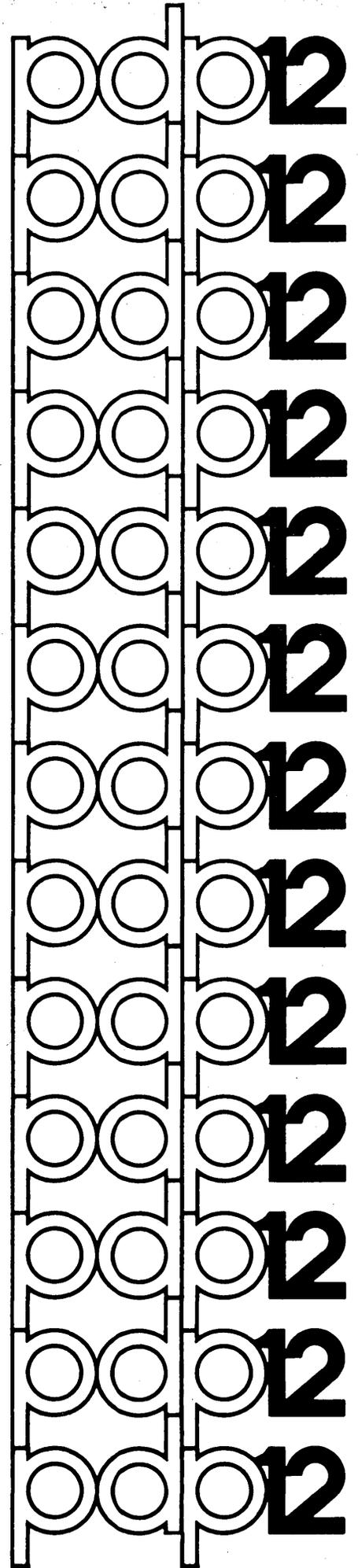


digital

MASH USER'S MANUAL

(VERSION 1)



DEC-12-SQ2A-D

First Printing July, 1971
Second Printing Oct., 1971
Third Printing Jan., 1972

MASH USER'S MANUAL

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Library, Digital Equipment Corporation, Maynard,
Massachusetts 01754 Price \$5.00

Your attention is invited to the last two pages of this document. The "How to Obtain Software Information" page tells you how to keep up-to-date with DEC's software. The "Reader's Comments" page, when filled in and mailed, is beneficial to both you and DEC; all comments received are acknowledged and are considered when documenting subsequent manuals.

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1.0 GENERAL DESCRIPTION

The Mass Spectrometer Handler (MASH) is a complete interactive data acquisition, processing and report generating system, utilizing the interfacing of a PDP-12 computer to any single mass spectrometer (or mass spectrometer/gas chromatograph combination) at a user's site. Three programs provide for the specification of parameters and control of all instrumentation during an experiment. The programs are:

a. Calibration (CALIB)

The chemist can recalibrate the mass spectrometer to correct for drift. The calibration procedure is efficient, thorough, and easy to use, and enables the MASH System to determine spectrum mass numbers with an accuracy of .2 amu if 15 bits, .3 amu if 12 bits, at masses of up to 600.

b. Acquisition (ACQUI)

During the Acquisition program data can be acquired and processed in either multiple scan (useful if a gas chromatograph is attached to the mass spectrometer) or single scan mode. The data is sampled at high speed and processed in the computer's memory. Only the coordinates of the mass peaks are saved on tape or disk.

c. Report Generator (LOOK)

The Report program displays the results of the scan(s) to the chemist. Data is manipulated in a line spectra format, using any of the nineteen powerful Teletype¹ commands provided by the program. Report's response times for all commands are well under one second.

All three MASH programs are run under the standard AIPOS System, and all MASH files are compatible with standard AIPOS files. Thus, the AIPOS system now has the capability of controlling a mass spectrometer or mass spectrometer/gas chromatograph configuration.

It is suggested that the reader refer to the AIPOS User's Manual (DEC-12-SQA-D) for information on the Job Control program which is used to call the MASH programs.

¹Teletype is a registered trademark of Teletype Corporation.

2.0 HARDWARE REQUIREMENTS

2.1 Minimum Configuration

The minimum configuration on which the MASH program runs is a PDP-12/LDP which includes:

- a. PDP-12 Laboratory Computer with 8K of core memory
- b. Real Time Clock (KW12A or equivalent)
- c. AIP-12 Data Break A/D Sampling Hardware
- d. FPP-12 Floating Point Processor Hardware connected to:
- e. Low Resolution Mass Spectrometer (AEI MS12 or equivalent) or Quadropole Mass Spectrometer
- f. Hall Voltage Probe with Interface, or Quadropole voltage input.

2.2 Supported Devices

In addition, the following hardware devices are supported through the AIPOS I/O Handler:

- a. Additional tape drives
- b. Disk (RK8 or equivalent)

Optional hardware that the MASH system can handle independently of the AIPOS Monitor is:

- a. An X-Y Plotter (HOUSTON or equivalent)
- b. An Electrostatic Recorder (Versatec Model 100A or equivalent).

2.3 Interface Options

The MASH System is designed to interface to a wide variety of mass spectrometers. The following are options available to handle the majority of machines in the field.

- a. Quadropole
- b. Scan backward
- c. Noisy option (spikes in Hall Voltage must be eliminated by 5 point median).

- d. TIC Discontinuous [total ion current not available during scans]
- e. TIC Unavailable [total ion current never available]
- f. Scan triggered from mass spectrometer

3.0 CALIBRATION

3.1 Introduction

CALIBRATION, which permits two modes of operation, enables the mass spectroscopist to assign mass numbers to Hall Voltages obtained from a mass spectrometer. Initially, these assignments are made manually by the user; subsequent mass assignments are performed automatically by the computer. The choice of MANUAL or AUTOMATIC mode is specified at AIPOS Job Control time. (Refer to Appendix A of the AIPOS User's Manual DEC-12-SQ1A-D for steps to call Job Control).

3.2 MANUAL Calibration

The following AIPOS function call command to Job Control, specifying MANUAL calibration, is performed at system initialization time and only very infrequently thereafter:

```
CALIB outdev:outfile )
```

where outdev = output device
 outfile = output filename
) = carriage return

After verification is obtained for only one output file and no input files, the necessary header block information for the HALL TABLE is specified in the user's response to three consecutive frames displayed on the scope.

3.2.1 Parameter Specification¹

When carriage return is typed after the MANUAL call statement, the following display appears on the scope:

¹ During this part of the program, typing CTRL/R causes a return to the first of the three display frames, with all previous answers erased. Striking the altmode key causes all the answers of the current message to be erased.

INITIAL CALIBRATION

1. RESOLUTION ----

2. SAMPLE RATE --

Question 1: Answer question 1 with the 10% valley definition of resolution (see Glossary). The range permitted for this choice is a decimal number from 200 - 2000.

Question 2: Answer question 2 with the number of samples per second for both Hall Voltage and Intensity. The range of the sample rate is 1-10 decimal, which is then multiplied by 1000 internally. Sample rate for magnetic scan is 10,000 with no Hall Voltage smoothing or TIC correction; 8000 if Hall Voltage smoothing or TIC correction is done; and 5,000 if both Hall Voltage smoothing and TIC correction are done.

NOTE

If a Quadropole is being used, enter mass range instead of resolution. The mass range is 1-600. For example, to examine 400-600, enter 200. Sample rate for a Quadropole is a maximum of 3000. Enter a decimal number from 1-3.

The next frame is

```
3. H.V. RANGE ---  
4. TIC BASELN ----  
5. TIC THRESH ----
```

Question 3: The range of values is 0-999. This number is a measure of the tolerable drift for Hall Voltages between successive calibrations; a good value is 5 for a 12 bit A/D, 20 for A 15 bit A/D.

Questions

4 and 5: The range of values for both questions is 0-9999. The Total Ion Current (TIC) baseline is the current value at which no ion current occurs (null). The TIC threshold is the value of TIC below which no scan will take place.

NOTE

TIC baseline and/or threshold can also be assigned during an Acquisition program run by typing "B" or "T". When TIC vs. Time Plot is being displayed (refer to 4.3), the value of the last point just displayed on the scope becomes the baseline (B) or threshold (T) value.

After question 5 has been answered, the final frame is displayed:

```
6. QUADRAPOLE (Y OR N) -  
7. SCAN DIR (F OR B) -  
8. H.V. NOISE (Y OR N) -  
9. TIC DISCONTINUOUS (Y OR N) -  
10. SPLINE FIT (Y OR N) -
```

Question 6: If the mass spectrometer in use is a quadropole, type Y; otherwise, type N.

Question 7: If the scan direction is from low to high mass numbers, type F (forward); otherwise, type B (backward). (Backward scanning requires an extra pass to calculate baseline).

Question 8: If the Hall Voltage has high frequency noise associated with it, type Y; otherwise, type N.

Question 9: If the TIC is not present during scan time, type Y; otherwise, type N.

Question 10: Once all Hall Voltage/Mass points have been paired, a curve is fitted to these points. If a Spline fit is desired, type Y; if a linear fit is preferred, type N.

Following question 10 is a series of questions concerning acquisition (refer to 4.0 ACQUISITION). After these questions have been answered, a single scan is run, leaving a table of Hall Voltage/Intensity pairs in core.

3.2.2 Line Spectra Frames

Based on the Hall Voltage/intensity pairs just obtained, line spectra frames are generated on the scope, showing peak number, Hall Voltage, and intensity. A fourth column, headed by the word MASS, is initially blank.

An example of a line spectra data frame is as follows:

PEAK	HU	INT	MASS
1	1207	33000	-----
2	1750	2178	-----
3	2082	3273	-----
4	2232	10373	-----
5	2502	798	-----
6	2625	554	-----
7	2712	537	-----

3.2.2.1 Intensity Threshold

At this point, an intensity threshold should be specified to eliminate all peaks of lesser intensity when the Hall Voltage table is created. This is accomplished as follows:

User types: T)
Teletype responds: PEAK#
User types: a decimal number from 1-999, followed by a carriage return.

For example, if the following information is specified:

T)
PEAK#3

the above display becomes:

PEAK	HV	INT	MASS
1	1297	33000	-----
2	2082	9273	-----
3	2232	10379	-----
---	---	---	---
---	---	---	---
---	---	---	---
---	---	---	---

3.2.2.2 Mass Number

Next, the user assigns a mass number to each intensity peak which will be used to calibrate subsequent runs. (The maximum number of assigned masses is 95.) Assignment is accomplished as follows:

User types: P)
Teletype responds: PEAK#
User types: any unsigned decimal number from 1-999, followed by a carriage return.

Teletype responds: MASS#
User types: any unsigned decimal number from
 1-1999.9 followed by a carriage
 return.

If the following information is specified:

P ↵
PEAK#2
MASS#119.0

the above display now becomes:

PEAK	HD	INT	MASS
1	1207	33000	-----
2	2002	3273	119.0
3	2232	10373	-----
---	-----	-----	-----
---	-----	-----	-----
---	-----	-----	-----
---	-----	-----	-----

A mass value being entered should obey the following criteria:

- a. "Mass Peaks" chosen will be separated by at least 3 but no more than 50 mass units (for spline fits).
- b. "Mass Peaks" chosen will be the highest in a 3 amu "range".

3.2.2.3 Deletions

During MANUAL calibration, the assigned masses can be deleted by typing: \$. Or, a single assigned mass can be deleted by typing: S. The Teletype responds with: PEAK#. The user then types the number of the peak whose mass is to be deleted.

3.2.2.4 Curve Fit

Once each Hall Voltage of importance has been assigned to its corresponding mass, the user can type: X. The program does a curve fit for the Hall Voltage vs. the assigned mass. This curve fit is either a Linear fit or a Spline fit (depending on the answer to question 10). When the curve fit is completed, the Hall Voltage table is saved as the AIPOS output file specified at Job Control time. The program then returns to Job Control.

3.3 AUTOMATIC Calibration

The following AIPOS function call format statement specifies AUTOMATIC calibration, which is carried out daily, primarily to ensure that the Hall Voltage has not shifted significantly:

```
CALIB outdev:outfile=indev:infile↵
```

where

```
CALIB      = name of program (if unspecified, LTØ is  
            assumed)  
outdev     = output device  
outfile    = output filename  
indev      = input device  
infile     = input filename  
↵         = carriage return
```

In MASH, the output file will be designated as the most recently created Hall Voltage table, having used the input file as a basis for its creation. If the input Hall table was not the latest one created, the user is informed of this by the following scope message:

```
OLD HALL TBL  
CONTINUE? (Y OR N)
```

Typing N causes the program to return to Job Control; typing Y causes the program to continue with the AUTOMATIC Calibration.

After verification is obtained for exactly one output file and one input file, a series of questions pertaining to acquisition are asked (refer to 4.0 ACQUISITION). When these questions have been answered, a peak sensing scan of the spectrum to be calibrated is run. This includes saving the intensities and Hall Voltages of the peaks.

3.3.1 Line Spectra Frames

Because AUTOMATIC calibration is used to check Hall Voltage drift, it may be necessary to align Hall Voltages with mass numbers. This can be determined from the line spectra frames on the scope which show peak number, Hall Voltage, intensity, mass, and deviation. Deviation, a measure of the Hall Voltage drift, is found by taking the absolute value of the difference between the old Hall Voltage and the new one which replaces it in the Hall table.

All peaks whose Hall Voltages lie within the chosen range (see question 3 of MANUAL Calibration) of a given Hall Voltage value are found. The Hall Voltage corresponding to the highest intensity becomes the new Hall Voltage associated with that peak. The absence of a peak number from a display indicates that no peak could be found for the displayed Hall Voltage such that it would be within the Hall Voltage Range specified at MANUAL calibration time.

Consider the following example:

PEAK	HV	INT	MASS	DEV
1	2210	301	140.0	1
2	2219	4061	-----	-----
3	2250	166	153.0	2
	2310	-----	167.2	-----
4	2317	2710	-----	-----
5	2333	1027	251.8	-----

At this point, the user can move a mass at a given peak to a peak with no mass, provided there are no masses between the two peaks. This is accomplished as follows:

```

User types:           M )
Teletype responds:   PEAK#
User types:           the peak number containing the mass
                      followed by a carriage return
Teletype responds:   PEAK#
User types:           the peak number to which the mass
                      is to be moved followed by a car-
                      riage return
  
```

If the following is specified:

```

M )
PEAK#1 )
PEAK#2 )
  
```

the above display becomes:

PEAK	HV	INT	MASS	DEV
1	2210	301	-----	-----
2	2219	4061	140.0	8
3	2250	166	153.0	2
	2310	-----	167.2	-----
4	2317	2710	-----	-----
5	2333	1027	251.8	1

A mass that is not associated with a peak number can also be moved so it has a peak number as follows:

```

User types:           M )
Teletype responds:   PEAK#
User types:           the peak number immediately pre-
                      ceding the blank, followed by a
                      plus sign and then a carriage re-
                      turn.
  
```

Teletype responds:

PEAK#

User types:

the peak number to which the mass
is to be moved followed by a car-
riage return

For example, to move mass 167.2 to peak 4 the following is specified:

```
M )  
PEAK#3+ )  
PEAK#4 )
```

the above display now becomes

PEAK	HV	INT	MASS	DEV
1	2210	301	-----	-----
2	2219	4061	140.0	8
3	2250	166	153.0	2
4	2317	2710	167.2	6
5	2333	1027	251.8	1

When the desired mass reassignments have been completed, type X. This causes the same exit described in Section 3.2.2.4.

3.4 Calibration Commands

In addition to the commands which pertain to a particular mode of calibration, there are several other commands which apply to both modes. With these additional commands, the line spectra frame on the scope can be advanced or backed up by one line or one frame; Teletype print-out of the entire display or only those lines with assigned masses can be generated; or a given peak number along with six neighboring peaks can be located immediately.

MANUAL AND AUTOMATIC MODES

<u>Command</u>	<u>Action</u>
F	Move forward 1 frame
B	Move backward 1 frame
LINE FEED	Move forward 1 line
ALT MODE	Move backward 1 line
L	Locate to a given peak number
H	Print hard copy of peaks with assigned masses ¹
A	Print hard copy of entire display ¹
X	Exit this mode (proceed to Curve fit) ²

MANUAL MODE ONLY

<u>Command</u>	<u>Action</u>
P	Assign a mass to a given peak
T	Set an intensity threshold
\$	Delete all masses
S	Delete a single mass

AUTOMATIC MODE ONLY

<u>Command</u>	<u>Action</u>
M	Move a mass from one peak to another

Where necessary the computer prints the PEAK# message so that the user can enter the specific peak.

¹This command can be aborted at any time by typing any control character.

²In automatic calibration mode, the Hall Voltage header from INFILE is read into core. Specific header information is changed to indicate the newest automatic calibration file. In both modes, the Hall Voltage/mass ordered pairs are written out to the specified output unit.

4.0 ACQUISITION

4.1 Introduction

ACQUISITION is the data gathering/processing portion of the MASH system. Data can be obtained from a mass spectrometer at a wide variety of scan speeds (up to 2 seconds/mass decade) and processed to yield mass peaks with an intensity accurate to 5 percent and a mass accurate to .3 amu if 12 bit A/D, .2 amu if 15 bit A/D, at masses up to 6000.

4.2 Operating Procedures

4.2.1 User Dialogue

In order to acquire mass spec data (assuming the mass spectrometer has been previously calibrated - refer to 3.0 CALIBRATION) the following must be typed at Job Control time.

```
dev:ACQUIS outdev:outfile=indev:infile ↵
```

where

outdev and indev = the unit of the corresponding file following the colon.

ACQUIS = the name of the acquisition program.

outfile - the name of the sample to be scanned. This name can be up to six characters long, and must not duplicate the first six characters of any other file name (no matter what length) on that LDP unit, an error message will be generated if duplication occurs.

infile = the name of the Hall Voltage table (generated previously using the calibration program) against which subsequent scans are to be calibrated.

↵ = carriage return.

The ACQUISITION program checks that:

- a. Only one input and one output file were specified
- b. The input file is a Hall Voltage/mass table
- c. The six characters of the output filename are unique on its unit
- d. The WRITE ENABLE switch is ON for the appropriate output unit
- e. The output file is greater than seven blocks in length.

If any of the above is not true, an appropriate error message is displayed (refer to Appendix A) and in all but case "D" above, the program declares a fatal error, and returns to Job Control.

4.2.2 DYSP

Assuming a successful load, the ACQUISITION program switches to the AIPOS oriented display subroutine, DYSP: While using this subroutine the user can type any of the following keys to alter the current process:

<u>Key</u>	<u>Action</u>
CONTROL/C	Returns to Job Control
CONTROL/R	Returns to the first display (of Acquisition program)
RETURN	Terminates an answer field (the final character in a full answer field also terminates the field)
ALTMODE	Deletes all responses on a frame
RUBOUT	Rubs out the last character in a field.

The ACQUISITION program presents four messages. The first display asks:

```
ACQUISITION : TYPE

      1. AUTOMATIC
      2. MANUAL

CHOICE -
```

Manual mode enables the user to call for 1 to 9 scans when the TIC starts to rise by hitting the appropriate key (1-9) on the Teletype.

Automatic mode enables the user to call for "n" scans when the TIC starts to rise by typing "G" (GO), where "n" is a number less than 250, and defined through a subsequent display (see Total Number of Scans).

The next display is:

```
ACQUISITION : TIME (IN SECONDS)

SCAN:  --
DELAY:  --
```

where the lower limit on scanning time is a variable dependent upon the internal parameters of mass spectrometer resolution, sample rate and peak width. Note that the fastest scan time allowable will always be the same for a given machine resolution, and its value might be in the neighborhood of:

SPECTROMETER RESOLUTION	QUICKEST SCANNING/DECADE
600	2 seconds
1000	4 seconds

The lower limit on delay time [or flyback] is always 2 seconds, to allow for the possible tape output of peaks from the previous scan. The maximum value for both times is currently 40 seconds. Note that the time interval between successive computer triggered mass spectrometer scans will merely be scan time plus delay time.

The next display:

```
ACQUISITION : PARAMETERS

THRESHOLD (ABSOLUTE DECIMAL) : ----
```

allows the user to specify a minimum value of intensity below which no peak will be looked at.

The exact threshold value chosen has a great effect on the results of the subsequent scans, and the conditions under which they are taken. Too high a value causes loss of important peaks (they are ignored;) too low a value causes the Acquisition program to peak sense white noise (this causes the loss of good data and creates spurious noise peaks at report time). The ideal threshold value for a given mass spectrometer must be determined by trial and error. The allowable values are from 0 to 9999 (out of a total intensity range of 32,000).

The final display appears only if automatic scanning was chosen. The range is 1 to 250.

```
TOTAL NUMBER OF SCANS : ---
```

4.3 TIC vs. Time Plot (Only if TIC Available from Mass Spectrometer)

After the last user information has been entered, the Acquisition program displays on the scope the curve of Total Ion Current vs. Time; enabling the user to see immediately when the TIC starts rising (implying a scan should be taken). If TIC is .4% or less of full scale, the message "WAITING FOR ION BOMBARDMENT" appears until the TIC value rises.

The curve is a moving window with the most recent point at the extreme rightmost part of the screen. It is updated at a rate of 5 times/sec; the screen at all times shows the behavior of the curve over the last 100 seconds.

Prenormalization is done for this curve, so that no matter how small the TIC value (except for a narrow range that is considered equal to \emptyset), it "fills" most of the screen and peaks are easily seen. Because there is a finite number of displayable points in the oscilloscope, MASH scales (normalizes) the spectrum to a power of 2 so that a curve display on the scale 2^0 changes in small increments, whereas a curve on the scale 2^3 has a wider displayed distance between points. The scaling being done on the current point is shown on the screen in the upper left corner. Areas of rescaling are, in figure 4.1, points B and C.

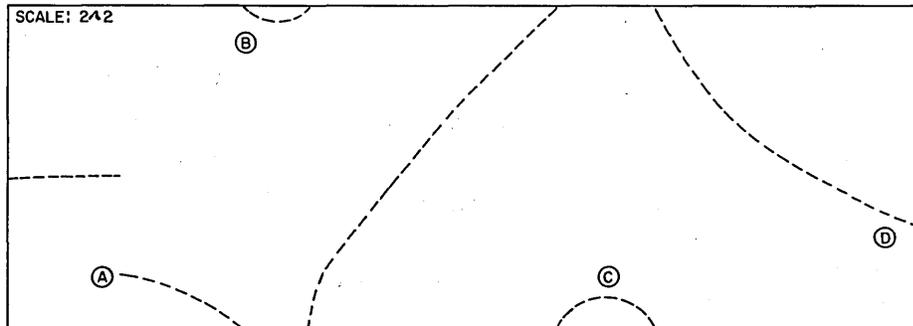


Figure 4.1 TIC vs. TIME Plot

Figure 4.1 point:

- A shows where TIC values had begun to be recorded (prior time is shown as a series of midscale points).
- B shows a "minimum" which required a change of scaling.
- C shows a maximum which required a change of scaling (a scan should have been taken here).
- D shows the current point. Since the scaling is 2^2 , this point (assuming a 12 bit AIP input of from +3777 to -3777) lies between -2000 and -2777.

<u>Input Value</u>	<u>Scaling Power of 2</u>	<u>Curve Value</u>	<u>Scaling Power</u>
±3777	scaled 0	4096	2 ⁰ or normal
0		2048	
-2000	scaled 1	1024	2 ¹
-3000	scaled 2	512	2 ²
-3400	scaled 3	256	2 ³
-3777	scaled 4 to 7	0	2 ⁴ to 7

The current TIC value times the current scale factor equals the TIC value in the upper half of the TIC range.

4.3.3 Acquisition Commands

The user can type various commands at this time. Some bring the user back to the display without an interrupt. They are:

<u>Command</u>	<u>Action</u>
B	Causes present value of TIC to be used as TIC baseline.
T	Causes present value of TIC (assuming B has been typed) to be used as the TIC threshold.

An illegal character (or illegal use of a legal character) causes an error message to be typed out.

Scan controlling user commands are:

<u>Command</u>	<u>Action</u>
O	Causes finalization processing and return to Job Control. This is the <u>only</u> acceptable exit from the Acquisition program. The data files created (assuming there were any) are accessible by REPORT and other AIPOS report programs.

<u>Command</u>	<u>Action</u>
G (in auto- matic mode)	Causes a specified number of scans to be taken sequentially if the current TIC value is above the TIC threshold. The user sees the display vanish and, in most cases, a return to an initial curve display (all previous TIC points are lost due to core limitations). The display will not reappear if:
1-9 (in manual mode)	
	<ol style="list-style-type: none"> 1. The total number of scans on this sample has reached 250 (in which case, the user types CTRL/C to exit back to Job Control). 2. Tape limitations (index or storage) have forced a premature exit.

5.0 REPORT GENERATOR

5.1 Introduction

MASH uses the line spectrum display program "LOOK" to generate hard copy and display up to 500 X,Y point pairs as a line spectrum. It allows the user to edit, print, visually manipulate and restore a MASH data file.

5.2 Operating Procedures

Once the AIPOS system is on the air, the user initiates LOOK by typing the following command

```
dev:LOOK outdev:outfile=indev:infile ↵
```

outdev and indev = the unit of the corresponding file following the colon.

LOOK = the name of the report program.

outfile = output file name

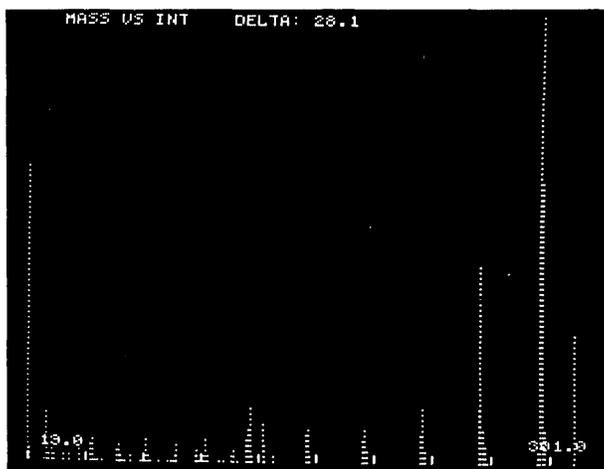
input = input file name

↵ = carriage return.

A line spectrum is initially displayed on the PDP-12's scope and an asterisk (*) is printed on the TTY after LOOK has been correctly loaded. The display features an eleven tick grid at the bottom and display identification at the top along with the actual line spectrum. The leftmost grid tick is labeled with the minimum X value of the file,

the rightmost grid tick with the maximum X value of the file.

For example, if the maximum value of a file is 301.0 and the minimum 19.0, the grid looks like this:



The ordinate and abscissa information is displayed on the top left corner of the scope. The options currently available are:

Hall Voltage VS. Mass
Scan Number VS. TIC
Mass Number VS. Intensity

The loaded MASH file determines which option is chosen.

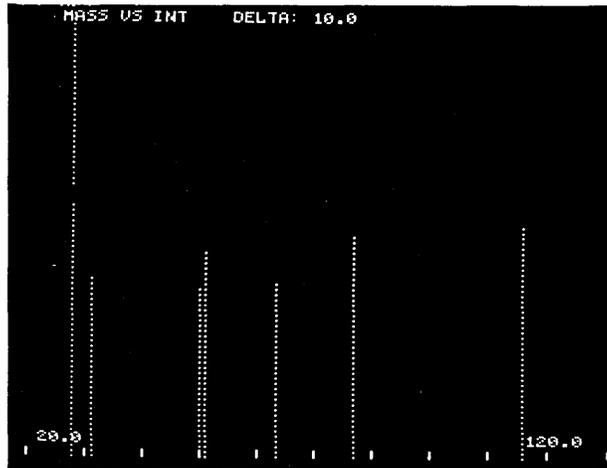
There is also a value labeled DELTA displayed on the top of the scope which is the distance between any two grid ticks. For the above grid, DELTA is 28.1.

The initial line spectrum display contains the complete file normalized to the new max peak.

For example, given the following point pairs:

20.0	100.00
31.2	41.15
50.0	39.56
51.0	47.71
63.4	40.15
77.0	51.29
105.9	52.88

the display would be as follows:



5.2.1 Commands

LOOK types an asterisk when it is ready to accept a command. If a command is illegal, a question mark is typed and the asterisk is re-typed.

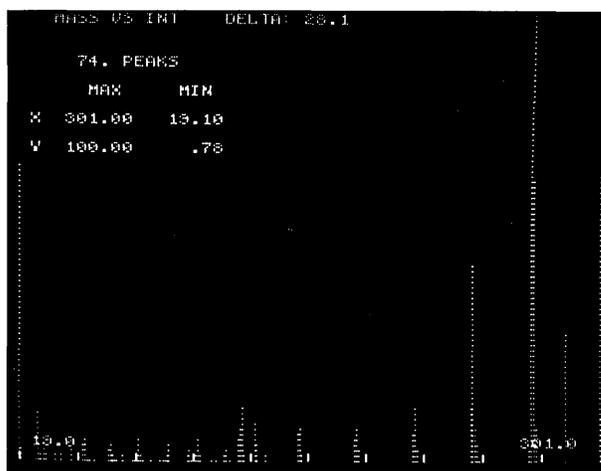
It types a colon when the requested command requires a parameter. If an illegal parameter is entered the colon is re-typed. All parameters are positive numeric values. If any character other than a number or a decimal is typed as a parameter, an asterisk is immediately typed. All parameters must be followed by a carriage return.

All commands are single alpha characters and are executed as soon as they are typed. The RUBOUT key may be used to eliminate a typed character while a parameter is being entered.

The commands accepted by the LOOK program are:

<u>Letter</u>	<u>Code</u>	<u>Explanation</u>
A	Adjust	Adjusts the display in the negative Y direction. This is effectively the same as scaling the display by a negative constant. The A command can be used to lower the display for visual purposes.
B	Backward	Moves the display one frame in the negative X direction. No move will take place if the displayed left limit is equal to the minimum X value of the file.

<u>Letter</u>	<u>Code</u>	<u>Explanation</u>
D	Delete	Deletes the specified peak. The user enters the desired peak number following the colon. (This is an excellent way of eliminating carrier gas peaks from a spectrum.)
E	Expand	Expands the distance between the points which make up the lines in the line spectrum. E may be used to reduce flicker on a full display.
F	Forward	Moves the display forward one frame in the X direction. No move is made if the displayed right limit is equal to the maximum X value of the file.
G	Go	Goes back to the original scale. G completely offsets all A's.
H	Highlight	Displays the important characteristics of the file. H would give the following results for the example file:



This message is displayed along with the line spectrum.

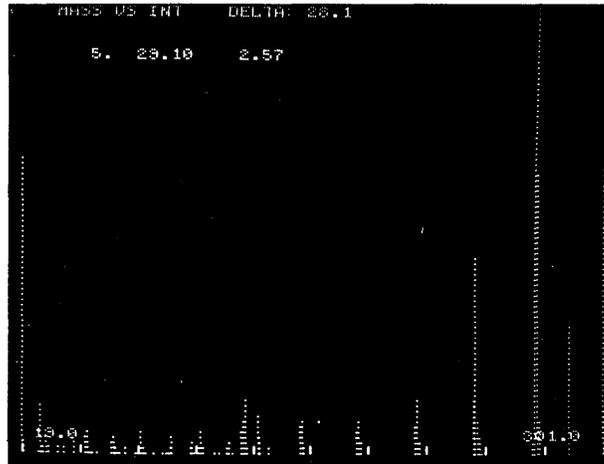
I	Indicate	Displays the coordinates of the specified peak. The peak number is entered following the colon. In the example:
---	----------	---

```
*I
:3
```

LetterCodeExplanation

would give the following display:

3 50.00 30.00



L	Left	Resets the left limit of the display. The new limit is entered following the colon and must be greater than or equal to the minimum X value of the file and less than the displayed right limit.
N	Normalize	Normalizes the spectrum to the defined peak. The desired peak number is entered following the colon. This can be used to effectively magnify the smaller peaks.
O		Displays the total file normalized to the max peak.
P	Print	Prints the total file.
R	Right	Resets the right limit of the display. The new limit is entered following the colon and must be less than or equal to the maximum X value of the file and greater than the displayed left limit.
S	Shrink	Reduces the distance between the displayed points which make up the lines of the line spectrum. This command has the opposite value of E.
T	Threshold	Eliminates all peaks with Y values less than the specified threshold peak from the file. The threshold peak number is specified following the colon. This can be used to quickly eliminate all but the key scans in a multi-scan run.
U		Indicates the peak number of the leftmost displayed peak on the scope.

<u>Letter</u>	<u>Code</u>	<u>Explanation</u>
V		Stores the current data file as OUTFIL and returns to the AIPOS Job Control. No storing takes place if no output file was specified at load time. This can replace the old data by the altered data.
X	Exit	Returns to the AIPOS Job Control. No storing takes place.

5.3 Use in MASH System

Assuming that the output file name typed in during acquisition mode was "SAMPLE", the MASH system has created files with the following names on the output unit.

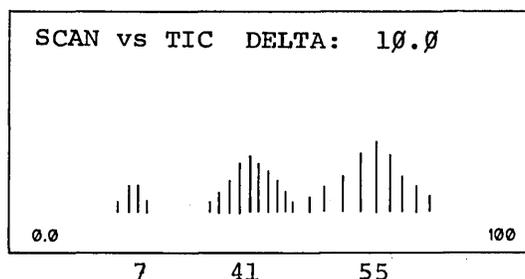
```
SAMPLE.SAM
SAMPLE.TIC
SAMPLE.001
```

```
⋮
```

```
SAMPLE. "n"
```

where "n" is the last scan requested.

To see which scans were "meaningful" (a high total ion current existed when the scans were taken), file "SAMPLE.TIC" must be examined. The display is:



Assuming a gas chromatograph was used, scans 7, 41, and 55 would be representative of the three chromatograph peaks. The files ("SAMPLE.7" "SAMPLE.41" and "SAMPLE.55") could then each be examined in turn. In this way, much spurious data can be eliminated.

APPENDIX A

ERROR MESSAGES

When an error is detected in the CALIBRATION or ACQUISITION routines, the appropriate message is immediately output on the scope, in the format:

```
ERROR XX
HIT RETURN.  TRY AGAIN
```

where XX = error code number. The sole exception to this rule is during the TIC vs. Time Plot of the Acquisition program. Here, rather than interrupt the display, the error in question is typed out preceded by a "?".

The errors, associated code numbers, and explanations are listed below:

?70 FPP ARITHMETIC ERROR

An FPP interrupt because of fraction overflow, exponent overflow, or exponent underflow has occurred.

?71 FPP DIVIDE BY 0

An FPP divide by 0 interrupt has occurred.

?72 HALL TABLE TOO SMALL

For a linear fit, the Hall table must have at least two Hall Voltage/Mass) pairs. For a spline fit, the Hall table must have at least thirty (HV, M) pairs if the spectrometer is not a quadropole and at least two pairs if it is a quadropole.

?73 HALL TABLE TOO BIG

During MANUAL calibration, a maximum number of 95 Hall Voltage - Mass pairs is allowed for any given Hall table. Thus, masses must be deleted until the total is 95 or less.

?74 ILLEGAL COMMAND

For a calibration command to be legal, it must be a defined command and certain specified conditions must prevail. For example, the threshold command, T, may be issued during initial calibration time, but may not be issued after a mass has been assigned to the Hall Voltage table. Also, certain commands are valid for only one mode of calibration. (See Section 3.4.)

?75 ILLEGAL PEAK

This error can occur in two cases:

1. The user has designated a peak number which is not in the range 1-999.
2. He has designated a peak number larger than the largest existing peak number.

?76 ILLEGAL MASS

This error occurs in a number of cases:

1. The designated mass lies outside the range 1-1999.9.
2. The user asks to delete a mass associated with some given peak when there is no mass there.
3. If the user requests a mass be moved to a different peak number, there must be a mass at the designated peak and no mass at the new location.
4. The mass being assigned or moved must satisfy the requirements mentioned in section 3.2.2.2.

?77 ILLEGAL INTENSITY

The user chose an intensity threshold which is not larger than the previous threshold.

?80 ILLEGAL CHARACTER

A Teletype reply is non-octal when it should be octal; or is non-numeric when a numeric reply is required; or an illegal non-numeric reply is given to a parameter specification question.

?81 ILLEGAL RANGE

Numeric replies to a parameter specification question are outside the required range. For example, the resolution must be in the range 200-2000.

?82 WORKING AREA TOO SMALL

The Calibration program needs at least six blocks of working area, the Acquisition program needs seven.

?83 AIPOS CALL ERROR

At Job Control time the wrong number or type of output or input files were specified. This error always leads back to Job Control.

?84 INPUT FILE NOT HALL TABLE

This is a specialized case of error ?83 for the Acquisition program. It subsequently exits.

- ?86 6 CHARACTER SAMPLE NAME NOT UNIQUE
- The first six characters [of a possible ten] of the output file name specified for the acquisition program via Job Control are not unique for the output volume. Acquisition exits.
- ?87 OUTPUT INDEX TOO SMALL
- There is not enough room in the output volume index for all the scan files requested. As many as possible are saved.
- ?88 ILLEGAL COMMAND AT THIS TIME
- The character typed is temporarily illegal because of existing conditions [ex: scan desired when TIC below threshold].
- ?90 AIP ERRORS
- AIP sampling errors occurred during scanning. Scan speed may have been too high.
- ?91 FPP ERROR ON SCAN
- FPP error occurred processing data. Scan is suspect.
- ?92 >500 SCAN PEAKS SEEN
- Intensity threshold was set too low; noise peaks were examined.
- ?93 HALL VOLTAGE UNSTABLE
- Disregard scan. Recalibrate.

APPENDIX B

CURVE FIT ALGORITHMS

Following are detailed descriptions of the two types of "fits" available for assigning masses to Hall Voltage values. Currently linear fits are only used with Quadropole mass spectrometers; all standard spectrometers require a spline fit because of the very nature of the Hall Voltage, which is not piecewise linear.

B.1 Linear Fit

Given: (H_k, M_k) and (H_{k+1}, M_{k+1})
Where: H = Hall Voltage
 M = corresponding assigned mass
Let: $H_k < H_a < H_{k+1}$

Finding M_a implies $M_a = AH_a + B$, where the given points are assumed to define the line.

So: $M_a = M_{k+1} + C_k (H_{k+1} - H_a)$ for all $M_k < M_a < M_{k+1}$
Where: $C_k = \frac{M_{k+1} - M_k}{H_{k+1} - H_k}$

B.2 Spline Fit

Given: (H_k, M_k) and (H_{k+1}, M_{k+1})
Let: $H_k < H_a < H_{k+1}$
Then: $M_k < M_a < M_{k+1}$ can be described by:
$$M_a = C_1 (H_{k+1} - H_a)^3 + C_2 (H_a - H_k)^3 + C_3 (H_{k+1} - H_a) + C_4 (H_a - H_k)$$

where C_1, C_2, C_3, C_4 are calculated by assuming continuous second derivatives through adjacent curve segments, as well as defining two arbitrary boundary conditions.

APPENDIX C

CONVENTIONS

The following conventions are assumed by the Acquisition program, and must be realized in every MASH interface with a mass spectrometer.

- a. If the computer initiates scanning:
 - Relay register 9: Takes control of Mass spectrometer
 - Relay register 11: Initiates scan
- b. If the mass spectrometer initiates scanning request:
 - External level \emptyset : Grounded if spectrometer is initiating scanning request:
- c. Channel 44 is the Hall Voltage (or Quadropole mass)
 - AIP input channel data is assumed 12 or 15 bits, reproducible, and monotonically related to mass number.
- d. Channel 45 is the intensity and input channel. Data is assumed 12 or 15 bits.
- e. If available, channel 46 is the AIP TIC channel. Data is assumed 12 or 15 bits, slowly changing.
- f. Channels 44, 45, and 46 are enabled to use the KW12A clock (internal to the PDP-12 LDP) as an external synchronization.

GLOSSARY

BASELINE

The \emptyset value of any parameter. This is subtracted from all subsequent values, and enables relative size to be calculated. For example, two values, 5 \emptyset : 1 $\emptyset\emptyset$ are related 1:2; but if the baseline is 25, the relationship is really 25:75 or 1:3.

FLYBACK (Or Delay)

The period in which the field recycles, usually considered "deadtime" between successive scans.

FRAME

The picture (display) on the scope.

HALL TABLE

An eight block file on LINtape having one header block, two blocks of Hall Voltage/Mass pairs, and five blocks of coefficients used in the linear or spline curve fits.

HALL VOLTAGE

Signal provided from Hall probe attached to mass spectrometer magnet that is proportional to field strength. Then for mass spectrometers that vary magnetic field and not voltage, this signal is related monotonically with mass, and the relationship will have drift noticeable only on a daily basis (if then).

INTENSITY

For a given mass, the relative number of ions out of all ions emerging from the source at scan time that weigh that mass. The sum of all intensities for a scan, then, equals the TIC.

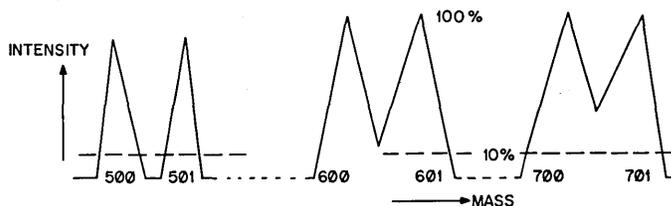
QUADROPOLE

A type of mass spectrometer where the electric field rather than the magnetic field is varied. The field voltage can be directly obtained, and as it is linear with mass, no Hall probe need be attached.

RESOLUTION

The 10 percent definition is used here. In other words, the highest mass number for which equal intensities at two adjacent masses drop to at least 10 percent of the peak height is considered the resolution of the mass spectrometer.

In the figure below, the resolution of the spectrometer is 6 $\emptyset\emptyset$.



SCAN

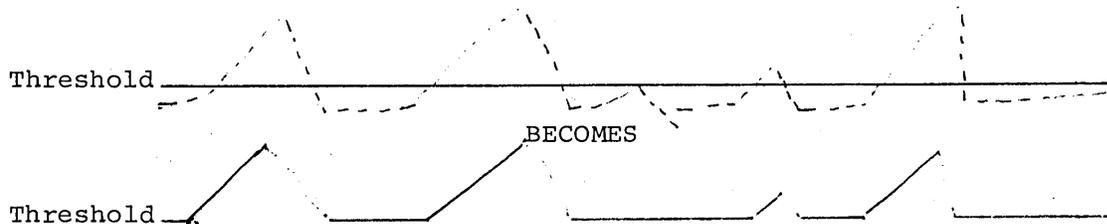
The bending and subsequent recording of ions emerging from the source, by varying either electric or magnetic field. The velocity of the heavier ions will be slower due to energy constraints, and the mass differentiation is made on this basis. The result of a scan is the relationship between intensity and Hall Voltage/exact mass at scan time.

SPLINE FIT

A relationship assumed to exist in some cases between Hall Voltage and mass, in which small increments are chosen, and their second derivatives are set equal. Such a relationship assumes nothing about linearity, although it is monotonic, and results in a curve rather like one drawn with a draftsman's spline.

THRESHOLD

A value of a parameter below which all readings will be ignored. If an intensity threshold is set, the smallest subsequent peak that could be looked at would be at least as high as the threshold value. This value is mainly used (as below) to reject spurious data:



TIC (Total Ion Current)

Signal from a gas chromatograph (or mass spectrometers so equipped) that represents the total ion current (or number of ions available) at any given moment.

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Product Name:	MASH - Correction to MASH User's Manual
Date Created:	December 30, 1971
Maintainer:	Software Support

First Printing
December, 1971

Second Printing
February, 1972

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The following information on automatic mode should be inserted in the MASH User's Manual (DEC-12-SQ2A-D), as the third paragraph on page 16.

If G is typed again, automatic mode initiates a series of scans that last until the chromatograph run is complete. Pressing one of the right switches on the console terminates scanning and returns the program to the TIC vs. Time plot.

IDENTIFICATION

Product Code:	DEC-12-SQ2A-DN1
Product Name:	MASH - Phase II Supplement to MASH User's Manual
Date Created:	October 18, 1971
Maintainer:	Development

First Printing
October, 1971

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PREFACE

It is suggested that the reader refer to the MASH User's Manual: Version I [DEC-12-SQ2A-D] for which this document is essentially a supplement. This document supersedes DEC-12-SQ2A-DN.

When MASH Phase III is developed, a new MASH User's Manual will be published which will include all previously published MASH documents.

◆◆◆◆◆◆◆◆

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1.0 INTRODUCTION

Phase II of the Mass Spectrometer Handler (MASH) greatly expands the data reporting facilities of Phase I, which was essentially a data acquisition system with minimum report capability. The expansion has been made in the following three major areas:

A. NEW REPORT GENERATOR FEATURES

1. Printed mass tables
2. Chaining facility for examining consecutive files
3. Normalizing to sum of intensities
4. Ordered printout of highest peaks
5. Ability to examine mass chromatographs [see below].
6. Ability to generate hard copy plotter output [see below].

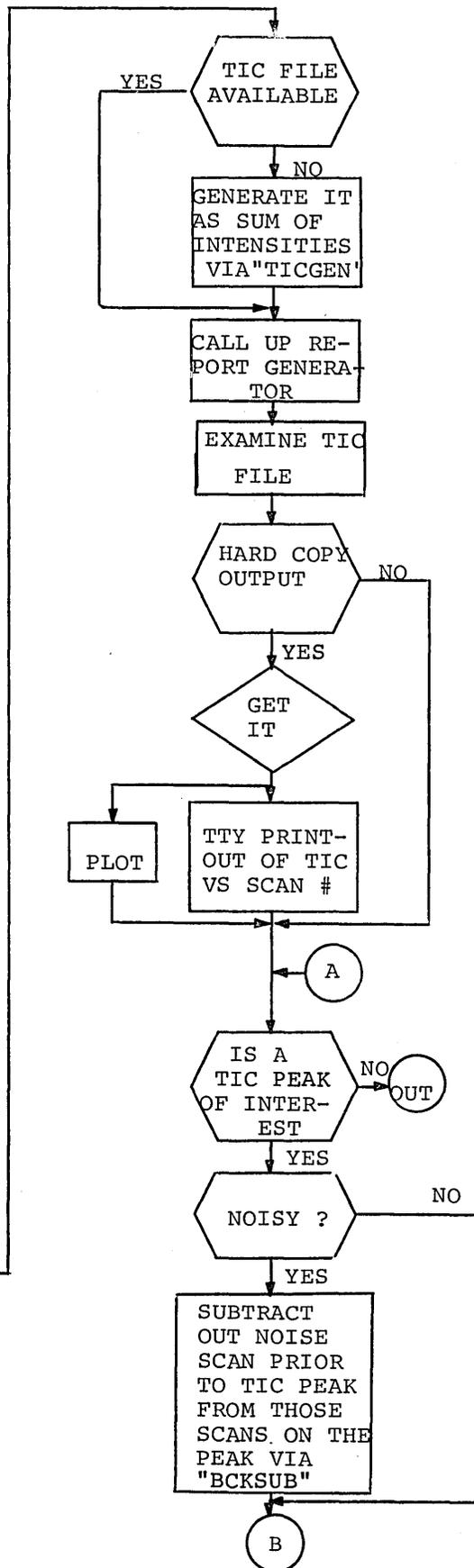
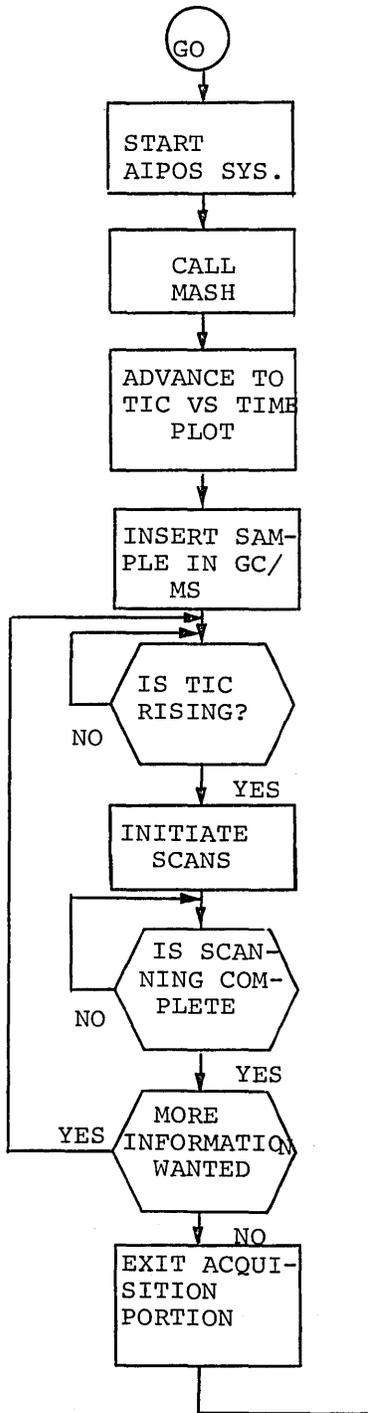
B. PLOTTER CAPABILITY

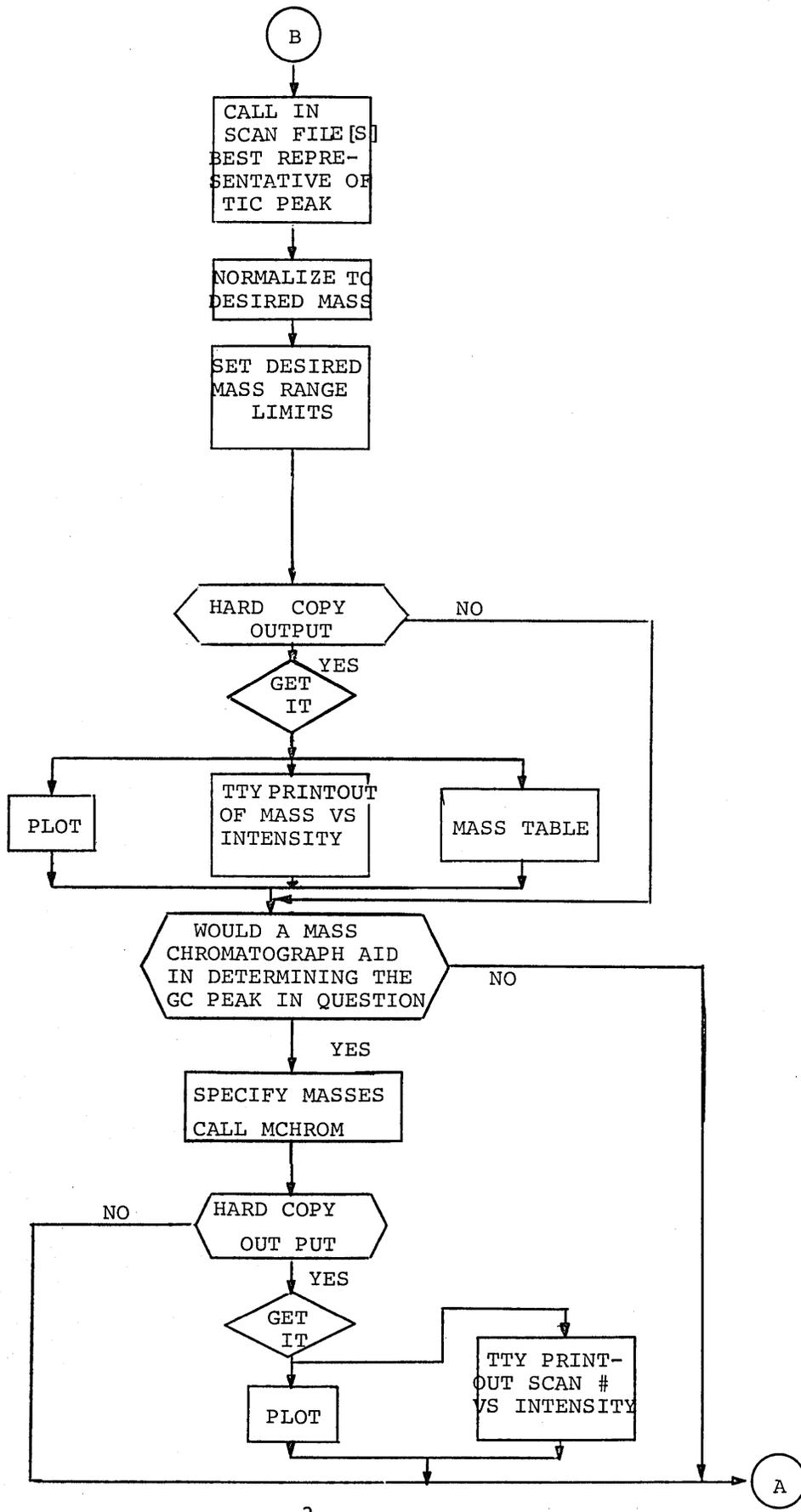
1. CALCOMP or Houston Plotter
2. Electrostatic Printer/Plotter

C. NEW FILE CREATIONS

1. Mass chromatographs [intensity vs. scan for given masses].
2. Total ion current [as a sum of intensities] vs. scan #.
3. Background subtraction of noise from scan data.

A flowchart of a typical chemist's usage of the MASH Subsystems is on page 2. This chart assumes that calibration has previously been done.





2.0 NEW REPORT GENERATOR FEATURES

2.1 General Description

All options explained in this Section assume that Report Generator [LOOK] has been correctly loaded and is examining a file of interest. Refer to Section 5.0 of the MASH User's Manual, Version 1 for both the loading procedure and the command list of Report Generator.

2.2 Mass Table

```

LOREM .001
  MASS TABLE
  STARTING MASS : 100

      0      1      2      3      4      5      6      7      8      9
0- 23.2  4.5   .0   .0   .0   .6   .0   .0   .0   .6
1-  .0   .0  3.4 10.9   .4   .5   .2  2.1   .0 ****
2-  2.2   .0   .0   .0  3.1   .6   .6   .9   .0   .0
3-  .0 ****  3.5  3.5   .0   .0   .4   .8   .0   .4
4-  .0   .0   .0  9.4  1.5  2.7   .0   .3   .4   .0
5-  4.8  7.2   .0   .0   .0  6.6   .4   .7   .0   .0
6-  .0   .0 11.1  6.2   .4   .0   .0  1.1   .6 60.6
7-  2.0   .0   .0   .0  1.4  1.6   .0   .5   .0   .8
8-  .0 72.4  3.3  1.7   .0   .0  3.4  1.1   .0   .0
9-  .0   .0   .0 12.2  1.2  1.4   .6  1.2  1.0   .9

      0      1      2      3      4      5      6      7      8      9
0-  1.1  2.2   .0   .0   .0  9.0   .8   .8   .0   .0
1-  .6   .0  4.8  3.1   .0   .0   .0  4.0   .8 23.9
2-  1.1   .0   .6   .4  1.9  1.8   .0   .0   .0   .9
3-  .0 34.0  1.9   .9   .0   .0  3.5  1.3   .4   .4
4-  3.5  1.7   .5 19.9  1.4   .8   .0   .0  1.0   .8
5-  .5  1.3   .0   .0  1.5  8.4   .9   .7   .0   .0
6-  .6   .0  1.2  1.8   .0   .2   .0  5.0   .7 10.7
7-  .7   .0   .4   .2  1.2  1.4   .0   .0   .0  1.2
8-  .0 21.9  1.4   .7   .0   .0  2.0  1.0   .0   .0
9-  .0   .9   .0 15.1  1.2   .5   .0   .0   .9   .6
  
```

Figure 1 - Mass Table

The following conditions must be met before a mass table for a given scan can be printed.

- A. The file being examined must be a scan file [i.e., Mass vs. Intensity].
- B. The file must be normalized to the desired peak [since all intensity values print out in normalized form if lower than 100%, or as *** if greater than or equal to 100%].
- C. The Mass Table range desired for printout must be the range currently shown on the scope [set via the L and R commands].
- D. If the Report Generator was loaded from LINCTape, the WRITE ENABLE switch must be enabled on the loading unit.

The sequence of steps to generate a Mass Table from the scope image is:

1. Type "M". The display vanishes, and a ":" is printed. [No ":" probably means that the WRITE ENABLE switch is off. Turn it on, and the ":" should follow.]
2. Type the number of columns desired (2-14), where the number is the atomic weight of the group suspected of forming the basic building block of the unknown compound. [For example, 14 would imply CH_2 was suspect.] If the number is correctly chosen, the Mass Table shows the concentration of all ions differing only by such building blocks, as the elements of a given column.
3. Type carriage return to generate the Mass Table. To find the normalized intensity of any given mass, subtract the starting mass of the table [as typed], from the given mass, and divide the difference by the number typed for the column length. The quotient is the row # [on the extreme left of the typeout], and the remainder is the column number [on the top of the typeout] of the intensity "element". [For example, if the starting mass is 100, the desired mass is 131, and the number of columns is 10, look in Row 3, Column 1. Note that for the PFK mass table peak 131 is saturated.] The intensity value output for mass "M" will be the highest value between mass $M-.3$ and $M+.3$.
4. To stop printout at any point after the Mass Table header is printed, type CTRL/R¹. The program returns to the scope display.
5. When printout is completed, the program, as in the CTRL/R case, returns to the scope display, and awaits new command.

¹CTRL/R is typed by holding down the CTRL key while typing R.

2.3 The Y Command

The Y command allows the operator to chain MASH files, normalize or print stored data. When Y command is typed, the display vanishes and a ":" is printed (for LINtape loaded programs, the WRITE ENABLE switch must be ON). The operator now has five choices:

2.3.1 Type S [for "SHOW ME"] to print a list of the other four options in the form:

TYPE 1	for chaining facility
TYPE 2	for normalization to sum of intensities
TYPE 3	for normalization to highest sum of intensities
TYPE 4	for printout of ten highest peaks
TYPE S	for SHOW ME

Type CTRL/R to stop typeout and return to the display.

Upon completion of the typeout another colon is printed.

2.3.2 Type 1 to call the chaining facility.

Previously, when the information in a given scan was exhausted, the operator was forced to exit, return to job control, type a new "load" line of the form:

```
LTa: LOOK LTb:OUTPUT = LTc:INPUT
```

and wait for the tape to stop shuffling before he could see the next MASH file.

The chaining facility allows the operator to type 1 , to go directly to the next MASH file.

Before 1 is typed, the following condition must be met:

- a. The next file after the current input file must be a MASH file, exclusive of the ".SAM" variety. If not, an error message occurs and the program returns to job control.

If this condition is met, type Y and then 1 to go from MASH file to MASH file. Example - to go from PFK.005 to PFK.006, type Y , 1 .

- 2.3.3 Type 2 to call for a normalization to the sum of the intensities in the current scan. In this case, the file being examined must be a MASH scan file, or the program returns to the display. Such normalization is useful in providing a measure of the extent of distribution of ions throughout a given spectrum. All intensities will, until a renormalization or exit is taken, be effectively reported as a percent of total ion current.
- 2.3.4 Type 3 to call for a normalization to the highest sum of intensities in the current scan provided the following conditions are met:
- a. The file being examined is a MASH scan file
 - b. At the time Report Generator was called, the T.I.C. file associated with this scan file [same first six characters, followed by .TIC] was given as a second input file.

If successful, all intensities in the scan are normalized to the highest sum of intensities for the experiment. If used consistently in the reporting of each scan, it means that the intensity percentage reported for every mass is directly proportional to the number of ions having that mass at the time the scan was taken. As an example, scans taken when the gas chromatograph was at or near a peak will report higher intensity percentages than other scans further away from a peak. This would apply even if the compound involved was the same, simply because the quantity of the compound was different.

If this feature is to be used consistently, a suggestion to speed up reporting would be to move the TIC file to a new tape unit prior to calling Report Generator. This would save "tape spinning" each time this type of normalization was called for a new scan file.

Assuming the scan data was on unit 1, and the name of the experiment was called "sample", the procedure might be to use the job control commands:

a) LT0:MOVE SAMPLE.TIC = LT1:SAMPLE.TIC

to move the file and:

b) LTØ: LOOK OUTPUT=LT1:SAMPLE.ØØ1,SAMPLE.TIC

to call Report Generator with this normalization feature enabled.

2.3.5 Type 4 to call for an ordered printout of the ten largest peaks in the file [which may be stopped by ↑R causing a return to the display], which is identical to the form of printouts generated by the "P" and "V" commands -- for many purposes [such as library identification], the ten highest peaks are of major importance. Also, the highest peak can thus be quickly identified for normalization purposes.

2.4 Examining Mass Chromatographs

A Mass Chromatograph file created via MCHROM (see below) can be examined via Report Generator. Use the Mass Chromatograph file name and unit as the input file name and unit when issuing the call to the AIPOS Monitor, as, for example:

```
LTa: LOOK LTb:OUTPUT=LTC:M69
```

where M69 is a Mass Chromatographic file.

A Mass Chromatograph file can also be examined using the "Y" command if it is the next file in a sequence of MASH files.

2.5 Generating Hard Copy Plotter Output

The Plot option in Report Generator is an exceedingly powerful one because of the extent of control the operator maintains over what is plotted. The operator can take a basic file and, before plotting:

1. Delete specific peaks
2. Perform thresholding to retain only significant peaks
3. Set the range of X [masses, scan numbers] through which the plot is desired via the "L" and "R" commands.
4. Set the range of Y [intensities, T.I.C.'s] by normalizing to a peak which will cause most peaks of interest to be in mid-range via the "N" command.

When the Q command is given to the Report Generator program (assuming conditions B, C, and D, of Section 2.2 are met) the scope image is plotted out. The plotter may be on or off at this point.

The Teletype prints:

TYPE

SPACING:

HEADER:

:

The operator types the spacing desired: 2-20 for the electrostatic plotter and 0-9 for the X-Y plotter. The spacing is proportional to the X-axis length. If a wide range of X is being examined in an over-view [see Figure 2], spacing should be small. If a small range is being studied closely, spacing should be wider [see Figures 3 and 4]. If a number out of limits or a non-number is typed, it is equivalent to hitting CTRL/R.

Upon receiving the spacing, the program prints another ":". The operator types in the one line "HEADER" (up to 68 characters) to appear on the plot. For example:

"HIGH BOILING PFK NORMALIZED TO MASS 131 - MARCH 1971"

Be sure the plotter is turned on before typing carriage return.

When carriage return is typed, the scope goes dark and plotting commences. The routine returns to display the scope image of the file being plotted only if:

1. the plotter was initially off;
2. ↑R is typed (in which case, the plot is incomplete);
3. the plot is completed.

Examples of Mass vs. Intensity plots are given in Figures 2, 3, and 4. Another type of possible plot is shown in Figure 5. Note that all X values are rounded to unity. The Y value plotted at X value "m", for example, is the highest Y value for any X between $m-.3$ and $m+.3$.

24 PFK FULL FILE NORMALIZED TO MASS 131

LOREM .001

MASS VS INT

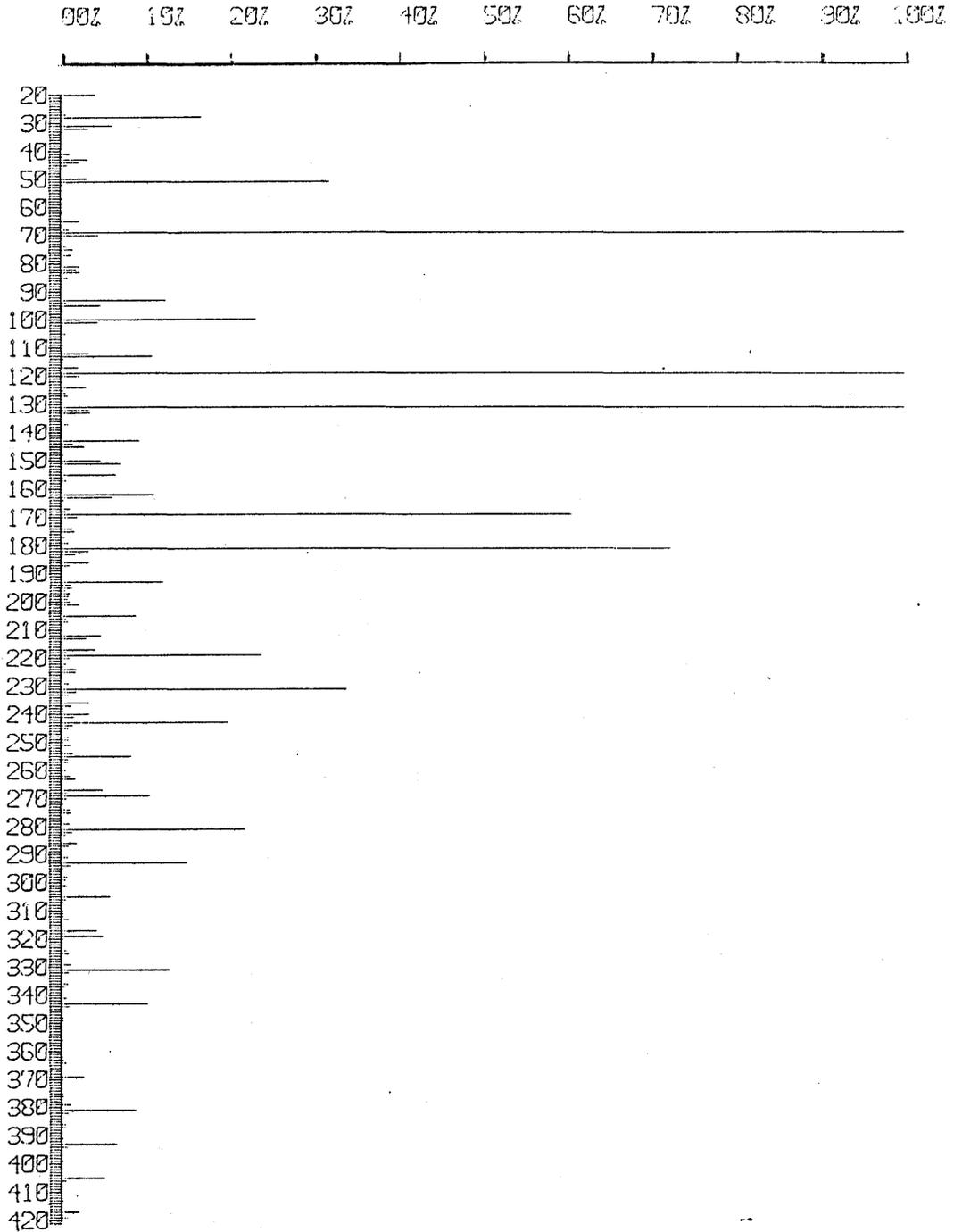


Figure 2 - Plot of Entire File (Spacing = 0)

PFK LIMITED RANGE NORMALIZED TO MASS 131

LOREM .001

MASS VS INT

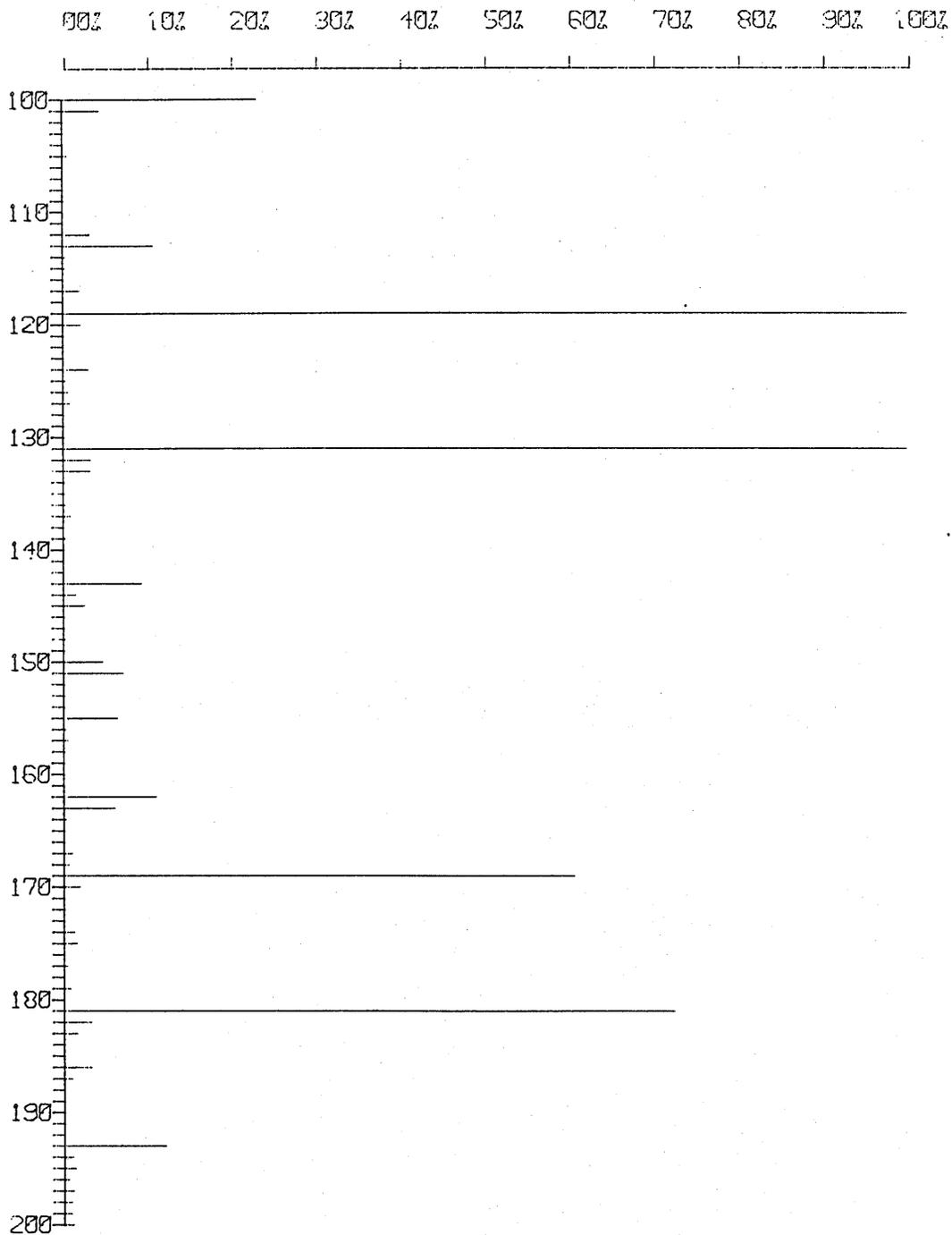


Figure 3 - Plot of Mass Region of Interest (Spacing = 3).

24 PFK FULL FILE NORMALIZED TO MASS 131

LOREM .001

MASS VS INT

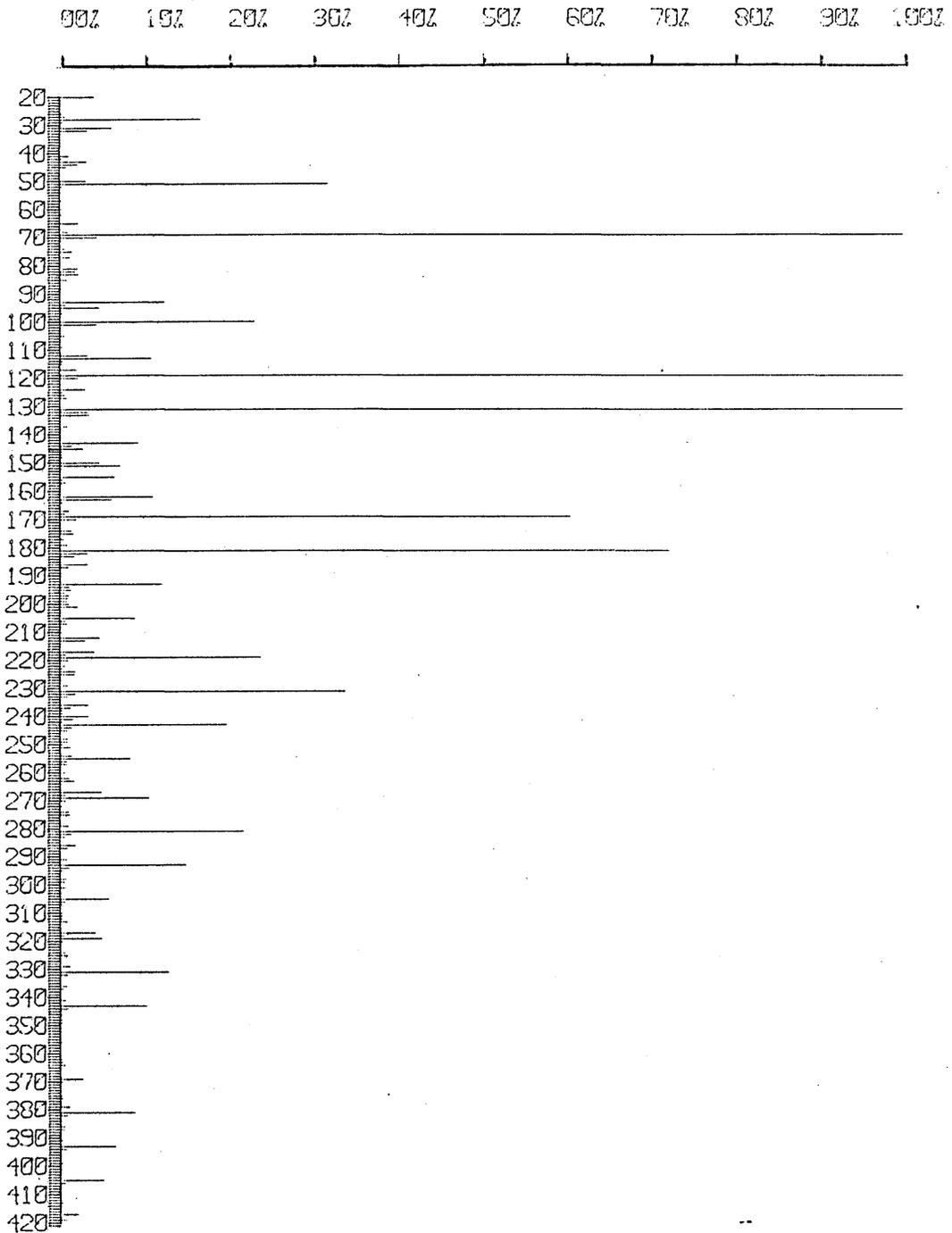


Figure 2 - Plot of Entire File (Spacing = 0)

PFK LIMITED RANGE NORMALIZED TO MASS 131

LOREM .001

MASS VS INT

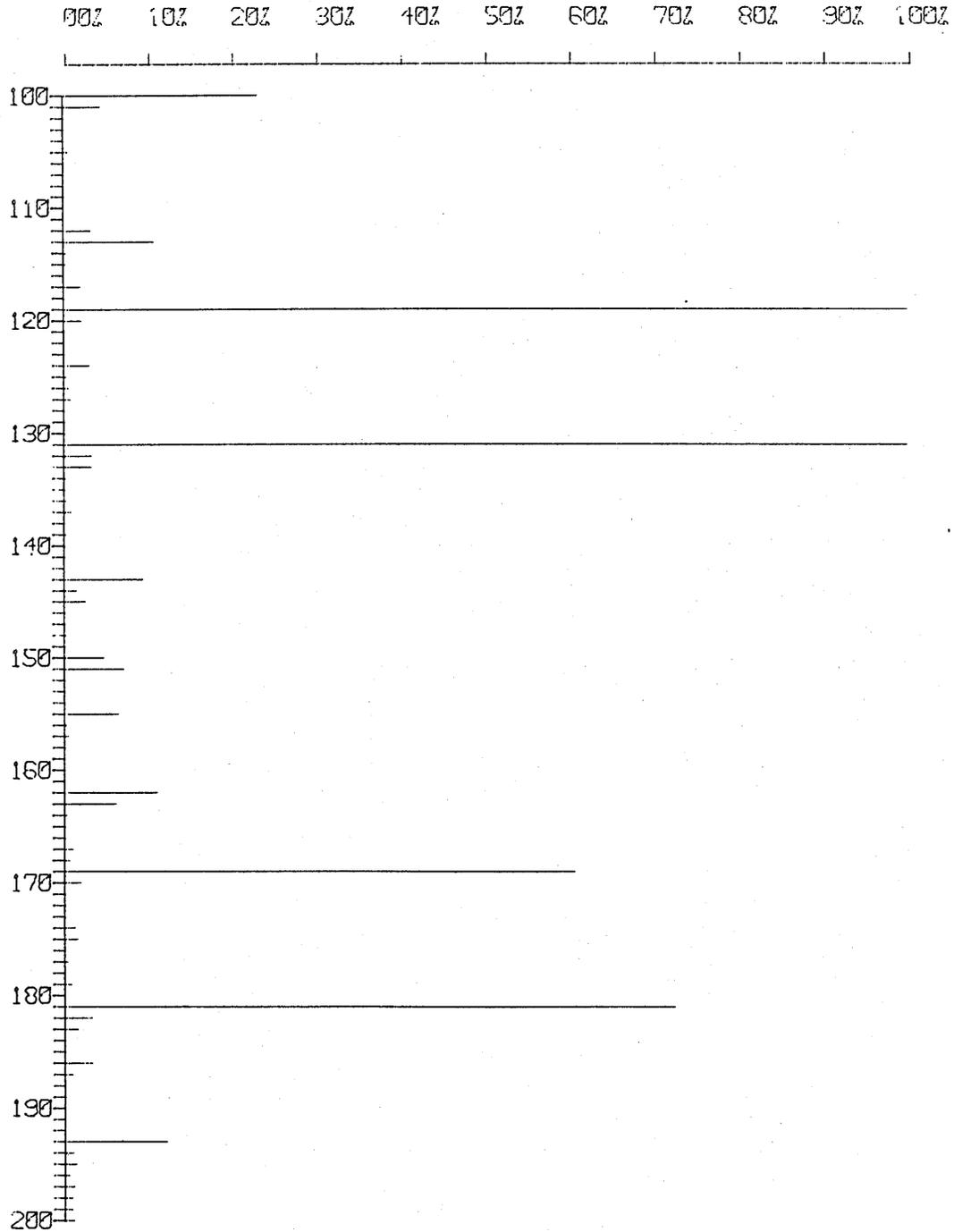


Figure 3 - Plot of Mass Region of Interest (Spacing = 3).

PFK LIMITED RANGE NORMALIZED TO MASS 200

LOREM .001

MASS VS INT

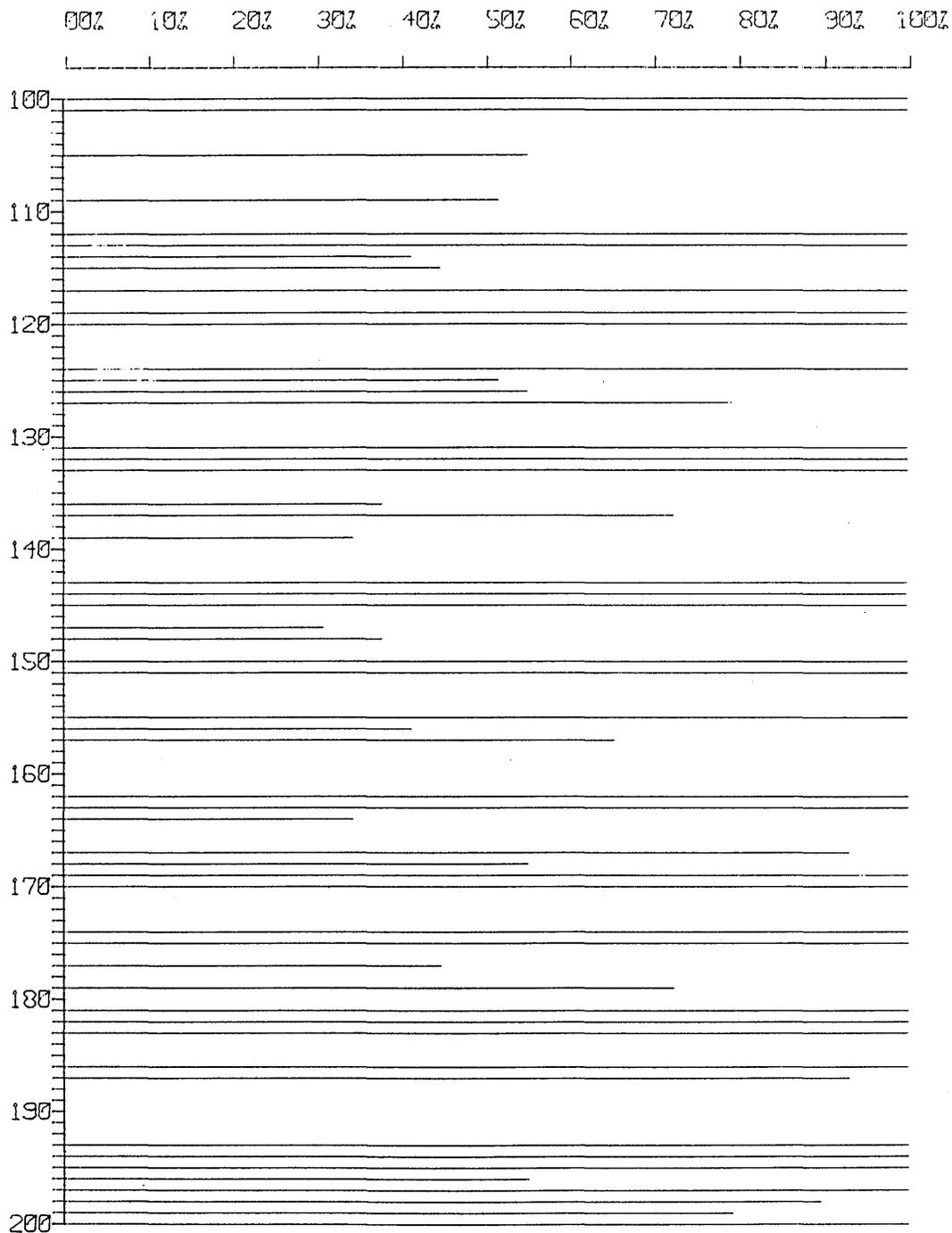


Figure 4 - Plot Emphasizing Small Peaks in the Mass Region of Interest

MASS CHROMATOGRAPH OF PFK FOR MASSES 69 AND 131

MCHROM

SCAN VS INT

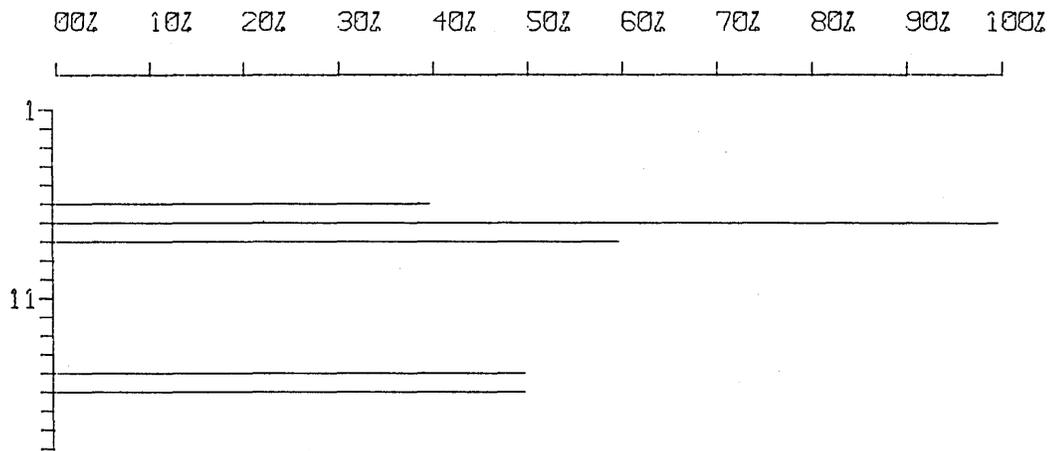


Figure 5 - X-Y Recorder Plot of Mass Chromatograph

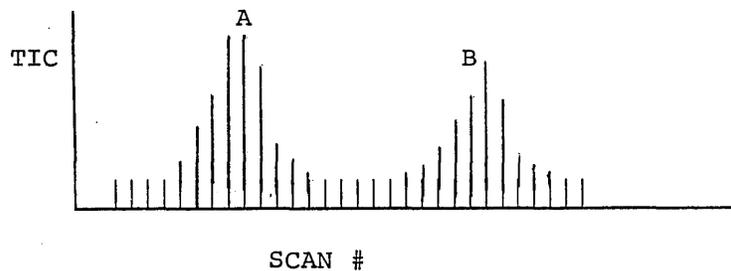
3.0 NEW FILE CREATIONS

In all programs which follow, it is assumed that the order of the MASH acquisition generated files has been left untouched on an AIPOS tape since the experiment involved was run. Violation of this assumption could cause catastrophic error.

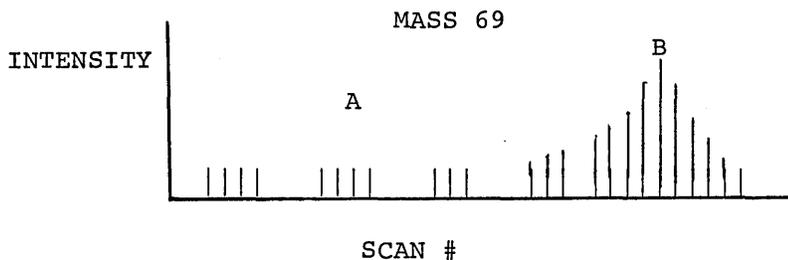
3.1 Mass Chromatographs

MASH uses the program "MCHROM" to process a sequence of mass vs. intensity scans to generate an output file consisting of the averaged intensities [of the specified masses] in a given scan vs. the scan number. The output file created can be examined by Report Generator.

Such files of intensity vs. scan number for given mass[es] have proved to be of value in determining the compounds involved in GC peaks. For example, in a given experiment, if the TIC vs. scan number file looked like:



and the intensity vs. scan number plot looked like:



then an ion of Mass 69 did not appear in the compound causing Gas Chromatograph peak A, but was a major component of peak B.

The operator can specify up to five masses whose intensities are to be averaged [of use when a particular grouping is suspected as a prime GC peak component] when the program "MCHROM" is called from the AIPOS Monitor. The calling statement takes the form of:

```
LTa:MCHROM LTb:MA6970=LTc:EXPERM.SAM;69,70
```

where:

MA6970 = File created, to be examined by Report Generator.

EXPERM = Six character name of series of MASH files created during the Acquisition mode of MASH.

For example, an index of LTc shows:

```
EXPERM.SAM
EXPERM.TIC
EXPERM.001
.
.
EXPERM.nnn
```

and "69" and "70" are the masses whose intensities are to be averaged.

Upon completion of the call statement, MCHROM generates the output file as a Mass Chromatograph, and exits to Job Control with no further operator input required.

Possible errors are:

80 = Parameter error [in calling statement]
83 = I/O file error
84 = Error in scan files

All errors cause a return to Job Control. Errors 80 and 83 are terminal. Error 84 allows creation of a partial Mass Chromatograph.

3.2 Total ION Current As a Sum of Intensities vs. Scan Number

The program "TICGEN" is used with those GC-MS systems for which the total ion current [T.I.C] is not available during scanning. Upon identification of the experiment, TICGEN sums all the intensities of a given scan, and saves the sum and the scan number. When all scans in the experiment have been examined, the intensity values are

scaled and saved in the TIC file previously created by Acquisition [and previously filled, if the TIC was available].

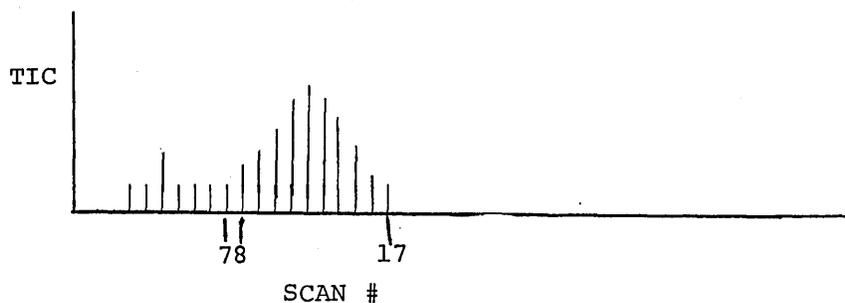
The calling sequence is:

```
LTa:TICGEN=LTb:EXPERM.SAM
```

The TIC file is stored in a previously created slot called "EXPERM.TIC". Possible errors are the same as for MCHROM. All errors cause a return to the AIPOS Monitor.

3.3 Background Subtraction of Noise from Scan Data

A common problem in GC-MS analysis is contamination of a peak on a GC by peaks that have occurred previously. A background subtraction program [BCKSUB], was created to handle this problem in the MASH system. For example, in the plot below:



If scan 7 were subtracted from scans 8-17, the resulting scans would be freer of the GC "prehistory", and give truer values for the component causing the G-C peak.

"BCKSUB" is called from the AIPOS Monitor via a calling statement of the form:

```
LTa:BCKSUB=LTb:EXPERM.007,EXPERM.008,EXPERM.017
```

where:

EXPERM is the name of the experiment.

EXPERM.007 [the first input file] is the scan to be subtracted.

EXPERM.008 [the second input file] is the first scan to be "cleaned up".

EXPERM.017 [the third input file], is the last scan to be "cleaned up".

The mass peak heights at the start of the GC peak [SCAN, EXPERM.007], are subtracted from each scan in the GC peak [SCANS EXPERM.008 - EXPERM.017], the results becoming the new mass peak heights of the GC peak scans. Error messages are the same as MCHROM. All errors cause a return to AIPOS Job Control.

4.0 MASH ASSEMBLY INSTRUCTIONS

This Section provides the assembly instructions for the six programs which make up the MASH Phase II system.

- a. Calibration
- b. Acquisition
- c. Report Generation
- d. Mass Chromatograph
- e. TIC As Sum of Intensities
- f. Background Subtract

4.1 Assembly Instructions: Calibration and Acquisition

1. Assemble "OVLYC4" via DIAL-MS Assembler¹. Save Binary with command:

```
→SB nameA,unit,P10400 ↵
```

2. Assemble "PREAC" via FPP Assembler². Save Binary with command:

```
→SB nameB,unit ↵
```

3. Assembler "ACQ27" via FPP Assembler. Save Binary with command:

```
→SB nameC,unit ↵
```

4. Assemble "ACFPPT" via FPP Assembler. Make sure "MASHFPPN" is on the same unit, and that the unit is either "LT1" or "R11". Save Binary with command:

```
→SB nameD,unit ↵
```

5. Assemble "PACPU2" via FPP Assembler. Make sure "PAFPP" is on the same unit, and that the unit is either "LT1" or "R11". Save Binary with command:

```
→SB nameE,unit ↵
```

¹Refer to LAP6-DIAL Programmer's Reference Manual (DEC-12-SE2D-D).

²Refer to FPP Assembler User's Guide (DEC-12-AQ2A-D).

6. Assemble "CURFIT4" via FPP Assembler. Save Binary with command:
 →SB nameF,unit ↵
7. Assemble "MASHEC" via FPP Assembler. Save Binary with command:
 →SB nameG,unit ↵
8. Load AIPOS¹. Order:
 BUILD CALIB ↵
9. Give "nameA" through "nameG" as successive overlays in exactly the order above. No scratch area or working areas are required.
10. Do an ALIAS on CALIB.BIN calling it ACQUI.BIN. Both should be 74₈ blocks long.

4.2 Assembly Instructions: Report Generator

1. Assemble "REPORTC" via FPP Assembler. Make sure that both "MLB1S" and "MLB2S" are on the same unit, and that the unit is either "LT2" or "R12". Save Binary with command:
 →SB name1,unit,P110000 ↵
2. Assemble "MASSTB10" via FPP Assembler. Save Binary with command:
 →SB name2,unit ↵
3. Assemble "YOVLV" via FPP Assembler. Save Binary with command:
 →SB name3,unit ↵
4. Assemble "EPLOT4" via FPP Assembler. Save Binary with command:
 →SB name4A,unit ↵

¹Refer to AIPOS User's Manual (DEC-12-SQ1A-D).

5. Assemble "XYPLOTT" via FPP Assembler. Save Binary with command:

→SB name4B1, unit)

6. Assemble "XYFPPI" via FPP Assembler. Save Binary with command:

→SB name4B2,unit)

7. Load AIPOS. Order:

BUILD LOOK)

8. Give "name1" through "name3" as successive overlays in exactly the order above. If the installation has a Calcomp plotter, a Houston plotter, or no plotter, finish with overlays "name4B1" and "name4B2". If the installation has a digital plotter (Versatic, for example), finish with overlay "name4A."

9. In either case, four blocks of scratch area and one working area are required.

4.3 Assembly Instructions: Mass Chromatograph

1. Assemble "MCHRM5" via FPP Assembler. Save Binary with command:

→SB name1,unit,P100000)

2. Load AIPOS. Order:

BUILD MCHROM)

3. Give "name1" as the only overlay. No scratch area or working area is needed.

4.4 Assembly Instructions: TIC As Sum of Intensities

1. Assemble "TICGENC" via FPP Assembler. Save Binary with command:

```
+SB namel,unit,P106000 ↵
```

2. Load AIPOS. Order:

```
BUILD TICGEN ↵
```

3. Give "namel" as the only overlay. No scratch area or working area is required.

4.5 Assembly Instructions: Background Subtract

1. Assemble "BCKSUBC" via FPP Assembler. Save Binary with command:

```
+SB namel,unit,P106000 ↵
```

2. Load AIPOS. Order:

```
BUILD BCKSUB ↵
```

3. Give "namel" as the only overlay. No scratch area or working area is required.