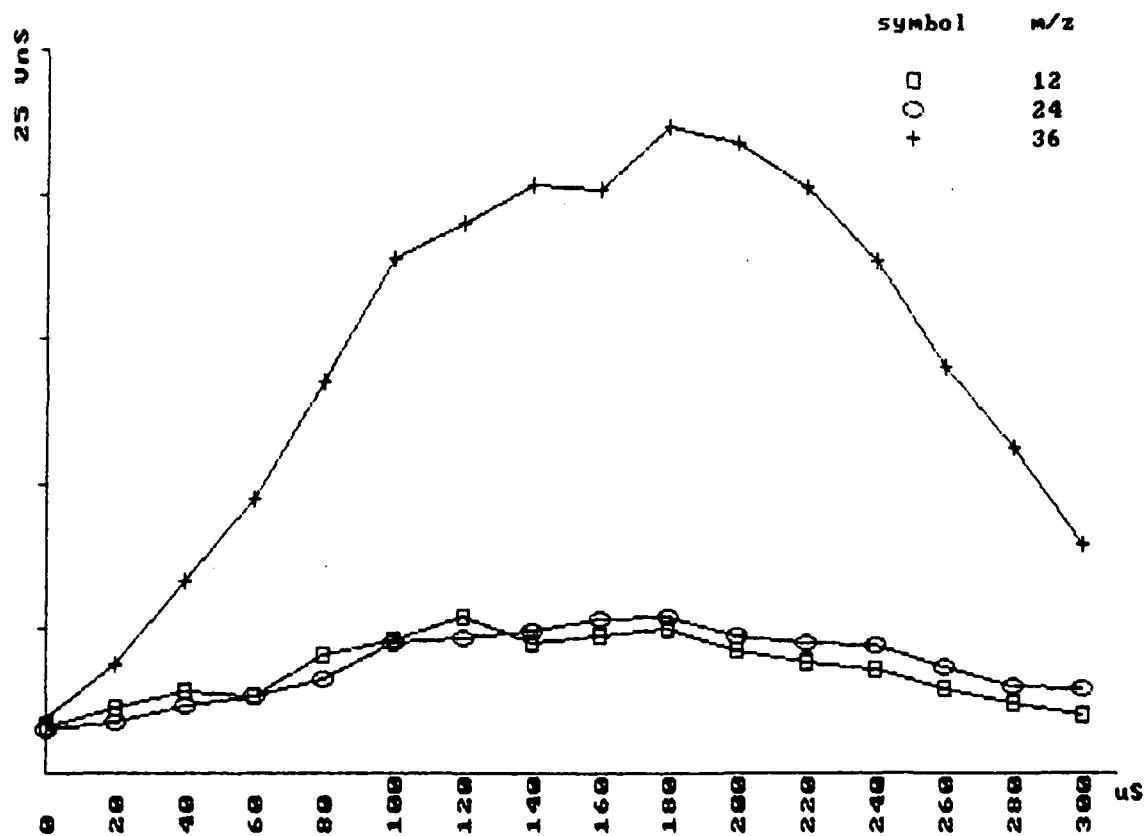


Fig. 5. Individual mass expansions: Intensity vs. time

TEST  
04-27-67  
14:32:09  
SHOT 1

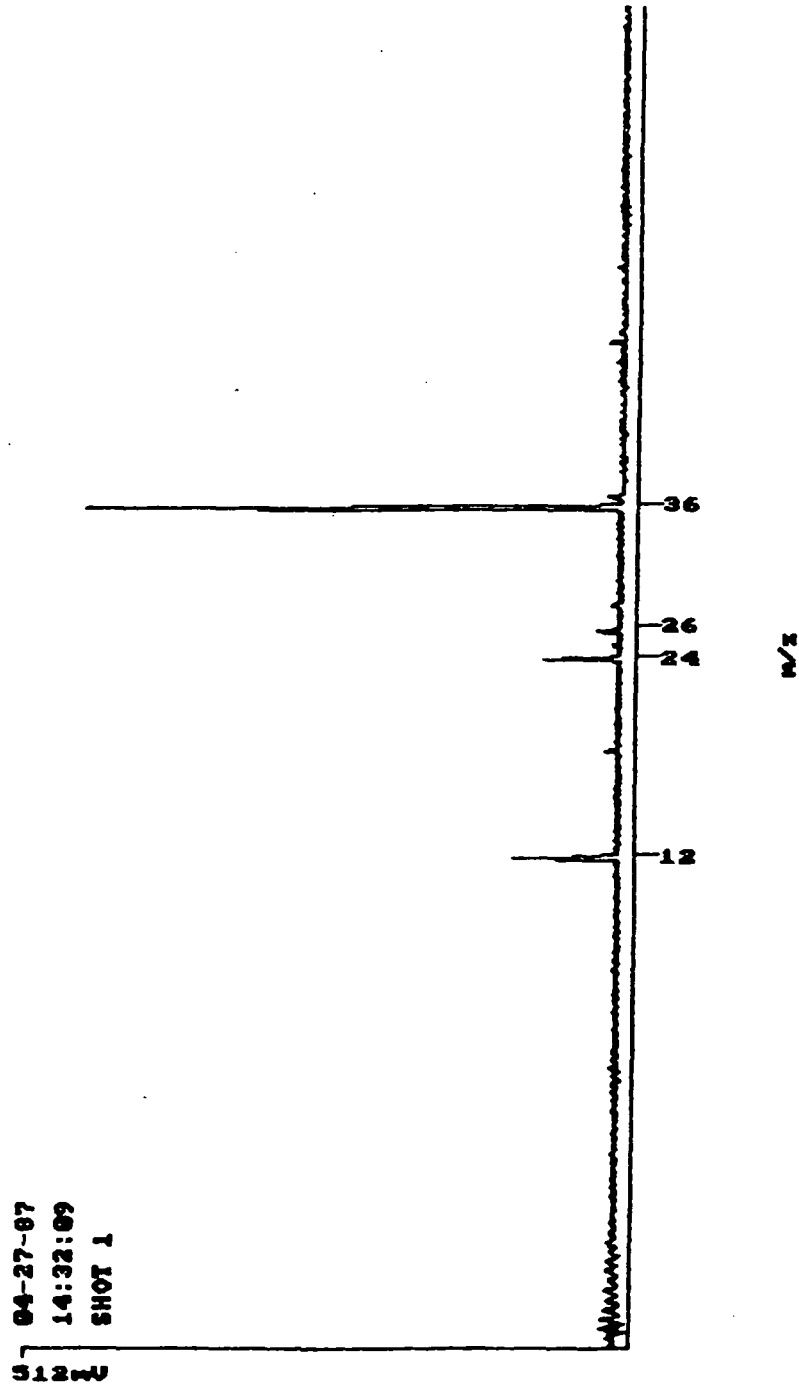


Fig. 6. Screen printout of a single spectrum from a 3-D array

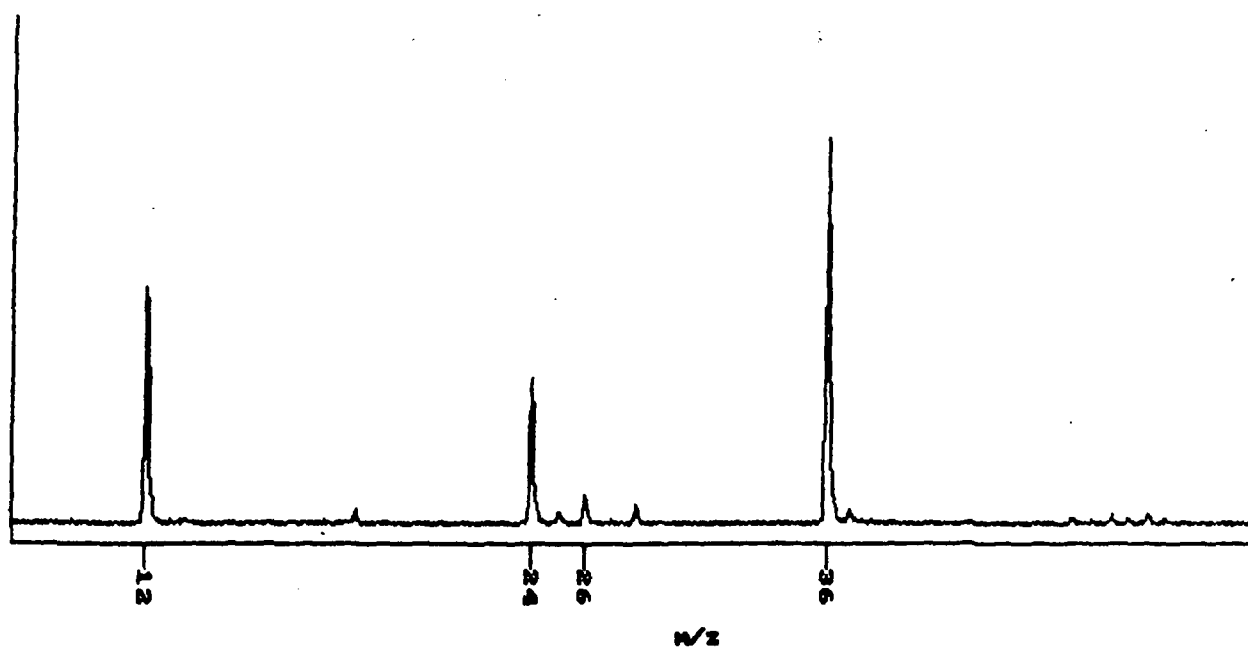
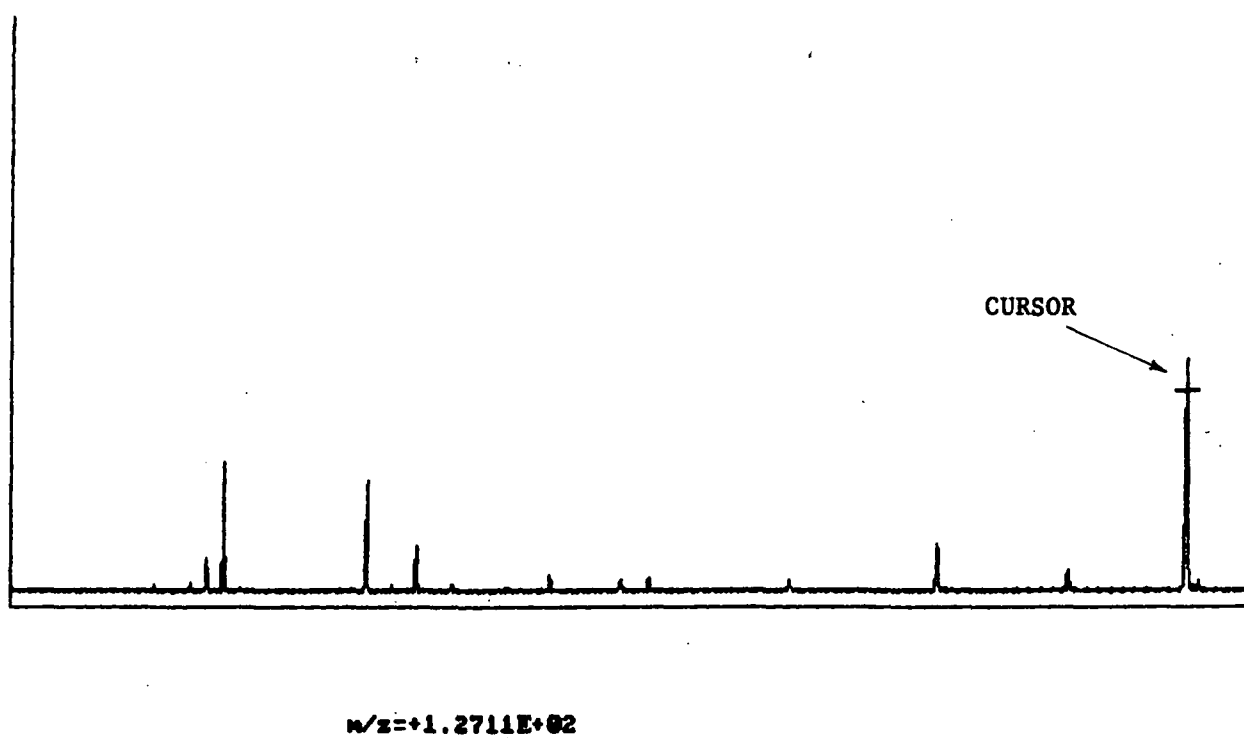


Fig. 7. Screen printout of the spectrum resulting from averaging the 3-D spectra from a single laser pulse.

CHANNEL 01	RADIOMETER	-5.3642E-02	
CHANNEL 02	-----	+5.4088E+00	V
CHANNEL 03	PS VOLTAGE	-4.6304E+00	KV
CHANNEL 04	PRESSURE	-9.6424E-03	TORR
CHANNEL 05	EXPONENT	-1.3551E-01	
CHANNEL 06	ELECTRON E	-7.0627E+00	eV
CHANNEL 07	TRAP CURRENT	+3.2397E-02	uA
CHANNEL 08	MCP VOLTS	+1.6719E+00	KV
CHANNEL 09	TMC	-2.0953E-01	nA
CHANNEL 10	DUTY CYCLE	+1.5247E-01	
CHANNEL 11	ION DEFLECTOR	-1.1728E+00	KV
CHANNEL 12	-----	+3.1335E-02	V
CHANNEL 13	-----	+1.0673E-03	V
CHANNEL 14	-----	-5.4907E-02	V
CHANNEL 15	-----	-1.8743E-01	V

Figure 8. Sample DVM Output





F1=LEFT F2=RIGHT F3=ENTER F4=DEL F5=1 F6=10 F7=100 F8=CAL F9=EXIT

Fig. 9. Sample calibration using  $SF_6$  calibration gas. Cursor is located at the maximum of the mass 127 peak ( $\cdot SF_5$ ).



# Report Documentation Page

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16. Abstract <p>Briefly described are the essential features of a computer program designed to interface a personal computer with the fast, digital data acquisition system of a time-of-flight mass spectrometer. The instrumentation was developed to provide a time-resolved analysis of individual vapor pulses produced by the incidence of a pulsed laser beam on an ablative material. The high-repetition rate spectrometer coupled to a fast transient recorder captures complete mass spectra every 20 to 35 microseconds, thereby providing the time resolution needed for the study of this sort of transient event. The program enables the computer to record the large amount of data generated by the system in short time intervals, and it provides the operator the immediate option of presenting the spectral data in several different formats. Furthermore, the system does this with a high degree of automation, including the tasks of mass labeling the spectra and logging pertinent instrumental parameters.</p>					
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