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Title: DIGITAL RECORDING AND ANALYSIS OF MASS SPECTRA

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A method has been devised for the digital recording of mass spectra and for reduction of the data by means of the CDC-3300 digital computer. The computer program *MASSPEC was developed to reduce the digital data obtained from a rare-gas mass spectrometer. The author devised a method of determining peak height values that approach values obtained by the eye of a skilled operator. In a majority of cases, the results due to the machine method of calculations were found to be within 2% of the results of the hand methods. Precision was improved by a factor of two by using the digital method of calculations.

Digital Recording and Analysis of Mass Spectra

by

David Robert Standley

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DIGITAL RECORDING AND ANALYSIS OF MASS SPECTRA

I. INTRODUCTION

Many analytical instruments used in chemistry record data by means of an analog device such as the strip chart recorder. The analog records must then be interpreted by a person to obtain usable data. This procedure can introduce human error and bias into the data. This source of error could be eliminated by obtaining a digital record of the data from the instrument in question. This record can be analyzed with the aid of a digital computer. Digital processing of analytical records can produce more reliable data with savings of time and effort. An additional advantage of digital recording and processing is possible improved sensitivity as a result of enhanced signal to noise ratios produced by digital filtering. The only bias introduced with this method is that of the programmer.

A way to digitally record and reduce mass spectra is discussed in this thesis. The computer program *MASSPEC was developed for the processing of rare-gas mass spectra. *MASSPEC was designed for argon isotopic analyses used in potassium-argon dating, but it can be applied to any mass spectrometer data, and possibly to other types of spectral analysis. *MASSPEC was programmed, using the FORTRAN and COMPASS programming languages, on a CDC-3300 digital computer under the OS-3 timesharing system.

Fritts and Peattie (1956) made an early step toward automation in collection of digital data. Their procedure uses a manually set wire on the chart recorder at the top of each peak. Closing a switch prints the digitized peak heights on prepared calculations. Three automated data collection systems were discussed by Dudenbostel and Klaas (1959) which again only recorded selected points of the spectrum.Thomason (1963) described a solid state digitizing system using computer circuitry. Weichert *et al.* (1967) devised a method for digital recording of mass spectra and for their reduction by an IBM 7040 digital computer.

Chapter II discusses the digital recording system, the methods of recording data, and the calculations to be performed. Chapter III contains descriptions of the subroutines used in the program. Chapter IV is a discussion of the main programs *MASSPEC and *ASCBCD. Chapter V includes the instructions to the operator for recording the digital data, and instructions to the user on how to run *MASSPEC and *ASCBCD. Chapter VI contains results pertaining to the comparison of hand calculations to machine calculations.

Two terms that are used throughout this paper are operator and user. The operator is the person who runs the mass spectrometer and facilitates collection of the digital data. The user is the person who uses the program *MASSPEC to reduce the digital data.

II. RECORDING SYSTEM AND METHODS

Description of Hardware

Components for the digital recording system discussed in this paper cost less than $5, 000, and therefore, could be used by laboratories with limited equipment budgets.

Figure 1 shows a block diagram of the digital recording system. The components are listed in Table 1. The system digitizes the analog output from the electrometer and provides both analog hardcopy and computer readable paper tape output. A full scale output from the electrometer is converted to a megahertz frequency by the digitizer and subsequently counted by the counter. Without the data buffer 1484A (see Figure 1) the dead time of the system during printout would be approximately one second per output. This would result in data taken once every two seconds. By adding the data buffer, the minimum integrating time is one second. While the teletype is printing what was in the data buffer, the next piece of data is being digitized.

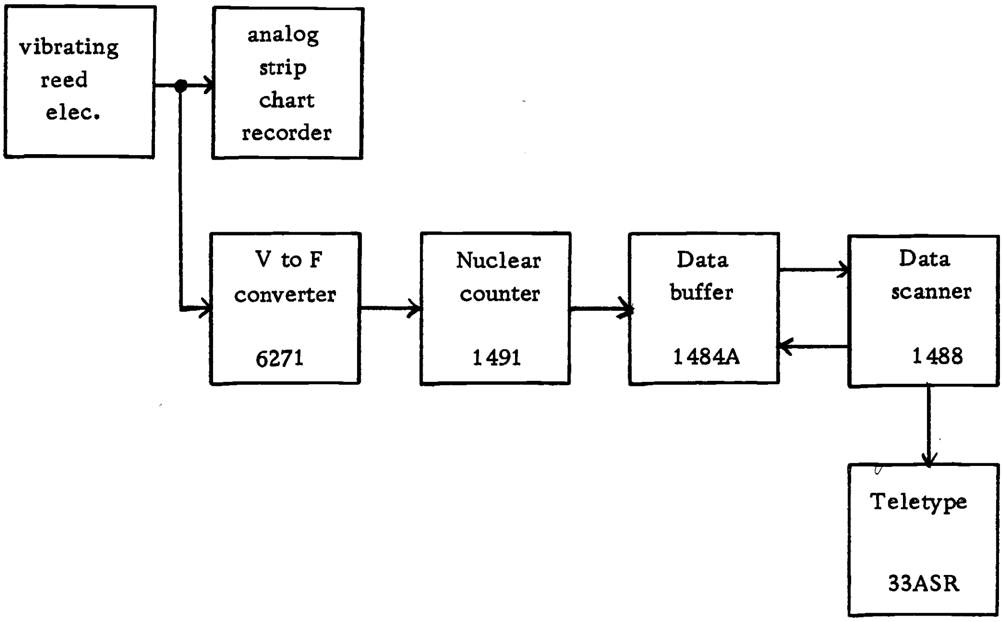

Figure 1. Block diagram of analog-digital recording system.

Table 1. Components of digital recording system.

Manufacturer	Model No.	Description	Price
Canberra Ind.	6271	Voltage to frequency converter (digitizer)	$ 750.00
Canberra Ind.	1491	Nuclear counter	1100.00
Canberra Ind.	1484A	Data buffer	500.00
Canberra Ind.	1488	Teletype data scanner	850.00
Teletype Corp.	33ASR	Teletype	1050.00
Canberra Ind.	1400	AEC Bin/power supply[1]	575.00
Canberra Ind.		3 width blank power[2]	20.00
		TOTAL	$4895.00

[1,2] These components do not appear in Figure 1 since they are supportive hardware.

Methods of Recording and Calculations

The method for acquiring the data for a typical argon run is discussed here. The operator scans back and forth over masses 40, 38, and 36 while the chart recorder records the peaks as they occur. Simultaneously the digital data is recorded on paper tape. The instructions for doing this are given in Chapter V. The operator must change scales on the vibrating reed electrometer to keep all of the peaks on the chart. One complete sequence of peaks is shown in Figure 2.

The vibrating reed electrometer has several scales, each expressed in terms of voltage. The precision of these scales with respect to each other must be checked periodically. Scale correction factors can thus be measured and inserted in *MASSPEC for the isotopic ratio calculations.

The peak heights must be measured from the chart in order to compute the isotopic ratios. The usual method of determining peak heights is illustrated in Figure 2. Straight lines are drawn to connect the baselines of the two mass 40 peaks. This is also done with the mass 38 peaks. In Figure 2 it happens that the mass 40 and mass 38 peaks have the same baseline. Now the tops of the mass 40 peaks are connected by straight lines (see Figure 2) as are the mass 38 peaks. A horizontal line is drawn through the top of each mass 36 peak at the estimated summit (the noise must be averaged). These are points c

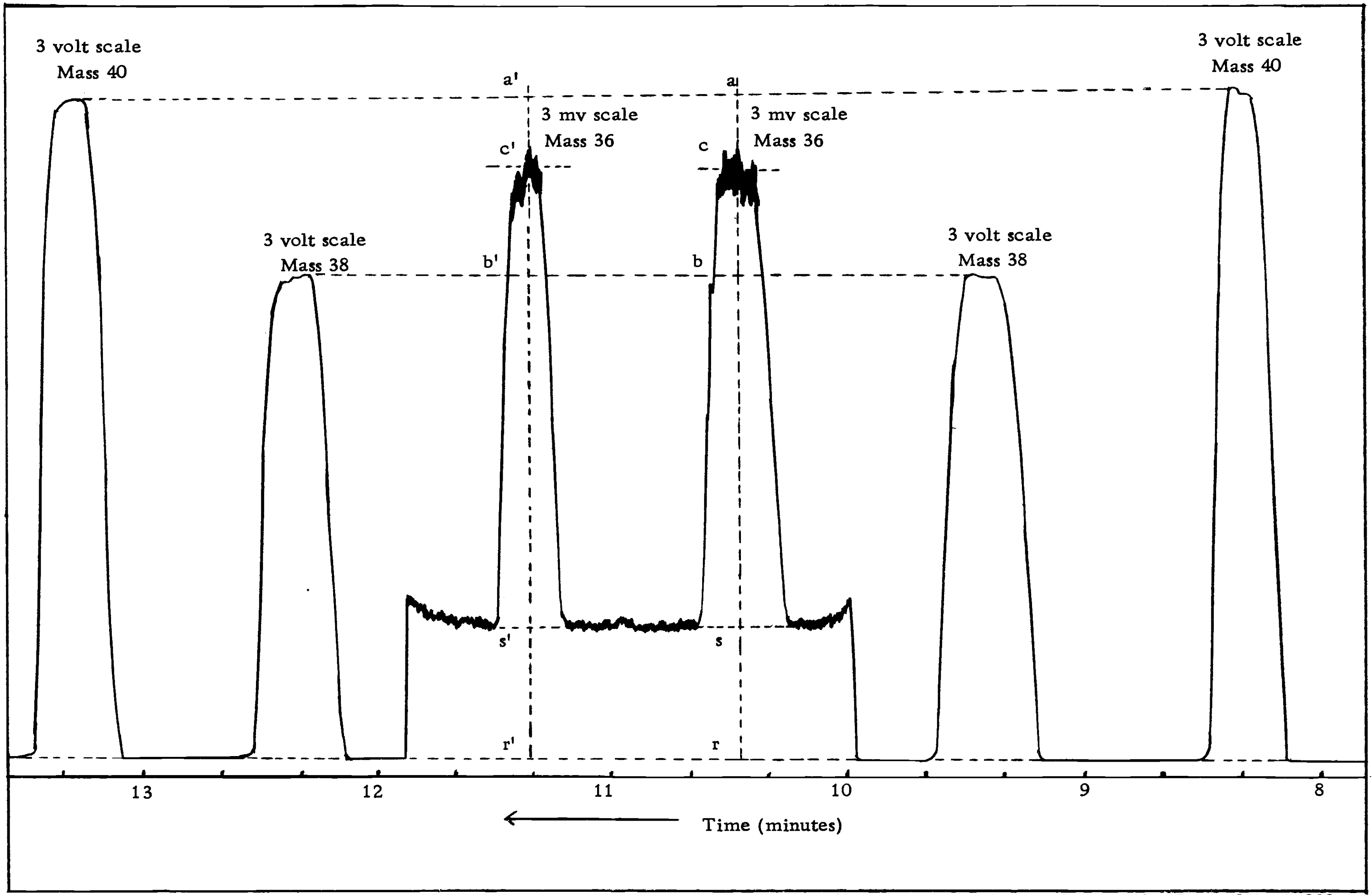

Figure 2. One sequence of peaks with the sweep going from mass 40 through mass 36 and from mass 36 back through mass 40. From chart A-323 Klamath 2B.

and c' in Figure 2. A vertical line is now drawn through the mass 36 peaks at the points in time where the summit values were picked. The interpolated heights of the mass 40 and mass 38 peaks must be measured at these vertical lines before calculation of ratios. For example the heights of mass 40 and mass 38 at 10.4 minutes (Figure 2) would be ra and rb, respectively. The corresponding values at 11.3 minutes would be r'a' and r'b'. The heights of mass 36 peaks are measured as sc and s'c'.

We now have the necessary values to calculate the ratios (in this case Ar^{40}/Ar^{38} and Ar^{38}/Ar^{36}) at 10.4 minutes and 11.3 minutes. These ratios are shown in Table 2.

Table 2. Isotopic ratios calculated for Figure 2.

Time (minutes)	Ar^{40}/Ar^{38}	Ar^{38}/Ar^{36}
10.4	ra/rb	rb/sc
11.3	r'a'/r'b'	r'b'/s'c'

The ratios in Table 2 are for just one sequence of peaks. There are usually three or four more sets of ratios calculated for one run.

Once all of the ratios have been recorded, they must be plotted against time and extrapolated to time zero. This is necessary to correct for machine "memory" caused by residual gas from the previous sample. Time zero is the point in time when the sample was first let into the mass spectrometer. The extrapolated values of the ratios

Ar^{40}/Ar^{38} and Ar^{38}/Ar^{36} are used in the age calculations.

*MASSPEC calculates the final extrapolated ratios but uses a slightly different method. First, all of the peak heights are determined and stored with their corresponding time values. Then (see Figure 3) the mass 38 peaks are fit to a power series polynomial in time. Ratios are computed using interpolated values for mass 38. Instead of calculating both the Ar^{40}/Ar^{38} and Ar^{38}/Ar^{36} ratios at one value of time, *MASSPEC will compute the individual ratios at the time when each peak occurred. For example (see Figure 3) Ar^{40}/Ar^{38} is computed at ${}^{t}40_1$, ${}^{t}40_2$, ${}^{t}40_3$, and ${}^{t}40_4$ while Ar^{38}/Ar^{36} is computed at ${}^{t}36_1$, ${}^{t}36_2$, ${}^{t}36_3$, and ${}^{t}36_4$. The ratios are linearly extrapolated to time zero as was done manually.

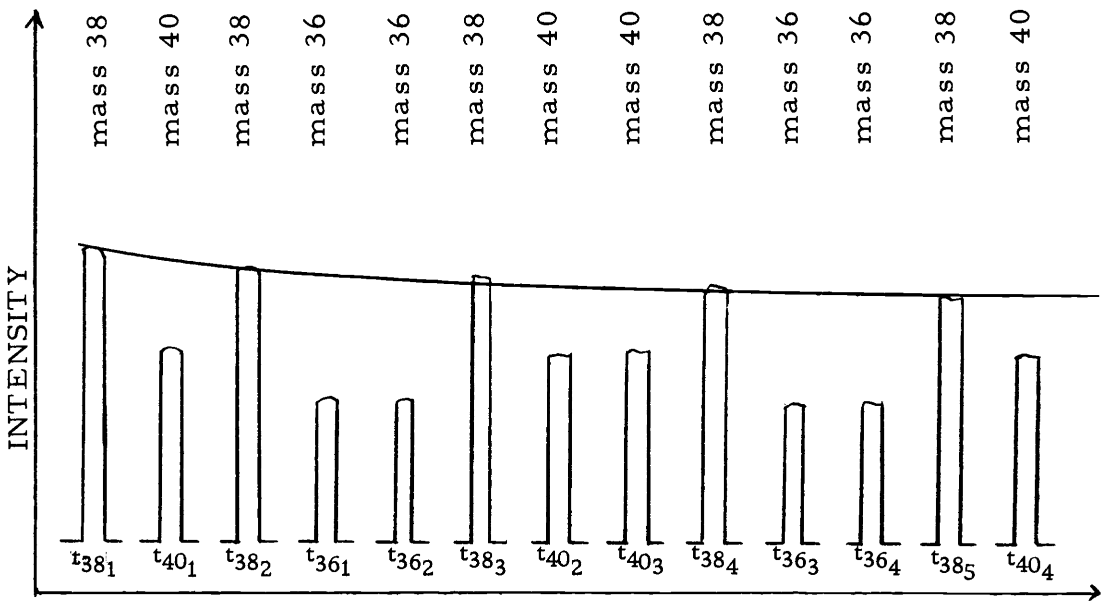

Figure 3. Interpolation criterion used by *MASSPEC for calculating isotopic ratios. In this case the peaks of mass 38 are fitted to a power series polynomial. The interpolated mass 38 peak values are then used to compute isotopic ratios at the mass 40 and mass 36 peaks.

III. SUBROUTINES

CANCEL

This COMPASS subroutine scans an 80 character line of data and checks for cancellation characters. The cancellation character, or backup character, is the backslash \. The subroutine corrects the line by deleting the character immediately preceding the backslash. An example of a line before and after correction is:

Before: ABCC \ DEEFG \ \ \ FG

After: ABCDEFG

A correction method similar to this is used by some systems programs. Since a subroutine was not readily available, CANCEL was written specifically for use in *MASSPEC. This subroutine is useful while typing in identifiers and comments.

The same subroutine can be used to detect the operator error code. The operator error code consists of two or more consecutive colons typed by the operator. The subroutine will scan a corrected line (from above) and if the proper sequence of colons occurs, the error flag is set to 1. If no error, the flag is set to 0. The FORTRAN calling sequence is:

CALL CANCEL(LINE, IFLAG)

where LINE is a 20 word array and FLAG is the error flag. If the second parameter is omitted, the error code is not searched for.

COMPRESS

COMPRESS is a COMPASS subroutine which takes a two word variable and eliminates all the blanks from within the variable. The variable is returned with the characters left-justified and blank fill to the right. As used in *MASSPEC an example is the peak identifier as entered by the operator or by the user.

A 40	is returned as	A40
NE 20	is returned as	NE20

This facilitates recognition by the program of the identifiers during execution of the program.

MISBJP

MISBJP is a utility subroutine, written in COMPASS by the author, to utilize the capabilities of the operating system. The calls to the subroutine are:

1: CALL MISET

2: CALL SBJP

The first call sets the manual interrupt flag for the OS-3 user. This is used to reenter the program if a mistake is made or if for any reason the user gets into control mode and wants to return to the program. It is cheaper to reenter the program by typing MI than by starting over. MI is an OS-3 control mode instruction.

The second call to this subroutine returns the user to system control mode when execution of the program is complete. This eliminates the END OF FORTRAN EXECUTION normally supplied by the FORTRAN run time subroutines.

PARA

PARA is a COMPASS subroutine which serves two purposes.

1. It processes a parameter when starting the program. The only legal parameter must begin with a C. (e.g., #*MASSPEC,C or #*MASSPEC,CONSTANT). The C parameter indicates that the user wants to examine or change the scale correction factors. If no parameter is entered, the program functions properly but does not ask the user about the stored constants.
2. It equips the file (* MASS *) which contains the scale correction factors.

The calling sequence for PARA is:

```
CALL PARA(L)
```

where L is set to

0 if no parameter

1 if a parameter

-1 if (* MASS *) does not exist.

The error messages produced by PARA are:

1. ILLEGAL PARAMETER.

   The parameter does not begin with C.

2. CONSTANT FILE HAS BEEN DELETED.

   The file does not exist. It must be recreated for use in the future.

3. CONSTANT FILE IS BUSY NOW, TRY AGAIN SOON.

   The file is presently equipped by another user. This is usually just temporary.

4. CONSTANT FILE IS PROTECTED.

   The file is protected meaning that it cannot be written on. It is now a read-only file. Protection should be removed before the constants can be changed.

READATA

READATA is the COMPASS subroutine that performs the chore of reading in the data for each peak. It reads data for one peak at a time, checking format and checking for error conditions.

READATA has two parameters, LUN and ANAME. ANAME is a two word variable which contains the correct peak identifier for the current peak being read in. LUN serves two purposes: (a) to signify the logical unit number the data is on, and (b) if any errors are detected, to return a special code to the calling program. The error codes are:

-1: End of file or end of data on data input unit.

-2: Peak identifier error.

-3: Operator error sensed.

READATA calls the FORTRAN subroutine READCARD which reads a 20 word line from the data unit. READCARD will read data that has been compressed by COSY (15).

If an end of file or end of data is sensed upon reading the data, -1 is stored in LUN and the routine will exit. If a blank line is read it is ignored and another line is read. After the line is read in it is scanned by CANCEL to correct cancellations and detect the operator error code. If the operator error code is present, -3 is stored in LUN and the subroutine exits.

Now if the line contains less than five words, the peak identifier code must be checked for. If more than five words were read, the numbers are converted to internal binary with DECBIN. If a number does not have six digits it is considered invalid and rejected. Once all of the numbers on this line have been converted, the routine goes on to read another line.

If the first two words of a line contain only numeric characters, no peak identifier is assumed and the line is converted as just mentioned. If not numeric and one peak identifier has been read already, this indicates the beginning of another peak and the routine exits. If a "/" exists in the identifier, this indicates a scale factor is present.

If the format of the scale factor is present (V or MV) the number is stored in the SCALE position in COMMON. V is converted to 0 or MV to -3 and stored into the FACTOR position in COMMON. If the incorrect format is used an error message is printed and 0 is stored in both SCALE and FACTOR. At this point the peak identifier is compared with ANAME and if it is the same a flag is set signifying the first peak is being read in. If the identifiers differ an error message is printed, -2 is stored in LUN, and the routine exits.

SMOOTH

This subroutine does a five-point moving smoothing of the raw data. The mathematical description of this process is:

$$Y_j^* = \frac{1}{N} \sum_{i=-m}^{i=+m} C_i \, Y_{i+j} \qquad (2.1)$$

where

Y: original data points

Y*: smoothed data points

C: convoluting integers

N: normalizing factor

m: such that 2_{m+1} points are used to compute Y*

j: the running index of the ordinate data in the original set of data

The values of the constants from Savitzky and Golay (1964) are:

$C_{\pm 2} = -3$

$C_{\pm 1} = 12$

$C_0 = 17$

$N = 35$

$m = 2$

The use of equation 2.1 is equivalent to fitting the data with a second degree polynomial. The smoothed first derivative is computed and used by the PEAK subroutine to determine the correct bounds on each peak. The first derivative is generally small in regions of a spectrum where there are no peaks.

Yule (1967) found that five-point smoothing was superior to seven or nine-point smoothing. The latter two tend to flatten peaks and fill in valleys thereby distorting the original spectrum. Yule's findings were verified when various smoothing routines were tried by the author on mass spectrometer data.

POLFIT

POLFIT is a FORTRAN subroutine to calculate the coefficients $a_0, a_1, a_2, \ldots, a_n$ for a least-squares fit to an array of data points with the polynomial curve:

$$Y = a_0 + a_1X + a_2X^2 + \ldots + a_nX^n$$

With these coefficients Y can be interpolated at new values of X. This is especially useful in determining isotopic ratios (see Figure 3). It is also used to determine the intercept value for a group of ratios.

Several curve fitting programs available on the OS-3 system were investigated, but due to lack of complete documentation they were dropped from consideration. Bevington (1969) described a subroutine which fit data to a Legrendre polynomial. Using this as an example, POLFIT was developed and written by the author to serve the purpose of *MASSPEC.

The author adapted MATINV which is used by POLFIT to invert a symmetric matrix and calculate its determinant, from Bevington (op. cit.)

STDEV

The calling program passes an array Y of n numbers to subroutine STDEV. Two arrays, SIGMA and MEAN, are created by STDEV. Each element of SIGMA from SIGMA(2) through SIGMA(n-2) is calculated as:

SIGMA(I) = standard deviation of the group of points Y(I-2) through Y(I+2)

and each element of MEAN from MEAN(2) through MEAN(n-2) is calculated as:

MEAN(I) = arithmetic mean of the group of points Y(I-2) through Y(I+2).

An example is shown in Table 3. Here the array Y is used to compute the arrays MEAN and SIGMA by the methods just mentioned. Note that the first two elements and last two elements of MEAN and SIGMA are zero since they cannot be calculated.

SIGMA is known as a five-point moving standard deviation and MEAN as a five-point moving mean. These means and standard deviations are used by the PEAK subroutine to determine a value at the summit of each peak.

PEAK

This subroutine is the so-called "heart" of the program as it detects the bounds of the peaks and determines a value for each peak.

Array DY contains the smoothed first derivative from SMOOTH in the form of tangents. SLOPE is the tangent of the legal threshold angle. CHANUP is the minimum number of points allowed for an acceptable uphill slope. TOPMAX is the maximum number of points allowed on the top of a peak. CHANDOWN is the minimum number of points allowed for an acceptable downhill slope.

The Searching Algorithm

This algorithm is similar to one used by Corliss (1969).

START position:

Look at successive derivatives until one is found that is greater than SLOPE. The index of this point is saved in LEFT. This is assumed to be the start of the uphill scan.

UP position:

Now look for the top of the peak by sensing a change in DY from exceeding SLOPE to less than SLOPE. If this happens before CHANUP this peak is assumed to be a false peak and the search must be returned to the START position.

TOP position:

When the top is found, a search is made for a negative derivative with absolute value greater than SLOPE. If such a derivative is not found before TOPMAX is reached, the search must be re-initialized since this top may have been an elevated baseline. If, while searching for the downhill slope, an uphill slope is encountered and TOPMAX is exceeded, the pointer is reset and the uphill slope is scanned in the START position.

DOWN position:

When a legal downhill scan is found, the right tail is detected by finding a change in $|DY|$ from greater than to less than SLOPE.

The index of this point is saved in RIGHT. If this occurs before CHANDOWN the pointer is set back to the TOP position and the search continued. If a peak is not found before the data is exhausted, an error is flagged and control is returned to the calling program.

Once the right tail is verified, no more of the current data is looked at. If the operator neglects to enter a peak identifier, two peaks will appear in one set of data. Only the first one would be detected by the program. It is imperative that a peak identifier be placed before each peak to be read. This method would not be practical for data from a fast-scanning mass spectrometer like that used by Hites and Biemann (1967). Their spectrometer scans from mass 20 through mass 500 in one to three seconds. It would be impossible for the operator to manually enter a peak identifier before each peak in such an application.

20° has been set as the SLOPE angle after many cases were studied. It was found that varying SLOPE has little effect on the threshold point. The angle increases rapidly within two or three points.

Determining the Peak Value

Now that the bounds are known, the program determines a value for the summit of the peak. The five-point moving standard deviations computed in subroutine STDEV are in an array called SIGMA and their corresponding means are in an array called MEAN.

The smallest point in the middle two thirds of the array SIGMA is found. This minimum is at the flattest part of the peak and the index of this minimum value is the position of the summit. Now using the summit position as the center of five points, all points that differ by more than one standard deviation from the mean at the summit are eliminated. From the remaining points in this group of five a new mean is calculated and this is used as the value at the summit.

The values for the left and right tails of the peak are taken as MEAN(LEFT-3) and MEAN(RIGHT+3), respectively. By moving back three points on each side, the weight due to the higher points is lessened. Using these values for the right and left tails of the peak, the baseline for the peak can be determined. The baseline is not always horizontal and may be sloping as is the case in Figure 5. To obtain a correct value for the baseline of a peak the program must, in essence, draw a straight line from the left tail to the right tail. The interpolated value at the index of the summit is then used as the value for the baseline.

Location of peaks by smoothing the data and using first derivatives has been used by others (7, 12). Hites and Biemann (1967) used smoothed values and took a maximum to determine a summit value. It was found that this would not present a representative value in some of the author's cases. There are some noise spikes that, if smoothed, would increase the summit value. Excluding these points by the statistical method mentioned gives a value nearer to the value obtained by eye by a skilled operator. For example in Figure 4 the method of Hites and Biemann would pick the peak summit at "a" while the statistical method of the author would pick the summit value at "b". The author's method would not be of such great importance in the case of the fast-scan used by Hites and Biemann.

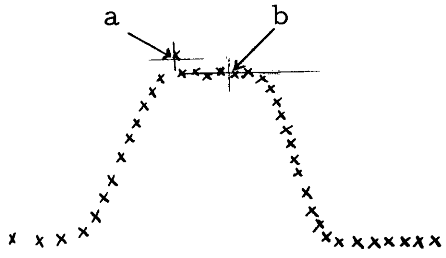

Figure 4. Comparison of the method of Hites and Biemann at point "a" to the author's method at point "b".

Figure 5 is an example of a peak and the values picked for it by the PEAK subroutine. Table 3 shown with the plot contains the time (I), digital reading (Y(I)), smoothed first derivative (DIFFERENCE), five-point moving mean (MEAN), and five-point moving standard deviation (SIGMA). The flags (*** in Table 3) denote the LEFT index, SUMMIT index, and RIGHT index. The summit value is at "s" (see Figure 5) and "b" is the baseline value interpolated between "a" and "c". The value for the peak height is (s-b).

DECBIN

DECBIN is a *SYSLIB[3] routine that converts a BCD decimal integer to an internal binary integer. DECBIN is used by READATA for number conversion.

ARMYTIME

This subroutine, developed by Gemperle and Keeling (6), computes the time of day (between 0000 and 2400) as it is supplied by a millisecond clock. The time is returned to the calling program in the format:

bbHHMMbb

where "b" is a blank, "H" is an hour digit and "M" is a minute digit.

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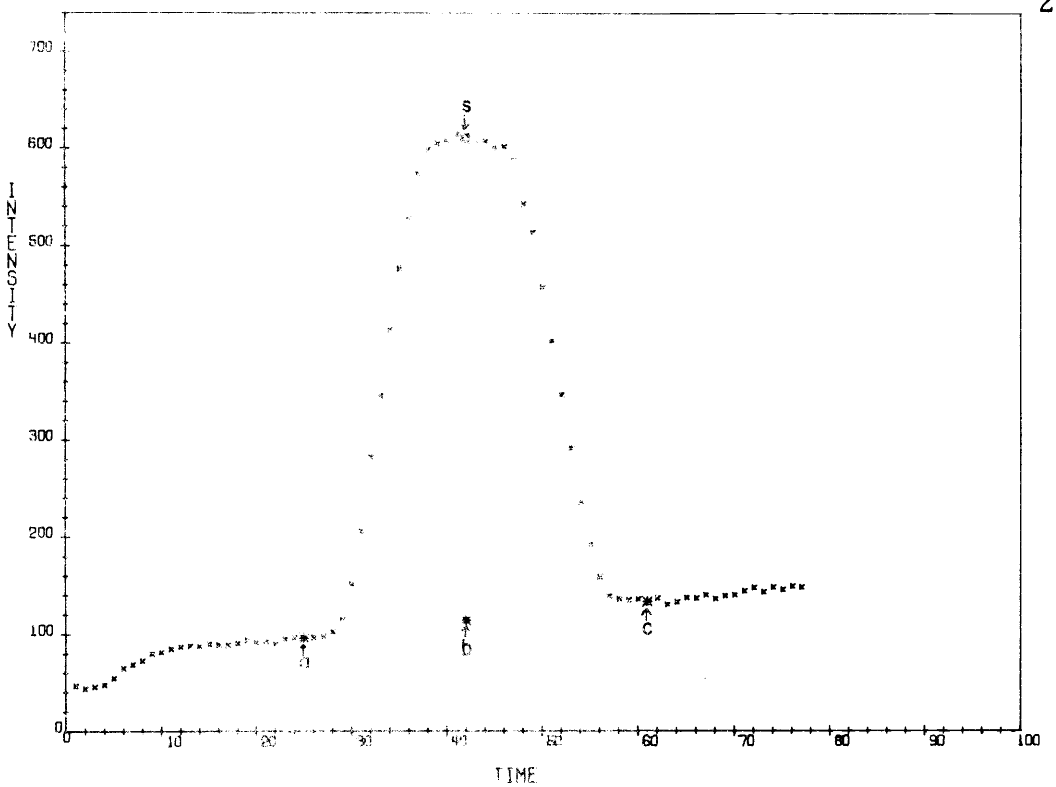
[3] *SYSLIB is a library of subroutines used by the systems programming classes at Oregon State University.



A-358 FØURTH 38 PEAK

FIGURE 5. AN EXAMPLE OF A PEAK AND THE VALUES PICKED FOR IT BY THE PEAK SUBROUTINE.

TABLE 3. NUMERICAL VALUES FOR THE POINTS IN FIGURE 5.

I	Y(I)	DIFFERENCE	MEAN	SIGMA
1	45877	0	0	0
2	43173	0	0	0
3	44900	.3363	47077	3687
4	47555	.7218	50824	7795
5	53882	.8019	55800	9166
6	64610	.5437	61137	9071
7	68055	.4671	67692	8484
8	71834	.3035	[illegible]	[illegible]
9	79627	[illegible]	77339	[illegible]
10	81233	.2443	80756	5966
11	84744	.2276	83877	2985
12	86343	.0318	[illegible]	[illegible]
13	87436	[illegible]	86333	[illegible]
14	86753	.0536	[illegible]	1115
15	89391	[illegible]	[illegible]	885
16	88442	-0.1558	[illegible]	[illegible]
17	88120	[illegible]	89047	[illegible]
18	90095	.1603	[illegible]	[illegible]
19	93687	[illegible]	[illegible]	[illegible]
20	91237	-0.[illegible]	[illegible]	1576
21	92476	.0764	92248	1834
22	89325	.1861	92692	2331
23	94514	.2450	93510	2395
24	95908	.5803	[illegible]	[illegible]
25	95338	.0042	[illegible]	[illegible]
26	96281	.1172	97421	2369
27	97171	.3538	[illegible]	6389
28	101905	1.54[illegible]	112489	9042***
29	114206	3.5535	123796	40174
30	150881	5.3550	170626	65920
31	204759	6.3397	219143	94719
32	281381	6.9999	278731	93710
33	344490	6.[illegible]	343639	95124
34	411393	[illegible]	[illegible]	[illegible]
35	475573	[illegible]	[illegible]	[illegible]
36	526273	[illegible]	[illegible]	[illegible]
37	572791	[illegible]	[illegible]	[illegible]
38	596980	[illegible]	[illegible]	[illegible]
39	603225	[illegible]	[illegible]	[illegible]
40	606680	.3676	606108	5647
41	612844	-0.2342	607171	4124
42	610811	-0.3793	607574	3804***
43	602295	-0.3670	605982	5240
44	605240	.0225	603437	4294
45	598721	-0.2587	598565	6446
46	600120	-1.8777	586275	23538
47	586448	-3.1969	567656	35135
48	540846	-4.3001	539075	52214
49	512146	-4.7439	499209	64932
50	455814	-5.7773	451067	71323
51	400790	-5.4740	401124	73081
52	345741	-5.5931	345818	77790
53	291130	-5.3224	292947	74843
54	235616	-4.5690	244346	67580
55	191457	-3.3086	202894	55084
56	157788	-1.8113	171735	37670
57	138479	-0.5746	151440	21764
58	135335	.0645	140151	8940***
59	134140	-0.1559	134782	2416
60	135012	.0798	134316	1806
61	130942	-0.1506	133109	2575
62	136151	-0.0733	132646	2556
63	129298	.0089	132954	2893
64	131825	.3327	133990	2915
65	136552	.2617	134629	3591
66	136125	-0.0477	135903	2409
67	139347	.0166	137206	1402
68	135668	-0.0123	137803	1616
69	138337	.2653	139172	2347
70	139538	.3603	140681	3893
71	142968	.0916	141975	2980
72	146895	.0669	143746	2927
73	142137	-0.0560	144824	2029
74	147194	.2197	145849	2124
75	144928	0	145918	2162
76	148089	0	0	0
77	147244	0	0	0

TELIO

The TELIO function is an OS-3 conversational aid for teletypes. This function is used in *MASSPEC quite often for asking the user questions requiring YES or NO for answers. It is also used for input of free-formatted numerical data from the teletype. This subroutine was developed by the O. S. U. Computer Center and is available on the OS-3 system but documentation has not been published as yet by the computer center.

STAT

STAT is a subroutine written by the author that computes the arithmetic mean and standard deviation of k data points.

WRITEIO

WRITEIO combines intermediate data from two scratch files (LUN1 and LUN2) and writes it on the line printer file (LPLUN). The author wrote this subroutine to combine the data in this way and reduce the number of pages of line printer output to an acceptable number.

An array, XLINE, is filled with a line from LUN1 and a line from LUN2. XLINE is then written onto LPLUN. This is done until there is no more data on LUN1 or LUN2.

XLINE	from LUN1	blanks	from LUN2
	12 words	8 words	12 words

IV. THE MAIN PROGRAMS

MASSPEC

MASSPEC is the main program that calls the various subroutines mentioned previously to help complete its task. The author designed the program to have a minimum of response from the user and yet tell him what he needs to know. The program is written in a conversational mode for use at teletypes only. The data must be available on an OS-3 file.

A convenient way to discuss the program is to use a list of steps and explain each one in order.

Algorithm for MASSPEC

1. Call the PARA subroutine to equip the file containing the scale correction factors and detect if the user wants to alter this file.
2. Initialize flags and print the greeting.
3. If PARA returned a -1, indicating the file does not exist, set the correction factors to default values. Otherwise read the values from the file.
4. If a "C" parameter was entered by the user, ask the user if he wishes to enter new scale correction factors. If he does, the user enters the factors and after any corrections the program writes them onto the file.

5. The manual interrupt flag is set here. Ask the user if he has started calculations for this data set. The purpose for this is to enable the user to bypass some steps if he wishes to restart the program.

6. Equip the users data file and ask for delta T. Delta T is the time interval, in seconds, from when the operator turned on the high voltage to when the digitizer was started on the first peak.

7. Read the header record from the data file and print it. If the program was restarted by the user having typed MI, and the user indicated he was starting over, transfer control to 12.

8. Ask the user if the preset peak identifiers are all right. If they are not, go to 10.

9. List the preset sequence of when the peaks should occur. Ask the user if this is all right. If they are go to 12. Otherwise go to 11.

10. Ask how many peak names there are and have the user enter them.

11. Have the user enter the correct sequence (one complete cycle) in which the peaks should occur. This sequence is used in the main loop to process the peaks in the correct order.

12. If an end of file has been read on the data file go to 22.

13. Set the peak identifier for the next peak to be read in.

14. Call READATA to have the next peak read into memory. If an error is noted go to 21.

15. Determine scale factors, if any were entered with the data. The corrected scale factors will be substituted here for the ones read from the data file. Increment the total time by the number of points read in the data plus five seconds. Five seconds was found to be an average time for the operator to stop the digitizer, enter the next peak identifier and restart the digitizer.

16. Complete the five-point moving means and standard deviations by calling STDEV.

17. Call SMOOTH for a set of smoothed first derivatives and convert these to tangents for use by the PEAK subroutine.

18. Constants must be entered here if the program is on its first pass or has been restarted. If not, go to 19. Have the user enter CHANUP, TOPMAX, and CHANDOWN to be used by the PEAK subroutine. If too many peaks were rejected before restarting, these constants must be changed. This is usually caused by the operator's having scanned the peak too rapidly on the uphill or downhill slopes. Also a peak can be rejected if the operator has scanned the top of the peak longer than TOPMAX counts.

19. Now call the PEAK subroutine to determine values for the summit and tails of the peak. If a peak was not found using the

above criteria print an error message and go to 12.

20. DO a straight line interpolation as discussed on page 21. Now a value for this peak can be calculated by subtracting the interpolated value on the baseline (at the point where the summit was determined in step 19) from the summit value. Multiply the value for the peak by its corresponding scale factor and store the result in an array which has been set aside for the successive peak values. If no scale factors have been entered with the data, the program will set a scale factor of one. The time index for the peak at the summit value is also stored, for future use, into the same array at an index corresponding to the index for the peak. The peakname, time, value, scale factor, and scaled value are now printed for the user to see.

21. READATA is programmed to indicate the following errors if they occur[4].

    (a) If an end of file has been read set the appropriate flag and go to 15.

    (b) If an operator error was noted print a message, increase the elapsed time and go to 14.

---

[4]The author has run the program at least 50 times and in none of the cases was there a set of data which was not handled properly by the program without one of these error conditions being detected. This of course does not mean that such an eventuality cannot occur.

(c) If an identifier has occurred ask the user if he wants to change the peak identifier. This occurs if the operator has made a mistake in typing and the identifier has been spelled incorrectly. The only way READATA will read the next peak is to accept the identifier given in the data. If the user wants to change it the program requests him to enter the acceptable identifier. Control is transferred to 14. The operator may have skipped a peak or scanned a peak too many times. In this case the user can change the sequence in which the peaks are read. Now the value for this peak will be stored in the correct array. Go to 13.

22. Equip and label a line printer file with the header record from the data file. Print lists of the peak values and corresponding times on the line printer. List them on the teletype and ask the user if he wants to omit or correct any of them. If the user elects to omit a value, the program sets that particular value to zero. Later the array is recreated omitting the zero values. At this point the user may also correct any obvious mistakes made by the operator in entering scale factors[5].

---

[5] If the user does not detect an operator error, the program is incapable, at this time, of making the necessary correction. This, however, does not mean that the capability of making automatic decisions is forever denied to the automation.

23. The data should now be in a form for calculating isotopic ratios. The manual interrupt is set now since the data are in their final form to compute ratios. If the program is restarted now using MI it will not have to start at the beginning.

24. Ask the user which variable he wants fit by a polynomial.

25. Fit the variable to a polynomial of a degree the user specifies. This is done with POLFIT. The coefficients and goodness of fit are listed for the user. Also the mean and standard deviation of the data are listed.

26. If this fit is not satisfactory, as determined by the user's response to a question, go to 25 and calculate a higher degree polynomial.

27. Ask the user if he wants ratios. If not, go to 32.

28. The user can enter a scale factor here to be multiplied by the ratios he wants. This is helpful in the case that no scale factors were entered in the original data. Compute the isotopic ratios that the user wants. Any combination of the available data can be used. The coefficients from step 25 are used to generate interpolated values at the new points to be used in the ratios. The ratios are printed on both the teletype and line printer.

29. To clean up the data, the user can now eliminate any ratios he wishes.

30. Now the ratios may be fit to a polynomial just as was done previously. Usually a first degree polynomial is used as the extrapolated ratio at time zero is of interest. The results of this fit are also printed on the line printer. If the user does not want to fit the ratios again go to 31. Else go to 30.

31. Ask the user if he wants to fit another variable. If he does, go to 24. If not, go to 27.

32. Ask the user if he has more data to process. If he does, go to 5. If not, the program will terminate.

*ASCBCD

This program was written for the purpose of converting the data tapes, coded in ASCII[6], to internal BCD code recognized by *MASSPEC.

When the data tapes are read onto a file by the high speed paper tape reader the OS-3 system stores the data in 62 word records. *ASCBCD reads each ASCII record and converts it to BCD records. When a line feed code is sensed this indicates a new BCD record must be started. Each ASCII record contains approximately two BCD records.

[6] ASCII is the same as USASCII (USA Standard Code for Information Interchange).

The teletype data scanner (see Figure 1) produces a special code between each six digit number it sends. The original purpose for this was to tell a special circuit to start the teletype and print the next number. This remote starting circuit was bypassed since it was deemed unnecessary for the teletype to be started and stopped between each number. The special code still remains in the data and the computer center routines will just convert it to an unwanted BCD character. To alleviate this problem the author wrote *ASCBCD which will convert all legal characters and yet pass over the special ASCII code mentioned.

Before the high speed reader was available, one normal sized data tape was copied onto a file from a teletype. This took about one half hour to complete and cost about $7.50. The high speed reader does the task much faster and at a cost of about $.80 per tape.

V. IMPLEMENTATION

Instructions to the Operator

Note: Steps one through four should be done before the sample is admitted to the spectrometer.

1. Switch the teletype to the digitizer position.

2. Turn on the paper tape punch. Make a leader by pressing the HERE IS key once or twice.

3. Type in the header record (one line usually consisting of sample identification). CRLF[7]

   Any number of CRLF's may be entered when typing, as they are ignored by the program.

   If a mistake in typing is made it can be corrected by typing a backslash for each preceding character to be corrected.

   An example would be:

   A-463 AER \ \ IR SAMPP\ LE

   The corrected line would be:

   A-463 AIR SAMPLE

4. Type the identifier for the first peak to be digitized and its scale factor if desired. Scale factors do not have to be entered unless the operator so desires. CRLF

---

[7]CRLF: Type RETURN and then LINE FEED in that order.

The scale factor (from the electrometer) need only be entered once for each peak class. If the scale is changed during the run the new factor must then be entered.

The format of the peak identifier is:

NAME/NUMBERSYMBOL

NAME: Any symbol starting with a non-numeric character used to identify this peak class. It may be up to eight characters long. Abbreviation of the element and its isotope are usually used.

/: The / must be included if a scale factor is to be entered.

NUMBER: An integer denoting the scale factor.

SYMBOL: Only two symbols are allowed.

V for volts and MV for millivolts.

Again, if any mistakes in typing occur they can be corrected with a backslash as mentioned previously. Some examples of peak identifiers are:

(a) A 38

(b) NE 21/100MV

(c) A 40/100 \ V

The identifier in (a) signifies argon 38. The scale factor may or may not have been set previously. The peak identifier in (b) is neon 21 at 100 millivolts and in (c) is argon 40 at 10 volts.

5. When the scan is on the baseline of the desired peak, start the digitizer. The digitized values will now be punched on the paper tape.

6. Upon completion of this peak, press STOP and press RESET on the digitizer. CRLF

7. If the run is not complete, type the next peak identifier and CRLF. Then go to 5.

8. Upon completion of the run make a trailer on the paper tape by pressing the HERE IS key.

9. Turn off the paper tape punch. The tape can now be rolled up and is ready for processing.

Errors

If an error is made by the operator (i. e. , wrong peak identifier or wrong peak digitized) this can be corrected by typing a series of colons on the next line. There must be at least two consecutive colons to be recognized by the program as an error code. The data from up through the preceding peak identifier will be ignored by the program. An example is:

```
            A 40
                         { data }
            A 36
(a)         : : : : : : : : : : :
            A 38
                         { data }
            A 36
                              { data }
(b)         : : : : : : : : : : :
            A 36
                         { data }
```

The identifier A 36 will be ignored at point (a). At point (b) the data and the preceding identifier (A 36) will be ignored.

<u>Instructions for use of *ASCBCD</u>

The data tapes are coded in ASCII and must be converted to internal BCD code to be recognized by *MASSPEC. The paper tapes must be submitted to the I/O desk in the computer center to be read onto a file by the high speed paper tape reader. After a tape has been read onto a file it is ready to be converted to BCD by *ASCBCD. To use the program, type:

*ASCBCD, I=<lun or name>, 0=<lun or name>

The I parameter is the file to be converted. The converted data is placed in the file with the 0 parameter. The data contained in the new file is now ready to be processed by *MASSPEC.

Instructions for use of *MASSPEC

The flow chart in Figure 6 shows all of the alternatives given the user during execution of *MASSPEC. The questions that the program asks are typed in capital letters while any other comments or questions are lower case. Most of the questions are self explanatory but some of them that are not underlined are explained here.

HAVE YOU STARTED THE CALCULATIONS FOR THIS DATA SET?

This question is answered YES only if this set of data has been started on and the user wishes to change the peak acceptance constants. The program is restarted here and some steps will be bypassed the next time through.

ENTER DELTA T IN SECONDS:

Delta T is the time interval from when the operator admitted the sample to the mass spectrometer to when the digitizer was started on the first peak.

ENTER PEAK NAMES, ONE PER LINE.

The peak names may be up to eight characters long. This is asked for if the user has data other than the usual argon.

ENTER THE SEQUENCE IN WHICH THE PEAKS SHOULD OCCUR.

Each peak name is assigned a number and an example of a sequence is given. The user then types in the correct sequence. When the sequence has been entered, type CTRL W which enters an end of file code. The program needs this to sense completion of the sequence.

DO YOU WISH TO ENTER CONSTANTS?

This question is asked if the program is on its first set of data or has been restarted. These constants are the criteria for peak acceptance.

(a) MINIMUM CHANNELS UP = usually 5

(b) MAX CHANNELS ON TOP = usually 20

(c) MINIMUM CHANNELS DOWN = usually 5

If too many peaks are rejected the program should be stopped by pressing the BREAK key and then restarted by typing MI. This is when the user should answer YES to the question: HAVE YOU STARTED THE CALCULATIONS FOR THIS DATA SET? When too many peaks are rejected, they are rejected for one of three reasons. The reasons are given here and the changes to the acceptance constants (a, b, and c), if any, are noted.

(1) The scan was too fast on the uphill or downhill slope of the peak. This creates a discontinuity in the data and the routine will not recognize the peak. The values of (a) and (c) should be changed to 1 or 2. If the discontinuity is too great this will not help and the peak will be lost.

(2) The peak scan lasted longer than the value set in (b) so the search for a peak was reinitialized and no peak was found.

This can be corrected by increasing the value of (b) to about 30.

(3) There was not digital data for the whole peak and no matter how the criteria are changed it would not be accepted.

PEAK IDENTIFIERS DIFFER: A40 VS A38

INPUT RECORD: A38/10V

DO YOU WANT TO CHANGE THE PEAK ID?

The data is either out of sequence or the operator has made a typing error. The only way the next peak will be read in is for the program to accept the identifier given in the data. There are two ways this can be done. If the peak identifier is spelled wrong the user must change it, or if the data is out of sequence the user must indicate where in the sequence the peak should be.

ANSWER THE QUESTIONS BELOW WITH THESE VALUES.

1 = A40[8]

2 = A38

3 = A36

WHICH VARIABLE DO YOU WANT TO FIT?

This question is answered by using the value for the variable the user wants to fit. For example, if he wishes to fit the A38 data he would type 2 for an answer.

---

[8]These are the preset peak names. Steps 9 and 10 in the algorithm for MASSPEC on page 28 let the user enter any names for peaks he wishes. If different peak names had been entered, they would be used here instead of the three preset names.

DO YOU WANT TO FIT AGAIN?

The user can tell by looking at the coefficients, standard error and the goodness of fit (CHI SQUARE) if he wants to fit the data again. Usually the third degree polynomial is as far as the user should fit the data since there are only eight or nine points to fit.

DO YOU WANT RATIOS? YES

RATIO WILL BE 1: A38/X OR 2: X/A38

ANSWER 1 or 2: 2

X =

Here when X is asked for, the user must enter one of the values given for the peak names. If he wishes A40/A38 he would type 1 for an answer.

SCALE FACTOR? YES

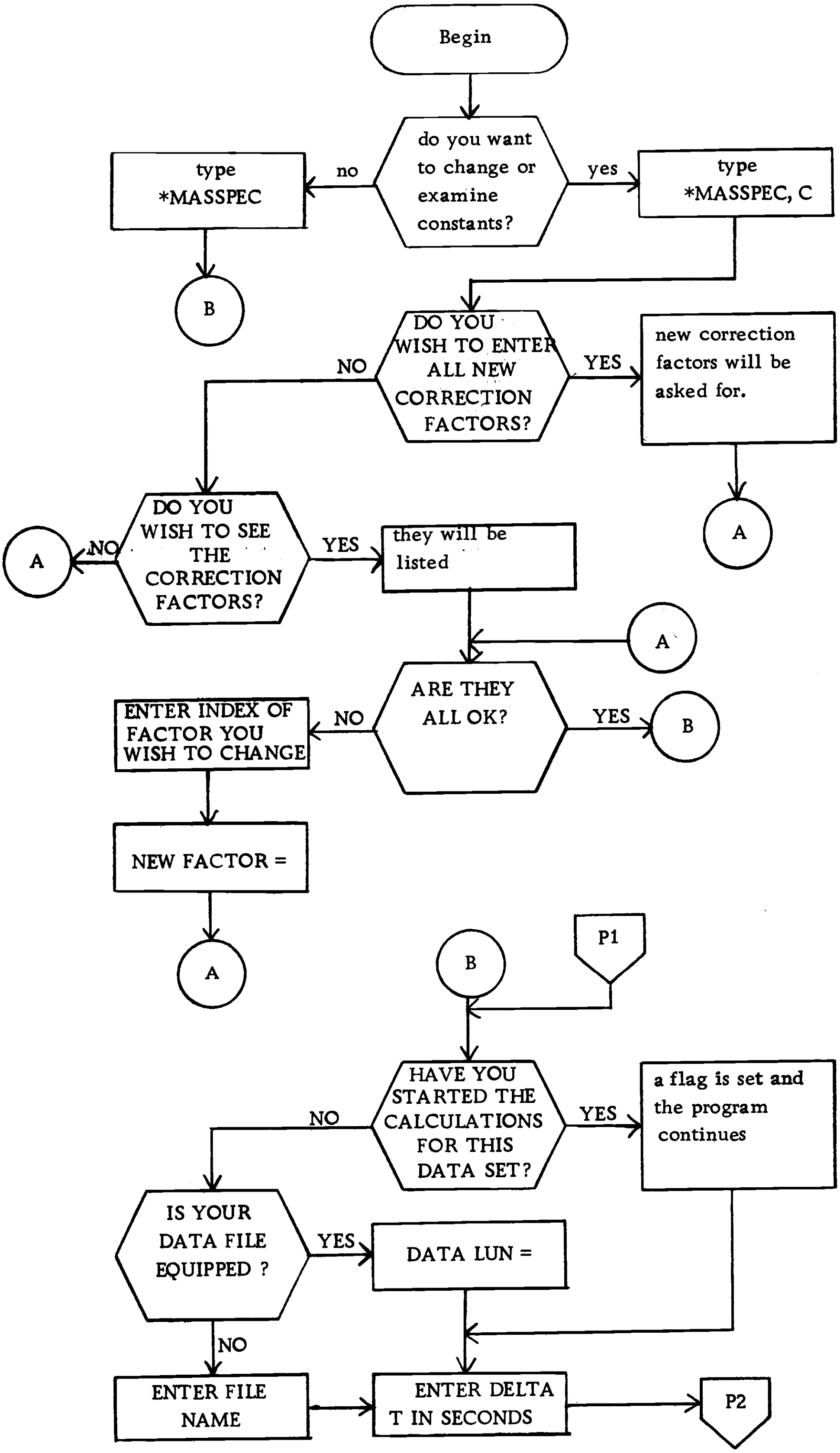
FACTOR =

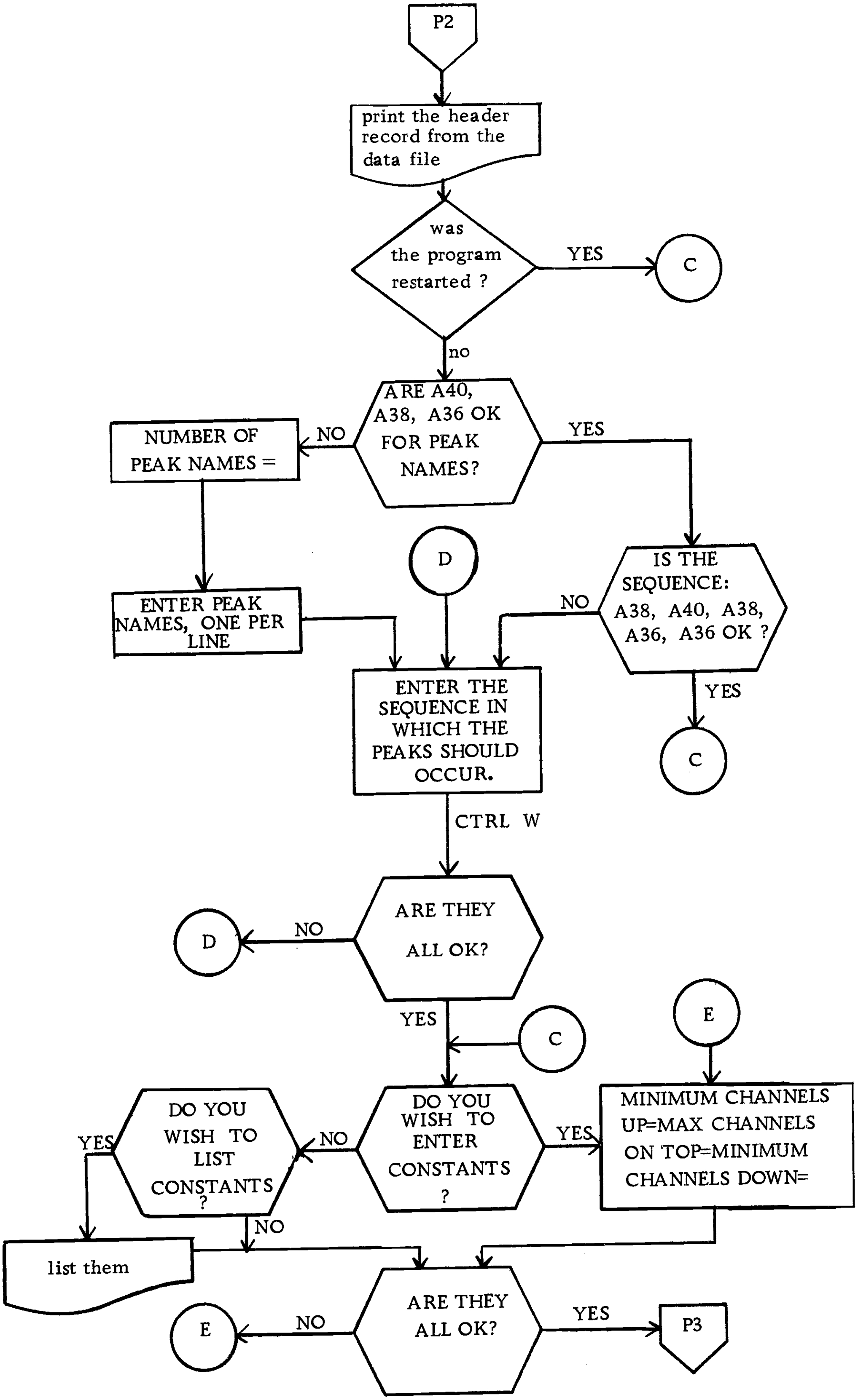
This is helpful if no scale factors were entered in the original data. The factor the user enters here will be multiplied by the ratios he has just chosen.

DO YOU WISH TO FIT ANOTHER VARIABLE?

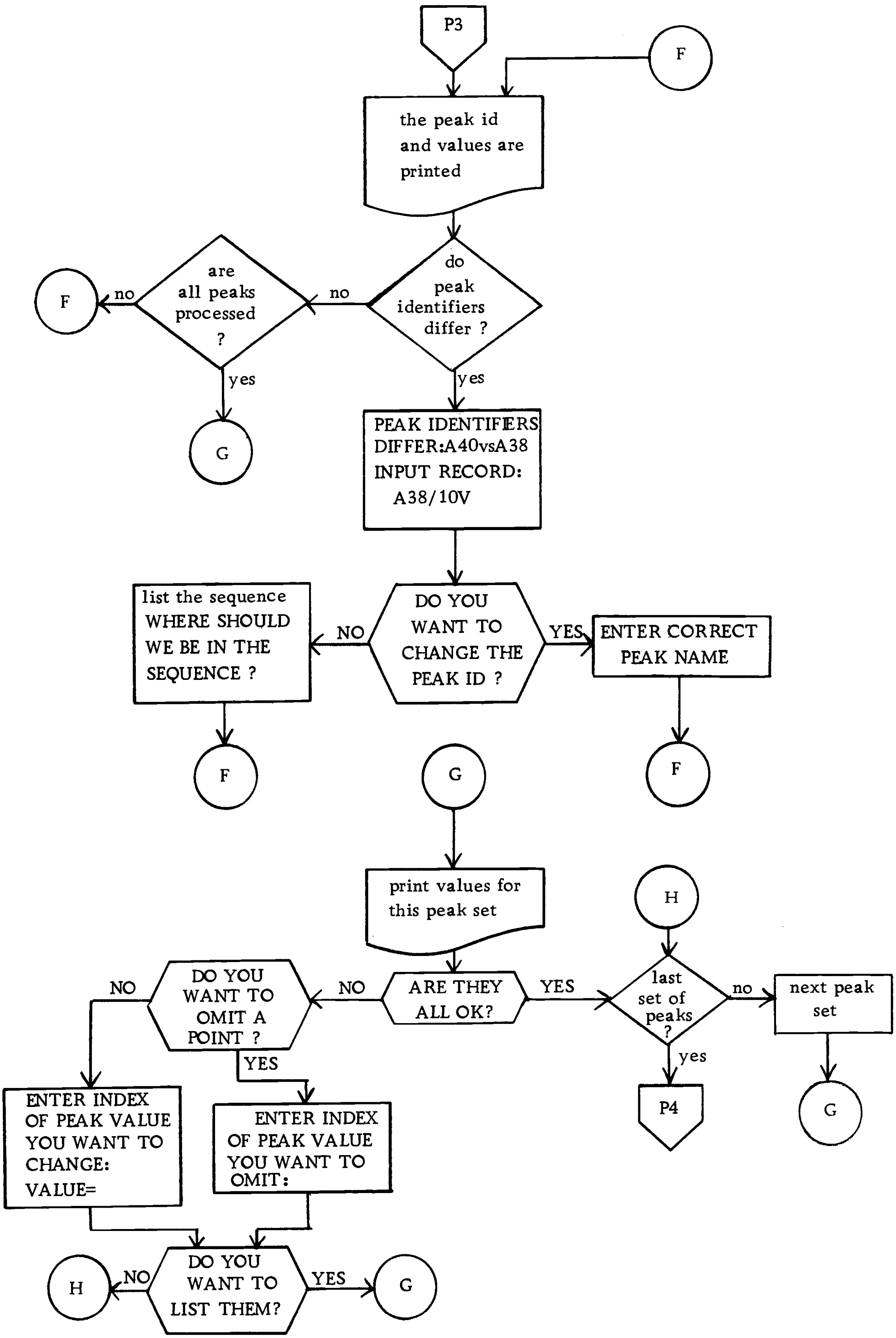
If the user needs ratios involving a different variable, he must type YES for an answer.

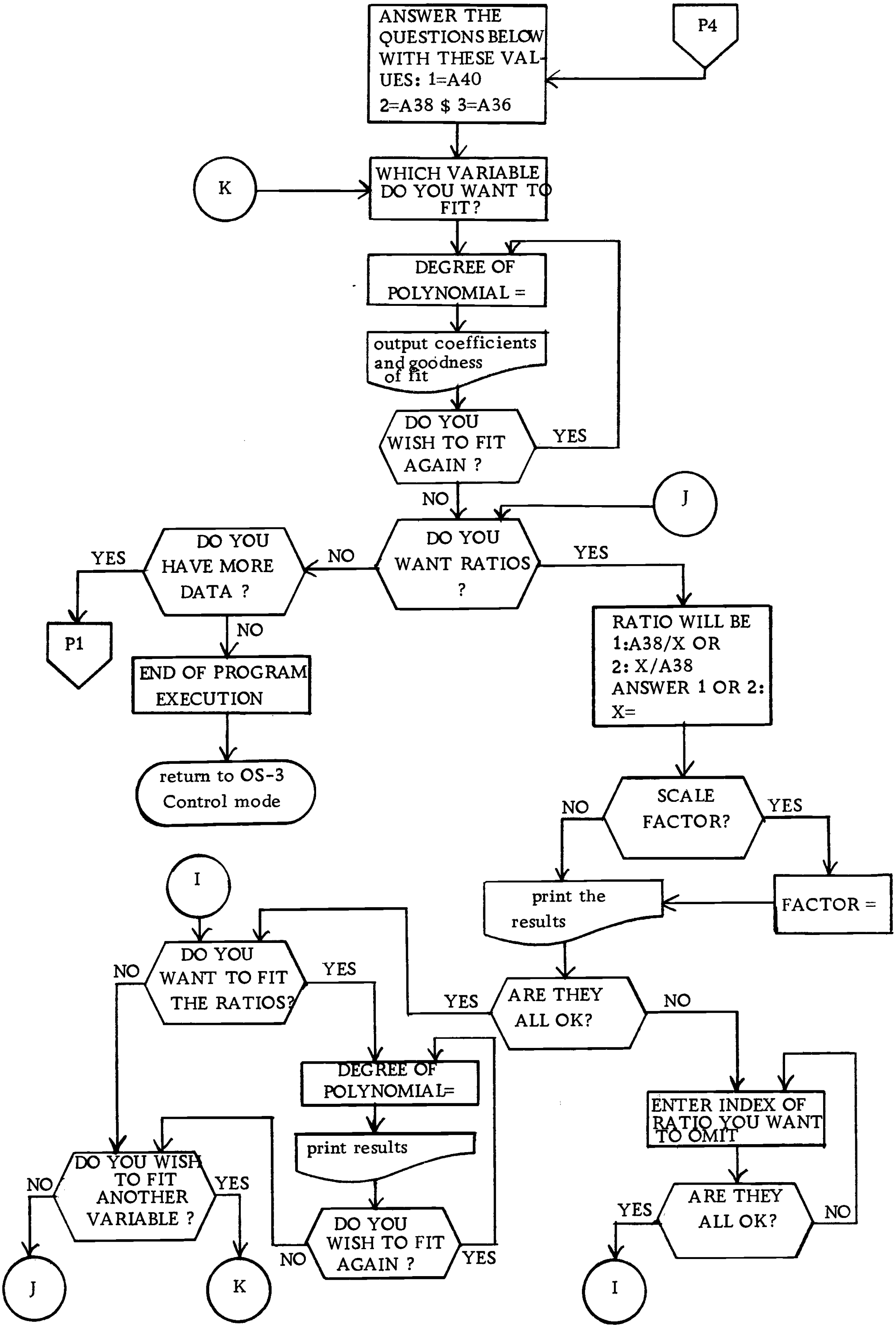
Some examples of the program being executed are shown in APPENDIX I.


Begin
do you want to change or examine constants?
no
yes
type *MASSPEC
type *MASSPEC, C
B
DO YOU WISH TO ENTER ALL NEW CORRECTION FACTORS?
NO
YES
new correction factors will be asked for.
A
DO YOU WISH TO SEE THE CORRECTION FACTORS?
NO
A
YES
they will be listed
A
ARE THEY ALL OK?
NO
YES
B
ENTER INDEX OF FACTOR YOU WISH TO CHANGE
NEW FACTOR =
A
B
P1
HAVE YOU STARTED THE CALCULATIONS FOR THIS DATA SET?
NO
YES
a flag is set and the program continues
IS YOUR DATA FILE EQUIPPED ?
YES
DATA LUN =
NO
ENTER FILE NAME
ENTER DELTA T IN SECONDS
P2



P2
print the header record from the data file
was the program restarted ?
YES
C
no
ARE A40, A38, A36 OK FOR PEAK NAMES?
NO
NUMBER OF PEAK NAMES =
YES
ENTER PEAK NAMES, ONE PER LINE
D
IS THE SEQUENCE: A38, A40, A38, A36, A36 OK ?
NO
YES
C
ENTER THE SEQUENCE IN WHICH THE PEAKS SHOULD OCCUR.
CTRL W
ARE THEY ALL OK?
NO
D
YES
C
E
DO YOU WISH TO LIST CONSTANTS ?
YES
NO
DO YOU WISH TO ENTER CONSTANTS ?
NO
YES
MINIMUM CHANNELS UP=MAX CHANNELS ON TOP=MINIMUM CHANNELS DOWN=
list them
ARE THEY ALL OK?
NO
E
YES
P3


P3
F
the peak id and values are printed
are all peaks processed ?
do peak identifiers differ ?
no
no
yes
yes
F
G
PEAK IDENTIFERS DIFFER:A40vsA38 INPUT RECORD: A38/10V
list the sequence WHERE SHOULD WE BE IN THE SEQUENCE ?
DO YOU WANT TO CHANGE THE PEAK ID ?
NO
YES
ENTER CORRECT PEAK NAME
F
G
F
print values for this peak set
H
DO YOU WANT TO OMIT A POINT ?
ARE THEY ALL OK?
NO
NO
YES
last set of peaks ?
no
next peak set
yes
YES
ENTER INDEX OF PEAK VALUE YOU WANT TO CHANGE: VALUE=
ENTER INDEX OF PEAK VALUE YOU WANT TO OMIT:
P4
G
DO YOU WANT TO LIST THEM?
H
NO
YES
G



ANSWER THE QUESTIONS BELOW WITH THESE VALUES: 1=A40 2=A38 $ 3=A36
P4
K
WHICH VARIABLE DO YOU WANT TO FIT?
DEGREE OF POLYNOMIAL =
output coefficients and goodness of fit
DO YOU WISH TO FIT AGAIN ?
YES
NO
J
DO YOU WANT RATIOS ?
YES
NO
DO YOU HAVE MORE DATA ?
YES
NO
P1
END OF PROGRAM EXECUTION
return to OS-3 Control mode
RATIO WILL BE 1:A38/X OR 2: X/A38 ANSWER 1 OR 2: X=
SCALE FACTOR?
NO
YES
print the results
FACTOR =
I
DO YOU WANT TO FIT THE RATIOS?
NO
YES
ARE THEY ALL OK?
YES
NO
DEGREE OF POLYNOMIAL=
print results
DO YOU WISH TO FIT AGAIN ?
NO
YES
ENTER INDEX OF RATIO YOU WANT TO OMIT
ARE THEY ALL OK?
YES
NO
DO YOU WISH TO FIT ANOTHER VARIABLE ?
NO
YES
J
K
I

VI. RESULTS

Hand calculations can introduce bias and human error into the data. At least a machine is more consistent in its actions although it will only do what it is told to do and no more. If there is any bias in the way the machine does its task, it is due to the way the programmer instructed it.

Accuracy and Precision

A group of mean values for ratios calculated by hand[9] and by machine are compared in Figure 7. The mean values were used instead of extrapolated values since the extrapolated figures for the hand calculations were not at all available. In the group of comparisons 80 to 85 percent of the machine calculations fall within one percent of the corresponding manual calculations. With the 40/38 ratios the machine seems to pick values slightly smaller than the hand calculations provide. For the 36/38 ratios they are somewhat random as is the case of the 38/36 ratios. The 40/36 ratios indicate that the machine picks values slightly larger than by hand. It is difficult to test the accuracy of the methods because everything is compared to a standard.

---

[9]Note: The manually calculated ratios were done by several people other than the author. The hand results were obtained prior to the machine results which thus could not bias the hand results.

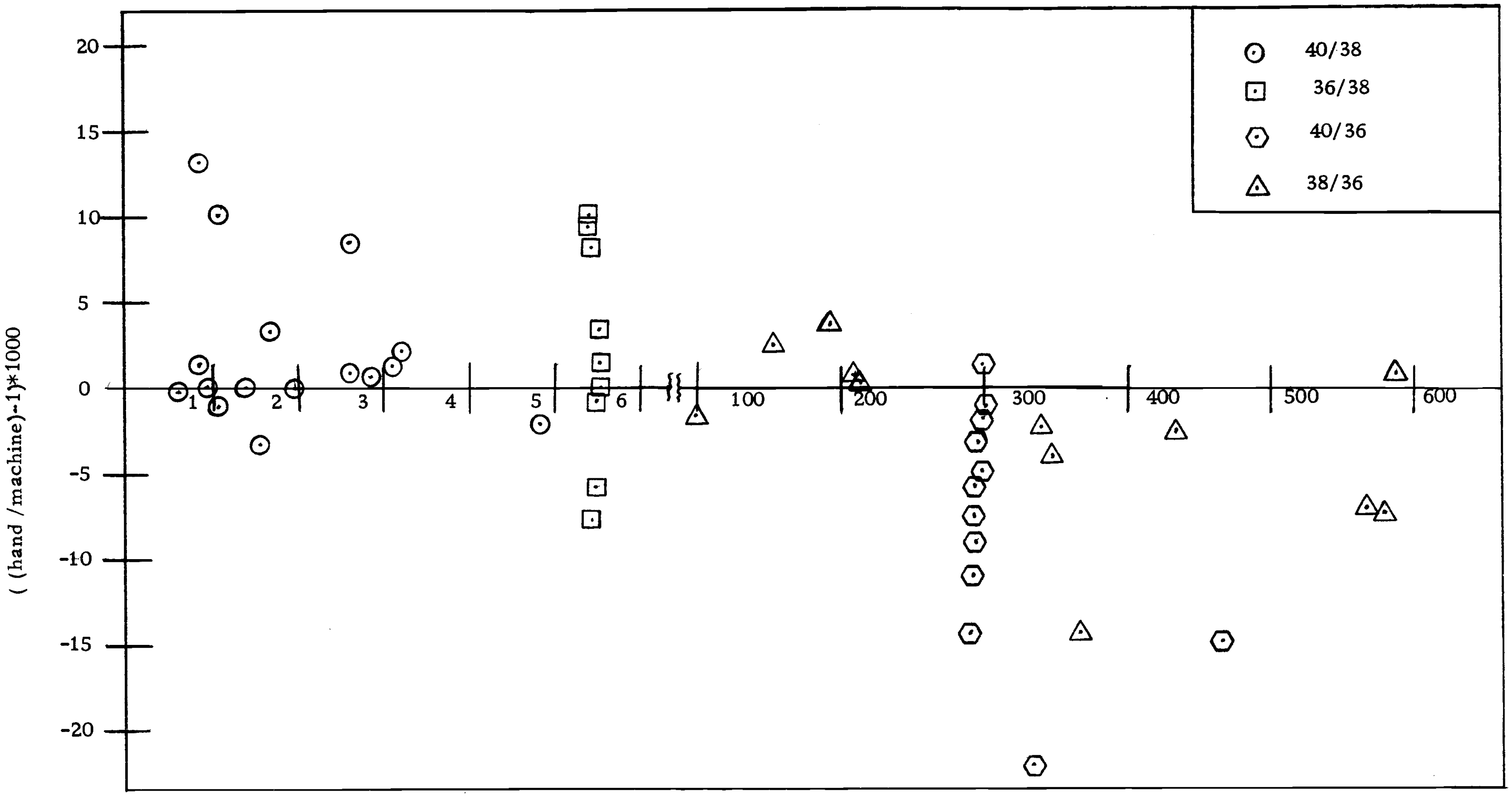


Figure 7. Comparison of hand and machine methods of calculating isotopic ratios. The ordinate values of $\pm$ 10 are $\pm$ 1 percent from perfect agreement (0).

The comparison between machine and hand determined isotopic ratios suggests that the accuracy of the machine computations is adequate. But perhaps even more important in rare gas analysis is precision as systematic errors can be corrected by comparison to a standard such as the rare gases in air. From a group of 40 ratios determined by both methods, the precision (standard error of the mean) was improved by a factor of two by using the machine method.

Costs

The cost per sample to have the paper tape read into the CDC-3300 and converted by *ASCBCD runs from $1.00 to $1.75, while processing by *MASSPEC costs from $1.60 to $2.25. This puts the total cost per sample at $2.60 to $4.00. The amount of time spent at the teletype processing the data is from 12 to 15 minutes per run if the traffic on the OS-3 timesharing system is not great. By using a Tektronix graphics display terminal, the processing time is cut from 12 to 15 minutes to 3 to 5 minutes per run. Manual processing of the data takes from 45 minutes to one hour to read a chart and to calculate the ratios.

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APPENDICES

APPENDIX I

Examples

This appendix contains two examples of digital data obtained and the use of *MASSPEC to reduce this data. The first set of data is for argon and the second is for neon.

```
A-492   HAWAIIAN SOIL SAMPLE, PALI  2-20  11/9/71

A38//10V
000558 000551 000557 000560 000565
 000571 000576 000583 000591 000603 000609 000627 000644 000670 000705
 000773 001378 052530 172588 241273 279058 305561 325453 337902 344458
 347142 348499 349364 350046 350705 351072 351199 350991 350410 348740
 344907 317513 208888 062806 003001 000843 000759 000711 000680 000650
 000625 000612 000604 000592 000583 000576 000492 000570 000532 00051

A40/10V
000561 000558 000563 000564 000570 000574 000579 000588 000597 000610
 000621 000645 000670 000711 000773 000934 001941 025095 079383 142607
 208660 274094 334114 377398 398479 408415 411805 413393 414387 415313
 415745 415578 414376 410671 401444 355011 176857 017684 000920 000790
 000718 000674 000642 000618 000602 000589 000576 000566 000557 000550
 000545 000526 000544

A40
000578 000575 000585 000592 000598 000608 000620
 000629 000648 000671 000691 000726 000764 000827 000923 004095 066898
 153151 201791 245225 286699 322138 350960 374112 390899 401911 408346
 411825 413426 413973 414029 413863 413485 412697 411897 410939 409423
 405332 386543 267075 085273 008440 001319 000917 000785 000721 000678
 000653 000632 000617 000608 000593

A38
000555 000552 000550 000551 000548
 000548 000546 000545 000548 000546 000550 000554 000558 000562 000566
 000571 000581 000587 000601 000617 000641 000672 000721 000800 002446
 058939 134626 195058 244512 285518 313160 331415 340807 344476 345373
 345880 345440 344765 344050 342832 338298 263640 078597 004504 000946
 000749 000679 000641 000611 000596 000581 000571 000560 000550 000546
 000542 000503 000538

A36/30MV
025300 024256 024067 023726 023061 022389 022457
 022184 022058 021646 021276 020914 020723 020875 020690 039606 209706
 335791 397372 432142 451003 455865 460302 458381 459822 460725 458842
 458159 447757 415016 291003 062433 020682 019593 019763 019504 019688
 019616 019206 019272 019254 019308 019069 019183 019029

A36
019436 019201
 019151 019167 019443 019692 019502 020128 019655 019823 019922 020130
 019914 020156 022341 045865 081143 118108 165182 218018 273732 332177
 378717 416672 437509 449521 450599 455633 453063 457446 460320 456587
 457887 460030 454312 449318 446356 410289 257636 072672 021306 021094
 021122 020730 021317 021188 020905 021205 021025 018285 021657

A38
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 339731 340443 341026 341500 341111 339669 334538 324005 265081 095518
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A40
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A40
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 406437 406296 405959 405353 404524 391380 154580 004669 001078 000848
 000746 000694 000665 000642 000626 000608 000597 000589 000579 000577

A36
037854 036766 036534 036109 035713 036836 037262 038248 039229 040496
 041215 043092 033709 038929
 !!!!!!!!!!!!!!!!!!!!!!!!
A38
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 000589 000600 000615 000642 000669 000723 000810 005028 080243 158264
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 337771 336523 334757 297397 123700 010710 001065 000772 000681 000638
 000611 000597 000580 000571 000560 000552 000547 000542 000535

A36
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 020972 020661 020926 020755 020405 021173 113514 263211 347462 382150
 399178 413782 425720 439639 449521 449656 450736 451476 450656 450609
 449740 449255 440841 411127 248086 049083 021069 020263 019997 019810
 019742 019505 019290 019534 019257 019198 019093 019115 018828 018754
 018547

A36
019295 019110 019114 018986 019073 019035 019310 019140 019124
 019071 019195 019171 019483 019533 019578 019680 019440 019921 021098
 039148 078836 120203 169150 227009 283285 338256 381911 415984 431809
 444048 447174 447874 451240 450509 449629 450205 449719 448837 448707
 442435 434312 392752 232805 056822 021270 020992 021033 021048 020991
 020972 021479 021509 021546

A38
000509 000508 000510 000510 000512 000514
 000516 000520 000522 000523 000527 000532 000535 000541 000546 000554
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 105609 171772 235369 284652 316420 329585 333280 334557 335377 336141
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A40
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A40
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A38
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333980 332044 316837 187140 029778 001538 000834 000709 000655 000624
000600 000585 000572 000564 000557 000550 000543 000539 000535

A36
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020771 020747 020438 020564 020521 026874 134526 216320 262503 316327
371469 411381 428115 438448 444240 444496 448183 446821 448596 448643
446734 450634 449747 450643 448893 447835 447468 443261 435174 383095
094014 020741 020386 020161 019773 019811 019566 019352 019412 019196
018975 019058 018978 018845

A36
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041023 074835 113572 157828 211402 262064 317105 366067 402738 425792
435283 444838 444845 444014 448701 449163 450304 451386 447168 446965
449501 443255 429957 418152 391409 356639 314582 267684 211435 158787
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021152 021355 021771

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000524 000527 000531 000536 000539 000544 000551 000554 000566 000578
000589 000609 000634 000679 000768 001050 010268 064757 133280 195309
249016 291123 317477 328523 331559 332684 333585 334617 334884 334788
333778 330472 320118 236260 061476 001233 000763 000691 000649 000622
000601 000589 000579 000570 000561 000557 000551

A40
000553 000549 000550
000549 000556 000557 000561 000567 000573 000585 000596 000611 000632
000659 000705 000806 001119 013088 171949 348723 380951 390022 393534
395998 397832 398939 400037 400755 401097 400333 397518 381311 257603
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000558 000551 000542 000535 000532 000531 000534 000538 000541 000548

A40
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375579 387304 394404 398387 400341 401231 401328 401395 400989 400496
399863 399112 397727 394925 387736 371524 343304 263575 033877 001031
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A38
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333927 334803 335006 334836 334010 333393 332101 328849 262365 078538
004278 000939 000740 000668 000631 000606 000591 000577 000566 000556
000550 000541 000538

A36
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447707 445646 449883 447174 449978 450625 450144 448858 448702 446936
444317 447256 446438 442128 434756 389403 097409 020442 019747 019395
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018513 018979 018921

A36
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019120 019765 019928 021478 043780 094740 143530 201633 255323 312255
361114 400858 425252 439453 441592 443547 442560 444892 447344 444858
447291 445177 448679 441678 431659 417706 393657 358622 316318 261046
210463 158000 108196 033425 020598 020198 020683 020513 020671 020988
020765 021439 021187 021756 021771

A38
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000523 000527 000530 000534 000538 000542 000545 000551 000559 000569
000579 000597 000612 000636 000675 000764 001048 010013 064003 129256
192275 248624 291449 316317 326943 330088 330565 331062 331588 332038
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000599 000583 000574 000566 000559 000556 000556 000551 000546 000547
000545 000547

A40
000567 000574 000576 000585 000596 000610 000630 000656
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398927 394990 384430 325524 126798 005074 000845 000745 000684 000650
000621 000603 000588 000573 000564 000556 000547 000543 000539 000531
000529 000525 000524 000523 000522 000522 000523

7/29/71 A-443 NE

NE 20

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000534 000509 000505 000503
 000502 000507 000507 000512 000514 000
512 000520 000523 000525 000523
 000527 000532 000540 000533 000544 000556 000558 000578 000410 001077
 014978 065446 137840 209025 259551 290181 306023 313576 316497 316975
 317499 316818 311444 275080 190887 102402 047494 019086 007098 003038
 001471 000548 000540 000518 000513 000504 000497 000498 000497 000491
 000486 000493 000488 000488
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NE 21

```
003494 003472 004483 010072 010466 010141
 008978 005429 004099 003575 003449 003412
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!!!!!!!!!!!

NE 21

```
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 042086 041156 041864 042504 041897 042439 041401 042030 042995 054462
 094496 110031 125467 134411 150494 168181 189016 203821 226828 247410
 256404 270052 290459 294046 298010 304928 308545 326161 319592 329518
 326564 336467 340932 329180 335591 338953 336511 344070 336103 340158
 336170 338081 345198 335129 340181 340834 338179 350106 348160 348030
 345526 338594 330473 342571 343853 344596 347905 351056 337850 346935
 338973 333555 337499 335012 322456 309144 289902 273442 230440 174006
 118422 073518 052440 043481 043004 041957 041460 043841 054562 076839
 101590 122499 142024 145167 134505 108083 085412 068535
```

NE 22

```
011812 011160
 011006 011047 011057 011072 011850 132932 482430 704097 812500 869959
 908422 928412 949183 952006 958949 964434 965026 961955 957940 963461
 966517 958141 962182 964167 961039 960551 969089 958116 943565 926425
 876547 799417 718591 621510 524071 425065 340945 265091 207900 161113
 119185 089005 068808 051520 038490 028427 023433 019176 016192 014824
 013477 012556 011526 011027 010505 010405 010415 010448 010471 010409
 010484 010592 010516 010540 010499 010122
```

NE 22

```
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 010015 010481 010418 010102 010447 010145 010041 010142 010122 010452
 010085 010445 010138 010547 010578 011577 014137 017184 023103 031174
 049136 078470 123129 190497 285844 416183 571118 732833 861409 930004
 941515 947117 957547 966011 963061 965014 976836 970022 967170 973054
 970471 970099 967572 973447 971519 973527 970162 969430 975010 963036
 971519 964561 964936 964024 965506 959166 953400 954116 950562 940408
 935813 930410 923489 902900 888466 875541 855188 816061 723883 602008
 442584 343176 206188 049448 013061 011160 011146 011133 010893 011003
 010870 010899 010916 010454 010489 010546 010411
```

NE 21

```
048122 045436 045098
 043870 044514 045496 045142 045583 044907 045448 045439 045196 045822
 047468 048184 050028 049005 050019 053120 056171 060837 066896 073108
 085425 100576 114437 129071 142477 141108 131111 119036 103466 085464
 066182 051471 045848 044578 043519 044557 043892 045529 043957 046903
 049425 058140 075466 107103 157481 233585 293992 332425 337448 341148
 344407 343034 341544 348502 333895 319169 296874 251565 185917 118895
 065517 046517 045156 044157 044914 044857 044413 045011 043033 044956
 044168 043553 044824
```

NE 20

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 000488 000487 000484 000490 000491 000491 000495 000495 000490 000494
 000496 000497 000495 000489 000495 000496 000494 000496 000496 000493
 000492 000497 000496 000495 000498 000500 000491 000497 000501 000505
 000493 000499 000505 000505 000504 000510 000500 000509 000509 000509
 000509 000515 000519 000523 000516 000529 000536 000542 000574 000480
 000940 001557 003520 007059 016504 038932 081816 157876 240542 295430
 309420 311542 312929 313156 313434 313416 313489 313491 314422 313550
 313461 313482 312596 312122 310464 309596 308099 305434 301092 293088
 270840 226470 151056 072417 021034 004134 000997 000596 000544 000534
 000522 000526 000520 000523 000511 000518 000522 000514 000516 000507
 000508 000511 000516
```

NE 20

```
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 000542 000539 000551 000567 000402 000502 001810 008555 025552 056130
 096409 141876 188513 230437 260056 281173 295085 303005 308118 310528
 312113 314126 313553 314009 314469 313833 313517 310572 301012 276525
 231091 177019 125014 082557 043568 015113 005468 002093 001014 000417
 000541 000530 000517 000511 000507 000498 000499 000498 000501 000491
 000483
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NE 21

```
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 042073 042422 042989 042182 041535 041910 042173 041113 039142 041474
 040874 041494 042163 042450 041969 041962 041067 041086 039962 040953
 040489 042428 041179 043132 041501 042995 081437 169427 230511 285579
 306502 322572 329563 332910 339005 331012 331909 337527 327981 326114
 294501 236185 162427 115953 076041 059576 050877 046808 043480 041922
 040586 041087 042593 041823 040929 041869 040113 043139
```

NE 22

```
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 854041 882992 910010 914882 934414 945993 955122 955436 958835 962842
 969114 968438 963962 966816 969009 969110 969153 961416 966482 965018
 965040 961831 950520 935881 933559 898003 791517 572932 335596 162972
 068496 029418 015503 011530 011130 010981 010956 010899 010801 010428
 010428 010452 010577 010559 010571 010443 010570
```

NE 22

```
010589 010086 010084
 010052 010185 010128 010539 010079 010081 010078 010088 010082 010031
 010146 010117 010108 010030 010415 011417 013514 016420 022155 032137
 051058 081475 131094 200952 297443 432012 592955 759488 873118 935551
 955425 960056 961019 962477 963996 964872 963895 960054 952535 948170
 935456 903197 851003 785157 663091 401505 136486 024092 012085 011032
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011069 011064 010867 010891 010864 010821 010516 010473 010478 010582

NE 21

050564 047184 060565 093477 148082 189020 219025 245038 266141 277523
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325927 307456 288508 253559 194104 100436 048940 043100 043845 043983
043039 043101 043181 043447 046057 044058 043531 044995 043895 045039
044157 044875

NE 20

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000487 000497 000493 000498 000496 000491 000494 000497 000501 000505
000503 000522 000514 000527 000550 000593 002425 008156 021881 054108
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287492 253089 190141 108103 040579 009521 001932 000565 000442 000403
000567 000565 000553 000546 000549 000545 000543 000548 000535 000539
000537 000530 000526 000531 000534 000528 000535 000525 000528 000527
000522 000521 000525 000530 000522

NE 20

000543 000523 000528 000531 000529
000527 000542 000554 000567 000571 000406 000473 001118 006088 021021
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309173 310579 311540 312494 312839 313067 312950 312420 310495 306013
291505 262025 216435 160129 097453 038554 012463 004404 001860 000846
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000485 000487

NE 21

046417 040960 039503 040056 039192 040174 039526 040173
041007 039469 039598 040043 040145 040077 040421 044167 060184 091443
153443 213131 267136 293197 312810 323057 325804 319937 324545 330532
335939 332444 332059 303965 260081 183087 125140 081067 061469 050452
046933 042973 042026 042103 041527 040491 040463 040540 039452 041418

NE 22

011173 010502 010531 010449 010814 010520 010548 010923 010867 011065
014420 067454 158565 242122 319917 387527 457013 525847 589567 660806
716980 760409 810462 835558 858536 891153 905128 921179 938541 940541
951593 954560 953033 955994 959518 964936 959981 970049 969067 965466
976134 967586 968134 965533 971017 971094 975188 969553 966162 958538
948580 932190 903516 866069 798899 724007 518599 292102 151168 071033
028586 015020 011466 011185 011027 011040 010561 010584 010556 010822
010529 010573 010483 010554 010413+

NE 22

010530 010422 010527 010446 010471
010143 010579 010597 010545 010433 010190 010479 011118 012415 015013
019937 024443 035137 058421 093883 152802 235582 337971 469466 615025
764031 871801 936103 953422 959562 966828 965541 967584 960160 962013
962489 953432 949526 949511 913547 882838 791836 581498 280880 072979
016162 011478 011024 011132 010974 010917 010804 010454 010467 010592
010551 010407

NE 21

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176106 236013 295575 325828 337451 333007 334932 327502 326980 330899
328563 311598 304897 272192 214495 110013 051919 042461 043024 042197
041464 041421 043801 043450 043472 043069 041974 042533 043584 042880
043183

NE 20

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279421 305103 309143 310007 309176 308812 306536 301581 291989 269432
227072 159078 073811 009590 000896 000592 000561 000542 000531 000522
000526 000513 000510 000506 000499 000510 000492

```
[redacted]
NOVEMBER 26, 1971  2:=9 PM TERMINAL 034

#*MASSPEC

HI THERE !
LETS CALCULATE MASS SPECTRA
DATE PROCESSED 11/26/71          1459
HAVE YOU STARTED THE CALCULATIONS FOR THIS DATA SET ? NO
IS YOUR DATA FILE EQUIPPED ? NO
ENTER FILE NAME
A492
ENTER DELTA T IN SECONDS : 140

*****************************************************
A-492   HAWAIIAN SOIL SAMPLE, PALI  2-20  11/9/71

*****************************************************
ARE A40 , A38 , A36  OK FOR PEAK NAMES ?YES
IS THE SEQUENCE : A38, A40, A40, A38, A36, A36 OK ?YES
DO YOU WISH TO ENTER CONSTANTS ?YES
MINIMUM CHANNELS UP    = 5
MAX CHANNELS ON TOP    = 20
MINIMUM CHANNELS DOWN = 5
ARE THEY ALL OK  ? YES
ERROR IN PEAK   A38
ERROR IN PEAK   A40
ERROR IN PEAK   A40
E
#MI
HAVE YOU STARTED THE CALCULATIONS FOR THIS DATA SET ? YES
ENTER DELTA T IN SECONDS : 140

*****************************************************
A-492   HAWAIIAN SOIL SAMPLE, PALI  2-20  11/9/71

*****************************************************
DO YOU WISH TO ENTER CONSTANTS ?YES
MINIMUM CHANNELS UP    = 2
MAX CHANNELS ON TOP    = 25
MINIMUM CHANNELS DOWN = 2
ARE THEY ALL OK  ? YES
A38        177     350250  10.000      3.50250
A40        235     414758  10.000      4.14758
A40        293     413174  10.000      4.13174
A38        355     344539  10.000      3.44539
A36        407     439356    .030       .01318
A36        464     437059    .030       .01311
A38        522     340205  10.000      3.40205
A40        576     405564  10.000      4.05564
A40        640     405442  10.000      4.05442

 PEAK IDENTIFIERS DIFFER : A38      VS  A36
INPUT RECORD : A36

DO YOU WANT TO CHANGE THE PEAK ID ? YES
ENTER CORRECT PEAK NAME
A36
OPERATOR ERROR NOTED

 PEAK IDENTIFIERS DIFFER : A36      VS  A38
INPUT RECORD : A38

DO YOU WANT TO CHANGE THE PEAK ID ? YES
ENTER CORRECT PEAK NAME
A38
A38        708     337880  10.000      3.37880
A36        763     430389    .030       .01291
A36        827     429140    .030       .01287
A38        885     335548  10.000      3.35548
A40        938     401460  10.000      4.01460
A40        996     402014  10.000      4.02014
A38       1047     335414  10.000      3.35414
A36       1103     428178    .030       .01285
A36       1166     429323    .030       .01288

 PEAK IDENTIFIERS DIFFER : A38      VS  A40
INPUT RECORD : A40

DO YOU WANT TO CHANGE THE PEAK ID ? YES
ENTER CORRECT PEAK NAME
A4

 PEAK IDENTIFIERS DIFFER : A4       VS  A40
INPUT RECORD : A40

DO YOU WANT TO CHANGE THE PEAK ID ? NO
  1 : A38
  2 : A40
  3 : A40
  4 : A38
  5 : A36
  6 : A36
WHERE SHOULD WE BE IN THE SEQUENCE ? 2
A40       1278     399715  10.000      3.99715
A40       1336     400570  10.000      4.00570
A38       1396     334177  10.000      3.34177
A36       1455     430229    .030       .01291
A36       1523     425009    .030       .01275
A38       1591     332785  10.000      3.32785
A40       1642     398705  10.000      3.98705

*****************************************************
         TIME        A40
  1      235      4.14758269
  2      293      4.13173818
  3      576      4.05563786
  4      640      4.05441600
  5      938      4.01460123
  6      996      4.02013819
  7     1278      3.99714688
  8     1336      4.00570300
  9     1642      3.98705107
ARE THEY ALL OK ? YES

         TIME        A38
  1      177      3.50250161
  2      355      3.44538933
  3      522      3.40205178
  4      708      3.37880431
  5      885      3.35547896
  6     1047      3.35414223
  7     1396      3.34176778
  8     1591      3.32785007
ARE THEY ALL OK ? YES

         TIME        A36
  1      407      .01318067
  2      464      .01311176
  3      763      .01291166
  4      827      .01287420
  5     1103      .01284534
  6     1166      .01287970
  7     1455      .01290688
  8     1523      .01275027
ARE THEY ALL OK ? YES

*****************************************************

ANSWER THE QUESTIONS BELOW WITH THESE VALUES
 1 = A40
 2 = A38
 3 = A36
WHICH VARIABLE DO YOU WANT TO FIT ? 2
DEGREE OF POLYNOMIAL = 1

COEFFICIENTS           STD. ERROR
 3.47944E 00           1.96572E-02
-1.08893E-04           2.05913E-05

CHI SQUARE            =  7.25537E-04
MEAN                  =  3.38850E 00
STANDARD DEVIATION =  5.93339E-02
DO YOU WISH TO FIT AGAIN ? YES
DEGREE OF POLYNOMIAL = 2

COEFFICIENTS           STD. ERROR
 3.54538E 00           1.34256E-02
-3.12778E-04           3.51774E-05
 1.14480E-07           1.92426E-08

CHI SQUARE            =  1.07769E-04
MEAN                  =  3.38850E 00
STANDARD DEVIATION =  5.93339E-02
DO YOU WISH TO FIT AGAIN ? YES
DEGREE OF POLYNOMIAL = 3

COEFFICIENTS           STD. ERROR
 3.58635E 00           7.70791E-03
-5.39959E-04           3.68742E-05
 4.26705E-07           4.85281E-08
-1.18905E-10           1.83227E-11

CHI SQUARE            =  1.16853E-05
MEAN                  =  3.38850E 00
STANDARD DEVIATION =  5.93339E-02
DO YOU WISH TO FIT AGAIN ? NO
DO YOU WANT RATIOS ? YES

RATIO WILL BE  1: A38       / X   OR   2: X /A38
ANSWER 1 OR 2 : 2
 X = 1
SCALE FACTOR ? NO

*****************************************************

                TIME       A40       / A38
         1       235      1.19133E 00
         2       293      1.19353E 00
         3       576      1.19488E 00
         4       640      1.19798E 00
         5       938      1.19583E 00
         6       996      1.19848E 00
         7      1278      1.19495E 00
         8      1336      1.19822E 00
         9      1642      1.19954E 00

*****************************************************
ARE THEY ALL OK ? YES
DO YOU WANT TO FIT THE RATIOS ? YES
DEGREE OF POLYNOMIAL = 1

COEFFICIENTS           STD. ERROR
 1.19236E 00           1.35578E-03
 4.21727E-06           1.36578E-06

CHI SQUARE            =  3.49640E-06
MEAN                  =  1.19608E 00
STANDARD DEVIATION =  2.68820E-03
STD. ERROR OF MEAN =  8.96068E-04
```

```
DO YOU WISH TO FIT AGAIN ? NO
DO YOU WISH TO FIT ANOTHER VARIABLE ? NO
DO YOU WANT RATIOS ? YES

RATIO WILL BE  1: A38      / X   OR  2: X /A38
ANSWER 1 OR 2 : 1
 X = 3
SCALE FACTOR ? NO
*****************************************************

                TIME      A38       / A36
           1     407      2.60173E 02
           2     464      2.60514E 02
           3     763      2.61001E 02
           4     827      2.61328E 02
           5    1103      2.60822E 02
           6    1166      2.59975E 02
           7    1455      2.58606E 02
           8    1523      2.61461E 02

*****************************************************
ARE THEY ALL OK ? YES
DO YOU WANT TO FIT THE RATIOS ? YES
DEGREE OF POLYNOMIAL = 1

COEFFICIENTS        STD. ERROR
 2.60871E 02        9.15996E-01
-3.99880E-04        8.80412E-04

CHI SQUARE          =  9.55809E-01
MEAN                =  2.60485E 02
STANDARD DEVIATION =  9.20561E-01
STD. ERROR OF MEAN =  3.25468E-01
DO YOU WISH TO FIT AGAIN ? NO
DO YOU WISH TO FIT ANOTHER VARIABLE ? NO
DO YOU WANT RATIOS ? NO
DO YOU HAVE MORE DATA ? YES
HAVE YOU STARTED THE CALCULATIONS FOR THIS DATA SET ? NO
IS YOUR DATA FILE EQUIPPED ? NO
ENTER FILE NAME
A443
ENTER DELTA T IN SECONDS : 90

*****************************************************
7/29/71   A-443  NE

*****************************************************
ARE A40 , A38 , A36  OK FOR PEAK NAMES ?NO
NUMBER OF PEAK NAMES = 3

ENTER PEAK NAMES, ONE PER LINE.
NE 20
NE 21
NE 22

ENTER THE SEQUENCE IN WHICH THE PEAKS SHOULD OCCUR.
 1 = NE20
 2 = NE21
 3 = NE22
AN EXAMPLE IS
  1 2 3 3 2 1
<> 1 2 3 3 2 1
<>   1  2  3  3  2  1
ARE THEY ALL OK?YES
NE20       128    316323       0       .31632
OPERATOR ERROR NOTED
ERROR IN PEAK   NE21
NE22       297    948891       0       .94889
ERROR IN PEAK   NE22
NE21       469     86777       0       .08678
NE20       594    312712       0       .31271
NE20       667    313251       0       .31325
NE21       744    292335       0       .29234
ERROR IN PEAK   NE22
NE22       883    952420       0       .95242
NE21       931    277595       0       .27760
NE20       995    311439       0       .31144
NE20      1069    312174       0       .31217
NE21      1126    283688       0       .28369
NE22      1197    956921       0       .95692
NE22      1267    952395       0       .95239
NE21      1322    286380       0       .28638
NE20      1393    308104       0       .30810

*****************************************************

      TIME        NE20
  1    128       .31632340
  2    594       .31271225
  3    667       .31325080
  4    995       .31143920
  5   1069       .31217353
  6   1393       .30810390
ARE THEY ALL OK ? YES

      TIME        NE21
  1    469       .08677700
  2    744       .29233523
  3    931       .27759505
  4   1126       .28368805
  5   1322       .28637957
ARE THEY ALL OK ? NO
DO YOU WANT TO OMIT A POINT ? NO
ENTER INDEX OF PEAK VALUE YOU WANT TO CHANGE : 1
VALUE = .260331
DO YOU WANT TO LIST THEM ? NO
ARE THEY ALL OK ? YES
```

```
      TIME        NE22
  1    297       .94889124
  2    883       .95241985
  3   1197       .95692057
  4   1267       .95239499
ARE THEY ALL OK ? YES

*****************************************************

ANSWER THE QUESTIONS BELOW WITH THESE VALUES
 1 = NE20
 2 = NE21
 3 = NE22
WHICH VARIABLE DO YOU WANT TO FIT ? 1
DEGREE OF POLYNOMIAL = 1

COEFFICIENTS        STD. ERROR
 3.16986E-01        8.33812E-04
-5.76009E-06        9.23063E-07

CHI SQUARE          =  8.30812E-07
MEAN                =  3.12334E-01
STANDARD DEVIATION =  2.66905E-03
DO YOU WISH TO FIT AGAIN ? YS ERR YES
DEGREE OF POLYNOMIAL = 2

COEFFICIENTS        STD. ERROR
 3.16515E-01        1.36311E-03
-4.00597E-06        3.85422E-06
-1.16089E-09        2.45812E-09

CHI SQUARE          =  1.03109E-06
MEAN                =  3.12334E-01
STANDARD DEVIATION =  2.66905E-03
DO YOU WISH TO FIT AGAIN ? YES
DEGREE OF POLYNOMIAL = 3

COEFFICIENTS        STD. ERROR
 3.18544E-01        1.25513E-03
-2.04691E-05        7.66202E-06
 2.57063E-08        1.19296E-08
-1.17574E-11        5.17392E-12

CHI SQUARE          =  4.31783E-07
MEAN                =  3.12334E-01
STANDARD DEVIATION =  2.66905E-03
DO YOU WISH TO FIT AGAIN ? NO
DO YOU WANT RATIOS ? YES

RATIO WILL BE  1: NE20     / X   OR  2: X /NE20
ANSWER 1 OR 2 : 1
 X = 2
SCALE FACTOR ? YES
FACTOR =333.3333

*****************************************************

        TIME      NE20      / NE21
    1    469     1.20380E 00      4.01265E 02
    2    744     1.06967E 00      3.56557E 02
    3    931     1.12495E 00      3.74984E 02
    4   1126     1.09734E 00      3.65781E 02
    5   1322     1.07985E 00      3.59948E 02

*****************************************************
ARE THEY ALL OK ? NO
ENTER INDEX OF RATIO YOU WANT TO OMIT : 1
ARE THEY ALL OK ? YES
DO YOU WANT TO FIT THE RATIOS ? YES
DEGREE OF POLYNOMIAL = 1

COEFFICIENTS        STD. ERROR
 3.64160E 02        2.41193E 01
 1.52345E-04        2.29037E-02

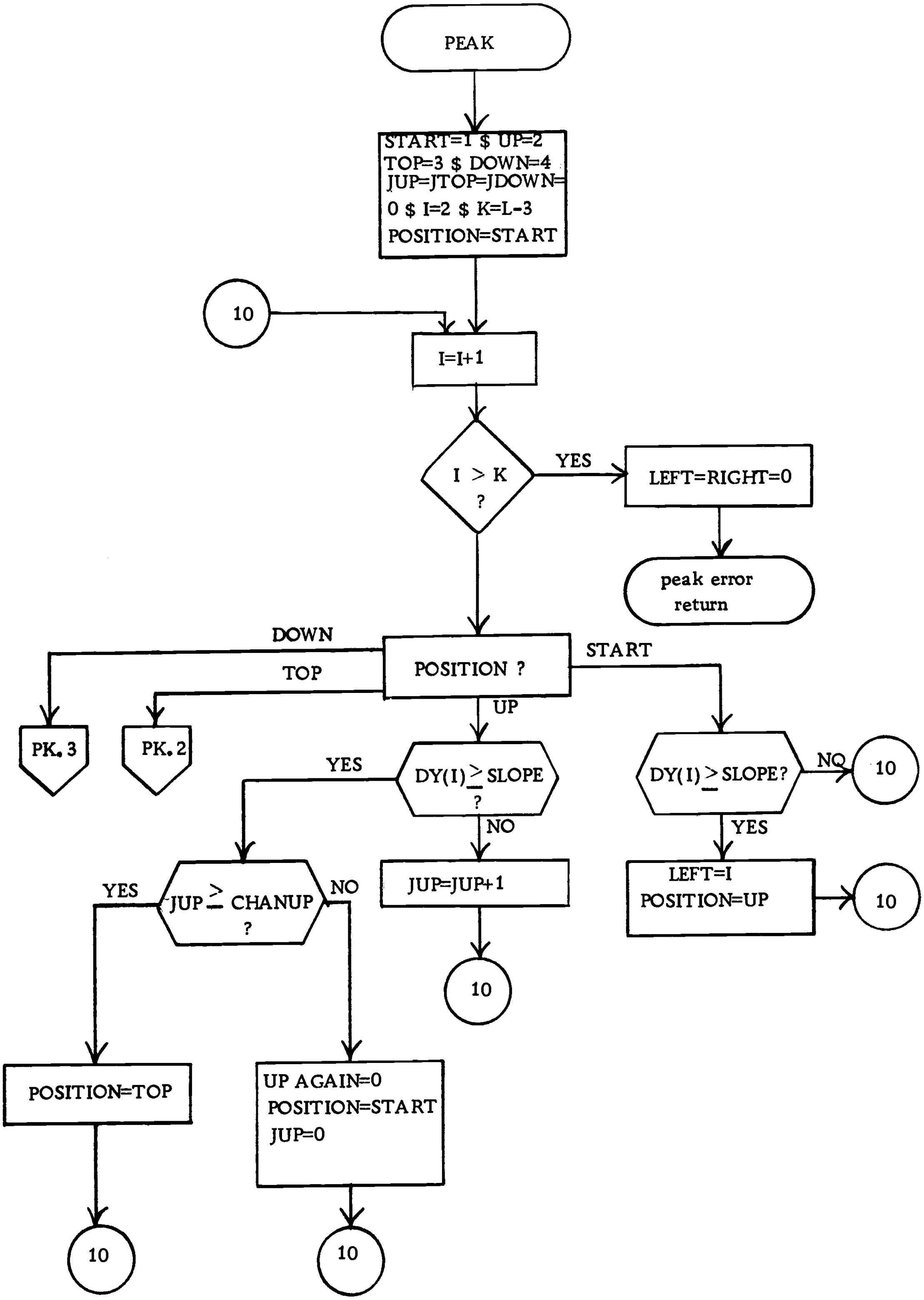
CHI SQUARE          =  9.76110E 01
MEAN                =  3.64317E 02
STANDARD DEVIATION =  8.06693E 00
STD. ERROR OF MEAN =  4.03347E 00
DO YOU WISH TO FIT AGAIN ? NO
DO YOU WISH TO FIT ANOTHER VARIABLE ? NO
DO YOU WANT RATIOS ? NO
DO YOU HAVE MORE DATA ? NO

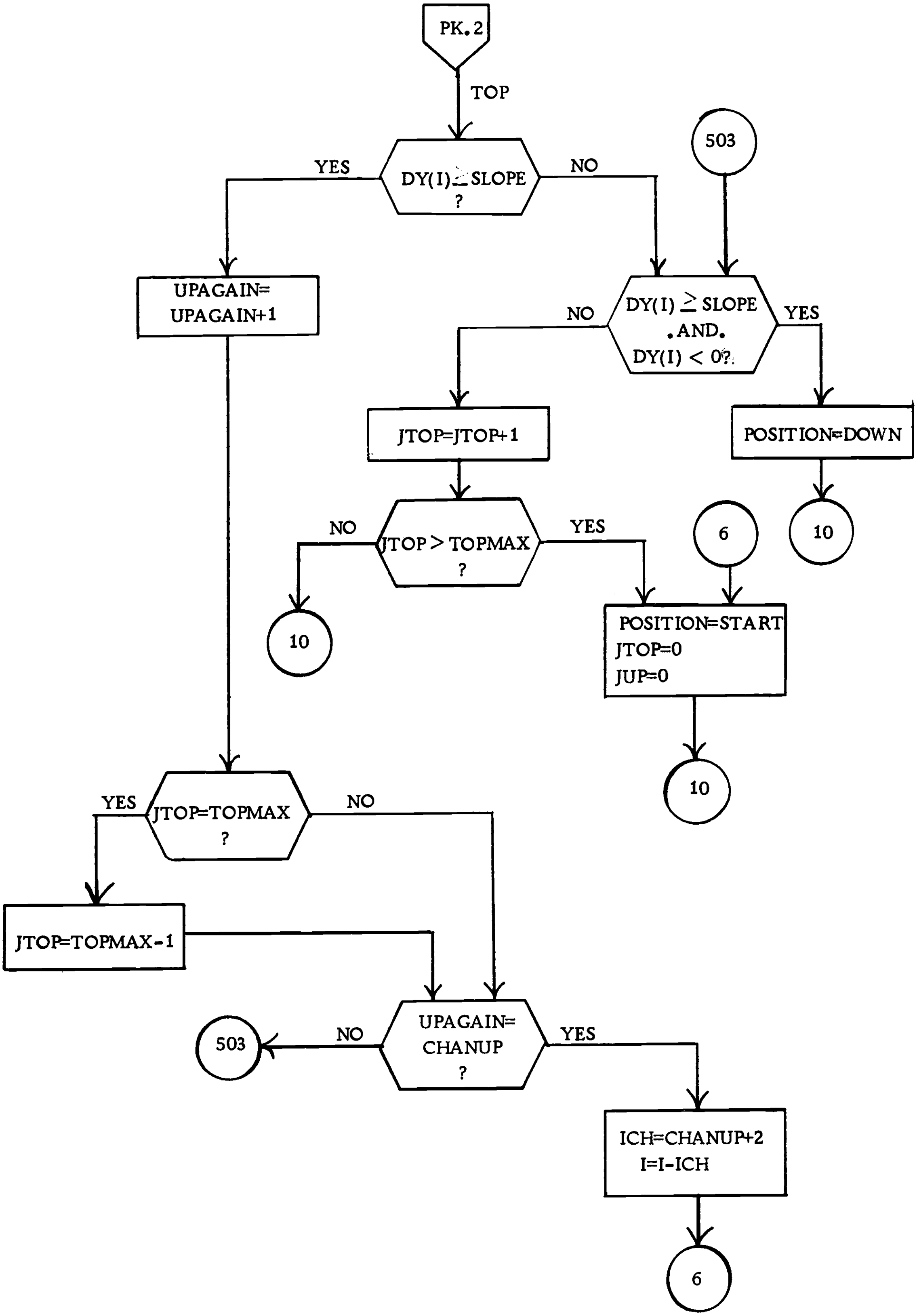
END OF PROGRAM EXECUTION.

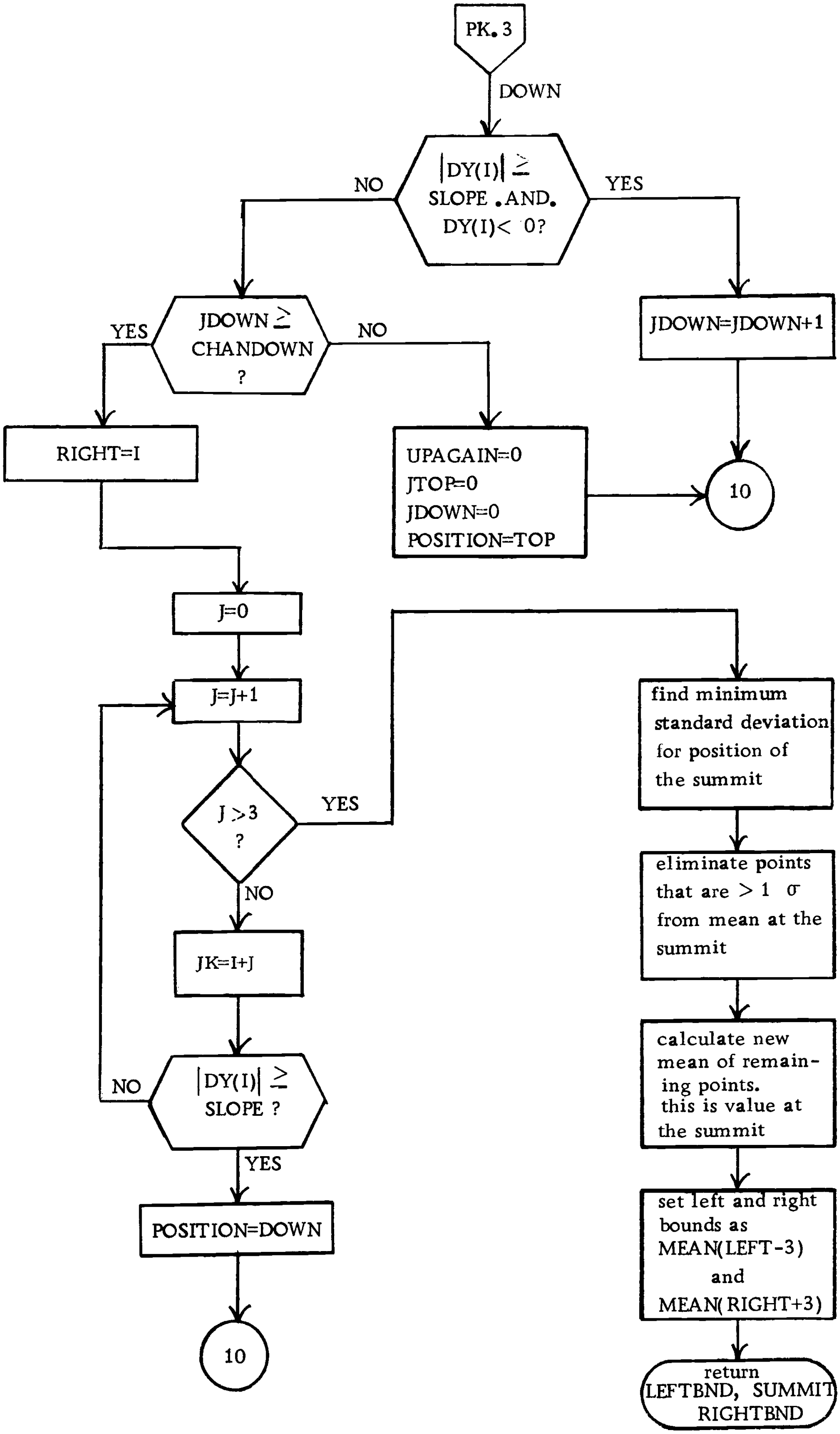
#LOGOFF
TIME 32.124 SECONDS  MFBLKS 4  COST $3.88
```

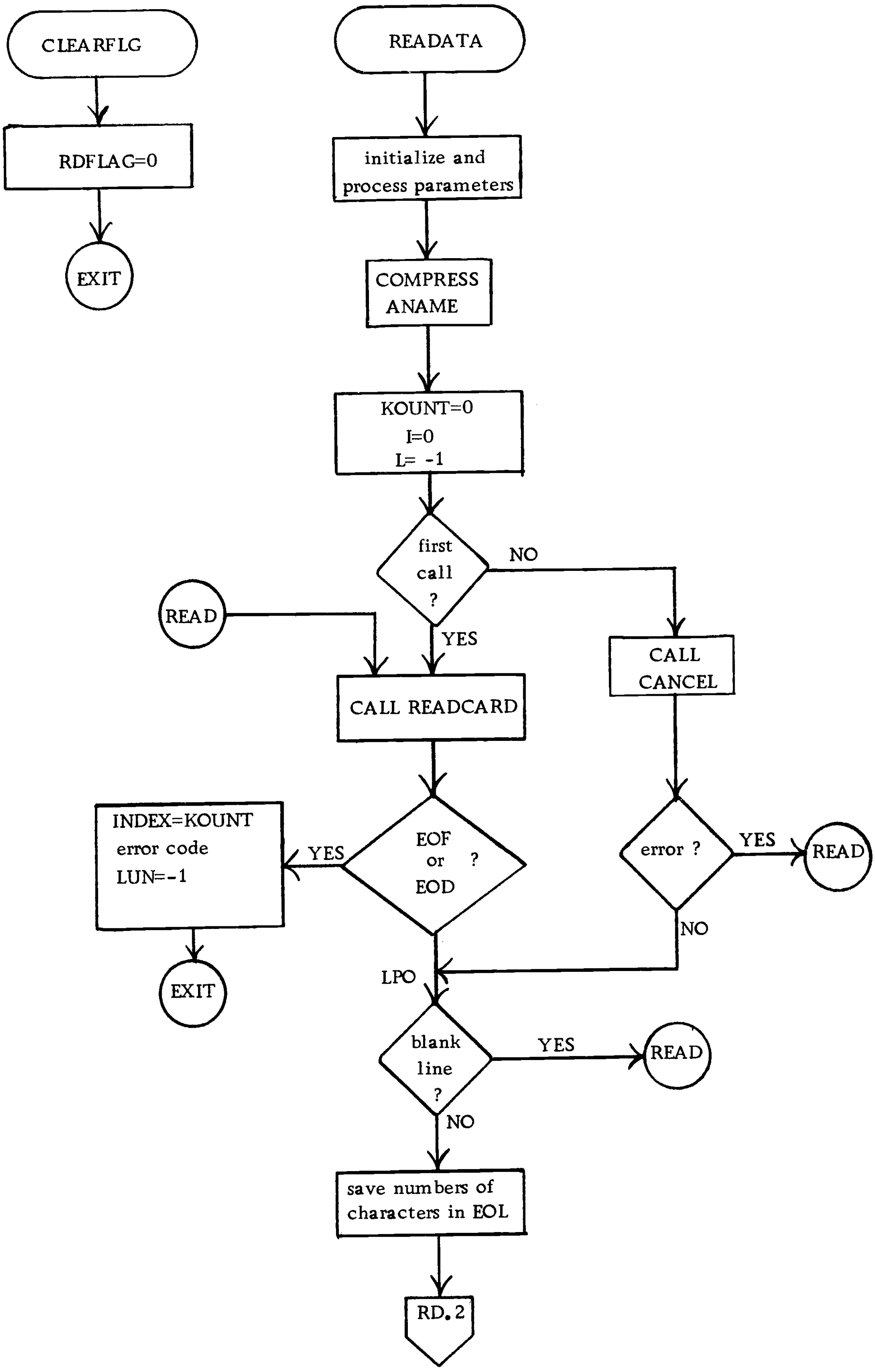
APPENDIX II

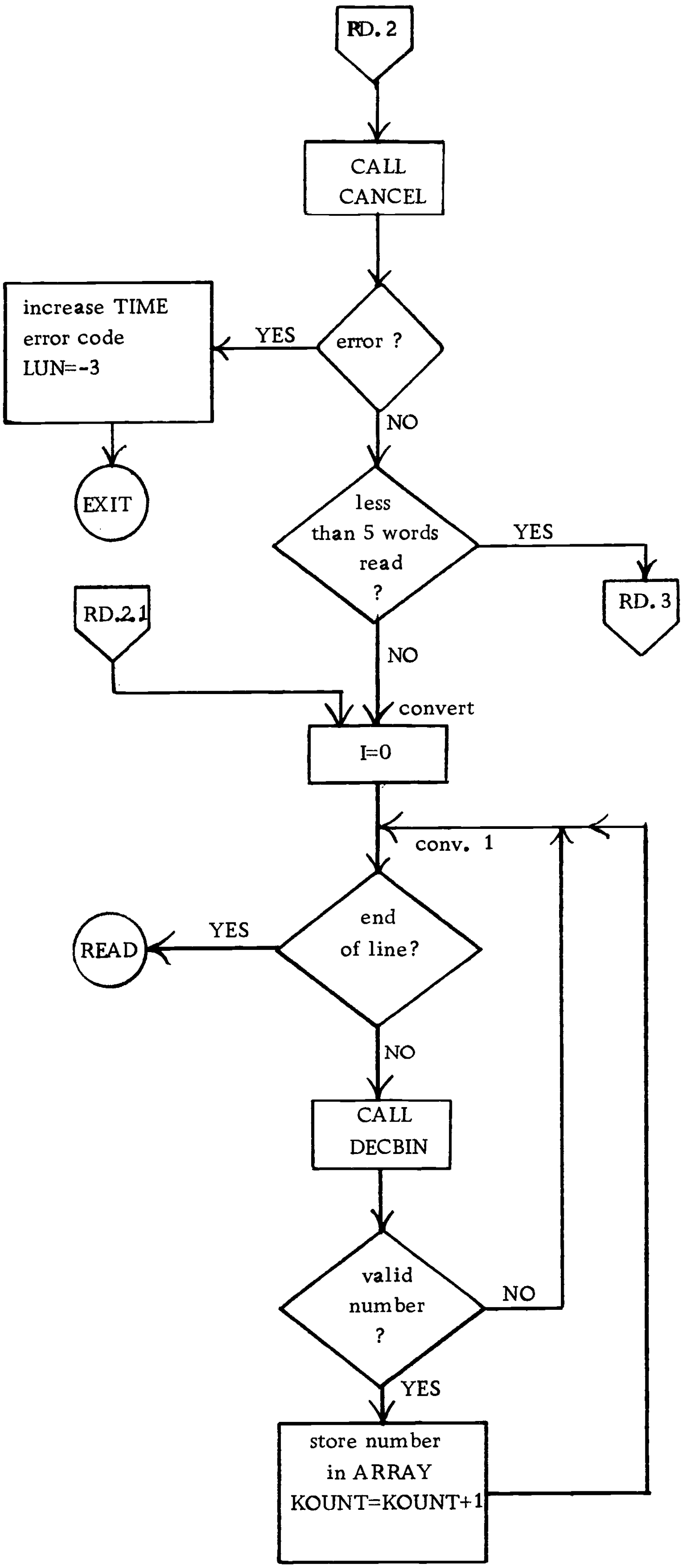
Flowcharts

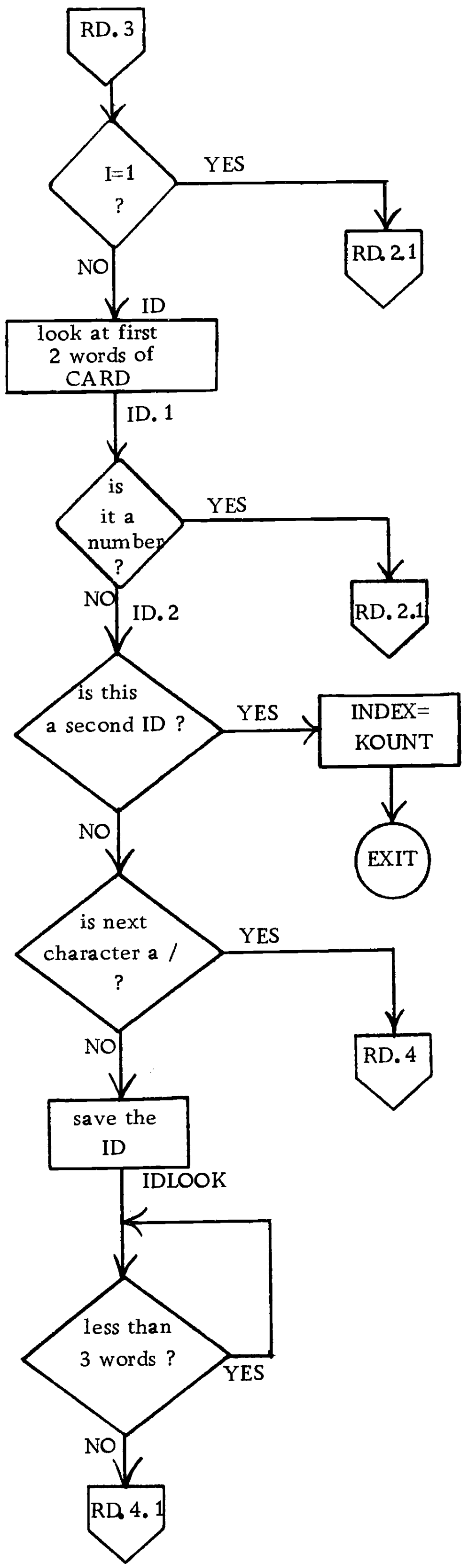

PEAK
START=1 $ UP=2
TOP=3 $ DOWN=4
JUP=JTOP=JDOWN=
0 $ I=2 $ K=L-3
POSITION=START
10
I=I+1
I > K ?
YES
LEFT=RIGHT=0
peak error return
DOWN
TOP
POSITION ?
START
UP
PK. 3
PK. 2
YES
DY(I) ≥ SLOPE ?
DY(I) ≥ SLOPE?
NO
10
NO
YES
YES
JUP ≥ CHANUP ?
NO
JUP=JUP+1
LEFT=I
POSITION=UP
10
10
POSITION=TOP
UP AGAIN=0
POSITION=START
JUP=0
10
10

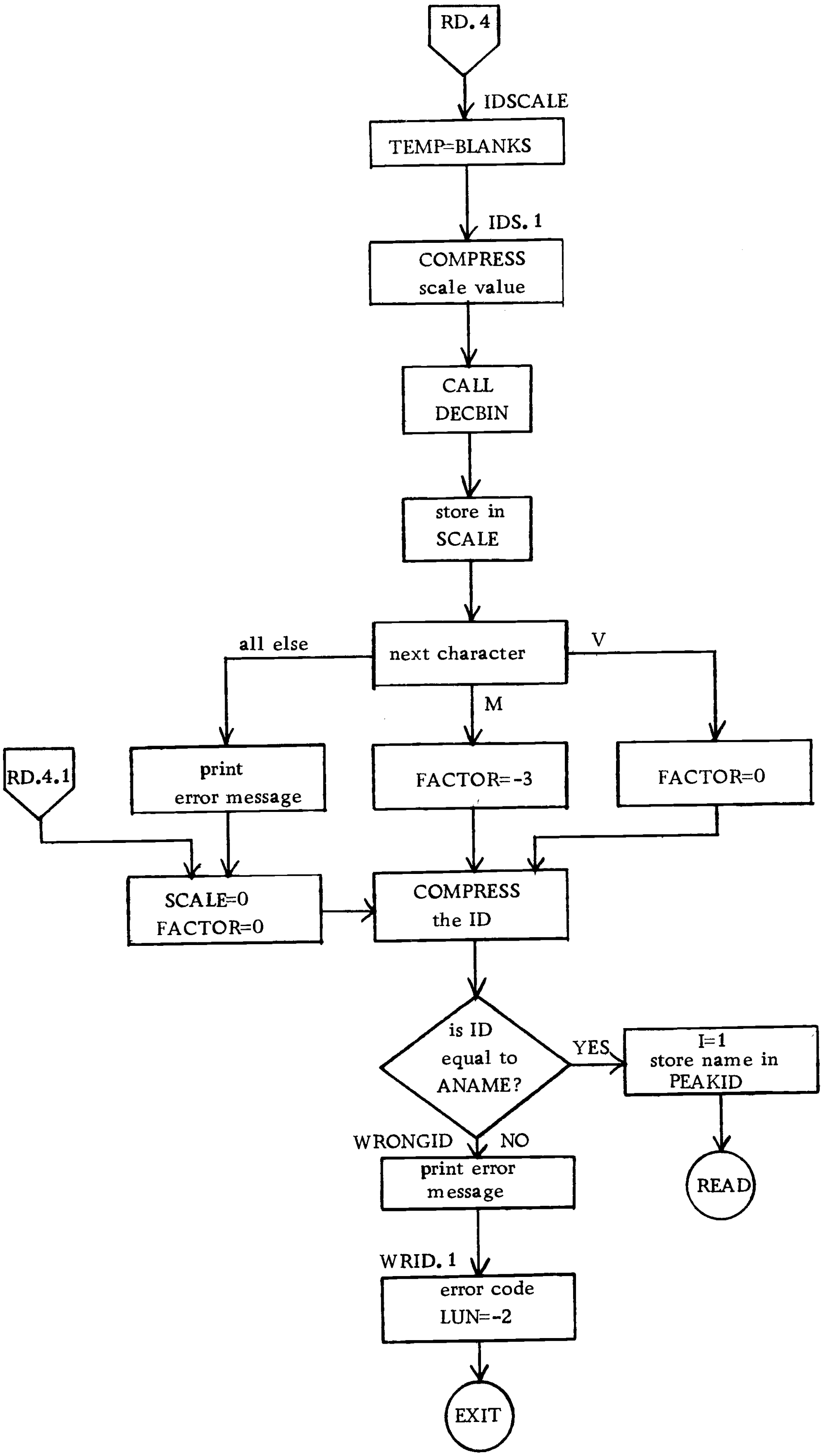

PK. 2
TOP
DY(I) ≥ SLOPE ?
YES
NO
503
UPAGAIN= UPAGAIN+1
DY(I) ≥ SLOPE .AND. DY(I) < 0?
NO
YES
JTOP=JTOP+1
POSITION=DOWN
10
JTOP > TOPMAX ?
NO
YES
6
10
POSITION=START
JTOP=0
JUP=0
10
JTOP=TOPMAX ?
YES
NO
JTOP=TOPMAX-1
UPAGAIN= CHANUP ?
503
NO
YES
ICH=CHANUP+2
I=I-ICH
6


PK. 3
DOWN
|DY(I)| ≥ SLOPE .AND. DY(I) < 0?
NO
YES
JDOWN=JDOWN+1
10
JDOWN ≥ CHANDOWN ?
YES
NO
RIGHT=I
UPAGAIN=0
JTOP=0
JDOWN=0
POSITION=TOP
10
J=0
J=J+1
J > 3 ?
YES
NO
JK=I+J
|DY(I)| ≥ SLOPE ?
NO
YES
POSITION=DOWN
10
find minimum standard deviation for position of the summit
eliminate points that are > 1 σ from mean at the summit
calculate new mean of remaining points. this is value at the summit
set left and right bounds as MEAN(LEFT-3) and MEAN(RIGHT+3)
return LEFTBND, SUMMIT RIGHTBND

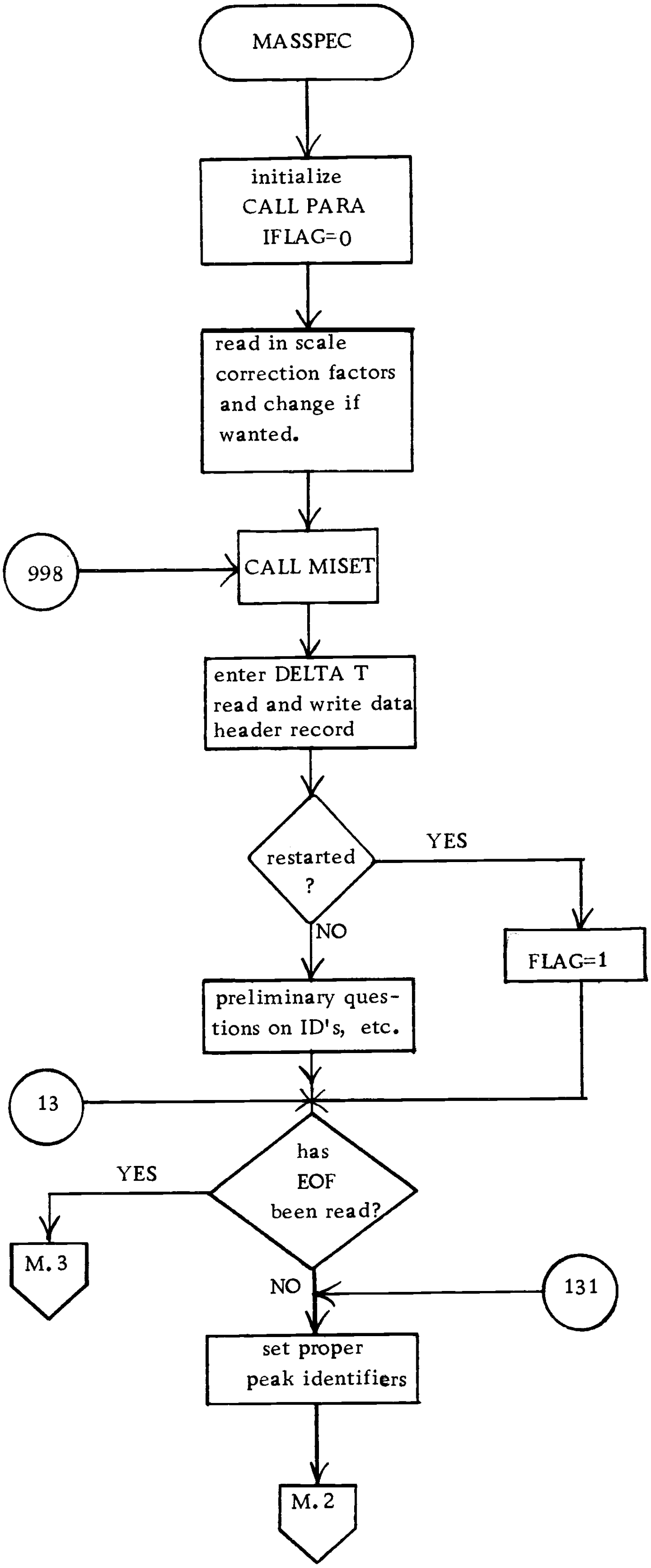

CLEARFLG
RDFLAG=0
EXIT
READATA
initialize and process parameters
COMPRESS ANAME
KOUNT=0
I=0
L= -1
first call ?
NO
YES
READ
CALL CANCEL
CALL READCARD
INDEX=KOUNT
error code
LUN=-1
YES
EOF or EOD ?
error ?
YES
READ
NO
EXIT
LPO
blank line ?
YES
READ
NO
save numbers of characters in EOL
RD. 2

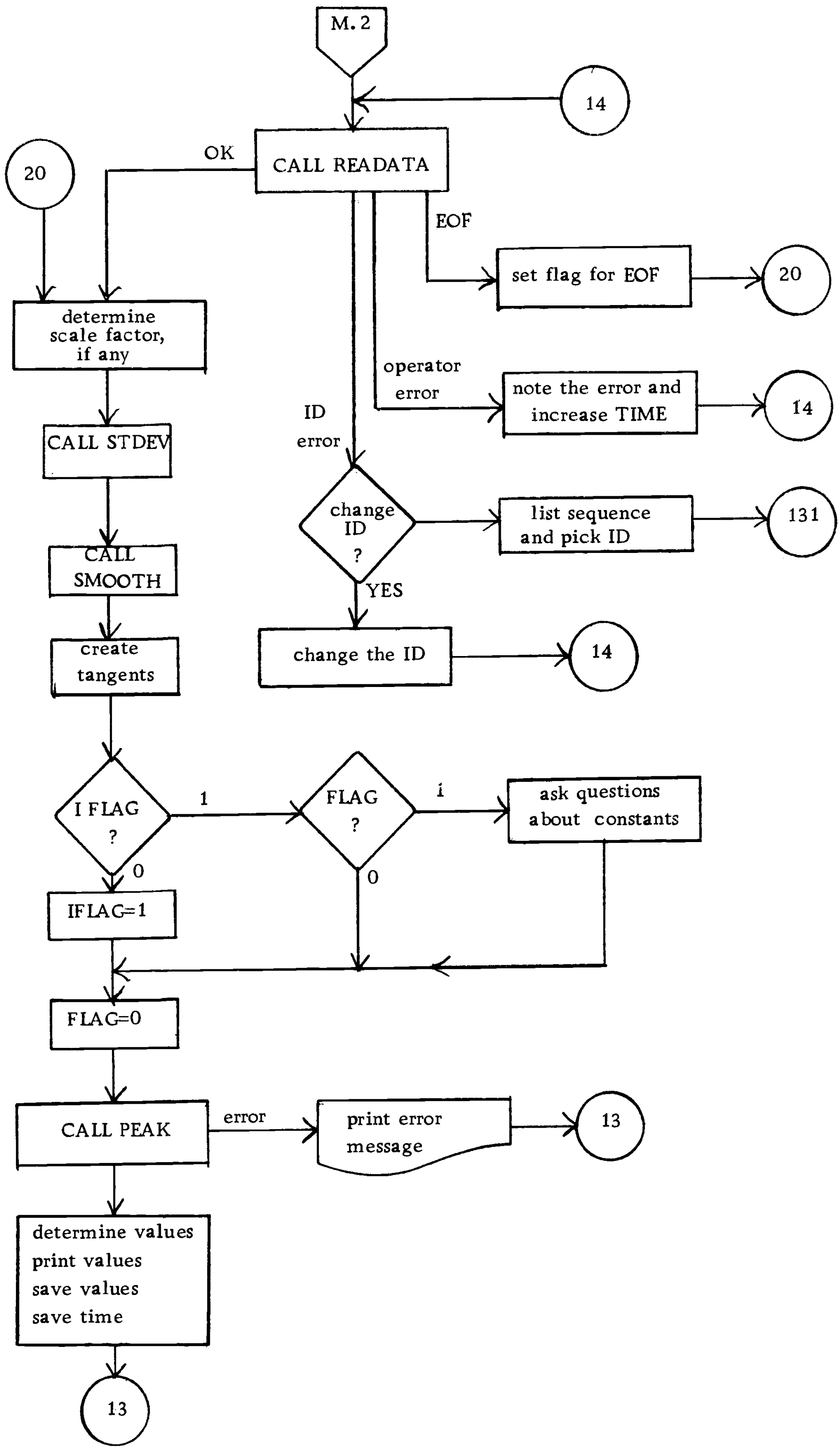

RD. 2
CALL
CANCEL
error ?
YES
increase TIME
error code
LUN=-3
EXIT
NO
less
than 5 words
read
?
YES
RD. 3
RD.2.1
NO
convert
I=0
conv. 1
end
of line?
YES
READ
NO
CALL
DECBIN
valid
number
?
NO
YES
store number
in ARRAY
KOUNT=KOUNT+1

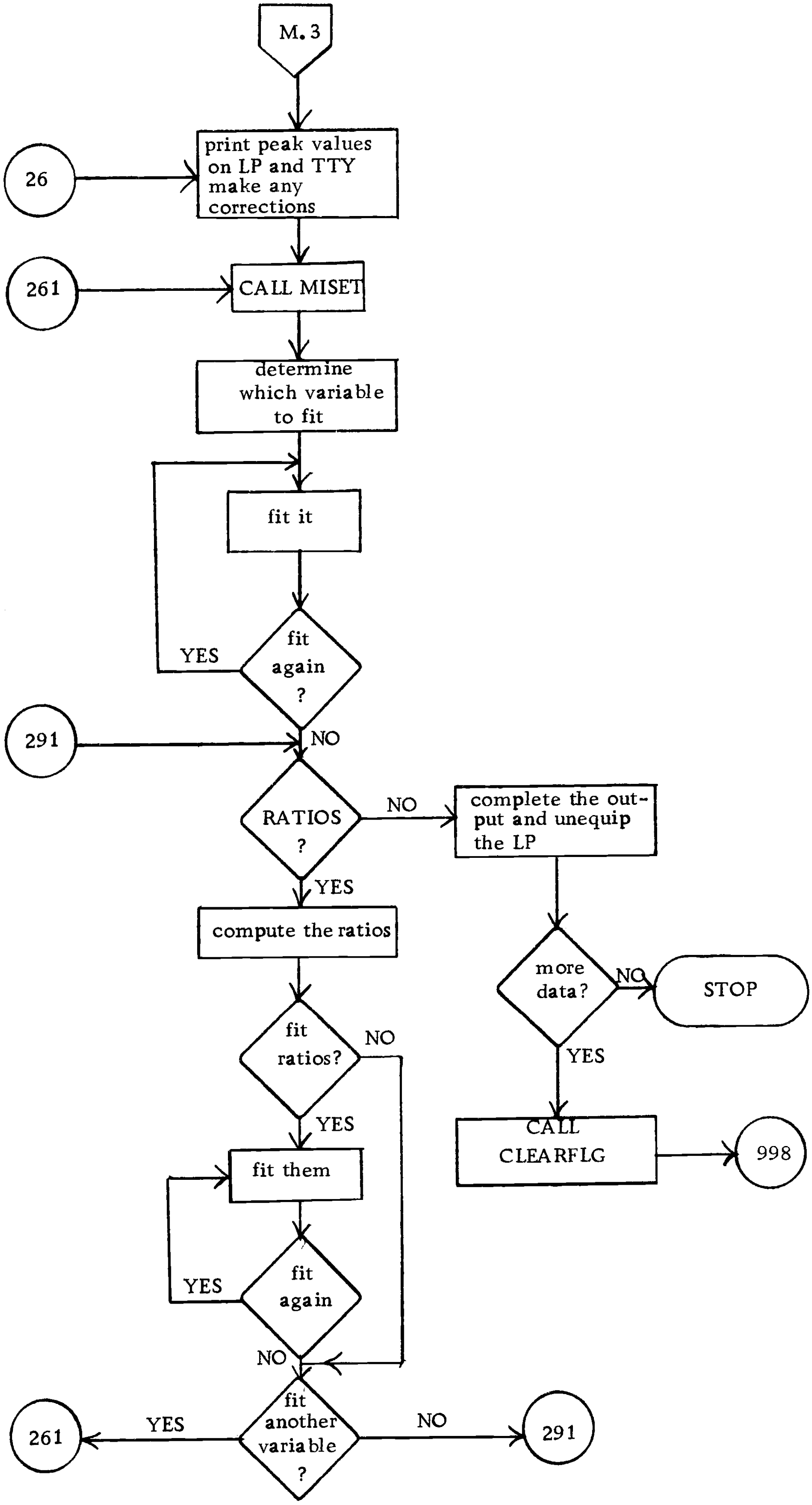

RD. 3
I=1
?
YES
RD. 2.1
NO
ID
look at first
2 words of
CARD
ID. 1
is
it a
number
?
YES
RD. 2.1
NO
ID. 2
is this
a second ID ?
YES
INDEX=
KOUNT
EXIT
NO
is next
character a /
?
YES
RD. 4
NO
save the
ID
IDLOOK
less than
3 words ?
YES
NO
RD. 4. 1



RD.4
IDSCALE
TEMP=BLANKS
IDS.1
COMPRESS scale value
CALL DECBIN
store in SCALE
next character
all else
V
M
RD.4.1
print error message
FACTOR=-3
FACTOR=0
SCALE=0 FACTOR=0
COMPRESS the ID
is ID equal to ANAME?
YES
I=1 store name in PEAKID
READ
WRONGID
NO
print error message
WRID.1
error code LUN=-2
EXIT


MASSPEC
initialize
CALL PARA
IFLAG=0
read in scale correction factors and change if wanted.
998
CALL MISET
enter DELTA T
read and write data header record
restarted ?
YES
NO
FLAG=1
preliminary ques- tions on ID's, etc.
13
has EOF been read?
YES
M. 3
NO
131
set proper peak identifiers
M. 2


M. 2
14
OK
CALL READATA
20
EOF
set flag for EOF
20
determine scale factor, if any
operator error
note the error and increase TIME
14
ID error
CALL STDEV
change ID ?
list sequence and pick ID
131
YES
CALL SMOOTH
create tangents
change the ID
14
I FLAG ?
1
FLAG ?
i
ask questions about constants
0
0
IFLAG=1
FLAG=0
CALL PEAK
error
print error message
13
determine values
print values
save values
save time
13


M. 3
26
print peak values on LP and TTY make any corrections
261
CALL MISET
determine which variable to fit
fit it
YES
fit again ?
291
NO
RATIOS ?
NO
complete the output and unequip the LP
YES
compute the ratios
more data?
NO
STOP
fit ratios?
NO
YES
YES
CALL CLEARFLG
998
fit them
YES
fit again
NO
261
YES
fit another variable ?
NO
291

APPENDIX III

Program Listings

```
      PROGRAM MASSPEC
      COMMON TIME, PKID, SCALE, FACTOR, NPTS, IY(200)
      COMMON/DATA/XLAB(5), FMT(5)
      DATA(XLAB =8H SAVE FO,8HR J. DYM,8HOND, OCE,8HANOGRAPH,8HY X-2135
     1)
      DATA(FMT=8H( / ,    ,8H         ,8H≠ TIME ≠,8H,4X,A8,≠,8H / ≠,A8))
      DIMENSION INDEX(5), VAR(5,100), COMMENT(10), PID(5), IDSEQ(20)
      DIMENSION Y(200), YM(200), SIG5(200), DY(200), PKSCALE(20)
      DIMENSION DTMES(5), ITIME(3), SCCOR(10), FLINE(15)
      DIMENSION NPKS(5), COEFF(10), X1(20), Y1(20), X2(20), Y2(20)
      DIMENSION XFT(20), YFT(20), RATIO(20), COEF(10), IBLNKS(5)
      DIMENSION YFIT(20), SIGMAA(10), RFIT(20), SIGA(10)
      EQUIVALENCE (DTMES(4),ITIME(1)), (FLINE,Y), (YM,IBLNKS)
      EQUIVALENCE (BLANKS,IPLANK)
      INTEGER TIME, SCALE, FACTOR, DELT, RIGHT, PEAKTOP, FLAG
      INTEGER CHANUP, TOPMAX, CHANDOWN
      REAL LEFTBND
C***********************************************************************
C
C         INITIALIZE
C
C***********************************************************************
      CALL PARA(L)
      IZ = 0
      ZERO = 0.
      IFLAG = IZ
      BLANKS = 8H
      OMIT = 8HOMITTED
      DO 200 I=1,5
  200 DTMES(I) = BLANKS
      DTMES(1) = 8H DATE PR
      DTMES(2) = 8HOCESSED
      CALL DATE(DTMES(3))
      CALL ARMYTIME(ITIME(2))
      WRITE(61,201)DTMES
  201 FORMAT(≠0HI THERE ≠,/,≠ LETS CALCULATE MASS SPECTRA≠,/,5A8)
      LUN = 52
      IF(L .LT. IZ)GO TO 204
      DO 203 I =1,10
      IF(EOF(LUN) .OR. EOD(LUN))GO TO 2033
      READ(LUN,2031)SCCOR(I)
      IF(EOF(LUN) .OR. EOD(LUN))GO TO 2033
  203 CONTINUE
 2031 FORMAT(F8.5)
      IF(L)205, 997
 2033 WRITE(61,2034)
 2034 FORMAT(≠ CONSTANT FILE IS NOT ALL THERE.≠)
      IF(L)205,204
  204 SCCOR(1) =.001     $    SCCOR(6) =  .300
      SCCOR(2) =.003     $    SCCOR(7) = 1.000
      SCCOR(3) =.010     $    SCCOR(8) = 3.000
      SCCOR(4) =.030     $    SCCOR(9) = 10.000
      SCCOR(5) =.100     $    SCCOR(10) = 30.000
      GO TO 997
  205 GO TO (208,2051)TELIO(8HDO YOU W,8HISH TO E,8HNTER ALL,8H NEW COR
     1                ,8HRECTION ,8HFACTORS ,8H$ 000000)
 2051 GO TO (206,2062)TELIO(8HDO YOU W,8HISH TO S,8HEE THE C,
     1                8HCRRECTIO,8HN FACTOR,8HS $ 0000)
  206 WRITE(61,2061)((I,SCCOR(I)),I=1,10)
 2061 FORMAT(X,I2,2X,≠1MV    =≠,F8.5,/,X,I2,2X,≠3MV    =≠,F8.5,/,
```



```
     1          X,I2,2X,≠10MV  =≠,F8.5,/,X,I2,2X,≠30MV  =≠,F8.5,/,
     2          X,I2,2X,≠100MV =≠,F8.5,/,X,I2,2X,≠300MV =≠,F8.5,/,
     3          X,I2,2X,≠1V    =≠,F8.5,/,X,I2,2X,≠3V    =≠,F8.5,/,
     4          X,I2,2X,≠10V   =≠,F8.5,/,X,I2,2X,≠30V   =≠,F8.5)
 2062 GO TO (209,207)TELIO(8HARE THEY,8H ALL OK ,8H$ 000000)
  207 IND = TELIO(8HENTER IN,8HDEX OF F,8HACTOR YO,8HU WISH T,
     1                8HO CHANGE,8H $ 00000)
      IF(IND .GT. 10)GO TO 207
      SCCOR(IND) = TELIO(8HNEW FACT,8HOR = 000)
      GO TO 2062
  208 SCCOR(1) = TELIO(8H  1MV = )
      SCCOR(2) = TELIO(8H  3MV = )
      SCCOR(3) = TELIO(8H 10MV = )
      SCCOR(4) = TELIO(8H 30MV = )
      SCCOR(5) = TELIO(8H100MV = )
      SCCOR(6) = TELIO(8H300MV = )
      SCCOR(7) = TELIO(8H   1V = )
      SCCOR(8) = TELIO(8H   3V = )
      SCCOR(9) = TELIO(8H  10V = )
      SCCOR(10) = TELIO(8H  30V = )
      GO TO 2062
  209 REWIND LUN
      WRITE(LUN,2031)(SCCOR(I),I=1,10)
      ENDFILE LUN
  997 CALL UNEQUIP(LUN)
  998 CALL MISET
      GO TO (500,501)TELIO(8HHAVE YOU,8H STARTED,8H THE CAL,
     S                       8HCULATION,8HS FOR TH,8HIS DATA ,8HSET $ 00)
  500 FLAG = 1
      GO TO 9983
  501 FLAG =IZ
      GO TO(9981,9982)TELIO(8HIS YOUR ,8HDATA FIL,8HE EQUIPP,8HED $ 000)
 9981 LUN = TELIO(8HDATA LUN,8H = 00000)
      GO TO 9983
 9982 WRITE(61,9970)
 9970 FORMAT(≠ ENTER FILE NAME≠)
      READ(60,100)COMMENT
      CALL CANCEL(COMMENT)
      CALL UNEQUIP(51)
      CALL EQUIP(51,COMMENT(1))
      LUN = 51
 9983 ILUN = LUN
      REWIND LUN
      DELT = 5
      TIME = TELIO(8HENTER DE,8HLTA T IN,8H SECONDS,8H $ 00000)
      DYSHIFT = 1.0E-4
      LUNEOF = IZ
    1 READ (LUN, 100) COMMENT
  100 FORMAT( 10A8)
      IF( EOF( LUN ))GO TO 9999
      IF ( COMMENT(2) .EQ. 8H COSY/  ) 1, 2
    2 DO 3 I=1, 10
      IF ( COMMENT(I) .NE. BLANKS ) GO TO 4
    3 CONTINUE
      GO TO 1
    4 CALL CANCEL( COMMENT )
      WRITE(61,116)
      WRITE( 61, 101 ) COMMENT
      WRITE(61,116)
      DO 401 I=1,5
```

```
      INDEX(I) = 1
      NPKS(I) = IZ
      DO 401 J = 1,100
  401 VAR(I,J) = ZERO
      CALL CLEARFLG
      IF(FLAG)GO TO 13
  101 FORMAT(≠ ≠, 10A8)
C*****************************************************************
C
C        INITIALIZE  ID≠S ACCEPTED FOR NORMAL USE.
C
C*****************************************************************
      DO 4001 I=1,20
 4001 PKSCALE(I) = ZERO
      SCALE = FACTOR = IZ
      NID =3 $IDLIMITS = 6
      PID(1) = 8HA40         $PID(2) = 8HA38        $PID(3) = 8HA36
      IDSEQ(1)=IDSEQ(4)=2$IDSEQ(2)=IDSEQ(3)=1$IDSEQ(5)=IDSEQ(6)=3
      GO TO (5,6) TELIO(8HARE A40 ,8H, A38 , ,8HA36  OK ,8HFOR PEAK,
     X                  8H NAMES $)
    5 GO TO (13,8) TELIO(8HIS THE S,8HEQUENCE ,8H: A38, A,8H40, A40,,
     X         8H A38, A3,8H6, A36 O,8HK $00000)
    6 NID = TELIO(8HNUMBER O,8HF PEAK N,8HAMES = 0)
      WRITE(61,102)
  102 FORMAT(≠0ENTER PEAK NAMES, ONE PER LINE.≠)
  103 FORMAT(A8)
      DO 7 I=1,NID
      READ(60,103) PID(I)
    7 CALL COMPRESS(PID(I))
    8 WRITE(61,104)
  104 FORMAT(≠0ENTER THE SEQUENCE IN WHICH THE PEAKS SHOULD OCCUR.≠)
      DO 9 I=1,NID
    9 WRITE(61,105)I, PID(I)
  105 FORMAT(≠ ≠, I2, ≠ = ≠, A8)
      WRITE(61,106)
  106 FORMAT(≠ AN EXAMPLE IS ≠,/,≠   1 2 3 3 2 1≠)
   10 DO 11 I=1,20
      IDSEQ(I) = FFIN(60)
      IF( EOF(60) ) GO TO 12
   11 CONTINUE
   12 I = I- 1
      IDLIMITS = I
      WRITE(61,107)( IDSEQ(I), I=1, IDLIMITS )
  107 FORMAT(X, 20I3)
      GO TO (13,10) TELIO(8HARE THEY,8H ALL OK$)
C*****************************************************************
C
C          SET UP THE MAIN LOOP
C
C*****************************************************************
   13 DO 1000 KK=1,IDLIMITS
      IF( LUNEOF ) GO TO 26
  131 IDUM = IDSEQ(KK)
      PEAKID = PID(IDUM)
   14 CALL READATA( LUN, PEAKID )
C*****************************************************************
C
C         CHECK FOR ERRORS
C
C*****************************************************************
```



```
      IF ( LUN .LT. IZ ) 15, 20
   15 LUN = LUN + 4
      GO TO (19, 17, 16) LUN
C*****************************************************************
C
C                      16  IS EOF OR EOD ON DATA LUN
C                      17  IS ID ERROR
C                      19  IS OPERATOR ERROR SIGNAL  !!!!!!!
C
C*****************************************************************
   16 LUNEOF = 1
      LUN = ILUN
      GO TO 20
   17 LUN = ILUN
      GO TO (181,182)TELIO(8HDO YOU W,8HANT TO C,8HHANGE TH,
     S                   8HE PEAK I,8HD $ 0000)
  181 WRITE(61,108)
  108 FORMAT(≠ ENTER CORRECT PEAK NAME≠)
      READ(60,103) PEAKID
      CALL COMPRESS(PEAKID)
      GO TO 14
  182 DO 183 IK=1,IDLIMITS
      IJ = IDSEQ(IK)
  183 WRITE(61,114)IK, PID(IJ)
  114 FORMAT(≠ ≠,I3,≠ : ≠,A8)
      KK = TELIO(8HWHERE SH,8HOULD WE ,8HBE IN TH,8HE SEQUEN,8HCE $ 000)
      GO TO 131
   19 WRITE(61,109)
  109 FORMAT(≠ OPERATOR ERROR NOTED≠)
      LUN = ILUN
      TIME = TIME + DELT + NPTS
      GO TO 14
C*****************************************************************
C
C                     PEAK IS READ IN AND OK SO FAR
C           SAVE SCALE FACTOR AND INCREMENT  TOTAL TIME HERE
C
C*****************************************************************
   20 DO 21 I=1,NPTS
   21 Y(I) = IY(I)
      IF( .NOT. SCALE) GO TO 22
      XFCT = 1.0
      IF(FACTOR .EQ. -3)XFCT = 1.E-3
      PKSCALE(IDUM) = SCALE * XFCT
      IF(PKSCALE(IDUM) .EQ. 0.001)PKSCALE(IDUM) = SCCOR(1)
      IF(PKSCALE(IDUM) .EQ. 0.003)PKSCALE(IDUM) = SCCOR(2)
      IF(PKSCALE(IDUM) .EQ. 0.010)PKSCALE(IDUM) = SCCOR(3)
      IF(PKSCALE(IDUM) .EQ. 0.030)PKSCALE(IDUM) = SCCOR(4)
      IF(PKSCALE(IDUM) .EQ. 0.100)PKSCALE(IDUM) = SCCOR(5)
      IF(PKSCALE(IDUM) .EQ. 0.300)PKSCALE(IDUM) = SCCOR(6)
      IF(PKSCALE(IDUM) .EQ. 1.000)PKSCALE(IDUM) = SCCOR(7)
      IF(PKSCALE(IDUM) .EQ. 3.000)PKSCALE(IDUM) = SCCOR(8)
      IF(PKSCALE(IDUM) .EQ.10.000)PKSCALE(IDUM) = SCCOR(9)
      IF(PKSCALE(IDUM) .EQ.30.000)PKSCALE(IDUM) = SCCOR(10)
   22 TIME = TIME + DELT + NPTS
C*****************************************************************
C
C          NOW TAKE THE MOVING STANDARD DEVIATIONS OF THE DATA
C
C*****************************************************************
```

```
 C
       CALL STDEV( Y, YM, SIG5 )
 C
 C*******************************************************************
 C
 C          SMOOTH THE DATA NOW AND RETURN WITH FIRST DERIVATIVE
 C
 C*******************************************************************
       CALL SMOOTH ( Y, DY )
 C      CHANGE DY TO TANGENTS
       DO 23 I=1,NPTS
    23 DY(I) = DY(I) * DYSHIFT
 C****  IFLAG IS 0 ON FIRST RUN
       IF( IFLAG ) 232, 231
   231 IFLAG = 1
       GO TO 233
   232 IF( FLAG ) 233, 2399
   233 GO TO (235,234) TELIO(8HDO YOU W,8HISH TO E,8HNTER CON,8HSTANTS $
      *)
   234 GO TO (236,238)TELIO(8HDO YOU W,8HISH TO L,8HIST CONS,8HTANTS  $)
   235 CHANUP=TELIO(8HMINIMUM ,8HCHANNELS,8H UP    = )
       TOPMAX=TELIO(8HMAX CHAN,8HNELS ON ,8HTOP    = )
       CHANDOWN=TELIO(8HMINIMUM ,8HCHANNELS,8H DOWN =  )
       GO TO 238
   236 WRITE(61,237)CHANUP,TOPMAX,CHANDOWN
   237 FORMAT(≠0MIN CHANNELS UP      = ≠,I4,/,
      *         ≠ MAX CHANNELS ON TOP = ≠,I4,/,
      *         ≠ MIN CHANNELS DOWN   = ≠,I4)
   238 GO TO(2399,235)TELIO(8HARE THEY,8H ALL OK ,8H $ 00000)
  2399 FLAG = IZ
 C
 C*******************************************************************
 C
 C                   NOW CALL THE PEAK SUBROUTINE
 C      .
 C*******************************************************************
       CALL PEAK(DY, SIG5, YM, LEFTBND, LEFT, RIGHTBND, RIGHT, SUMMIT,
      A  PEAKTOP, CHANUP, TOPMAX, CHANDOWN)
       IF( LEFT + RIGHT ) 25,24
 C    ERROR IF LEFT = RIGHT = 0
    24 WRITE(61,110)PKID
   110 FORMAT(≠ ERROR IN PEAK    ≠, A8)
       GO TO 1000
 C*******************************************************************
 C
 C                   DETERMINE VALUES FOR THIS PEAK
 C
 C*******************************************************************
    25 XIR = RIGHT + 3
       XIL = LEFT - 3
       BASELINE = ((RIGHTBND - LEFTBND)/(XIR - XIL)) *
      3          (PEAKTOP - XIL) + LEFTBND
 C*******************************************************************
 C
 C                   VALUE FOR THIS PEAK
 C
 C*******************************************************************
       VALUE = SUMMIT - BASELINE
       XSC = PKSCALE(IDUM)
       IF( .NOT. XSC) XSC = 1.
```



```
 C  SCVAL IS VALUE IN VOLTS
       SCVAL = VALUE * XSC * 1.E-6
       PKTIME = TIME - NPTS + PEAKTOP
       WRITE(61,111)PKID, PKTIME, VALUE, PKSCALE(IDUM), SCVAL
   111 FORMAT(≠ ≠, A8, F5.0, F10.0, 2X, F6.3, 2X, F13.5)
 C*******************************************************************
 C
 C                   NOW STORE THE VALUE AND ITS TIME
 C
 C*******************************************************************
       INV = INDEX(IDUM)
       VAR(IDUM,INV) = PKTIME
       VAR(IDUM,INV+1) = SCVAL
       INDEX(IDUM) = INDEX(IDUM) + 2
  1000 CONTINUE
       GO TO 13
 C*******************************************************************
 C
 C     NOW ALL THE PEAKS ARE CALCULATED
 C     LETS PRINT THEM OUT
 C
 C*******************************************************************
 C****   EQUIP  LP AND LABEL IT
    26 CALL UNEQUIP(52)
       CALL EQUIP(52,8HLP        )
       WRITE(52,2601)XLAB
  2601 FORMAT(5A8)
       CALL ARMYTIME(ITIME(2))
       WRITE(52,2602)DTMES
  2602 FORMAT(≠1≠,5A8)
       WRITE(52,2591)
  2591 FORMAT(≠0*****************************************************≠
      1,≠*******************************************************≠
      2,≠*********************≠)
       WRITE(52,101)COMMENT
       WRITE(52,2591)
       DO 2592 I=1,NID
  2592 IBLNKS(I) =IBLANK
       WRITE(52,2603)((IBLNKS(I),PID(I)),I=1,NID)
  2603 FORMAT(≠0≠,3X,5(X,A4,≠TIME≠,7X,A8,3X))
 C****   PRINT PEAK VALUES ON THE LP
       L = IZ
       DO 263 I=1,100,2
       DO 2604 II=1,15
  2604 PLINE(II)=BLANKS
       K = 1
       JK = IZ
       DO 262 J =1,NID
       IF(VAR(J,I) .EQ. ZERO)GO TO 261
       ENCODE(24,2621,PLINE(K))VAR(J,I), VAR(J,I+1)
  2621 FORMAT(5X, F4.0, 2X, F13.8)
       GO TO 2613
   261 JK = JK + 1
       IF(JK .EQ. NID) GO TO 264
  2613 K = K + 3
   262 CONTINUE
       L = L + 1
       WRITE(52,2622) L,PLINE
  2622 FORMAT(X,I2,4(3A8,3X),3A8)
   263 CONTINUE
```

```
  264 WRITE(52,2591)
      WRITE(61,116)
      DO 28 J=1,NID
      M = IZ
  269 WRITE(61,112) PIO(J)
  112 FORMAT(≠0≠,6X,≠TIME≠,7X,A8)
      K =  IZ
      DO 27 I=1,100,2
      K = K + 1
      IF(VAR(J,I) .EQ. ZERO) GO TO 271
      IF (M) GO TO 2701
      NPKS(J) = NPKS(J) + 1
 2701 IF( VAR(J,I+1) .NE. ZERO) GO TO 2702
      WRITE(61,1131)K,VAR(J,I),CMIT
 1131 FORMAT(≠ ≠,I3,2X,F5.0,5X,A8)
      GO TO 27
 2702 WRITE(61,113)K, VAR(J,I), VAR(J,I+1)
  27  CONTINUE
  113 FORMAT(≠ ≠,I3,2X,F5.0,2X,F13.8)
  271 GO TO(28,272)TELIO(8HARE THEY,8H ALL OK ,8H$ 000000)
  272 GO TO (273,274)TELIO(8HDO YOU W,8HANT TO O,8HMIT A PO,8HINT $ 00)
  273 IND2 = 2 * TELIO(8HENTER IN,8HDEX OF P,8HEAK VALU,
    1              8HE YOU WA,8HNT TO OM,8HIT : 000)
      VAR(J,IND2) = ZERO
      GO TO 275
  274 IND1 = 2 * TELIO(8HENTER IN,8HDEX OF P,8HEAK VALU,8HE YOU WA,
    X              8HNT TO CH,8HANGE : 0)
      VAR(J,IND1) = TELIO(8HVALUE = )
  275 M = 1
      GO TO(269,271)TELIO(8HDO YOU W,8HANT TO L,8HIST THEM,8H $ 00000)
  28  CONTINUE
C*******************************************************************
C
C         LETS DO THE RATIOS NOW
C
C*******************************************************************
      WRITE(61,116)
      WRITE(61,300)
  300 FORMAT(≠0ANSWER THE QUESTIONS BELOW WITH THESE VALUES≠)
      DO 281 I=1,NID
  281 WRITE(61,105)I, PID(I)
      CALL MISET
      CALL UNEQUIP(53)
      CALL UNEQUIP(54)
      CALL EQUIP(53,8HFILE      )
      CALL EQUIP(54,8HFILE      )
      IFILE = IZ
 2811 IVAR = TELIO(8HWHICH VA,8HRIABLE D,8HO YOU WA,8HNT TO FI,
    X              8HT $ 0000)
      IFIT = IZ
      K = NPKS(IVAR)
  282 IDEG = TELIO(8HDEGREE O,8HF POLYNO,8HMIAL = 0)
      IF(IDEG .GE. K)283, 284
  283 WRITE(61,301)
  301 FORMAT(≠0DEGREE TOO LARGE≠)
      GO TO 282
  284 NTERMS = IDEG +1
      IF(IFIT) GO TO 287
      KK = K + K
      I = IZ
```

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      DO 286 J=1,KK,2
      IF (VAR(IVAR,J+1) .EQ. ZERO )285, 2851
  285 K = K - 1
      GO TO 286
 2851 I = I + 1
      XFT(I) = VAR(IVAR,J)
      YFT(I) = VAR(IVAR,J+1)
  286 CONTINUE
      IFIT = 1
C*******************************************************************
C
C         POLYNOMIAL FIT
C
C*******************************************************************
  287 CALL POLFIT(XFT, YFT, K, IDEG, IZ, YFIT, COEFF, SIGMAA, CHISQR)
      WRITE(61,302)
  302 FORMAT(/,≠ COEFFICIENTS          STD. ERROR≠)
      WRITE(61,303)(COEFF(I), SIGMAA(I), I=1,NTERMS)
  303 FORMAT(≠ ≠,E12.5,6X,E12.5)
      WRITE(61,306) CHISQR
      CALL STAT(YFT, K, SIG, YMEAN)
      WRITE(61,304)YMEAN, SIG
  304 FORMAT(≠ MEAN≠,15X,≠= ≠,E12.5,/,≠ STANDARD DEVIATION = ≠,E12.5)
  306 FORMAT(/,≠ CHI SQUARE           = ≠,E12.5)
      GO TO(282,291)TELIO(8HDO YOU W,8HISH TO F,8HIT AGAIN,8H $ 00000)
  291 GO TO (2911,1999)TELIO(8HDO YOU W,8HANT RATI,8HOS $ 000)
 2911 IF(IFILE .EQ. 54)8901, 8902
 8901 CALL WRITEIO(52,53,54)
      WRITE(52,101)DTMES
      WRITE(52,2591)
      WRITE(52,101)COMMENT
      WRITE(52,2591)
      IFILE = 53
      GO TO 8903
 8902 IF(IFILE .EQ. 53)IFILE = 54
      IF(IFILE .EQ. IZ) IFILE = 53
 8903 WRITE(61,3061) PID(IVAR), PID(IVAR)
 3061 FORMAT(≠0RATIO WILL BE  1: ≠,A8,≠ / X  OR  2: X /≠,A8)
      IR = TELIO(8HANSWER 1,8H OR 2 : )
29111 IXR = TELIO(8H X = 000)
      IF(IXR .GT. NID) 29112,29113
29112 WRITE(61,3062)
 3062 FORMAT(≠ X IS TOO BIG...SEE VALUES FOR PEAK NAMES.≠)
      GO TO 29111
29113 FMT(2) = 8H 17X,
      IFCTR = IZ
      XFCTR = 1.
      GO TO (2912,2913)TELIO(8HSCALE FA,8HCTOR $ 0)
 2912 XFCTR = TELIO(8HFACTOR =)
      IFCTR = 1
      FMT(2) = 8H 8X,
 2913 CONTINUE
      WRITE(61,116)
      GO TO(292,293)IR
  292 WRITE(61,FMT)PID(IVAR), PID(IXR)
      WRITE(IFILE,FMT)PID(IVAR), PID(IXR)
      GO TO 294
  293 WRITE(61,FMT) PID(IXR), PID(IVAR)
      WRITE(IFILE,FMT)PID(IXR), PID(IVAR)
C
```

```
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  C*********************************************************************
  C
  C        COMPUTE THE RATIOS
  C
  C*********************************************************************
    294 K = NPKS(IXR)
        KK = K + K
        J = IZ
        DO 295 I =1,KK,2
        IF( VAR(IXR,I+1) .EQ. ZERO )2941, 2942
   2941 K = K - 1
        GO TO 295
   2942 J = J + 1
        X1(J) = VAR(IXR,I)
        Y1(J) = VAR(IXR,I+1)
    295 CONTINUE
        DO 296 I=1,K
        Y2(I) = COEFF(1)
        DO 2952 J=2,NTERMS
        L = J - 1
   2952 Y2(I) = Y2(I) + COEFF(J)*(X1(I) ** L)
        GO TO(2953,2954)IR
   2953 RATIO(I) = Y2(I) / Y1(I)
        GO TO 2955
   2954 RATIO(I) = Y1(I) / Y2(I)
   2955 IF( IFCTR ) 2956, 2957
   2956 FRATIO = RATIO(I) * XFCTR
        WRITE(61,309) I, X1(I), RATIO(I), FRATIO
        WRITE(IFILE,309)I, X1(I), RATIO(I), FRATIO
        RATIO(I) = FRATIO
    309 FORMAT(≠ ≠,3X,I2,2X,F6.0,2(4X,E12.5))
        GO TO 296
   2957 WRITE(61,308) I, X1(I), RATIO(I)
        WRITE(IFILE,308)I, X1(I), PATIO(I)
    296 CONTINUE
        WRITE(61,116)
  C*****************************************************************
  C
  C        FIT THE RATIOS AND EXTRAPOLATE TO T 0
  C
  C*****************************************************************
        GO TO(399,390)TELIO(8HARE THEY,8H ALL OK ,8H$ 000000)
    390 INDRAT = TELIO(8HENTER IN,8HDEX OF R,8HATIO YOU,8H WANT TO,
      1                 8H OMIT : )
        RATIO(INDRAT) = ZERO
        GO TO (391,390)TELIO(8HARE THEY,8H ALL OK ,8H$ 000000)
    391 J = IZ
        DO 392 I =1,K
        IF(RATIO(I) .EQ.ZERO )GO TO 392
        J = J + 1
        RFIT(J) = RATIO(I)
        Y1(J) = X1(I)
    392 CONTINUE
        K = J
        DO 393 I =1,K
        RATIO(I) = RFIT(I)
    393 X1(I) = Y1(I)
    399 GO TO(400,2981)TELIO(8HDO YOU W,8HANT TO F,8HIT THE R,8HATIOS $ )
    400 IDEG = TELIO(8HDEGREE O,8HF POLYNO,8HMIAL = ()
        WRITE(IFILE,4010)IDEG
```

```
OS3 FORTRAN  VERSION 3.0  MASSPEC   11/23/71  1349
   4010 FORMAT(/,≠ DEGREE OF POLYNOMIAL = ≠,I2)
        NTM = IDEG + 1
        IF(NTM .GE. K)411,402
    411 WRITE(61,301)
        GO TO 400
    402 CALL POLFIT(X1, RATIO, K, IDEG, 0, RFIT, COEF, SIGA, CHISQR)
        WRITE(61,302)
        WRITE(IFILE,302)
        WRITE(61,303)(COEF(I), SIGA(I),I=1,NTM)
        WRITE(IFILE,303)(COEF(I), SIGA(I), I=1,NTM)
        WRITE(IFILE,306)CHISQR
        WRITE(61,306)CHISQR
        CALL STAT(RATIO, K, SIG, YMEAN)
        STERR = SIG / SQRT(FLOAT(K))
        WRITE(61,304)YMEAN, SIG
        WRITE(61,310)STERR
        WRITE(IFILE,304)YMEAN, SIG
        WRITE(IFILE,310)STERR
    310 FORMAT(≠ STD. ERROR OF MEAN = ≠,E12.5)
        GO TO (400,298)TELIO(8HDO YOU W,8HISH TO F,8HIT AGAIN,8H $ 00000)
    308 FORMAT(≠ ≠,11X,I2,2X,F6.0,4X,E12.5)
    298 ENDFILE IFILE
        GO TO 297
   2981 REWIND IFILE
        IF(IFILE .EQ. 53) IFILE = IZ
        IF(IFILE .EQ. 54) IFILE = 53
    297 GO TO(2811,291)TELIO(8HDO YOU W,8HISH TO F,8HIT ANOTH,8HER VARIA,
       X            8HBLE $ 00)
   1999 CALL WRITEIO(52,53,54)
        CALL UNEQUIP(52)
        GO TO (998,9999)TELIO(8HDO YOU H,8HAVE MORE,8H DATA $ )
    116 FORMAT(≠0****************************************************≠)
   9999 CALL UNEQUIP(51)
        CALL UNEQUIP(52)
        CALL UNEQUIP(53)
        CALL UNEQUIP(54)
        WRITE(61,115)
    115 FORMAT(≠0END OF PROGRAM EXECUTION.≠)
        CALL SBJP
        END
```

```
OS3 FORTRAN  VERSION 3.0              11/23/71  1136
        SUBROUTINE STDEV(Y,YM,SIG5)
  C*****  THIS SUBROUTINE DETERMINES 5 POINT MOVING
  C*****  MEANS AND STANDARD DEVIATIONS.
        DIMENSION Y(1),YSS(200),YS(200),YMS(200),YM(1),SIG5(1)
        COMMON ITIME,PEAKID,SCALE,L,IY(200)
  C*****  INITIALIZE AND COMPUTE SQUARES
        DO 2 I=1,L
        SIG5(I)=YM(I)=0.
      2 YS(I)=Y(I)*Y(I)
  C*****  STANDARD DEVIATIONS AND MEANS (5 POINTS)
        M=L-2
        DO 3 I=3,M
        YM(I)=(Y(I-2)+Y(I-1)+Y(I)+Y(I+1)+Y(I+2))/5.
        YMS(I)=YM(I)*YM(I)
        YSS(I)=(YS(I-2)+YS(I-1)+YS(I)+YS(I+1)+YS(I+2))/5.
      3 SIG5(I)=SQRTF(YSS(I)-YMS(I))
        RETURN
        END
```

```
OS3 FORTRAN  VERSION 3.0            11/23/71  1130
      SUBROUTINE PEAK(DY,SIGMA,MEAN,LEFTBND,LEFT,RIGHTBND,RIGHT,SUMMIT,
     *PEAKTOP, CHANUP, TOPMAX, CHANDOWN)
      COMMON TIME,PEAKID,SCALE,L,IY(200)
      DIMENSION DY(1),SIGMA(1),MEAN(1)
      INTEGER TIME, START, UP, TOP, DOWN, POSITION, UPAGAIN
      INTEGER PEAKTOP, TOPMAX, CHANUP, CHANDOWN, RIGHT
      REAL MEAN,LEFTBND
C***********************************************************************
C         DY IS SMOOTHED FIRST DERIVATIVE
C         SIGMA IS 5 POINT MOVING STANDARD DEVIATION
C         LEFTBND IS VALUE AT LEFT TAIL
C         LEFT IS INDEX OF LEFTBND
C         RIGHTBND IS VALUE AT RIGHT TAIL
C         RIGHT IS INDEX OF RIGHTBND
C         SUMMIT IS VALUE AT SUMMIT OF PEAK
C         PEAKTOP IS INDEX AT SUMMIT
C         CHANUP IS MINIMUM CHANNELS UP
C         TOPMAX IS MAXIMUM CHANNELS ON TOP
C         CHANDOWN IS MINIMUM CHANNELS DOWN
C***********************************************************************
      THETA = 20.
      SLOPE=TANF(THETA/57.29577951)
C*******  POSITION OF SCAN
      START = 1
      UP    = 2
      TOP   = 3
      DOWN  = 4
C******  INITIALIZE
      JUP = JTOP = JDOWN = 0
      K=L-3
      POSITION = START
      DO 10 I=2,K
      GO TO (1,3,5,7) POSITION
C*****  LOOK FOR BEGINNING OF UPHILL SCAN
    1 IF(DY(I) .GE. SLOPE)2,10
    2 LEFT = I
      POSITION = UP
      GO TO 10
C******  LOOK FOR TOP ON UPHILL SCAN
    3 IF(DY(I) .GE. SLOPE)4,41
    4 JUP = JUP + 1
      GO TO 10
C********  IS LEFT SLOPE LONG ENOUGH
C****  ELIMINATE SMALL PEAKS
   41 IF (JUP .GE. CHANUP )42,43
   42 POSITION = TOP
      UPAGAIN = 0
      GO TO 10
   43 POSITION = START
      JUP = 0
      GO TO 10
    5 IF( DY(I) .GE. SLOPE )501, 503
C****   OOPS WE ARE STARTING UP AGAIN
  501 UPAGAIN = UPAGAIN + 1
      IF( JTOP .EQ. TOPMAX )JTOP = TOPMAX-1
      IF( UPAGAIN .EQ. CHANUP )502, 503
  502 ICH = CHANUP + 2
C****   MOVE POINTER BACK CHANUP+2 PLACES
      I = I - ICH
      IF( I .LT. 2) I = 2
```

```
OS3 FORTRAN  VERSION 3.0  PEAK       11/23/71  1130
C****   START OVER AGAIN
      GO TO 6
C*****   LOOK FOR START OF STEEP DOWNHILL SLOPE
  503 IF(ABSF(DY(I)) .GE. SLOPE .AND. DY(I) .LT. 0. ) 51,52
   51 POSITION = DOWN
      GO TO 10
   52 JTOP = JTOP + 1
      IF ( JTOP .GT. TOPMAX )6,10
C****  IF TOP IS TOO LONG START OVER
    6 POSITION = START
      JTOP = JUP = 0
      GO TO 10
C*****  LOOK FOR RIGHT TAIL
    7 IF ( ABSF( DY(I) ) .GE. SLOPE .AND. DY(I) .LT. 0. ) 71,72
   71 JDOWN =JDOWN + 1
      GO TO 10
   72 IF ( JDOWN .GE. CHANDOWN ) 74,73
   73 JTOP = JDOWN
      POSITION = TOP
      UPAGAIN = 0
      GO TO 10
   74 RIGHT = I
      DO 9 J= 1,3
      JK = I + J
      IF ( ABSF( DY(JK) ) .GE. SLOPE ) 91,9
C*****  MAKE SURE WE ARE ON THE TAIL
   91 POSITION = DOWN
      GO TO 10
    9 CONTINUE
      GO TO 12
   10 CONTINUE
C***********************************************************************
C         IF LOOP TERMINATES THERE IS AN ERROR
C         ERROR IS SIGNIFIED BY SETTING THE
C         VALUES OF LEFT AND RIGHT TO 0
C***********************************************************************
   11 LEFT = RIGHT = 0
      RETURN
C**********************************************************************
C*****  NOW WE KNOW THE RIGHT AND LEFT BOUNDS OF THE PEAK
C*****  MINIMIZE THE STANDARD DEVIATIONS FOR THE SUMMIT VALUE
C**********************************************************************
   12 PEAKTOP = 0
      SIGMIN = 1.E10
C****   SEARCH UPPER 2/3 OF THE PEAK
      IPRANGE = RIGHT - LEFT
      KF = IPRANGE / 6
      LFT = LEFT + KF
      IRT = RIGHT - KF
      DO 20 I=LFT,IRT
      IF ( SIGMA(I) .LT. SIGMIN )19,20
   19 SIGMIN = SIGMA(I)
      PEAKTOP = I
   20 CONTINUE
C*****  POSITION OF PEAK IS NOW PEAKTOP
      IF(PEAKTOP .EQ. LFT .OR. PEAKTOP .EQ. IRT)GO TO 11
C****   COULDNT FIND TOP BY MINIMIZING SIGMA SO ABORT
      M = PEAKTOP - 2
      N = PEAKTOP + 2
      J = ISUM = 0
```

```
OS3 FORTRAN  VERSION 3.0  PEAK       11/23/71  1130
      DO 25 I=M,N
      IF (ABSF(IY(I) - MEAN(PEAKTOP)) .LT. SIGMA(PEAKTOP) ) 22,25
   22 J=J+1
      ISUM = ISUM + IY(I)
   25 CONTINUE
C******* CALCULATE NEW MEAN    ( VALUE AT SUMMIT )
      SUMMIT = ISUM/J
      I = LEFT - 3
      J = RIGHT + 3
      IF(I .LT. 3)I = 3
      IF(J .GT. (L - 2))J = L - 2
C****   LEFT TAIL
      LEFTBND = MEAN(I)
C****  RIGHT TAIL
      RIGHTBND = MEAN(J)
      RETURN
      END
```

```
3300 COMPASS/OS3 VER 2.0                          COMPRESS                                   11/23/71  1140  PAGE    2
                                          COMPRESS COSY/     01                  11/23/71  1140
                                          ***************************************************************
                                          *    THIS SUBROUTINE TAKES A TWO WORD VARIABLE AND             *
                                          *     COMPRESSES ALL BLANKS FROM IT.                           *
                                          *     THE CALLING SEQUENCE IS                                  *
                                          *        RTJ       COMPRESS                                    *
                                          *        77        ANAME                                       *
                                          *                                                              *
                                          *OR IN FORTRAN IT IS     CALL COMPRESS(ANAME)                  *
                                          ***************************************************************
                                                   ENTRY     COMPRESS
00000  01077777 01 0  77777 0  COMPRESS UJP       **
00001  47100037 47 0 P00037 1           STI       B1,1
00002  47200040 47 0 P00040 2           STI       B2,2
00003  20000000 20 0 P00000 0           LDA       COMPRESS
00004  44000010 44 0 P00010 0           SWA       COM1
00005  44000036 44 0 P00036 0           SWA       COM2
00006  15400001 15 1  00001 0           INA,S     1
00007  44000041 44 0 P00041 0           SWA       XIT                 SET UP EXIT
00010  25477777 25 1  77777 0  COM1     LDAQ,I    **                  PICK UP PARAMETER
00011  45000042 45 0 P00042 0           STAQ      T1                  PUT IT IN T1
00012  14700060 14 1  00060 3           ENQ       60B                 BLANK IN Q
00013  14177776 14 0  77776 1           ENI       -1,1
00014  14200000 14 0  00000 2           ENI       0,2                 INITIALIZE
00015  15100001 15 0  00001 1  LOOP     INI       1,1
00016  04100010 04 0  00010 1           ISE       8,1
00017  01000021 01 0 P00021 0           UJP       *+2
00020  01000027 01 0 P00027 0           UJP       DONE
00021  22400210 22 1 P00042 0           LACH      T1,1                LOOK AT A CHARACTER
00022  03500024 03 1 P00024 1           AQJ,NE    *+2
00023  01000015 01 0 P00015 0           UJP       LOOP
00024  42400220 42 1 P00044 0           SACH      T2,2                STORE THE CHARACTER
00025  15200001 15 0  00001 2           INI       1,2
00026  01000015 01 0 P00015 0           UJP       LOOP
00027  14600060 14 1  00060 2  DONE     ENA       60B
00030  01000033 01 0 P00033 0           UJP       *+3
00031  42400220 42 1 P00044 0           SACH      T2,2                FILL REST OF WORD WITH BLANKS
00032  15200001 15 0  00001 2           INI       1,2
00033  05200010 05 0  00010 2           ISG       8,2
00034  01000031 01 0 P00031 0           UJP       *-3
00035  25000044 25 0 P00044 0           LDAQ      T2                  PICK UP ANSWER
00036  45477777 45 1  77777 0  COM2     STAQ,I    **                  STORE IT
00037  14177777 14 0  77777 1  B1       ENI       **,1
00040  14277777 14 0  77777 2  B2       ENI       **,2
00041  01077777 01 0  77777 0  XIT      UJP       **                  RETURN TO CALLING PROGRAM
00042                          T1       BSS       2
00044                          T2       BSS       2
                                        END

                                   NUMBER OF LINES WITH DIAGNOSTICS          0
```

```
OS3 FORTRAN  VERSION 3.0          11/23/71  1123
      SUBROUTINE POLFIT(X, Y, NPTS, NORDER, NEVEN, YFIT, A, SIGMAA,
     1    CHISQR)
C*****************************************************************
C         PURPOSE
C     MAKE A LEAST-SQUARES FIT TO  DATA WITH A POWER SERIES POLYNOMIAL
C
C         DESCRIPTION OF PARAMETERS
C     X          - ARRAY OF DATA POINTS FOR INDEPENDENT VARIABLE
C     Y          - ARRAY OF DATA POINTS FOR DEPENDENT VARIABLE
C     NPTS       - NUMBER OF PAIRES OF DATA POINTS
C     NORDER     - HIGHEST ORDER OF POLYNOMIAL (NUMBER OF TERMS - 1)
C     NEVEN      - DETERMINES ODD OR EVEN CHARACTER OF POLYNOMIAL
C                  +1  FITS ONLY TO EVEN TERMS
C                   0  FITS TO ALL TERMS
C                  -1 FITS ONLY TO ODD TERMS
C     YFIT       - ARRAY OF CALCULATED VALUES OF Y
C     A          - ARRAY OF COEFFICIENTS OF POLYNOMIAL
C     SIGMAA     - ARRAY OF STANDARD DEVIATIONS FOR COEFFICIENTS
C     CHISQR     - REDUCED CHI SQUARE FOR FIT
C*****************************************************************
C
      DIMENSION X(1), Y(1), YFIT(1), A(1), SIGMAA(1), P(100,10),
     1         BETA(10), ALPHA(10,10)
C
C         ACCUMULATE POLYNOMIALS
C
   11 NTERMS = NCOEFF = 1
      JMAX = NORDER + 1
   20 DO 40 I=1, NPTS
      P(I,1) = 1.
      P(I,2) = X(I)
      DO 40 L=2, NORDER
   40 P(I,L+1) = X(I) ** L
C
C         ACCUMULATE MATRICES ALPHA AND BETA
C
   51 DO 54 J=1, NTERMS
      BETA(J) = 0.
      DO  54 K=1, NTERMS
   54 ALPHA(J,K) =0.
      DO 60 I =1, NPTS
      DO 60 J =1, NTERMS
      BETA(J) = BETA(J) + P(I,J) * Y(I)
      DO 60 K=J, NTERMS
      ALPHA(J,K) = ALPHA(J,K) + P(I,J) * P(I,K)
   60 ALPHA(K,J) = ALPHA(J,K)
C
C         DELETE FIXED COEFFICIENTS
C
   70 IF(NEVEN)71, 91, 81
   71 DO 76 J=3, NTERMS, 2
      BETA(J) = 0.
      DO 75 K=1, NTERMS
      ALPHA(J,K) = 0.
   75 ALPHA(K,J) = 0.
   76 ALPHA(J,J) = 1.
      GO TO 91
   81 DO 86 J=2, NTERMS, 2
      BETA(J) = 0.
      DO 85 K=1, NTERMS
```

```
OS3 FORTRAN  VERSION 3.0  POLFIT    11/23/71  1120
      ALPHA(J,K) = 0.
   85 ALPHA(K,J) = 0.
   86 ALPHA(J,J) = 1.
C
C         INVERT CURVATURE MATRIX ALPHA
C
   91 DO 95 J=1, JMAX
      A(J) = 0.
   95 SIGMAA(J) = 0.
      DO 97 I=1, NPTS
   97 YFIT(I) = 0.
  101 CALL MATINV(ALPHA, NTERMS, DET)
      IF(DET) 111, 103
  103 CHISQR = 0.
      GO TO 170
C
C         CALCULATE COEFFICIENTS ,FIT, AND CHI SQUARE
C
  111 DO 115 J=1, NTERMS
      DO 113 K=1, NTERMS
  113 A(J) = A(J) + BETA(K) * ALPHA(J,K)
      DO 115 I =1, NPTS
  115 YFIT(I) = YFIT(I) + A(J)* P(I,J)
      CHISQ = 0.
      DO 123 I =1, NPTS
      DEL = Y(I)-YFIT(I)
  123 CHISQ = CHISQ + DEL * DEL
      FREE = NPTS - NCOEFF
      CHISQR = CHISQ / FREE
C
C         TEST FOR END OF FIT
C
  131 IF(( NTERMS - JMAX ) .GE. 0) 151, 132
  132 IF (( NCOEFF - 2 ) .GE. 0) 134, 133
  133 IF (NEVEN .GT. 0) 135, 137
  134 IF (NEVEN) 135, 137
  135 NTERMS = NTERMS + 2
      GO TO 138
  137 NTERMS = NTERMS + 1
  138 NCOEFF = NCOEFF + 1
      GO TO 51
C
C         CALCULATE REMAINDER OF OUTPUT
C
  151 DO 152 J=1, NTERMS
  152 SIGMAA(J) = SQRT(CHISQR * ALPHA(J,J))
  170 RETURN
      END
```

```
OS3 FORTRAN  VERSION 3.0          11/26/71  1600
      SUBROUTINE READCARD(LUN,LINE)
C****  THIS SUBROUTINE ALLOWS COSY DECKS TO BE READ
C****  BY A COMPASS ROUTINE.
      DIMENSION LINE(20)
    1 FORMAT(20A4)
      READ(LUN,1)LINE
      END
```

```
OS3 FORTRAN  VERSION 3.0             11/23/71  1129
      SUBROUTINE MATINV ( ARRAY, NORDER, DET)
C*********************************************************************
C
C         PURPOSE
C      INVERT A SYMMETRIC MATRIX AND CALCULATE ITS DETERMINANT
C
C         DESCRIPTION OF PARAMETERS
C      ARRAY    - INPUT MATRIX WHICH IS REPLACED BY ITS INVERSE
C      NORDER   - DEGREE OF MATRIX (ORDER OF DETERMINANT)
C      DET      - DETERMINANT OF INPUT MATRIX
C
C*********************************************************************
      DIMENSION ARRAY(10,10), IK(10), JK(10)
   10 DET = 1.
   11 DO 100 K=1, NORDER
C
C         FIND LARGEST ELEMENT ARRAY(I,J) IN REST OF MATRIX
C
      AMAX = 0.
   21 DO 30 I=K, NORDER
      DO 30 J=K, NORDER
   23 IF (ABSF(AMAX) - ABSF(ARRAY(I,J))) 24,24,30
   24 AMAX = ARRAY(I,J)
      IK(K) = I
      JK(K) = J
   30 CONTINUE
C
C         INTERCHANGE ROWS AND COLUMNS TO PUT AMAX IN ARRAY(K,K)
C
   31 IF(AMAX) 41, 32
   32 DET = 0.
      GO TO 140
   41 I = IK(K)
      IF(I-K) 21, 51, 43
   43 DO 50 J=1, NORDER
      SAVE = ARRAY(K,J)
      ARRAY(K,J) = ARRAY(I,J)
   50 ARRAY(I,J) = -SAVE
   51 J = JK(K)
      IF (J-K) 21, 61, 53
   53 DO 60 I=1, NORDER
      SAVE = ARRAY(I,K)
      ARRAY(I,K) = ARRAY(I,J)
   60 ARRAY(I,J) = -SAVE
C
C         ACCUMULATE ELEMENTS OF INVERSE MATRIX
C
   61 DO 70 I=1, NORDER
      IF (I-K) 63,70
   63 ARRAY(I,K) = -ARRAY(I,K) / AMAX
   70 CONTINUE
   71 DO 80 I=1, NORDER
      DO 80 J=1, NORDER
      IF (I-K) 74, 80
   74 IF(J-K) 75, 80
   75 ARRAY(I,J) = ARRAY(I,J) + ARRAY(I,K) * ARRAY(K,J)
   80 CONTINUE
   81 DO 90 J=1, NORDER
      IF (J-K) 83, 90
   83 ARRAY(K,J) = ARRAY(K,J)/AMAX
```

```
OS3 FORTRAN  VERSION 3.0  MATINV     11/23/71  1129
   90 CONTINUE
      ARRAY(K,K) = 1. / AMAX
  100 DET = DET * AMAX
C
C         RESTORE ORDERING OF MATRIX
C
  101 DO 130 L=1, NORDER
      K = NORDER - L + 1
      J = IK(K)
      IF((J-K) .GT. 0) 105, 111
  105 DO 110 I=1, NORDER
      SAVE = ARRAY(I,K)
      ARRAY(I,K) = - ARRAY(I,J)
  110 ARRAY(I,J) = SAVE
  111 I = JK(K)
      IF((I-K) .GT. 0) 113, 130
  113 DO 120 J=1, NORDER
      SAVE = ARRAY(K,J)
      ARRAY(K,J) = - ARRAY(I,J)
  120 ARRAY(I,J) = SAVE
  130 CONTINUE
  140 RETURN
      END
```

```
OS3 FORTRAN  VERSION 3.0             11/23/71  1132
      SUBROUTINE WRITEIO(LPLUN,LUN1,LUN2)
      DIMENSION XLINE(16)
      REWIND LUN1
      REWIND LUN2
      IEOF1 = IEOF2 = 0
    1 DO 2 I=1,16
    2 XLINE(I) = 8H
      IF(IEOF1)GO TO 3
      IF( EOF(LUN1) .OR. EOD(LUN1) )21,22
   21 IEOF1 = 1
      GO TO 3
   22 READ(LUN1,100)(XLINE(I),I=1,6)
  100 FORMAT(6A8)
      IF(EOF(LUN1).OR.EOD(LUN1))IEOF1 = 1
    3 IF(IEOF2)GO TO 4
      IF( EOF(LUN2) .OR. EOD(LUN2) )31, 32
   31 IEOF2 = 1
      GO TO 4
   32 READ(LUN2,100)(XLINE(I),I=11,16)
      IF(EOF(LUN2).OR.EOD(LUN2))IEOF2 = 1
    4 WRITE(LPLUN,101)XLINE
  101 FORMAT(16A8)
      IF(IEOF1.AND.IEOF2)5,1
    5 WRITE(LPLUN,102)
  102 FORMAT(1H1)
      CALL UNEQUIP(LUN1)
      CALL UNEQUIP(LUN2)
      CALL EQUIP(LUN1,8HFILE      )
      CALL EQUIP(LUN2,8HFILE      )
      RETURN
      END
```

```
3300 COMPASS/OS3 VER 2.0                    CANCEL                                   11/23/71  1352     PAGE      2
                                     CANCEL   COSY/        01                  11/23/71  1352
                                     ****************************************************************
                                     *        THIS SUBROUTINE CHECKS A LINE FOR CANCELLATION            *
                                     *        CHARACTERS (BACK SLASH) AND DOES THE CORRECTIONS.         *
                                     *        ALSO IT CHECKS FOR THE ERROR CODE (!!) IF WANTED.         *
                                     *        TO USE                                                    *
                                     *                     CALL CANCEL(CARD)                            *
                                     *        OR                                                        *
                                     *                     CALL CANCEL(CARD,L)                          *
                                     *                                                                  *
                                     *        WHERE L IS THE ERROR FLAG.                                *
                                     ****************************************************************
                                              ENTRY        CANCEL
      00000  01077777 01 0  77777 0  CANCEL   UJP          **
      00001  47100105 47 0 P00105 1           STI          B1,1                SAVE B1
      00002  47200106 47 0 P00106 2           STI          B2,2                SAVE B2
      00003  14600000 14 1  00000 2           ENA          0
      00004  40000110 40 0 P00110 0           STA          ERROR               INITIALIZE ERROR
      00005  20000000 20 0 P00000 0           LDA          CANCEL
      00006  44000030 44 0 P00030 0           SWA          PAR1                ADDRESS OF FIRST PARAMETER
      00007  15400001 15 1  00001 0           INA,S        1
      00010  44000107 44 0 P00107 0           SWA          XIT                 SET UP EXIT FOR 1 PARAMETER
      00011  44000021 44 0 P00021 0           SWA          PAR2                ADDRESS OF SECOND PARAMETER
      00012  44000024 44 0 P00024 0           SWA          PAR2.1
      00013  44000014 44 0 P00014 0           SWA          *+1
      00014  20077777 20 0  77777 0           LDA          **                  LOOK AT WORD
      00015  12000006 12 0  00006 0           SHA          6
      00016  17600077 17 1  00077 2           ANA          77B
      00017  04600077 04 1  00077 2           ASE          77B                 SKIP IF IT IS A JUMP
      00020  01000030 01 0 P00030 0           UJP          PAR1                ONLY ONE PARAMETER
      00021  14677777 14 1  77777 2  PAR2     ENA          **                  IS A SECOND PARAMETER
      00022  15400001 15 1  00001 0           INA,S        1
      00023  44000107 44 0 P00107 0           SWA          XIT                 SET UP EXIT
      00024  20077777 20 0  77777 0  PAR2.1   LDA          **
      00025  44000104 44 0 P00104 0           SWA          PAR2BACK
      00026  14600001 14 1  00001 2           ENA          1
      00027  40000110 40 0 P00110 0           STA          ERROR               WILL CHECK FOR ERRORS
      00030  20077777 20 0  77777 0  PAR1     LDA          **
      00031  44000063 44 0 P00063 0           SWA          PAR1BACK
      00032  17677777 17 1  77777 2           ANA          77777B
      00033  12000002 12 0  00002 0           SHA          2
      00034  46000040 46 0 P00040 0           SCHA         LACH                SAVE ADDRESS FOR LATER
      00035  14177776 14 0  77776 1           ENI          -1,1
      00036  14200000 14 0  00000 2           ENI          0,2
      00037  15100001 15 0  00001 1  CHECK    INI          1,1
      00040  22777777 22 1  77777 3  LACH     LACH         **,1                LOOK AT A CHARACTER
      00041  04600075 04 1  00075 2           ASE          75B                 SKIP IF CANCELLATION OCCURS (\)
      00042  01000046 01 0 P00046 0           UJP          STORE
      00043  04200000 04 0  00000 2           ISE          0,2                 DONT GO BELOW 0
      00044  15277776 15 0  77776 2           INI          -1,2
      00045  01000037 01 0 P00037 0           UJP          CHECK
      00046  05100120 05 0  00120 1  STORE    ISG          80,1                IF CARD IS FULL
      00047  01000051 01 0 P00051 0           UJP          *+2
      00050  01000054 01 0 P00054 0           UJP          DONE


3300 COMPASS/OS3 VER 2.0                    CANCEL                                   11/23/71  1352     PAGE      3
      00051  42400444 42 1 P00111 0           SACH         CARD,2              STORE CHARACTER
      00052  15200001 15 0  00001 2           INI          1,2
      00053  01000037 01 0 P00037 0           UJP          CHECK               GO LOOK AT MORE
      00054  14600060 14 1  00060 2  DONE     ENA          60B
      00055  42400444 42 1 P00111 0           SACH         CARD,2
      00056  15200001 15 0  00001 2           INI          1,2
      00057  05200121 05 0  00121 2           ISG          81,2
      00060  01000055 01 0 P00055 0           UJP          *-3
      00061  14100023 14 0  00023 1           ENI          19,1
      00062  20100111 20 0 P00111 1           LDA          CARD,1
      00063  40177777 40 0  77777 1  PAR1BACK STA          **,1                PUT CORRECTED LINE BACK
      00064  02500062 02 1 P00062 1           IJD          *-2,1
      00065  20000110 20 0 P00110 0           LDA          ERROR
      00066  03000105 03 0 P00105 0           AZJ,EQ       B1                  QUIT IF NO ERROR PARAMETER
      00067  14100023 14 0  00023 1           ENI          19,1                CHECK 20 CHARS FOR ERROR CODE !!
      00070  14700012 14 1  00012 3           ENO          12B                   THE ERROR SIGNAL
      00071  22400444 22 1 P00111 0           LACH         CARD,1              LOOK AT A CHARACTER
      00072  03400075 03 1 P00075 0           AQJ,EQ       ER
      00073  02500071 02 1 P00071 1  IJD      IJD          *-2,1               GO LOOK SOME MORE
      00074  01000105 01 0 P00105 0           UJP          B1                  NO ERROR CODE SO EXIT
      00075  04100000 04 0  00000 1  ER       ISE          0,1                 IF LAST CHARACTER
      00076  01000100 01 0 P00100 0           UJP          *+2
      00077  01000105 01 0 P00105 0           UJP          B1                  ONLY ONE !(NOT ENUF FOR AN ERROR)
      00100  15177776 15 0  77776 1           INI          -1,1
      00101  22400444 22 1 P00111 0           LACH         CARD,1              LOOK AT NEXT CHARACTER
      00102  03500073 03 1 P00073 1           AQJ,NE       IJD                 IF NOT AN ERROR CODE
      00103  14600001 14 1  00001 2           ENA          1
      00104  40077777 40 0  77777 0  PAR2BACK STA          **                  PUT A 1 IN THE PARAMETER
      00105  14177777 14 0  77777 1  B1       ENI          **,1                RESTORE B1
      00106  14277777 14 0  77777 2  B2       ENI          **,2                RESTORE B2
      00107  01077777 01 0  77777 0  XIT      UJP          **                  RETURN TO CALLING PROGRAM
      00110                           ERROR   BSS          1
      00111                          CARD     BSS          21
                                              END

                                      NUMBER OF LINES WITH DIAGNOSTICS       0
```

```
                                          READATA  COSY/      01                        11/23/71  1141
                                                   ENTRY      READATA,CLEARFLG
                                                   EXT        COMPRESS,CANCEL,DECBIN,READCARD
00000  01077777 01 0  77777 0  CLEARFLG UJP        **                     CLEAR THE INPUT FLAG
00001  14600000 14 1  00000 2           ENA        0
00002  40000350 40 0 P00350 0           STA        RDFLAG
00003  01400000 01 1 P00000 0           UJP,I      CLEARFLG
00004  01077777 01 0  77777 0  READATA  UJP        **
00005  47100275 47 0 P00275 1           STI        B1,1                   SAVE
00006  47200276 47 0 P00276 2           STI        B2,2                   THE
00007  47300277 47 0 P00277 3           STI        B3,3                   INDEXES
00010  20000004 20 0 P00004 0           LDA        READATA
00011  44000016 44 0 P00016 0           SWA        R1                     PARAMETER 1
00012  15400001 15 1  00001 0           INA,S      1
00013  44000020 44 0 P00020 0           SWA        R2                     PARAMETER 2
00014  15400001 15 1  00001 0           INA,S      1
00015  44000302 44 0 P00302 0           SWA        XIT                    FIX UP RETURN ADDRESS
00016  20477777 20 1  77777 0  R1       LDA,I      **                     PICK UP FIRST PARAMETER
00017  40000305 40 0 P00305 0           STA        LUN
00020  25477777 25 1  77777 0  R2       LDAQ,I     **                     PICK UP SECOND PARAMETER
00021  45000306 45 0 P00306 0           STAQ       ANAME
00022  00777777 00 1 X77777 3           RTJ        COMPRESS
00023  77000306 77 0 P00306 0           77         ANAME                  COMPRESS THE BLANKS OUT
00024  14600000 14 1  00000 2           ENA        0
00025  40000315 40 0 P00315 0           STA        KOUNT                  INITIALIZE WORD COUNT
00026  40000303 40 0 P00303 0           STA        I                      INITIALIZE ID TAG
00027  14477776 14 1  77776 0           ENA,S      -1
00030  40000316 40 0 P00316 0           STA        L                      INITIALIZE ID COUNT
00031  14300000 14 0  00000 3           ENI        0,3                    INITIALIZE ARRAY
00032  20000350 20 0 P00350 0           LDA        RDFLAG                 CHECK FOR FIRST CALL
00033  03200042 03 0 P00042 2           AZJ,GE     READ                   IF FIRST CALL
00034  00777777 00 1 X77777 3           RTJ        CANCEL                 LOOK FOR ::::::
00035  77000323 77 0 P00323 0           77         CARD
00036  77000304 77 0 P00304 0           77         J                      ERROR CODE PRESENT IF J=1
00037  20000304 20 0 P00304 0           LDA        J
00040  03100042 03 0 P00042 1           AZJ,NE     READ                   IF ERROR READ ANOTHER LINE
00041  01000053 01 0 P00053 0           UJP        LP0                    SKIP THE READ
00042  00777777 00 1 X77777 3  READ     RTJ        READCARD               READ A LINE
00043  77000305 77 0 P00305 0           77         LUN
00044  77000323 77 0 P00323 0           77         CARD
00045  14700000 14 1  00000 3           ENQ        0
00046  72400305 72 1 P00305 0           CNTL,I     LUN                    STATUS OF LUN
00047  12000002 12 0  00002 0           SHA        2
00050  03300250 03 0 P00250 3           AZJ,LT     EOF                    EOD
00051  12000001 12 0  00001 0           SHA        1
00052  03300250 03 0 P00250 3           AZJ,LT     EOF                    EOF
00053  20000371 20 0 P00371 0  LP0      LDA        =H
00054  14100023 14 0  00023 1           ENI        19,1
00055  21100323 21 0 P00323 1  LOOP     LDQ        CARD,1
00056  03500061 03 1 P00061 1           AQJ,NE     LP1                    LOOK AT BLANK WORDS
00057  02500055 02 1 P00055 1           IJD        LOOP,1
00060  01000062 01 0 P00062 0           UJP        *+2
00061  15100001 15 0  00001 1  LP1      INI        1,1
00062  53100000 53 0  00000 1           TIA        1
00063  13000030 13 0  00030 0           SHAQ       24                     Q CONTAINS NUMBER OF WORDS READ
00064  04700000 04 1  00000 3           QSE        0
00065  01000067 01 0 P00067 0           UJP        *+2
00066  01000042 01 0 P00042 0           UJP        READ                   READ ANOTHER CARD IF ALL BLANK
00067  12400002 12 1  00002 0           SHQ        2
00070  41000347 41 0 P00347 0           STQ        EOL                    NUMBER OF CHARACTERS
00071  14600000 14 1  00000 2           ENA        0
00072  40000304 40 0 P00304 0           STA        J                      INITIALIZE ERROR FLAG
00073  00700034 00 1 X00034 3           RTJ        CANCEL                 REMOVE CANCELLATIONS
00074  77000323 77 0 P00323 0           77         CARD
00075  77000304 77 0 P00304 0           77         J                      ERROR CODE PRESENT IF J=1
00076  20000304 20 0 P00304 0           LDA        J
00077  03100244 03 0 P00244 1           AZJ,NE     ERROR
00100  20000347 20 0 P00347 0           LDA        EOL
00101  12000026 12 0  00026 0           SHA        22
00102  15477772 15 1  77772 0           INA,S      -5
00103  03300105 03 0 P00105 3           AZJ,LT     *+2                    IF LESS THAN 5 WORDS WERE READ
00104  01000254 01 0 P00254 0           UJP        CONVERT                GO CONVERT THE LINE
00105  20000303 20 0 P00303 0           LDA        I
00106  03000110 03 0 P00110 0           AZJ,EQ     ID                     CHECK IF PREVIOUS ID READ
00107  01000254 01 0 P00254 0           UJP        CONVERT
00110  14100007 14 0  00007 1  ID       ENI        7,1
00111  14700060 14 1  00060 3           ENQ        60B                    BLANK
00112  22401514 22 1 P00323 0  ID.1     LACH       CARD,1
00113  03400116 03 1 P00116 0           AQJ,EQ     *+3                    IF BLANK
00114  15477765 15 1  77765 0           INA,S      -10                    SUBTRACT 10
00115  03200120 03 0 P00120 2           AZJ,GE     ID.2                   NOT A NUMBER
00116  02500112 02 1 P00112 1           IJD        ID.1,1
00117  01000254 01 0 P00254 0           UJP        CONVERT                IS A NUMBER
00120  20000316 20 0 P00316 0  ID.2     LDA        L                      NUMBER OF ID#S READ
00121  15600001 15 1  00001 2           INA        1
00122  40000316 40 0 P00316 0           STA        L                      INCREASE BY ONE
00123  03100223 03 0 P00223 1           AZJ,NE     ID.3                   IF SECOND ID WAS READ
00124  14200000 14 0  00000 2           ENI        0,2
00125  14100000 14 0  00000 1           ENI        0,1
00126  14700061 14 1  00061 3           ENQ        61B                    SLASH  /
00127  22401514 22 1 P00323 0  IDLOOK   LACH       CARD,1                 LOOK AT A CHARACTER
00130  03400142 03 1 P00142 0           AQJ,EQ     IDSCALE                IF A / EXISTS
00131  42401440 42 1 P00310 0           SACH       TEMP,2                 SAVE ID
00132  15100001 15 0  00001 1           INI        1,1
00133  15200001 15 0  00001 2           INI        1,2
00134  05100014 05 0  00014 1           ISG        12,1                   SKIP IF .GT. 3 WORDS
00135  01000127 01 0 P00127 0           UJP        IDLOOK
00136  14600000 14 1  00000 2  IDL      ENA        0
00137  14700000 14 1  00000 3           ENQ        0
00140  45000003 45 0 C00003 0           STAQ       SCALE                  NO SCALE FACTOR HERE
00141  01000206 01 0 P00206 0           UJP        ID.21                  GO PROCESS ID
00142  14600060 14 1  00060 2  IDSCALE  ENA        60B                    BLANK
00143  42401440 42 1 P00310 0           SACH       TEMP,2                 FILL REST OF TEMP
00144  15200001 15 0  00001 2           INI        1,2                    WITH BLANKS
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00145  05200010 05 0  00010 2            ISG       8,2
00146  01000143 01 0 P00143 0            UJP       *-3
00147  14200000 14 0  00000 2            ENI       0,2
00150  15100001 15 0  00001 1            INI       1,1              NEXT CHARACTER
00151  22401514 22 1 P00323 0  IDS.1     LACH      CARD,1
00152  42401454 42 1 P00313 0            SACH      TEMP2,2          SAVE IN TEMP2
00153  15100001 15 0  00001 1            INI       1,1
00154  15200001 15 0  00001 2            INI       1,2
00155  05200010 05 0  00010 2            ISG       8,2              SKIP IF .GT. 2 WORDS
00156  01000151 01 0 P00151 0            UJP       IDS.1
00157  00700022 00 1 X00022 3            RTJ       COMPRESS         COMPRESS THE SCALE
00160  77000313 77 0 P00313 0            77        TEMP2
00161  14100000 14 0  00000 1            ENI       0,1
00162  11001454 11 0 P00313 0            ECHA      TEMP2
00163  00777777 00 1 X77777 3            RTJ       DECBIN           CONVERT NUMBER TO BINARY
00164  40000003 40 0 C00003 0            STA       SCALE            SAVE THE NUMBER
00165  14700044 14 1  00044 3            ENQ       44B              M
00166  22401454 22 1 P00313 0            LACH      TEMP2,1          LOOK AT NEXT CHARACTER
00167  03400201 03 1 P00201 0            AQJ,EQ    MV               IF MILLIVOLTS
00170  14700065 14 1  00065 3            ENQ       65B              V
00171  03400204 03 1 P00204 0            AQJ,EQ    VOLT             IF VOLTS
00172  14600365 14 1 P00365 2            ENA       SCMESS            ERROR MESSAGE
00173  14700004 14 1  00004 3            ENQ       4
00174  76000075 76 0  00075 0            WRITE     61
00175  14600317 14 1 P00317 2            ENA       CMES
00176  14700030 14 1  00030 3            ENQ       24
00177  76000075 76 0  00075 0            WRITE     61               PRINT INPUT RECORD
00200  01000136 01 0 P00136 0            UJP       IDL              PUT ZEROS IN SCALE FACTOR
00201  14477774 14 1  77774 0  MV        ENA,S     -3
00202  40000004 40 0 C00004 0            STA       FACTOR           PUT -3 IN FACTOR
00203  01000206 01 0 P00206 0            UJP       ID.21
00204  14600000 14 1  00000 2  VOLT      ENA       0
00205  40000004 40 0 C00004 0            STA       FACTOR           PUT 0 IN FACTOR
00206  00700157 00 1 X00157 3  ID.21     RTJ       COMPRESS
00207  77000310 77 0 P00310 0            77        TEMP             SUPPRESS THE BLANKS
00210  20000306 20 0 P00306 0            LDA       ANAME
00211  21000310 21 0 P00310 0            LDQ       TEMP
00212  03500226 03 1 P00226 1            AQJ,NE    WRONGID
00213  20000307 20 0 P00307 0            LDA       ANAME+1
00214  21000311 21 0 P00311 0            LDQ       TEMP+1
00215  03500226 03 1 P00226 1            AQJ,NE    WRONGID
00216  14600001 14 1  00001 2            ENA       1
00217  40000303 40 0 P00303 0            STA       I                SET ID TAG
00220  25000310 25 0 P00310 0            LDAQ      TEMP
00221  45000001 45 0 C00001 0            STAQ      PEAKID           STORE THE NAME
00222  01000042 01 0 P00042 0            UJP       READ             GO READ ANOTHER CARD
00223  20000315 20 0 P00315 0  ID.3      LDA       KOUNT
00224  40000005 40 0 C00005 0            STA       INDEX            SAVE THE WORD COUNT
00225  01000275 01 0 P00275 0            UJP       B1               TIME TO EXIT
00226  25000306 25 0 P00306 0  WRONGID   LDAQ      ANAME
00227  45000360 45 0 P00360 0            STAQ      MESS+7
00230  25000310 25 0 P00310 0            LDAQ      TEMP
00231  45000363 45 0 P00363 0            STAQ      MESS+10
00232  14600351 14 1 P00351 2            ENA       MESS
00233  14700014 14 1  00014 3            ENQ       12
00234  76000075 76 0  00075 0            WRITE     61               WRITE ERROR MESSAGE
00235  14600317 14 1 P00317 2            ENA       CMES
00236  14700030 14 1  00030 3            ENQ       24
00237  76000075 76 0  00075 0            WRITE     61               PRINT INPUT RECORD
00240  14477775 14 1  77775 0            ENA,S     -2
00241  54700004 54 1 P00004 3  WRID.1    LDI,I     READATA,3
00242  40300000 40 0  00000 3            STA       0,3              PUT -2 IN LUN TO SIGNIFY ERROR
                                                                    OR -1 TO SIGNIFY EOF OR EOD
                                                                    OR -3 TO SIGNIFY OPERATOR ERROR
00243  01000275 01 0 P00275 0            UJP       B1               EXIT
00244  20000315 20 0 P00315 0  ERROR     LDA       KOUNT            OPERATOR ERROR
00245  40000005 40 0 C00005 0            STA       INDEX            SAVE THE TIME LOST
00246  14477774 14 1  77774 0            ENA,S     -3
00247  01000241 01 0 P00241 0            UJP       WRID.1           STORE ERROR CODE AND EXIT
00250  20000315 20 0 P00315 0  EOF       LDA       KOUNT
00251  40000005 40 0 C00005 0            STA       INDEX            STORE THE WORD COUNT
00252  14477776 14 1  77776 0            ENA,S     -1
00253  01000241 01 0 P00241 0            UJP       WRID.1           STORE IT IN LUN AND EXIT
00254  14600000 14 1  00000 2  CONVERT   ENA       0
00255  40000303 40 0 P00303 0            STA       I                CLEAR ID TAG
00256  14100000 14 0  00000 1            ENI       0,1              INITIALIZE FOR DECBIN
00257  21000347 21 0 P00347 0  CONV.1    LDQ       EOL
00260  53100000 53 0  00000 1            TIA       1
00261  03600042 03 1 P00042 2            AQJ,GE    READ             GO READ ANOTHER CARD IF EOL
00262  11001514 11 0 P00323 0            ECHA      CARD
00263  00700163 00 1 X00163 3            RTJ       DECBIN           CONVERT DECIMAL TO BINARY
00264  13000030 13 0  00030 0            SHAQ      24
00265  53200000 53 0  00000 2            TIA       2
00266  04600006 04 1  00006 2            ASE       6
00267  01000257 01 0 P00257 0            UJP       CONV.1           NOT VALID
00270  41300006 41 0 C00006 3            STQ       ARRAY,3          STORE THE NUMBER IN ARRAY
00271  15300001 15 0  00001 3            INI       1,3
00272  14600001 14 1  00001 2            ENA       1
00273  34000315 34 0 P00315 0            RAD       KOUNT            INCREASE WORD COUNT
00274  01000257 01 0 P00257 0            UJP       CONV.1           GO GET ANOTHER NUMBER
00275  14177777 14 0  77777 1  B1        ENI       **,1             RESTORE
00276  14277777 14 0  77777 2  B2        ENI       **,2             THE
00277  14377777 14 0  77777 3  B3        ENI       **,3             INDEXES
00300  14477777 14 1  77777 0            ENA,S     -0
00301  40000350 40 0 P00350 0            STA       RDFLAG           SET FLAG
00302  01077777 01 0  77777 0  XIT       UJP       **               RETURN TO CALLING PROGRAM
00303                                  I         BSS       1
00304                                  J         BSS       1
00305                                  LUN       BSS       1
00306                                  ANAME     BSS       2
00310                                  TEMP      BSS       3
00313                                  TEMP2     BSS       2
00315                                  KOUNT     BSS       1
00316                                  L         BSS       1
00317  60314547                        CMES      BCD       4, INPUT RECORD :
00320  64636051
00321  25234651
```

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00322  24601260
00323                              CARD     BSS      20
00347                              EOL      BSS      1
00350  00000000                    RDFLAG   OCT      0                      FLAG INDICATING FIRST CALL
00351  00604725                    MESS     BCD      12,0 PEAK IDENTIFIERS DIFFER :        VS
00352  21426031
00353  24254563
00354  31263125
00355  51626024
00356  31262625
00357  51601260
00360  60606060
00361  60606060
00362  65626060
00363  60606060
00364  60606060
00365  00622321                    SCMESS   BCD      4,0SCALE ERROR ***
00366  43256025
00367  51514651
00370  60545454
                                            COMMON
00000                              TIME     BSS      1
00001                              PEAKID   BSS      2
00003                              SCALE    BSS      1
00004                              FACTOR   BSS      1
00005                              INDEX    BSS      1
00006                              ARRAY    BSS      1000
                                            END

 LITERALS
00371           60606060

                                   NUMBER OF LINES WITH DIAGNOSTICS        0
```

```
3300 COMPASS/OS3 VER 2.0                    MISBJP                          11/23/71  1137    PAGE    2
                                            ENTRY     MISET,SBJP
      00000  01077777 01 0  77777 0  MISET  UJP       **
      00001  20000000 20 0 P00000 0         LDA       MISET
      00002  40000013 40 0  00013 0         STA       13B
      00003  01400000 01 1 P00000 0         UJP,I     MISET
      00004  14000000 14 0  00000 0  SBJP   NOP       0
      00005  14200000 14 0  00000 2         ENI       0,2
      00006  77620000 77 1  20000 2         SBJP
                                            END

                                   NUMBER OF LINES WITH DIAGNOSTICS        0
```

```
OS3 FORTRAN  VERSION 3.0           11/23/71  1137
      SUBROUTINE STAT(Y, K, SIG, YMEAN)
      DIMENSION Y(1)
      SUM = 0
      DO 1 I=1,K
    1 SUM = SUM + Y(I)
      YMEAN = SUM / K
      SUM = 0
      DO 2 I=1,K
      X = Y(I) - YMEAN
    2 SUM = SUM + X * X
      SIG = SQRT(SUM / (K-1))
      RETURN
      END
```

```
OS3 FORTRAN  VERSION 3.0           11/23/71  1137
      SUBROUTINE SMOOTH(Y,ZZ)
C***** 5 POINT SMOOTH
C**** FIRST DIFFERENCES OF SMOOTHED DATA ARE RETURNED
      COMMON ITIME,PEAKID,SCALE,L,IY(200)
      DIMENSION ZZ(1),Y(1)
      DO 1 I=1,L
    1 ZZ(I)=0.
      K=L-2
      DO 2 I=3,K
      SUM=-3.*Y(I-2)+12.*Y(I-1)+17.*Y(I)+12.*Y(I+1)-3.*Y(I+2)
    2 ZZ(I)=SUM/35.
      K=L-3
C****   GENERATE FIRST DERIVATIVE
      DO 3 I=3,K
    3 ZZ(I)=ZZ(I+1)-ZZ(I)
      ZZ(1)=ZZ(2)=ZZ(L)=ZZ(L-1)=ZZ(L-2)=0.
      END
```

```
                                     ASCIIBCD COSY/      01               11/23/71  1358
                                     ******************************************************************
                                     *          D. STANDLEY                                           *
                                     *          2-17-71                                               *
                                     * THIS PROGRAM TAKES ASCII RECORDS UP TO 64 WORDS LONG AND       *
                                     * CONVERTS THEM TO BCD RECORDS.                                  *
                                     * EACH WORD OF THE INPUT RECORD MUST CONTAIN 2 ASCII CHARACTERS  *
                                     ******************************************************************
                                              ENTRY    IO
                                              EXT      IOLUNS
00000                                INLUN    BSS      1
00001                                OUTLUN   BSS      1
00002  00777777 00 1 X77777 3        IO       RTJ      IOLUNS              PROCESS PARAMETER STRING
00003  45000000 45 0 P00000 0                 STAQ     INLUN
00004  14600000 14 1  00000 2                 ENA      0
00005  53420040 53 1  20040 0                 TAM      40B                 DONE FLAG OFF
00006  14200000 14 0  00000 2                 ENI      0,2                 INITIALIZE BCD INDEX
00007  14600073 14 1 P00073 2        START    ENA      CARD
00010  14700100 14 1  00100 3                 ENQ      100B
00011  74400000 74 1 P00000 0                 READ,I   INLUN               READ A CARD
00012  12000002 12 0  00002 0                 SHA      2
00013  03300040 03 0 P00040 3                 AZJ,LT   DONE                IF EOD
00014  12000001 12 0  00001 0                 SHA      1
00015  03300040 03 0 P00040 3                 AZJ,LT   DONE                IF EOF
00016  16577777 16 1  77777 1                 XOQ,S    -0                  NEGATE Q
00017  15500100 15 1  00100 1                 INQ,S    100B
00020  13000030 13 0  00030 0                 SHAQ     24
00021  53700000 53 1  00000 3                 TAI      3
00022  47300035 47 0 P00035 3                 STI      ISG,3               SAVE NUMBER OF RECORDS
00023  14300000 14 0  00000 3                 ENI      0,3                 INITIALIZE INPUT INDEX
00024  14600000 14 1  00000 2                 ENA      0
00025  21300073 21 0 P00073 3        LOOK     LDQ      CARD,3
00026  13000014 13 0  00014 0                 SHAQ     12                  MOVE FIRST ASCII INTO LOWER A
00027  17600177 17 1  00177 2                 ANA      177B                MASK
00030  00700173 00 1 P00173 3                 RTJ      STORE               STORE VALID CHARACTER
00031  13000014 13 0  00014 0                 SHAQ     12                  MOVE SECOND ASCII INTO LOWER A
00032  17600177 17 1  00177 2                 ANA      177B                MASK IT
00033  00700173 00 1 P00173 3                 RTJ      STORE               STORE IT
00034  15300001 15 0  00001 3                 INI      1,3
00035  05377777 05 0  77777 3        ISG      ISG      **,3                SKIP IF GE WORDS READ
00036  01000025 01 0 P00025 0                 UJP      LOOK                GO LOOK AT ANOTHER 2 CHARS
00037  01000007 01 0 P00007 0                 UJP      START               READ ANOTHER RECORD
00040  14477777 14 1  77777 0        DONE     ENA,S    -0
00041  53420040 53 1  20040 0                 TAM      40B                 DONE FLAG ON
00042  01000217 01 0 P00217 0                 UJP      NEWLINE             OUTPUT THE LAST LINE
00043  14700002 14 1  00002 3        XIT      ENQ      2
00044  72400001 72 1 P00001 0                 CNTL,I   OUTLUN              WRITE FILE MARK
00045  14200000 14 0  00000 2                 ENI      0,2
00046  77620000 77 1  20000 2                 SBJP                         STOP HERE ******
00047  60606060                      LINE     BCD      20,
00073                                CARD     BSS      64
00173  01077777 01 0  77777 0        STORE    UJP      **
00174  55700000 55 1  00000 3                 AQE                          SAVE AQ
00175  14700015 14 1  00015 3                 ENQ      15B                 RET (215)
00176  03400215 03 1 P00215 0                 AQJ,EQ   OUT
00177  14700012 14 1  00012 3                 ENQ      12B                 LF (212)
00200  03400217 03 1 P00217 0                 AQJ,EQ   NEWLINE             GO OUTPUT A BCD LINE
00201  14700040 14 1  00040 3                 ENQ      40B                 BLANK (240)
00202  03700215 03 1 P00215 3                 AQJ,LT   OUT                 IF .LT. 240 SKIP IT
00203  14700140 14 1  00140 3                 ENQ      140B
00204  03600215 03 1 P00215 2                 AQJ,GE   OUT                 IF .GE. 340 SKIP IT
00205  53500000 53 1  00000 1                 TAI      1
00206  22401144 22 1 P00231 0                 LACH     TBL,1               PICK UP BCD CHARACTER
00207  42400234 42 1 P00047 0                 SACH     LINE,2              STORE IT
00210  15200001 15 0  00001 2                 INI      1,2
00211  05200120 05 0  00120 2                 ISG      80,2                END OF OUTPUT RECORD
00212  01000215 01 0 P00215 0                 UJP      OUT
00213  14700024 14 1  00024 3                 ENQ      20                  20 WORDS OUT
00214  01000227 01 0 P00227 0                 UJP      TBL-2               WRITE THE RECORD
00215  55300000 55 0  00000 3        OUT      EAQ
00216  01400173 01 1 P00173 0                 UJP,I    STORE               RETURN
00217  15200001 15 0  00001 2        NEWLINE  INI      1,2
00220  53200000 53 0  00000 2                 TIA      2
00221  17600003 17 1  00003 2                 ANA      3
00222  03000224 03 0 P00224 0                 AZJ,EQ   *+2                 MOVE UP TO FULL WORD
00223  01000217 01 0 P00217 0                 UJP      NEWLINE
00224  53200000 53 0  00000 2                 TIA      2
00225  13000030 13 0  00030 0                 SHAQ     24
00226  12477775 12 1  77775 0                 SHQ      -2                  DIVIDE BY 4
00227  14600047 14 1 P00047 2                 ENA      LINE
00230  76400001 76 1 P00001 0                 WRITE,I  OUTLUN              OUTPUT A BCD LINE
00231  53020050 53 0  20050 0        TBL      TMA      40B
00232  03300043 03 0 P00043 3                 AZJ,LT   XIT                 TIME TO QUIT****
00233  14100023 14 0  00023 1                 ENI      19,1
00234  20000261 20 0 P00261 0                 LDA      =H
00235  40100047 40 0 P00047 1                 STA      LINE,1              PUT BLANKS IN LINE
00236  02500235 02 1 P00235 1                 IJD      *-1,1
00237  14200000 14 0  00000 2                 ENI      0,2                 INITIALIZE FOR NEW LINE
00240  01000215 01 0 P00215 0                 UJP      OUT
00241  60523635                      TABLE    OCT      60523635
00242  53161514                               OCT      53161514
00243  74345420                               OCT      74345420
00244  73403361                               OCT      73403361
00245  00010203                               OCT      00010203
00246  04050607                               OCT      04050607
00247  10111237                               OCT      10111237
00250  32135777                               OCT      32135777
00251  56212223                               OCT      56212223
00252  24252627                               OCT      24252627
00253  30314142                               OCT      30314142
00254  43444546                               OCT      43444546
00255  47505162                               OCT      47505162
00256  63646566                               OCT      63646566
00257  67707117                               OCT      67707117
00260  75725576                               OCT      75725576
                                              END      IO
```