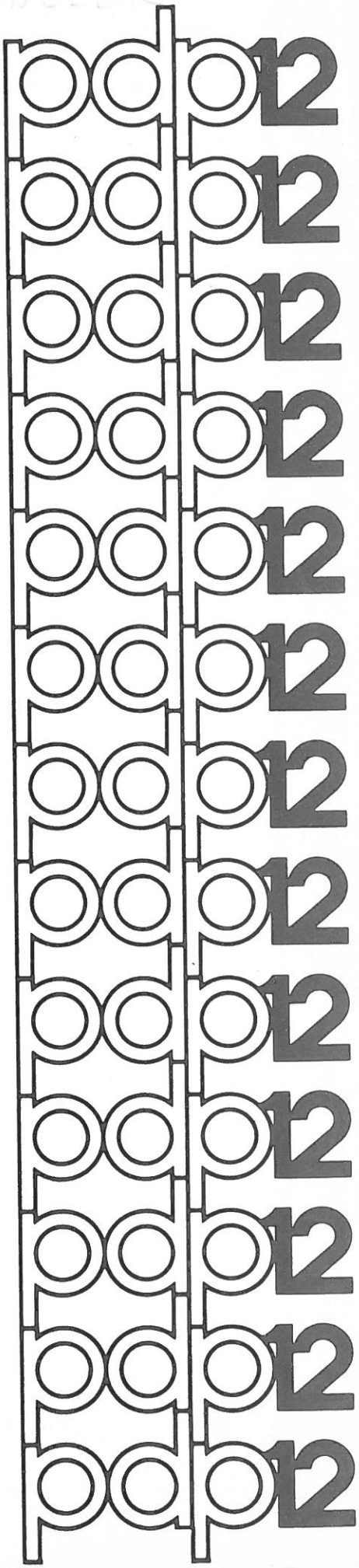
digital



MASH

USER'S MANUAL

(VERSION 1)

DEC-12-SQ2A-D
First Printing
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MASH USER'S MANUAL

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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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CONTENTS

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 Teletype[1] 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-SQ1A-D) for information on the Job Control program which is used to call the MASH programs.

[1]Teletype 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

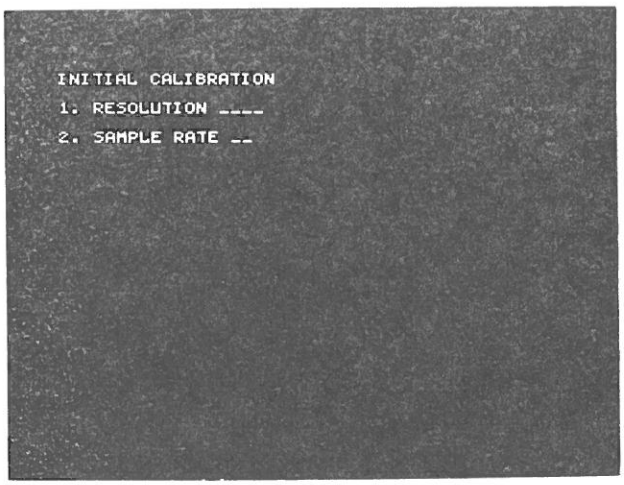
After verification is obtained for only one output file and no input files, the necessary header block information for the HALL TABLE is specified in the user's response to three consecutive frames displayed on the scope.

3.2.1 Parameter Specification[1]

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.



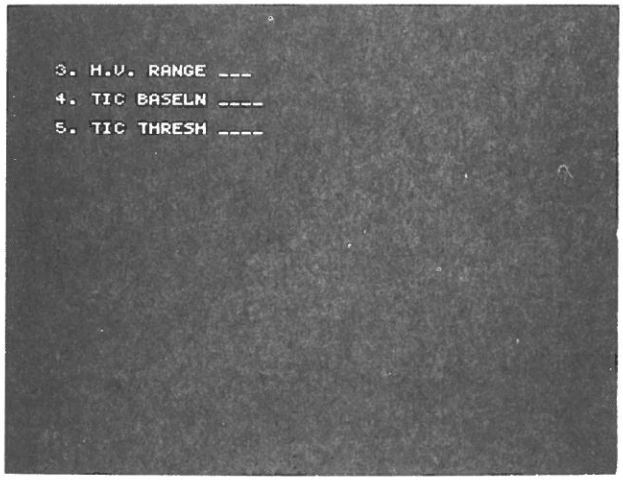
Question 1: Answer question 1 with the 10% valley definition of resolution (see Glossary). The range permitted for this choice is a decimal number from 2ØØ - 2ØØØ.

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 1-1Ø decimal, which is then multiplied by 1ØØØ internally. Sample rate for magnetic scan is 1Ø,ØØØ with no Hall Voltage smoothing or TIC correction; 8ØØØ if Hall Voltage smoothing or TIC correction is done; and 5,ØØØ 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 1-6ØØ. For example, to examine 4ØØ-6ØØ, enter 2ØØ. Sample rate for a Quadropole is a maximum of 3ØØØ. Enter a decimal number from 1-3.

The next frame is



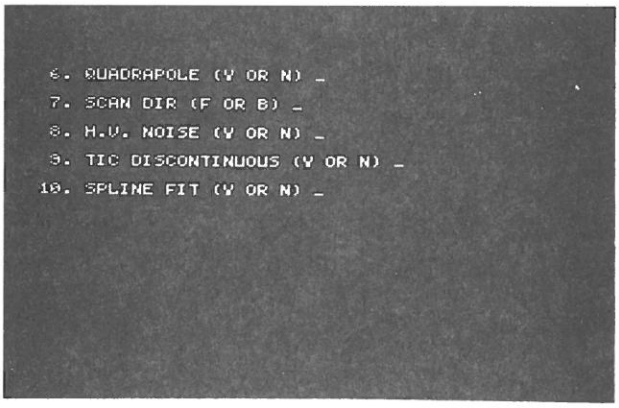
Question 3: The range of values is Ø-999. This number is a measure of the tolerable drift for Hall Voltages between successive calibrations; a good value is 5 for a 12 bit A/D, 20 for A 15 bit A/D.

Questions 4 and 5: The range of values for both questions is Ø-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:



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.

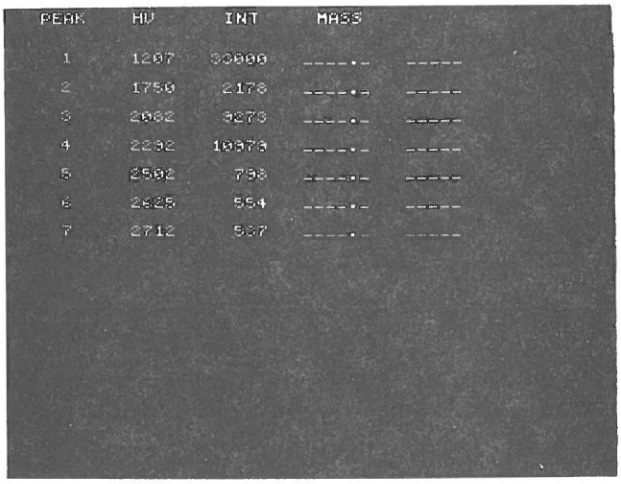
Question 10: Once all Hall Voltage/Mass points have been paired, a curve is fitted to these points. If a Spline fit is desired, type Y; if a linear fit is preferred, type N.

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:



3.2.2.1 Intensity Threshold

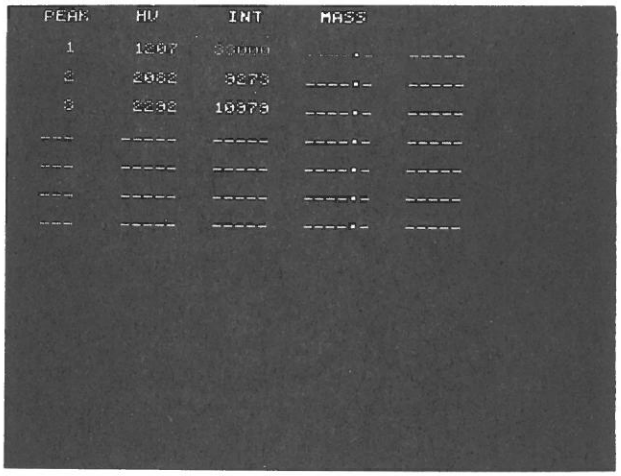
At this point, an intensity threshold should be specified to eliminate all peaks of lesser intensity when the Hall Voltage table is created. This is accomplished as follows:

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:



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.

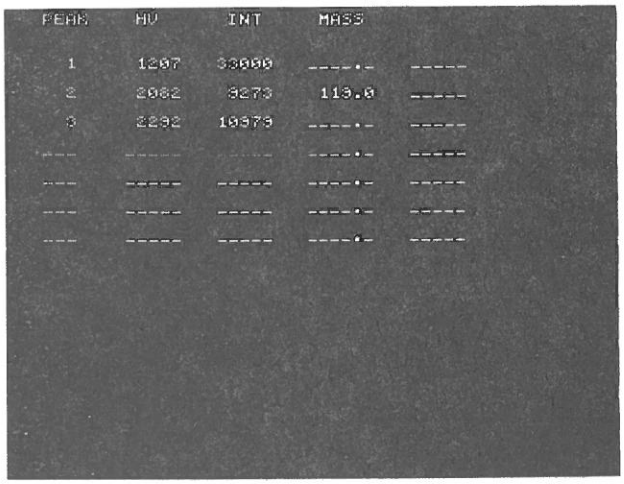
Teletype responds:	MASS#
User types:	any unsigned decimal number from 1-1999.9 followed by a carriage return.

If the following information is specified:

P↵

PEAK#2
MASS#119.0

the above display now becomes:



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

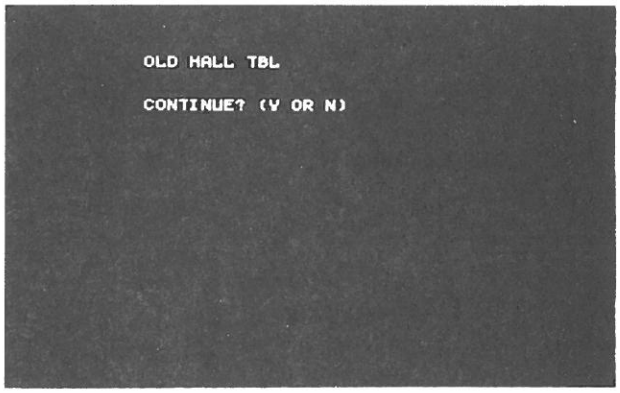
The following AIPOS function call format statement specifies AUTOMATIC calibration, which is carried out daily, primarily to ensure that the Hall Voltage has not shifted significantly:

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 <u>not</u> the latest one created, the user is informed of this by the following scope message:



Typing N casues 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	221Ø	3Ø1	14Ø.Ø	1
2	2219	4Ø61	----.-	-----
3	225Ø	166	153.Ø	2
	231Ø	-----	167.2	-----
4	2317	271Ø	----.-	-----
5	2333	1Ø27	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 carriage return

If the following is specified:

M ↵
PEAK#1 ↵
PEAK#2 ↵

the above display becomes:

PEAK	HV	INT	MASS	DEV
1	221Ø	3Ø1	----.-	-----
2	2219	4Ø61	14Ø.Ø	8
3	225Ø	166	153.Ø	2
	231Ø	-----	167.2	-----
4	2317	271Ø	----.-	-----
5	2333	1Ø27	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 preceding the blank, followed by a plus sign and then a carriage return.

Teletype responds:	PEAK#
User types:	the peak number to which the mass is to be moved followed by a carriage 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	221Ø	3Ø1	----.-	-----
2	2219	4Ø61	14Ø.Ø	8
3	225Ø	166	153.Ø	2
4	2317	271Ø	167.2	6
5	2333	1Ø27	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 printout 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

Command	Action
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

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

AUTOMATIC MODE ONLY

Command	Action
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.

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

[2]In 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 6ØØ.

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.

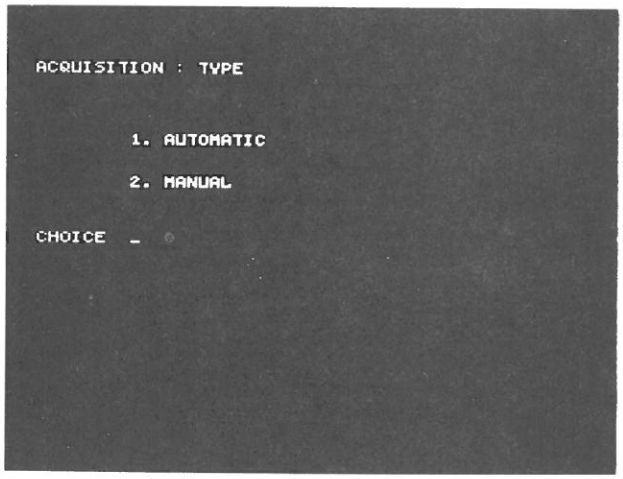
If any of the above is not true, an appropriate error message is displayed (refer to Appendix A) and in all but case "D" above, the program declares a fatal error, and returns to Job Control.

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:

Key	Action
CONTROL/C	Returns to Job Control
CONTROL/R	Returns to the first display (of Acquisitoon 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.

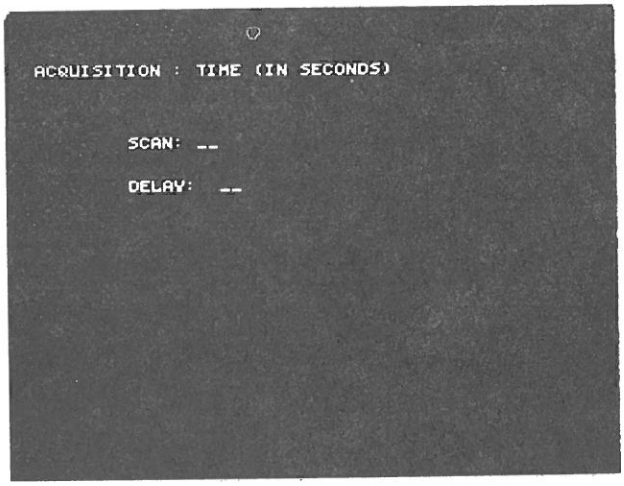
The ACQUISITION program presents four messages. The first display asks:



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 25Ø, and defined through a subsequent display (see Total Number of Scans).

The next display is:

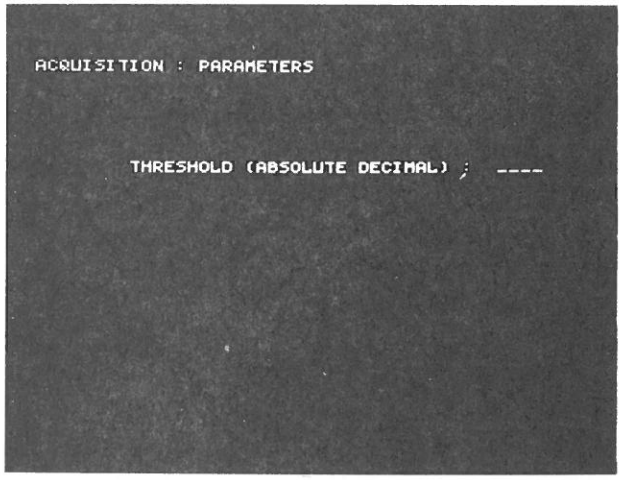


where the lower limit on scanning time is a variable dependent upon the internal parameters of mass spectrometer resolution, sample rate and peak width. Note that the fastest scan time allowable will always be the same for a given machine resolution, and its value might be in the neighborhood of:

SPECTROMETER RESOLUTION	QUICKEST SCANNING/DECADE
6ØØ	2 seconds
1ØØØ	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.

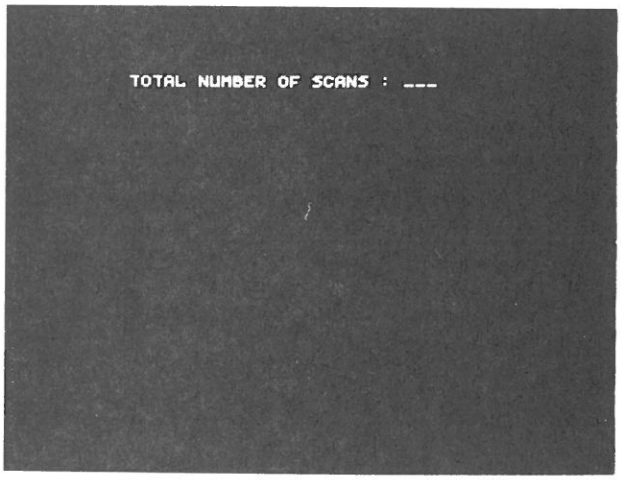
The next display:



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 Ø to 9999 (out of a total intensity range of 32,ØØØ).

The final display appears only if automatic scanning was chosen. The range is 1 to 25Ø.



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 Ø), 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.

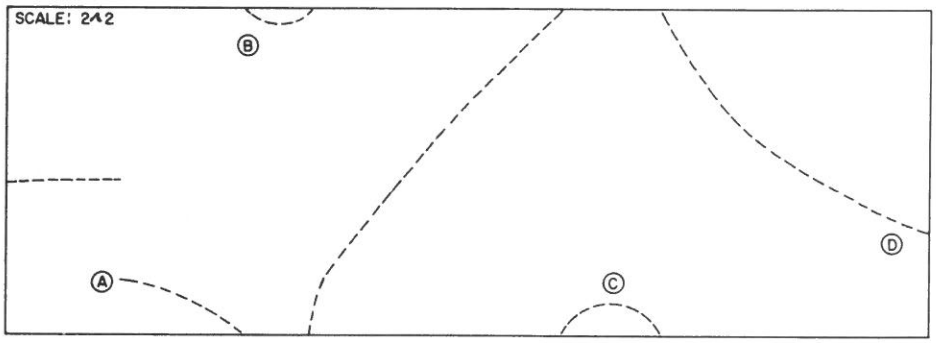


Figure 4.1 TIC vs. TIME Plot

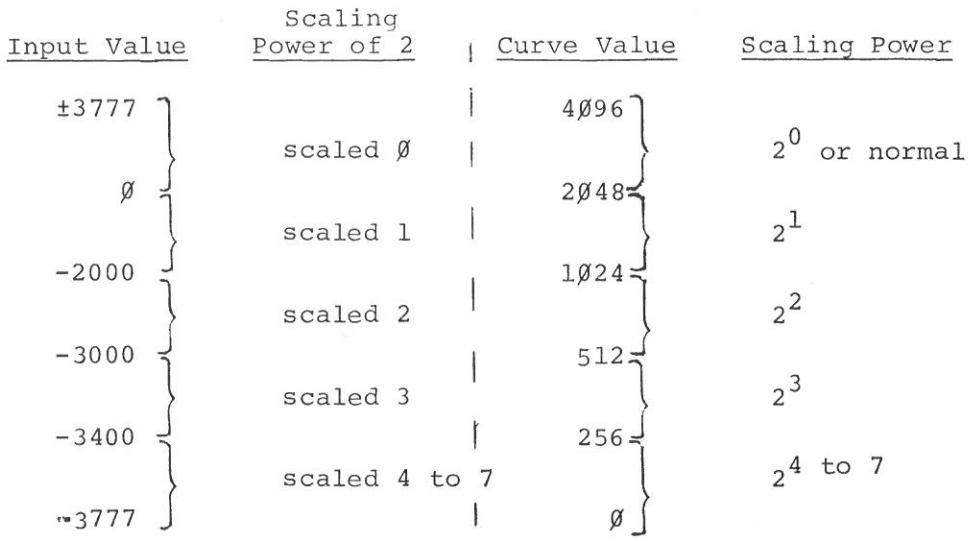
Figure 4.1 point:

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 -2ØØØ and -2777.



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:

Command	Action
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:

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

Command	Action
G (in automatic mode) 1-9 (in manual 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. The total number of scans on this sample has reached 25Ø (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 5ØØ 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

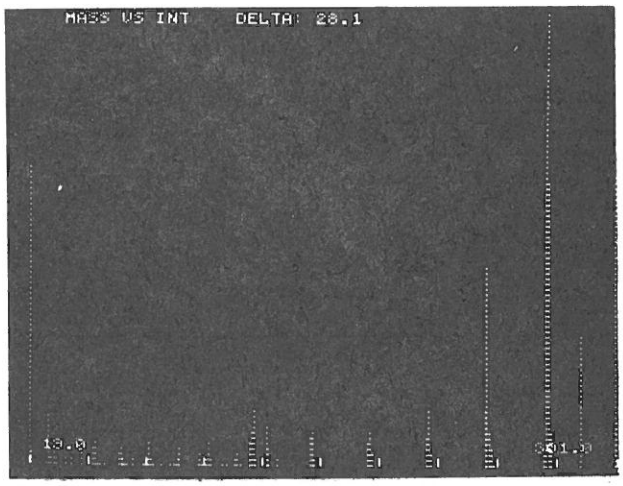
input = input file name

↵ = 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 3Ø1.Ø and the minimum 19.Ø, 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.

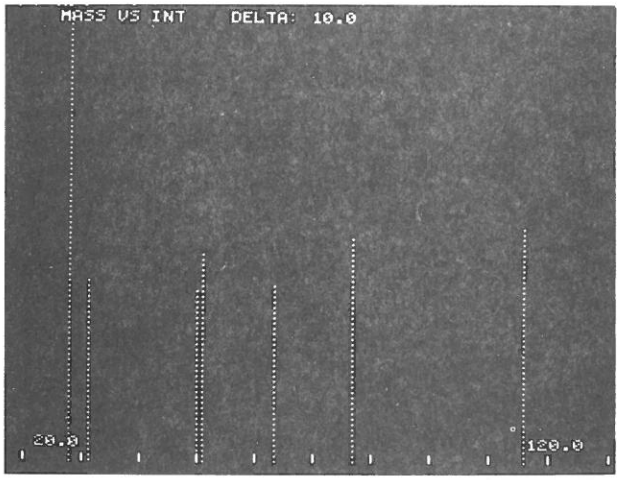
There is also a value labeled DELTA displayed on the top of the scope which is the distance between any two grid ticks. For the above grid, DELTA is 28.1.

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

For example, given the following point pairs:

2Ø.Ø	1ØØ.ØØ
31.2	41.15
5Ø.Ø	39.56
51.Ø	47.71
63.4	4Ø.15
77.Ø	51.29
1Ø5.9	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 retyped.

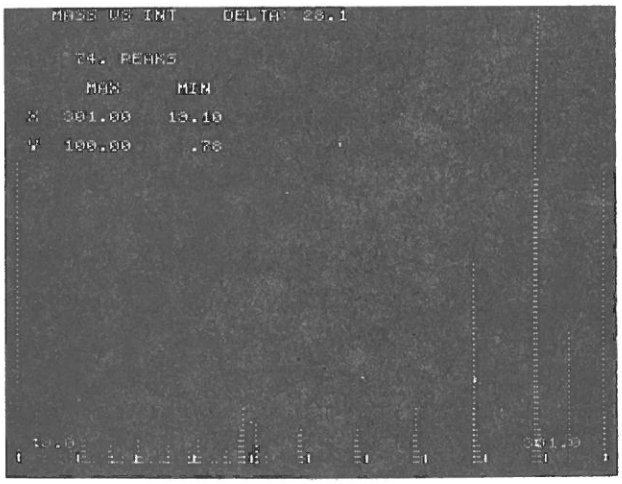
It types a colon when the requested command requires a parameter. If an illegal parameter is entered the colon is retyped. All parameters are positive numeric values. If any character other than a number or a decimal is typed as a parameter, an asterisk is immediately typed. All parameters must be followed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

Letter	Code	Explanation
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.

Letter	Code	Explanation
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
```

Letter	Code	Explanation
		would give the following display:
		3 5Ø.ØØ 3Ø.ØØ

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.

Letter	Code	Explanation
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.

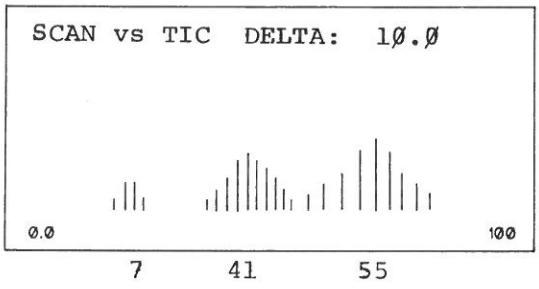
5.3 Use in MASH System

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.ØØ1
⋮
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:

?7Ø FPP ARITHMETIC ERROR

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

?71 FPP DIVIDE BY Ø

An FPP divide by Ø 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.

?8Ø 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 2ØØ-2ØØØ.

?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].

?9Ø 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 >5ØØ 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: $H_k \leq H_a \leq H_{k+1}$

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 C1, C2, C3, C4 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 Ø: 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 Ø value of any parameter. This is subtracted from all subsequent values, and enables relative size to be calculated. For example, two values, 5Ø: 1ØØ 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 LINCtape 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.

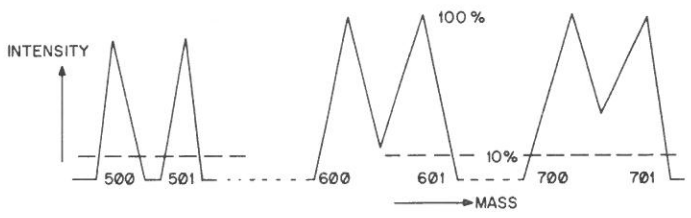
QUADROPOLE

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 6ØØ.



SCAN

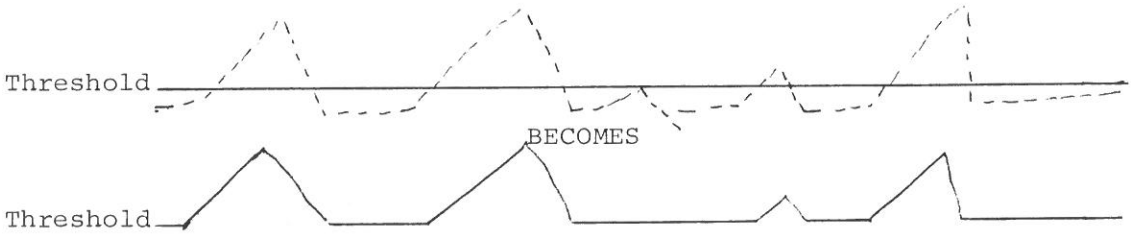
The bending and subsequent recording of ions emerging from the source, by varying either electric or magnetic field. The velocity of the heavier ions will be slower due to energy constraints, and the mass differentiation is made on this basis. The result of a scan is the relationship between intensity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