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CONVERSATIONAL HIGH-RESOLUTION MASS SPECTROGRAPHIC DATA REDUCTION

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16. Abstract

A FORTRAN IV program is described which reduces the data obtained from a high-resolution mass spectrograph. The program (1) calculates an accurate mass for each line on the photoplate, and (2) assigns elemental compositions to each accurate mass. The program is intended for use in a time-shared computing environment and makes use of the conversational aspects of time-sharing operating systems.

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SUMMARY

A FORTRAN IV program is described which reduces the data obtained from a high-resolution mass spectrograph. The program (1) calculates an accurate mass for each line on the photoplate, and (2) assigns elemental compositions to each accurate mass. The program is intended for use in a time-shared computing environment and makes use of the conversational aspects of time-sharing operating systems.

INTRODUCTION

Since the organic chemist first realized the potential of high-resolution mass spectrometry as an analytical tool (ref. 1), a great effort has been spent in developing computer software to process the large amounts of data generated (refs. 2, 3, and 4). The first programs were written for use on large batch computer systems. Recently, however, the emphasis has shifted to programing for relatively small, dedicated computer systems, with the data acquisition and reduction in real-time (refs. 5 and 6).

Obviously, a real-time data system has many advantages, the best of which is immediate data analysis and presentation. In the off-line schemes, typically a day or more separated the data acquisition and the computer analysis of the mass spectra. A disadvantage of the real-time systems is that it takes approximately 20 seconds (ref. 6) (for resolution of one part in 10,000) to acquire a mass spectrum. If greater resolution than one part in 10,000 is desired, even more time is neccessary to obtain the spectrum. For certain applications, for example, a directly coupled gas-chromatograph mass spectrometer, the sample concentration may be so small that it does not remain in the mass spectrometer long enough for the complete mass spectrum to be acquired. For these kinds of applications a photodetection system, which is an integrating detector, is superior to the real-time system.

In the mass spectrometers used in real-time systems (ref. 7), the beam of ions comes to focus at a point. The magnetic field or ion accelerating voltage of the mass spectrometer must be scanned to sweep all the ion types past an electron multiplier at the point of focus. For samples of small concentration, as mentioned above, there may not be enough time to complete the scanning process. On the other hand, in a mass spectrograph (ref. 7), the ion optics of the instrument bring the sample beam to focus in a plane, and a photoplate placed in this plane can continuously record all the ions of the entire mass spectrum. With this scheme, even for small sample quantities, a complete mass spectrum can be obtained. For most of the analytical problems encountered in this laboratory, a photoplate recording system is the preferred method of data acquisition.

The computer program described below is designed to reduce data acquired off-line from a photoplate, but, because it runs on a time-sharing computer, it has some of the advantages of a real-time program. A day or more still separates acquisition of the mass spectrum and its computer analysis, but after the program is in use, it communicates with the user at a conversational terminal and accepts various inputs from the user during execution. As will be discussed later, parameters that affect the calculations in the program must be selected on the basis of various characteristics of each photoplate. With this conversational program, the selections can be made and changed while the program is running, the same as in a real-time system.

SYSTEM OVERVIEW

The high-resolution mass spectrograph (CEC 21–110B) employed at Ames Research Center is of the Mattuch-Herzog geometry. The sample to be analyzed is introduced into the ion source chamber of the mass spectrograph, and is ionized and fragmented by a collimated beam of thermally emitted 70 volt electrons. The positively charged fragments of the sample are accelerated through a focusing slit and passed into a magnetic field where ion-type groupings separate according to their mass. Each charged fragment type forms a slit image on a photoplate placed in the focal plane of the instrument. The photoplate can record up to 45 exposures (mass spectra) of typically several hundred slit images (peaks) each.

Each mass spectrum is transcribed from the photoplate to seven track BCD magnetic tape by a custom-designed comparator-microphotometer interfaced with a tape writing unit. The exposed photographic plate is scanned past the optical density measuring photomultiplier on a precision driven table. When the circuitry senses a line on the photoplate, the table is slowed to tape writing speed, and optical transmittance data are passed to the digitizing circuitry every one-half micron. After the last optical density reading in a slit image profile is recorded, the distance of this last reading, in half microns from the low mass end of the photoplate, is encoded.

At the conclusion of one complete spectrum transcription, the data tape will contain a profile and a distance value for each peak in the mass spectrum. This mass spectrograph data tape is read into disk storage on the Ames Research Center, IBM 360 Model 67 computer under an IBM supplied time-sharing operating system (TSS) and becomes the input file for the data reduction program.

From the shape of the line profiles and the distances of the last optical density readings in each profile, the position of the center of each peak can be determined to within an error of less than one-half micron. The masses of each ion type are related to each other by the square of the distance that separates them. Peaks of known mass are interspersed in the sample spectra by having a mass standard (perfluoroalkane) always present in the ionizing chamber. These peaks of known mass are used to calculate a distance to mass relationship for the length of the photoplate. From this relationship, the masses of the ion types present in the sample spectrum can be determined to within an error of a few parts per million. This mass measurement accuracy is, for the vast majority of problems, sufficient to assign unambiguous elemental compositions to each fragment in the sample spectrum. The final output is a tabular listing of the accurate mass and elemental composition of each peak in the mass spectrum.

COMPUTER PROGRAM DESCRIPTION

The computer program can be logically divided into three sections: peak center calculation, standard mass identification, and accurate mass calculation and element fitting.

Peak Center Calculation

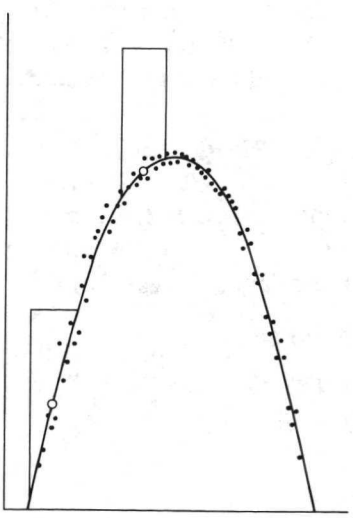
Because the accurate mass calculated for each peak in the mass spectrum can only be determined within the error of the peak center calculations, the determination of the center of each peak profile is the most important aspect of the data reduction process. For an ideal line profile, whose shape is a gaussian distribution curve, the accurate center is easily discerned. In general, however, not all profiles in a spectrum will have a gaussian shape. There will be profiles with complicated shapes that describe lines which are not completely separated, and there will be wide profiles with flat tops that correspond to overexposed lines on the photographic plate. In addition, always superimposed on each profile will be a certain amount of random error commonly referred to as noise. An algorithm for peak center calculation must first attempt to filter out mathematically as much random error as possible, without degrading the underlying profile data, before addressing itself to the determination of the center of each peak.

Data smoothing— On examining a plot of a peak profile, one would tend to draw through the points, a line which best fits them, thereby obtaining the best smooth curve through the points. Numerically, this can be done by fitting a least squares polynomial to the data profile.

The set of points to be smoothed is fit to some polynomial curve.

$$P(x) = \sum_{j=0}^{N} a_j x^j$$

The coefficients designated a are computed so that when the x values are substituted into the polynomial equation, the square of the differences between the computed values and the profile data points are a minimum. Methods used to calculate the a coefficients are described in most textbooks on numerical analysis (refs. 8 and 9). The degree of the polynomial (which can be varied from 1 to 10) and the number of points used (2 to 200) in the moving polynomial smoothing function can be selected and changed while the program is executing. The sketch shows how the smoothing process works, for an overlapping 11 point polynomial.



As in the first grouping in the sketch a new value for the central position in the group is calculated from the least squares polynomial. The point at the left is dropped and a new point added from the right. Again a central point is calculated from the new polynomial and the process is repeated until a smoothed curve is obtained for the entire profile. An intermediate grouping is also indicated in the sketch. All peak profiles in the mass spectrum are smoothed in this fashion.

Peak center calculation– The first derivative of each peak profile is calculated using overlapping polynomials as above. From the shape of the first derivative curve, the number of peaks and the center of each peak in the profile can be determined (ref. 10).

Not all line profiles are analyzed in this fashion. Narrow profiles which can only contain a single peak are analyzed by a scheme that uses less computer time. If the total number of points in the peak profile is below some minimum number (selected during the program execution), the profile is best fit to a gaussian curve and the center and height determined directly from this curve (ref. 4).

$$y = y_{max} \exp\left[-\frac{5.545(x - x_{max})^2}{2w^2}\right]$$

$$ln\, y = ln\, y_{max} - \frac{5.545(x - x_{max})^2}{2w^2}$$

$$ln\, y = \left(ln\, y_{max} - \frac{5.545}{2w^2} x^2_{max}\right) + \left(\frac{5.545 x_{max}}{w^2}\right) x - \left(\frac{5.545}{2w^2}\right) x^2$$

y intensity at position x

y_{max} intensity at the maximum

x_{max} position of the maximum

w half-width

This second degree polynomial can be fit to the entire profile to yield directly the center and height of a peak.

Occasionally, a peak is so overexposed on the photoplate that its shape cannot be properly analyzed by the methods described above. For this contingency a provision exists whereby a profile with an excessively large number of data points (the number is selected during program execution) will be displayed for editing on the conversational terminal. Long leading edges and tails (which are a phenomenon caused by the emulsion on the photoplate during an overexposure) can be eliminated and the profile can otherwise be edited before any further analysis.

Peak intensity calculation— With electrical ion detection, the abundance of each ion type can be accurately determined, but the intensity measurement capabilities of a photoplate are very limited (ref. 11). Because of this limitation, no attempt is made at accurate ion abundance measurements. The largest intensity reading in each profile is used to calculate an approximate relative abundance for each ion type.

A list of peak centers, in millimeters from the left edge of the photoplate, and high intensity values for each peak in the mass spectrum are passed to the standard mass identification portion of the program.

Standard Mass Identification

As mentioned above, not all the lines in a spectrum are due to the analyzed sample; some arise from an internal mass standard (perfluoroalkane). It is the task of this section of the program to identify which peaks correspond to masses from the mass standard and to use these to establish a distance-to-mass relationship for the length of the photoplate.

Mass identification— To begin with, the distances of the first 40 peaks in the list are displayed on the conversational terminal. At this point the program must be supplied the known mass of at least two lines in the table. Using these two (or more) lines, the program will calculate distances where it expects to find 160 of the most prominent peaks in the perfluoroalkane spectrum. Each time the program is successful in its search, it incorporates the new line into its standard mass table. At the end of one search iteration, the program will use the table of identified masses to calculate a distance-to-mass relationship.

Distance to mass conversion— Theoretically, there is a linear relationship between the square root of the mass of each ion type and the distance that separates the ions (ref. 7). In practice, because of inhomogeneous areas in the magnetic field used for separation, the relationship is not exactly linear, but is best approximated by overlapping polynomial functions that are fitted to the standard mass values spread throughout the length of the photoplate. The degree of and the number of points spanned by the polynomials may be selected during the program execution. Generally, the best results are obtained from a second degree polynomial fit to four standard masses. The coefficients of the polynomial are calculated and saved for each overlapping set of calibration masses. To assess the accuracy of the conversion relationship, these polynomials are used to recalculate the masses of the identified standard mass lines, and this information is displayed at the conversational terminal. The difference between the calculated mass and the known mass of the lines of the calibration compound gives a very good idea of the accuracy of the distance-to-mass relationship in the area of interest. At this point misidentified peaks in the list may be deleted, and missed peaks may be added from the conversation terminal. If there has been any input from the user, the program loops back to the standard mass search routine and a new conversion relationship is calculated. This process may be repeated until one is sure that the calculated distance-to-mass relationship is correct.

Element fitting parameters— If there are no additions to or deletions from the standard mass list, the program prompts the user for element fitting parameters. A tolerance for element fitting must be chosen; it is the variance in millimass units between the calculated mass and the mass of an acceptable elemental composition. Next the elements considered for possible compositions must be selected. Carbon, hydrogen, nitrogen, and oxygen are always included in the candidate element table, and as many as seven additional elements may be added for consideration at execution time.

After the element fitting parameters are entered, the user may choose either (1) to write all information calculated thus far into a disk file, where it may be accessed by a program that uses the computer center line printer for output, or (2) to let the program continue with the final results displayed at the conversational terminal. Usually there will be too much information for listing on the relatively slow conversational terminal.

Mass Calculation and Element Fitting

Mass calculation— The distance-to-mass relationship just obtained, is used to calculate an accurate mass for all the lines in the mass spectrum. Each mass is calculated using the polynomial that was fit to the nearest group of calibration masses. Next, all masses corresponding to ion species commonly found in the background of the mass spectrometer and all ion types of the marker compound are eliminated from the list of calculated masses. It is this abbreviated list of accurate masses that represents the mass spectrum of the unknown sample.

Element fitting— All possible permutations of the elements submitted for element fitting are considered as compositions for each of the masses calculated. The minimum number of each isotope considered is zero. The maximum number varies as follows: for carbon-12 it is the integer resulting from the division of the accurate mass by 12; for carbon-13 it is one; for hydrogen it is twice the maximum number of carbon atoms plus eight; for nitrogen-14 it is two; for oxygen-16 it is three. All other isotopes are entered during program execution and the maximum number of each is one of the input parameters. All permutations whose masses fall within the millimass unit tolerance specified are displayed along with the calculated accurate masses.

Output— The final output consists of a relisting of the standard mass table of part II and a table of all calculated masses and their associated elemental compositions. If no permutations of elements fall within the tolerance, the calculated mass is listed with an appropriate comment. There is no provision for special handling of multiply-charged ions in the mass spectrum. Generally, if an obviously multiply-charged species (calculated to be in the vicinity of half an integral mass unit) is doubled, the corresponding singly-charged ion can be found at this value. The accurate mass of the multiply charged ion species is listed with no associated elemental compositions.

CONCLUSIONS

A typical standard mass listing is shown in appendix A. The largest deviation from the exact mass in the entire list is less than five parts per million. This accuracy compares favorably with previously reported high resolution data analysis programs. In addition, for directly coupled gas-chromatograph mass spectrometery applications, a photoplate detection system used with the conversational data reduction system described here is more sensitive and more efficient than previously reported systems.

Ames Research Center
National Aeronautics and Space Administration
Moffett Field, Calif. 94035, March 22, 1973.

APPENDIX A

SAMPLE OF STANDARD MASS ACCURACY

	DISTANCE	CALCULATED MASS	EXACT MASS	DIFFERENCE IN MMU	DIFFERENCE IN PPM
1	15.3497	26.01569	26.01565	0.04	1.47
2	16.9022	27.02342	27.02347	-0.06	2.04
3	18.3888	28.00616	28.00615	0.01	0.29
4	22.7609	30.99844	30.99840	0.04	1.34
5	24.1629	31.98985	31.98983	0.02	0.51
6	29.5927	35.97659	35.97668	-0.09	2.44
7	34.7268	39.96239	39.96239	0.00	0.02
8	39.6593	43.98983	43.98983	-0.00	0.02
9	46.6147	49.99686	49.99680	0.06	1.10
10	47.7399	51.00465	51.00463	0.02	0.43
11	52.0936	54.99833	54.99840	-0.07	1.19
12	59.3566	61.99684	61.99680	0.04	0.71
13	67.1731	69.99841	69.99856	-0.15	2.20
14	70.9115	73.99688	73.99680	0.08	1.10
15	77.2184	80.99519	80.99521	-0.02	0.25
16	81.5609	85.99656	85.99681	-0.25	2.90
17	87.4290	92.99544	92.99521	0.23	2.52
18	93.0803	99.99501	99.99521	-0.20	2.00
19	96.9997	104.99532	104.99521	0.11	1.04
20	102.3302	111.99335	111.99361	-0.26	2.33
21	106.0392	116.99518	116.99521	-0.03	0.26
22	111.0970	123.99365	123.99361	0.04	0.34
23	116.0157	130.99141	130.99202	-0.61	4.68
24	116.7109	131.99539	131.99537	0.02	0.18
25	122.8240	140.99512	140.99521	-0.09	0.61
26	124.1546	142.99197	142.99201	-0.04	0.28
27	126.7720	146.96262	146.96248	0.14	0.95
28	128.7443	149.99033	149.99041	-0.08	0.54
29	131.9597	154.99195	154.99201	-0.06	0.41
30	136.3722	161.99051	161.99041	0.10	0.62
31	139.4679	166.99177	166.99201	-0.24	1.46
32	140.6919	168.98871	168.98882	-0.11	0.62
33	143.7246	173.99051	173.99041	0.10	0.59
34	146.7139	178.99164	178.99201	-0.37	2.08
35	146.8967	180.98895	180.98882	0.13	0.70
36	150.8293	185.99030	185.99041	-0.11	0.61
37	154.8685	192.98889	192.98882	0.07	0.37
38	158.8352	199.98709	199.98722	-0.13	0.65
39	161.6289	204.98894	204.98882	0.12	0.58
40	165.4817	211.98724	211.98722	0.02	0.08
41	168.1976	216.98875	216.98882	-0.07	0.30
42	171.9456	223.98732	223.98722	0.10	0.45
43	174.5880	228.98836	228.98882	-0.46	2.01
44	175.6358	230.98565	230.98562	0.03	0.14
45	178.2386	235.98724	235.98722	0.02	0.10
46	180.8154	240.98862	240.98882	-0.20	0.82
47	181.8369	242.98585	242.98562	0.23	0.95
48	184.3764	247.98717	247.98722	-0.05	0.22
49	187.8883	254.98563	254.98562	0.01	0.04
50	190.3679	259.98745	259.98722	0.23	0.90
51	191.3517	261.98396	261.98402	-0.06	0.24
52	193.8005	266.98578	266.98562	0.16	0.59
53	194.7711	268.98230	268.98242	-0.12	0.45
54	197.1875	273.98413	273.98402	0.11	0.41
55	199.5817	278.98529	278.98562	-0.33	1.17
56	200.5325	280.98243	280.98242	0.01	0.04
57	202.8978	285.98399	285.98402	-0.03	0.11
58	205.2427	290.98575	290.98562	0.13	0.46
59	206.1733	292.98258	292.98242	0.16	0.54
60	208.4914	297.98402	297.98402	-0.00	0.01
61	211.7035	304.98241	304.98242	-0.01	0.03
62	217.1272	316.98269	316.98242	0.27	0.86
63	218.0198	318.97910	318.97923	-0.13	0.41
64	220.2442	323.98096	323.98083	0.13	0.39
65	222.4508	328.98184	328.98242	-0.58	1.76
66	223.3280	330.97922	330.97923	-0.01	0.03
67	225.5114	335.98091	335.98083	0.08	0.25
68	227.6800	340.98186	340.98242	-0.56	1.65
69	228.5419	342.97977	342.97923	0.54	1.59
70	230.6881	347.98047	347.98083	-0.36	1.03
71	233.6681	354.97938	354.97922	0.16	0.44
72	235.7785	359.98078	359.98083	-0.05	0.13
73	238.7097	366.97938	366.97923	0.15	0.42
74	239.5406	368.97603	368.97603	0.00	0.01
75	243.6715	378.97910	378.97923	-0.13	0.34
76	244.4894	380.97594	380.97603	-0.09	0.24
77	246.5286	385.97791	385.97763	0.28	0.72
78	249.3603	392.97586	392.97603	-0.17	0.42
79	254.1604	404.97645	404.97603	0.42	1.05

	DISTANCE	CALCULATED MASS	EXACT MASS	DIFFERENCE IN MMU	DIFFERENCE IN PPM
80	257.3239	412.98206	412.98242	-0.36	0.86
81	258.8923	416.97604	416.97603	0.01	0.02
82	263.5553	428.97626	428.97603	0.23	0.54
83	264.3252	430.97260	430.97284	-0.24	0.55
84	266.2459	435.97467	435.97444	0.23	0.52
85	268.1541	440.97582	440.97603	-0.21	0.48
86	268.9139	442.97233	442.97284	-0.51	1.14
87	273.4419	454.97284	454.97284	0.00	0.01
88	277.9075	466.97284	466.97284	0.00	0.00
89	282.3171	478.97289	478.97284	0.05	0.10
90	283.0455	480.96973	480.96964	0.09	0.20
91	287.3917	492.96960	492.96964	-0.04	0.07
92	291.6849	504.96941	504.96964	-0.23	0.46
93	295.9264	516.96986	516.96964	0.22	0.43
94	300.1182	528.96730	528.96964	-2.34	4.43
95	300.8127	530.96465	530.96445	0.20	0.38
96	304.9507	542.96604	542.96645	-0.41	0.75
97	309.0428	554.96634	554.96645	-0.11	0.21
98	313.0897	566.96659	566.96645	0.14	0.25
99	317.0956	578.96471	578.96645	-1.74	3.01
100	317.7595	580.96341	580.96325	0.16	0.27
101	321.7162	592.96277	592.96325	-0.48	0.80
102	325.6343	604.96374	604.96325	0.49	0.80
103	329.5140	616.96308	616.96325	-0.17	0.27

APPENDIX B

PROGRAM LISTING

```
C     JANUARY 9,1973                                    MICHAEL ROMIEZ
C
C     THIS PROGRAM WILL CONTROL THE READING OF THE AMES HIGH RESOLUTION DATA TAPE INTO A
C     DISK FILE WHICH CAN BE ACCESSED BY THE MAIN DATA REDUCTION PROGRAM.
C
C     THE DATA ON THE TAPE IS ENCODED IN SEVEN TRACK BCD FORMAT; IT IS CONVERTED INTO EBCDIC
C     BY AN AMES LIBRARY SUBROUTINE ALBYTES. THE DATA IS CONVERTED TO INTEGER FORMAT BY AN
C     ASSEMBLY SUBROUTINE TAPERD. THE RAW DATA IN INTGER FORMAT IS WRITTEN INTO A DISK FILE.
C
C                                                       VARIABLES
C
C     IBYTES              - THE NUMBER OF BCD CHARACTERS FOUND IN ONE TAPE RECORD BY SUBROUTINE
C                         - ALBYTES
C     IHOLD(300)          - THE STRING OF CHARACTERS FOUND BY ALBYTES PACKED FOUR TO A WORD IN
C                         - ZONE DECIMAL FORMAT
C     INTTAB(400)         - TABLE OF INTEGER INTENSITY VALUES RETURNED BY SUBROUTINE TAPERD
C     PNTPER(40)          - TABLE OF THE NUMBER OF INTENSITY READINGS PER PEAK IN THE INTTAB
C                         - LIST
C     DISTAB(40)          - TABLE OF DISTANCE VALUES. ONE VALUE FOR EACH PEAK IN PNTPER
C     PEKNUM              - TOTAL NUMBER OF PEAKS IN THE TAPE RECORD
C     TOTP                - TOTAL NUMBER OF INTENSITY READINGS IN THE TAPE RECORD
C     ERR                 - AN ERROR FLAG RETURNED BY SUBROUTINE TAPERD. ERR=0 NORMAL RETURN
C                         - ERR=1 FOR TAPE FORMAT ERROR
C     RAWINT(25000)       - TABLE OF INTENSITY VALUES FOR THE ENTIRE TAPE FILE
C     NUMINT(1000)        - TABLE OF THE NUMBER OF INTENSITY READINGS PER PEAK IN THE ENTIRE
C                         - TAPE FILE
C     RAWDIS(1000)        - TABLE OF DISTANCE READINGS. ONE FOR EACH PEAK IN NUMINT
C     NEXINT              - POINTER TO NEXT VARIABLE IN THE RAWINT ARRAY
C     NEXDIS              - POINTER TO NEXT VARIABLE IN NUMINT AND RAWDIS ARRAYS
C     NOLIST              - LOGICAL VARIABLE TO OPT FOR RAW DATA LISTING. TRUE FOR NO LISTING
C                         - AND FALSE FOR A LISTING
C
C     XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
          LOGICAL NOLIST
          INTEGER DISTAB,PNTPER,PEKNUM,TOTP,ERR
          INTEGER RAWINT,NUMINT,RAWDIS
          COMMON/AMESTP/ IBYTES,IHOLD(300)
          COMMON/MASPEC/ INTTAB(400),PNTPER(40),DISTAB(40),PEKNUM,TOTP,ERR
          COMMON/FILE/RAWINT(25000),NUMINT(1000),RAWDIS(1000)
C  CLEAR ALL COMMON AREAS
          DO 500 N=1,25000
   500    RAWINT(N)=0
          DO 501 N=1,1000
          NUMINT(N)=0
   501    RAWDIS(N)=0
C  NOLIST IS THE LOGICAL VARIABLE TO OPT FOR A PRINTER LISTING OF THE
C  TAPE FILE
          READ(5,50) NOLIST
          NEXINT=1
          NEXDIS=1
  1000    DO 1001 I=1,300
  1001    IHOLD(I)=0
C  BYTES IS AN AMES LIBRARY SUBROUTINE THAT READS ONE RECORD OF A TAPE
C  FILE AT A TIME INTO THE IHOLD ARRAY IN ZONE DECIMAL FORMAT. IERR IS
C  AN ERROR FLAG:  0= NORMAL RETURN; 1= END OF FILE; 2=I/O ERROR
          CALL BYTES(IHOLD,IBYTES,IERR)
          IF(IERR.EQ.1) GO TO 100
          IF(IERR.EQ.2) GO TO 1000
C  TAPERD IS AN ASSEMBLY SUBROUTINE TO UNBLOCK THE DATA TAPE FORMAT
C  AND CONVERT THE ZONE DECIMAL NUMBERS TO INTEGER. ERR=0 FOR NORMAL
C  RETURN; ERR=1 FOR TAPE FORMAT ERROR
     1    CALL TAPERD
          IF(ERR.EQ.1) GO TO 1000
     2    IF(.NOT.NOLIST) GO TO 300
     3    IF(PEKNUM.EQ.0) GO TO 4
          LIMIT1=NEXINT+TOTP-1
          LIMIT2=NEXDIS+PEKNUM-1
          KOUNT1=0
          DO 4001 M=NEXINT,LIMIT1
          KOUNT1=KOUNT1+1
  4001    RAWINT(M)=INTTAB(KOUNT1)
          NEXINT=LIMIT1+1
          KOUNT2=0
          DO 4002 M=NEXDIS,LIMIT2
          KOUNT2=KOUNT2+1
          NUMINT(M)=PNTPER(KOUNT2)
  4002    RAWDIS(M)=DISTAB(KOUNT2)
          NEXDIS=LIMIT2+1
          GO TO 1000
C  UPON READING AN END OF FILE, THE CONTENTS OF THE RAW DATA COMMON
C  BLOCK ARE READ OUT INTO A DISK FILE NAMED IN THE DDEF STATEMENT
     4    NEXINT=NEXINT-1
          NEXDIS=NEXDIS-1
```

```
C    JANUARY 9,1973                                    MICHAEL ROMIEZ
C
       WRITE(7) NEXINT,(RAWINT(I),I=1,NEXINT),NEXDIS,(NUMINT(I),RAWDIS(I),I=1,NEXDIS)
       STOP
C  IF AN END OF FILE HAS BEEN READ THE VARIABLE PEKNUM IS SET TO ZERO
  100  PEKNUM=0
       GO TO 2
C  THIS SECTION WILL PRINT THE CONTENTS OF THE AMES DATA TAPE IF
C  REQUESTED BY SETTING NOLIST EQUAL TO FALSE
  300  IF(PEKNUM.EQ.0) GO TO 4
       LENGTH=IBYTES/4+1
       INTLN=IBYTES/3
       WRITE(6,16)
       WRITE(6,10) IBYTES
       WRITE(6,11) (IHOLD(J),J=1,LENGTH)
       WRITE(6,17)
       WRITE(6,12)(INTTAB(J),J=1,INTLN)
       WRITE(6,13) PNTPER
       WRITE(6,14) DISTAB
       WRITE(6,15) PEKNUM
       GO TO 3
   10 FORMAT(1X,'  THE NUMBER OF CHARACTERS IN THIS RECORD ARE  ',I4)
   11 FORMAT(1X,30A4)
   12 FORMAT(' ','  INTENSITIES',3014)
   13 FORMAT(1X,'PNTPER',2014)
   14 FORMAT(1X,'DISTAB',1018)
   15 FORMAT(1X,'PEKNUM',I4)
   16  FORMAT(1H0)
   17  FORMAT(1HX)
   50  FORMAT(L5)
       END
```

```
*    JANUARY 9,1973                                    MICHAEL ROMIEZ
*
*    THIS SUBROUTINE WILL CONVERT AN AMES HIGH RESOLUTION TAPE RECORD
*    IN EBCDIC FORMAT TO INTEGER FORMAT FOR THE MAIN DATA REDUCTION
*    PROGRAM TO USE.
*
*    XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
TAPE      CSECT
          ENTRY TAPERD
          USING TAPERD,15
TAPERD    SAVE  (14,12)
          LR    2,15
          DROP  15
          USING TAPERD,2
* LOAD AMES COMMON BLOCK ADDRESS INTO REG 3
          L     3,COM1
* LOAD MASPEC COMMON BLOCK ADDRESS INTO REG 4
          L     4,COM2
* THIS LOOP WILL CLEAR MASPEC COMMON BLOCK
          LR    5,4
          L     6,=F'482'
          L     7,=F'0'
CLEAR     ST    7,0(5)
          A     5,=F'4'
          BCT   6,CLEAR
* LOAD REGISTER 5 WITH IBYTES
          L     5,0(0,3)
* ADVANCE AMESTP ADDRESS A FULLWORD TO BEGINNING OF IHOLD ARRAY
          A     3,=F'4'
* INITALIZE THE TOTAL BYTE COUNTER IN REGISTER 5. THIS IS USED TO TEST
* FOR A NORMAL READ WITH THE FOLLOWING LOGIC. IF WE SUBTRACT SIX FROM
* THE TOTAL BYTES INITALLY AND THREE EVERY TIME WE READ AN INTENSITY
* OR SIX EACH TIME WE READ A DISTANCE THEN WHEN THE COUNTER EQUALS ZERO
* THERE SHOULD ONLY BE SIX ALPHABETIC CHARACTERS LEFT IN THE ARRAY.
* IF THIS IS NOT THE CASE WE TELL THE CALLING PROGRAM THAT THERE IS A
* FORMAT ERROR
          S     5,=F'6'
* LOAD REGISTER SIX AS THE TOTAL OPTICAL DENSITY READING COUNTER
          L     6,=F'0'
* LOAD REGISTER 8 AS THE OPICAL DENSITY PER PEAK COUNTER
          L     8,=F'0'
* LOAD REGISTER 9 WITH THE ADDRESS OF PNTPER
          LR    9,4
          A     9,=F'1600'
* LOAD REG 10 WITH THE ADDRESS OF DISTAB
          LR    10,9
          A     10,=F'160'
* LOAD REG 11 WITH THE ADDRESS OF PEKNUM
          LR    11,10
          A     11,=F'160'
* INITALIZE REG 12 AS DISTANCE READING COUNTER
          L     12,=F'0'
* WE BEGIN TO PROCESS THE TAPE RECORD
*
* END OF RECORD TEST
*
TESEND    C     5,=F'2'
          BNH   EXIT
* WE NOW ENTER THE TAPE READ LOGIC
*
TESTCH    TM    0(3),X'F0'
          BNO   DISTCE
          TM    2(3),X'F0'
          BNO   ERROR
* IF THE CHARACTER IS NUMERIC IT IS AN INTENSITY READING
* WE CONVERT IT TO BINARY AND STORE IT IN INTTAB
          PACK  DBL,0(3,3)
* IF THE INTENSITY IS NEGITIVE WE HAVE A TAPE FORMAT ERROR
          CP    DBL,=P'0'
          BNH   ERROR
          CVB   7,DBL
          ST    7,0(0,4)
* INCREMENT THE COUNTERS AND DATA BASE REGISTERS
          A     3,=F'3'
          A     4,=F'4'
          A     8,=F'1'
          A     6,=F'1'
* SUBTRACT THREE FROM TOTAL BYTE COUNTER
          S     5,=F'3'
          B     TESEND
* IF THE CHARACTER IS ALPHABETIC IT IS A DISTANCE READING
* WE CONVERT IT TO BINARY AND STORE IT IN DISTAB
DISTCE    TM    5(3),X'D0'
```

```
*    JANUARY 9,1973                                    MICHAEL ROMIEZ
*
          BNO   ERROR
          PACK  DBL,0(6,3)
* CONVERT THE DISTANCE READING TO A LEGITIMATE POSITIVE NUMBER
          OI    DBL+7,X'0F'
          CVB   7,DBL
          ST    7,0(0,10)
* ADVANCE THE DISTAB BASE REGISTER AND ADD 1 TO THE DISTANCE READING
* COUNTER,SUBTRACT SIX FROM THE TOTAL BYTE COUNTER
          A     10,=F'4'
          A     12,=F'1'
          A     3,=F'6'
          S     5,=F'6'
* STORE THE NUMBER OF OPTICAL DENSITY READINGS FOR THIS PEAK AND
* ADVANCE THE PNTPER BASE REGISTER
          ST    8,0(0,9)
          A     9,=F'4'
* RE INITALIZE THE INTENSITY NUMBER COUNTER
          L     8,=F'0'
          B     TESEND
* IF TAPE FORMAT IS INCORRECT GO TO ERROR EXIT
*
EXIT      TM    0(3),X'F0'
          BO    ERROR
          TM    5(3),X'F0'
          BO    ERROR
* FOR CORRECT TAPE FORMAT TAKE NORMAL EXIT
*
* STORE FINAL DISTANCE READING IN DISTAB
          PACK  DBL,0(6,3)
          OI    DBL+7,X'0F'
          CVB   7,DBL
          ST    7,0(0,10)
* INCREMENT DISTANCE READING COUNTER
          A     12,=F'1'
* STORE THE NUMBER OF OPTICAL DENSITY READINGS IN THE LAST RECORD
* IN PNTPER
          ST    8,0(0,9)
* STORE THE NUMBER OF PEAKS IN THIS RECORD IN PEKNUM
          ST    12,0(0,11)
* WE ADD FOUR TO THE ADDRESS OF PEKNUM TO GET TO TOTP
          A     11,=F'4'
* STORE THE TOTAL NUMBER OF OPTICAL DENSITY READINGS IN THIS RECORD
* IN TOTP
          ST    6,0(0,11)
* WE ADD FOUR TO THE ADDRESS OF TOTP TO GET TO THE ERROR FLAG
          A     11,=F'4'
* THIS IS A NORMAL EXIT STORE ZERO IN ERROR FLAG
          L     4,=F'0'
          ST    4,0(0,11)
          B     OUT
* WE ADD EIGHT TO THE ADDRESS OF PEKNUM TO GET TO THE ERROR FLAG
ERROR     A     11,=F'8'
* THIS IS AN ABNORMAL EXIT STORE ONE IN THE ERROR FLAG
          L     4,-F'1'
          ST    4,0(0,11)
          B     OUT
* RETURN CONTROL TO CALLING PROGRAM
OUT       RETURN (14,12)
          BR    14
DBL       DS    D
COM1      DC    V(AMESTP)
COM2      DC    V(MASPEC)
          END   TAPE
```

```
C     OCTOBER 10,1972                                    MICHAEL ROMIEZ
C
C     THIS IS THE PROGRAM WHICH CALLS THE VARIOUS SUBROUTINES TO REDUCE THE HIGH
C     RESOLUTION MASS SPECTRAL DATA.
C
C     XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
          CALL PARLST
          CALL PKLIST
          CALL STDFIT
          CALL ELELST
          STOP
          END
```

```
C     JANUARY 30,1973                                        MICHAEL ROMIEZ
C
C     THIS SUBROUTINE IS A GENERAL POLYNOMIAL FITTING ALGORITHM. IT WILL FIT UP TO 200
C     DATA POINTS TO A FROM FIRST TO TENTH DEGREE POLYNOMIAL. THE POLYNOMIAL IS BEST FIT
C     IN THE LEAST SQUARES SENSE.
C
C                                                            VARIABLES
C
C     X(200)              - UP TO 200 ABCISSA VALUES
C     Y(200)              - UP TO 200 ORDINATE VALUES
C     C(11)               - UP TO 11 COEFFICIENTS CALCULATED BY THIS SUBROUTINE
C     N                   - THE NUMBER OF DATA POINTS IN THE  X AND Y  ARRAYS
C     IDEG                - THE DEGREE OF THE POLYNOMIAL
C     SUMX(20)            - THE UP TO TWENTY VALUES OF THE SUMMATIONS OF  X  RAISED TO THE
C                         - POWERS OF ONE THROUGH TWICE IDEG INCLUSIVE.
C     SUMXY(10)           - THE UP TO TEN VALUES OF THE SUMMATIONS OF  Y  TIMES  X  RAISED
C                         - TO THE POWERS OF ONE THROUGH IDEG INCLUSIVE.
C     SUMY                - THE SUMMATION OF THE  Y  VALUES
C     A(11,11)            - THE IDEG+1 BY IDEG+1 SQUARE MATRIX OF SUMMATION VALUES FROM
C                         - THE NORMAL EQUATIONS OF THE LEAST SQUARE SYSTEM OF EQUATIONS
C     B(11)               - THE UP TO ELEVEN CONSTANT TERMS OF THE NORMAL EQUATIONS
C     DM(11)              - TEMP STORAGE
C
C     XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
        SUBROUTINE POLYFT
        DOUBLE PRECISION B(11),A(11,11),C(11),DM(11)
        DOUBLE PRECISION SUMX(20),SUMXY(10),SUMY,X(200),Y(200)
        COMMON/FIT/X,Y,N,IDEG,C
C CLEAR VARIABLES
        DO 1000 J=1,10
 1000   SUMXY(J)=0.
        DO 1001 J=1,11
        B(J)=0.
        DM(J)=0.
 1001   C(J)=0.
        DO 1002 J=1,20
 1002   SUMX(J)=0.
        DO 1003 J=1,11
        DO 1003 K=1,11
 1003   A(J,K)=0.
        SUMY=0.
C CALCULATE THE SUMMATION VALUES
        DO 2000 M=1,IDEG
        DO 2000 K=1,N
 2000   SUMXY(M)=SUMXY(M)+Y(K)*X(K)**M
        DO 2001 M=1,N
 2001   SUMY=SUMY+Y(M)
        N2=IDEG*2
        DO 2002 M=1,N2
        DO 2002 K=1,N
 2002   SUMX(M)=SUMX(M)+X(K)**M
C THIS SECTION ASSIGNS THE SUMMATION VALUES TO THE PROPER
C MATRIX ELEMENTS
        LIMIT=IDEG+1
        DO 3001 J=1,LIMIT
        DO 3000 K=1,LIMIT
        M=J+K-2
        IF(M.EQ.0) GO TO 3000
        A(J,K)=SUMX(M)
 3000   CONTINUE
        IF(J.EQ.1) GO TO 3001
        B(J)=SUMXY(J-1)
 3001   CONTINUE
        A(1,1)=N
        B(1)=SUMY
C THIS SECTION CALCULATES THE ELEMENTS OF THE TRIANGULAR MATRIX
        NN=0
        DO 4001 J=1,IDEG
        NN=NN+1
        DO 4001 K=NN,IDEG
        DM(K)=A(K+1,J)/A(J,J)
        DO 4000 L=1,LIMIT
 4000   A(K+1,L)=A(K+1,L)-DM(K)*A(J,L)
        B(K+1)=B(K+1)-DM(K)*B(J)
 4001   CONTINUE
C THIS SECTION CALCULATES THE COEFFICIENTS OF THE CURVE FITTING
C POLYNOMIAL FROM THE TRIANGULAR MATRIX
        M=LIMIT+1
        DO 5001 K=1,LIMIT
        DM(1)=0.DO
        IROW=M-K
        ICOL=M-K
 5000   ICOL=ICOL+1
```

```
C     JANUARY 30,1973                                    MICHAEL ROMIEZ
C
      IF(ICOL.GT.LIMIT) GO TO 5001
      DM(1)=DM(1)-A(IROW,ICOL)*C(ICOL)
      GO TO 5000
 5001 C(IROW)=(B(IROW)+DM(1))/A(IROW,IROW)
      RETURN
      END
```

```
C    FEBRUARY 5,1973                                    MICHAEL ROMIEZ
C
C    THIS MODULE SETS ALL THE VARIABLE PARAMETERS USED BY THE DECONVOLUTION, PEAK CENTER
C    DETERMINATION, AND DISTANCE TO MASS CONVERSION ROUTINES.
C
C    THE VARIABLES HAVE DEFALT VALUES GIVEN AT COMPILATION, BUT THEY MAY BE REVIEWED AND
C    CHANGED AT EXECUTION TIME.
C
C                                                    VARIABLES
C
C    DERDEG            - THE DEGREE OF THE FIRST DERIVATIVE POLYNOMIAL
C    DERNUM            - THE NUMBER OF DATA POINTS USED BY THE FIRST DERIVATIVE POLYNOMIAL
C    SMNUM             - THE NUMBER OF DATA POINTS USED BY THE SMOOTHING POLYNOMIAL
C    SMDEG             - THE DEGREE OF THE SMOOTHING POLYNOMIAL
C    CONNUM            - THE NUMBER OF POINTS USED BY THE DISTANCE TO MASS CONVERSION POLYNOMIAL
C    CONDEG            - THE DEGREE OF THE DISTANCE OF MASS CONVERSION POLYNOMIAL
C    CUTOFF            - IF THE TOTAL NUMBER OF DATA POINTS IN THE PEAK PROFILE IS LESS THAN OR
C                      - EQUAL THIS NUMBER, THE PEAK IS TREATED AS A SINGLE PEAK WITH NO
C                      - DECONVOLUTION ANALYSIS
C    INTMIN            - IF THE PEAK PROFILE CONTAINS NO INTENSITY READINGS ABOVE THIS VALUE, THE
C                      - PEAK IS IGNORED. THIS ABILITY IS USEFUL IN DISCRIMINATION AGAINST SUCH
C                      - ARTIFACTS AS SCRATCHES ON THE PHOTOPLATE
C    TOLFAC            - THIS IS A FACTOR USED BY THE STANDARD MASS SEARCHING ROUTINE TO CALCULATE
C                      - THE TOLERANCE WITHIN WHICH IT WILL ACCEPT A PEAK AS A STANDARD MASS.
C    EXPTOL            - LOWER LIMIT OF THE NUMBER OF INTENSITY VALUES CONSIDERED AN
C                      - OVEREXPOSURE.
C
C    XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      SUBROUTINE PARLST
      INTEGER DERDEG,DERNUM,SMNUM,SMDEG,CUTOFF,CONNUM,CONDEG,TOLFAC,EXPTOL
      INTEGER YES/'Y'/
      COMMON/PAR/DERDEG,DERNUM,SMDEG,SMNUM,CUTOFF,INTMIN,CONNUM,CONDEG,TOLFAC,EXPTOL
      DERDEG=3
      DERNUM=5
      SMNUM=25
      SMDEG=3
      CONNUM=4
      CONDEG=2
      CUTOFF=30
      INTMIN=90
      TOLFAC=7
      EXPTOL=180
      WRITE(6,100)
  100 FORMAT(1X'DO YOU WANT TO REVIEW THE PEAK POSITION PARAMETERS?')
      READ(6,101) I
  101 FORMAT(A1)
      IF(I.NE.YES) RETURN
      WRITE(6,102) DERDEG
  102 FORMAT(1X,'THE DEGREE OF THE FIRST DERIVATIVE POLYNOMIAL IS',13)
      CALL INTGER(M)
      IF(M.NE.0) DERDEG=M
      WRITE(6,103) DERNUM
  103 FORMAT(1X'THE NUMBER OF POINTS USED FOR THE FIRST DERIVATIVE IS',13)
      CALL INTGER(M)
      IF(M.NE.0) DERNUM=M
      WRITE(6,104) SMNUM
  104 FORMAT(1X,'THE NUMBER OF POINTS USED FOR THE SMOOTHING POLYNOMIAL IS',13)
      CALL INTGER(M)
      IF(M.NE.0) SMNUM=M
      WRITE(6,105) SMDEG
  105 FORMAT(1X,'THE DEGREE OF THE POLYNOMIAL USED FOR SMOOTHING IS'13)
      CALL INTGER(M)
      IF(M.NE.0) SMDEG=M
      WRITE(6,108) CONNUM
  108 FORMAT(1X,'THE NUMBER OF MASSES USED BY THE MASS CALCULATION POLYNOMIAL IS',13)
      CALL INTGER(M)
      IF(M.NE.0) CONNUM=M
      WRITE(6,109) CONDEG
  109 FORMAT(1X,'THE DEGREE OF THE MASS CALCULATION POLYNOMIAL IS',13)
      CALL INTGER(M)
      IF(M.NE.0) CONDEG=M
      WRITE(6,106) CUTOFF
  106 FORMAT(1X,'THE CUTOFF VALUE FOR A SINGLE PEAK IS',14)
      CALL INTGER(M)
      IF(M.NE.0) CUTOFF=M
      WRITE(6,107) INTMIN
  107 FORMAT(1X,'THE MINIMUM HIGH INTENSITY FOR A REAL PEAK IS',14)
      CALL INTGER(M)
      IF(M.NE.0) INTMIN=M
     :WRITE(6,110) TOLFAC
  110 FORMAT(1X,'THE SLIDING TOLERANCE FACTOR FOR STANDARD MASS IDENTIFICATION IS',13)
      CALL INTGER(M)
      IF(M.NE.0) TOLFAC=M
```

```
C    FEBRUARY 5,1973                                    MICHAEL ROMIEZ
C
      WRITE(6,111) EXPTOL
  111 FORMAT(1X,'THE NUMBER OF INTENSITY VALUES ABOVE WHICH A PEAK WILL BE EDITED IS',I4)
      CALL INTGER(M)
      IF(M.NE.0) EXPTOL=M
      RETURN
      END
```

```
C     JANUARY 11,1973                                         MICHAEL ROMIEZ
C
C     THIS SUBROUTINE SENDS RAW PEAK PROFILES TO SUBROUTINE PEAK WHICH IN TURN CONTROLS
C     THE SMOOTHING, DECONVOLUTION, AND PEAK CENTER CALCULATION ROUTINES. THIS MODULE
C     SENDS UP TO 400 DATA POINTS TO SUBROUTINE PEAK AND IS RETURNED UP TO TEN PEAK CENTERS
C     AND MAXIMUM INTENSITY VALUES. THESE CENTERS AND INTENSITIES ARE STORED FOR THE REST
C     OF THE DATA REDUCTION ROUTINES.
C
C                                                              VARIABLES
C
C     RAWINT(25000)       - TABLE OF INTENSITY VALUES FOR THE ENTIRE RAW DATA FILE
C     NUMINT(1000)        - TABLE OF THE NUMBER OF INTENSITY READINGS PER PEAK IN THE ENTIRE
C                         - RAW DATA FILE
C     RAWDIS(1000)        - TABLE OF DISTANCE READINGS. ONE FOR EACH PEAK IN NUMINT
C     CENTER(1500)        - DISTANCE OF PEAK CENTERS FROM THE LEFT EDGE OF THE PHOTOPLATE
C                         - IN MILLIMETERS
C     HIGHT(1500)         - MAXIMUM INTENSITY VALUE OF EACH PEAK
C     NUMPK               - NUMBER OF PEAKS IN THE PEAK LIST TABLE
C     LIST(400)           - HOLDING TABLE TO PASS ONE PEAK PROFILE BETWEEN MODULES
C     NUM                 - EITHER THE NUMBER OF INTENSITY VALUES IN THE PEAK PROFILE OR THE
C                         - NUMBER OF PEAK CENTERS RETURNED BY SUBROUTINE PEAK
C     DIS                 - THE DISTANCE IN HALF-MICRONS OF THE LAST INTENSITY READING IN THE
C                         - PEAK PROFILE MEASURED FROM THE LEFT END OF THE PHOTOPLATE
C     CENT(10)            - UP TO 10 PEAK CENTERS RETURNED TO THIS SUBROUTINE FOR EACH PEAK
C                         - PROFILE
C     HGT(10)             - UP TO TEN MAXIMUM INTENSITY VALUES, ONE FOR EACH PEAK IN CENT
C     LSTPAR(10)          - LIST OF PARAMETERS FROM THE PARLIST MODULE
C     PTINT               - POINTS TO NEXT INTENSITY READING IN RAWINT
C     PTDIS               - POINTS TO NEXT POSITION IN THE RAWDIS AND NUMINT ARRAYS
C     PTCENT              - POINTS TO NEXT POSITION IN THE CENTER AND HIGHT ARRAYS
C     INTMIN              - ALL INTENSITY READINGS IN A PROFILE MUST BE ABOVE THIS VALUE
C                         - OR THE PEAK IS IGNORED. THIS IS USEFUL IN DISCRIMINATING AGAINST
C                         - SCRATCHES ON THE PHOTOPLATE
C     IEDIT               - LOWER LIMIT OF THE NUMBER OF INTENSITY READINGS FOR EDITING
C
C     XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      SUBROUTINE PKLIST
      DOUBLE PRECISION CENTER,CENT(10)
      INTEGER RAWINT(25000),NUMINT(1000),RAWDIS(1000)
      INTEGER PTDIS,PTINT,LIST(400),PTCENT,DIS
      INTEGER YES/'Y'/
      DIMENSION HGT(10)
      COMMON/PKLST/ CENTER(1500),HIGHT(1500),NUMPK
      COMMON/PK/LIST,NUM,DIS,CENT,HGT
      COMMON/PAR/LSTPAR(10)
C SET THE INTMIN VALUE AS GIVEN BY THE PARAMETER LIST MODULE
      INTMIN=LSTPAR(6)
C SET THE LOWER LIMIT OF THE NUMBER OF INTENSITY READINGS FOR PROFILE EDITING
      IEDIT=LSTPAR(10)
C CLEAR VARIABLES
      DO 100 M=1,1500
      CENTER(M)=0.
  100 HIGHT(M)=0.
      DO 150 M=1,25000
  150 RAWINT(M)=0
      DO 151 M=1,1000
      RAWDIS(M)=0
  151 NUMINT(M)=0
C READ IN RAW DATA FROM DISK FILE
      READ(9) N,(RAWINT(I),I=1,N),M,(NUMINT(I),RAWDIS(I),I=1,M)
      PTINT=0
      PTDIS=1
      PTCENT=0
   10 DO 15 I=1,10
      HGT(I)=0.
   15 CENT(I)=0.
C RETURN IF THERE ARE NO MORE PROFILES IN THE RAW DATA FILE
      IF(NUMINT(PTDIS).EQ.0) GO TO 9999
C IF THERE ARE MORE THAN 400 POINTS IN A PARTICULAR PEAK PROFILE, THE PEAK IS
C IGNORED. A PEAK 200 MICRONS WIDE IS TOO WIDE TO BE A REAL PEAK.
      IF(NUMINT(PTDIS).GT.400) GO TO 11
      IF(NUMINT(PTDIS).GT.4) GO TO 200
C IF A PROFILE HAS FEWER THAN 5 INTENSITY READINGS IT IS DELETED AS A NOISE SPIKE
   11 PTDIS=PTDIS+1
      PTINT=PTINT+NUMINT(PTDIS-1)
      GO TO 10
C READ PEAK PROFILE AND DISTANCE INTO DATA PASSING ARRAYS
  200 NUM=NUMINT(PTDIS)
      DO 225 I=1,400
  225 LIST(I)=0
      DO 250 J=1,NUM
      PTINT=PTINT+1
  250 LIST(J)=RAWINT(PTINT)
      DIS=RAWDIS(PTDIS)
```

```
C    JANUARY 11,1973                                    MICHAEL ROMIEZ
C
C IF THE HIGHEST INTENSITY VALUE IS LESS THAN INTMIN IGNORE THE PEAK
      DO 275 J=1,NUM
      IF(LIST(J).GT.INTMIN) GO TO 290
  275 CONTINUE
      PTDIS=PTDIS+1
      GO TO 10
C IF THERE ARE MORE THAN IEDIT INTENSITY READINGS IN A PEAK PROFILE, IT IS AN
C OVEREXPOSURE AND IS DISPLAYED FOR POSSIBLE EDITING.
  290 IF(NUM.GT.IEDIT) CALL EDIT
C SEND PEAK PROFILE TO BE ANALYZED
      CALL PEAK
C KEEP PEAK CENTERS AND INTENSITIES IN CENTER AND HIGHT ARRAYS
      DO 299 M=1,NUM
      PTCENT=PTCENT+1
C THE PEAK CENTER VALUES ARE CONVERTED FROM HALF-MICRONS TO MILLIMETERS
      CENTER(PTCENT)=CENT(M)/2000.
C THE DISTANCE ENCODER RECYCLES AT 255 MILLIMETERS AND THIS TEST
C COMPENSATES FOR RECYCLING.
      IF(PTCENT.EQ.1) GO TO 299
      IF(CENTER(PTCENT).LT.CENTER(PTCENT-1).AND.CENTER(PTCENT-1)-
     X.GT.200) CENTER(PTCENT)=CENTER(PTCENT)+255.
  299 HEIGHT(PTCENT)=HGT(M)
C THIS TEST WILL TRUNCATE THE PEAK LIST IF IT APPROACHES WITHIN 10 VARIABLES OF
C THE END OF THE ARRAY
      IF(PTCENT.GT.1490) GO TO 400
      PTDIS=PTDIS+1
      GO TO 10
  400 WRITE(6,1)
    1 FORMAT('0','THE PEAK LIST WAS TRUNCATED AT',I6,' VALUES')
 9999 NUMPK=PTCENT
      RETURN
      END
```

```
C    JANUARY 17,1973                                    MICHAEL ROMIEZ
C
C    THIS SUBROUTINE CONTROLS DATA SMOOTHING, PEAK DECONVOLUTION, AND PEAK CENTER CALCULATION
C
C                                                         VARIABLES
C
C    LIST(400)          - HOLDING TABLE TO PASS ONE PEAK PROFILE BETWEEN MODULES
C    NUM                - EITHER THE NUMBER OF INTENSITY VALUES IN THE PEAK PROFILE OR THE
C                       - NUMBER OF PEAK CENTERS RETURNED BY SUBROUTINE ANAL
C    DIS                - THE DISTANCE IN HALF-MICRONS OF THE LAST INTENSITY READING IN THE
C                       - PEAK PROFILE MEASURED FROM THE LEFT END OF THE PHOTOPLATE
C    CENT(10)           - UP TO 10 PEAK CENTERS RETURNED TO THIS SUBROUTINE FOR EACH PEAK
C                       - PROFILE
C    HGT(10)            - UP TO TEN MAXIMUM INTENSITY VALUES, ONE FOR EACH PEAK IN CENT
C    LSTPAR(10)         - LIST OF PARAMETERS FROM THE PARLIST MODULE
C    NUMSM              - NUMBER OF POINTS USED BY THE SMOOTHING ROUTINE
C    CUTOFF             - MINIMUM NUMBER OF POINTS FOR A PROFILE TO BE ANALYZED FOR
C                       - MORE THAN ONE PEAK. PROFILES WITH LESS THAN CUTOFF DATA
C                       - POINTS WILL BE TREATED AS A SINGLE PEAK
C
C    XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      SUBROUTINE PEAK
      DOUBLE PRECISION CENT(10)
      INTEGER DIS,CUTOFF
      DIMENSION HGT(10),LIST(400)
      COMMON/PAR/LSTPAR(10)
      COMMON/PK/LIST,NUM,DIS,CENT,HGT
C SET THE PARAMETERS FOR THE NUMBER OF POINTS USED BY THE SMOOTHING ROUTINE AND
C THE MINIMUM NUMBER OF POINTS IN A PROFILE CONSIDERED FOR DECONVOLUTION ANALYSIS
      NUMSM=LSTPAR(4)
      CUTOFF=LSTPAR(5)
C IF THERE ARE LESS THAN CUTOFF DATA POINTS, THIS IS A SINGLE PEAK
      IF(NUM.GT.CUTOFF) GO TO 100
C IF THERE ARE ENOUGH RAW DATA POINTS IN THE PROFILE, SMOOTH THE DATA
C BEFORE SENDING IT TO MODULE ONEPK
      IF(NUM.GT.(NUMSM+10)) GO TO 150
      CALL ONEPK
      RETURN
  150 CALL SMOOTH
C THE DATA SMOOTHING ROUTINE RETURNS (NUMSM-1) LESS DATA POINTS THAN WAS IN THE
C RAW DATA. THE DISTANCE VALUE WHICH INDICATES THE DISTANCE OF THE LAST DATA POINT
C IN THE LIST MUST BE ADJUSTED
      DIS=DIS-((NUMSM-1)/2)
      CALL ONEPK
      RETURN
C SMOOTH THE DATA
  100 CALL SMOOTH
C THE DATA SMOOTHING ROUTINE RETURNS (NUMSM-1) LESS DATA POINTS THAN WAS IN THE
C RAW DATA. THE DISTANCE VALUE WHICH INDICATES THE DISTANCE OF THE LAST DATA POINT
C IN THE LIST MUST BE ADJUSTED
      DIS=DIS-((NUMSM-1)/2)
C SUBROUTINE ANAL USES THE FIRST DERIVATIVE TO DETERMINE IF THERE IS MORE THAN ONE
C PEAK IN A PARTICULAR SMOOTHED PROFILE
      CALL ANAL
      RETURN
      END
```

```
C     JANUARY 16,1973                                          MICHAEL ROMIEZ
C
C     THIS ROUTINE CALLS A GENERAL LEAST SQUARE POLYNOMIAL FITTING ROUTINE TO SMOOTH
C     THE PROFILE DATA. IT RETURNS NUM LESS (NUMSUM-1) SMOOTHED DATA POINTS. THE DEGREE
C     OF THE POLYNOMIAL AND THE NUMBER OF DATA POINTS USED FOR SMOOTHING IS SELECTED IN
C     PARAMETER SELECTING SUBROUTINE PARLST.
C
C                                                               VARIABLES
C
C     LIST(400)           - HOLDING TABLE TO PASS ONE PEAK PROFILE BETWEEN MODULES
C     NUM                 - THE NUMBER OF INTENSITY VALUES IN THE PEAK PROFILE
C     DIS                 - THE DISTANCE IN HALF-MICRONS OF THE LAST INTENSITY READING IN THE
C                         - PEAK PROFILE MEASURED FROM THE LEFT END OF THE PHOTOPLATE
C     CENT(10)            - UP TO 10 PEAK CENTERS
C     HGT(10)             - UP TO TEN MAXIMUM INTENSITY VALUES, ONE FOR EACH PEAK IN CENT
C     LSTPAR(10)          - LIST OF PARAMETERS FROM THE PARLIST MODULE
C     X(200)              - UP TO 200 ABCISSA VALUES TO BE PASSED TO THE POLYNOMIAL FITTING
C                         - ROUTINE
C     Y(200)              - UP TO 200 ORDINATE VALUES TO BE PASSED TO THE POLYNOMIAL FITTING
C                         - ROUTINE
C     N                   - NUMBER OF  X AND Y  VALUES PASSED
C     IDEG                - DEGREE OF THE POLYNOMIAL (UP TO TENTH POSSIBLE)
C     C(11)               - UP TO 11 COEFFICIENTS RETURNED BY THE POLYNOMIAL ROUTINE
C     DEGSM               - DEGREE OF THE SMOOTHING POLYNOMIAL, SUPPLIED BY THE PARLST MODULE
C     NUMSM               - NUMBER OF DATA POINTS USED BY THE SMOOTHING POLYNOMIAL, SUPPLIED
C                         - BY THE PARLST MODULE
C     HOLD(400)           - TEMPORARY STORAGE USED BY THIS MODULE
C
C     XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      SUBROUTINE SMOOTH
      DOUBLE PRECISION X(200),Y(200),C(11),CENT(10)
      DIMENSION LIST(400),HGT(10)
      INTEGER DIS,DEGSM,HOLD(400)
      COMMON/PAR/LSTPAR(10)
      COMMON/FIT/X,Y,N,IDEG,C
      COMMON/PK/LIST,NUM,DIS,CENT,HGT
C SET THE DEGREE AND NUMBER OF POINTS USED BY THE SMOOTHING POLYNOMIAL
      DEGSM=LSTPAR(3)
      NUMSM=LSTPAR(4)
C CLEAR TEMP STORAGE
      DO 100 M=1,400
  100 HOLD(M)=0
      LIMIT=NUMSM-1
      M=NUM-LIMIT
C LOAD RAW DATA POINTS INTO  X AND Y  ARRAYS
      DO 10 I=2,NUMSM
      J=I-1
   10 Y(I)=DFLOAT(LIST(J))
      DO 150 L=1,NUMSM
  150 X(L)=DFLOAT(L)
      IDEG=DEGSM
      N=NUMSM
C THIS DO LOOP (DOWN TO STMT 200) CONTROLS THE SENDING OF NUMSM RAW DATA POINTS TO THE
C POLYNOMIAL ROUTINE TO OBTAIN THE SMOOTHED DATA POINTS. ALL NUMSM DATA POINTS ARE USED
C TO CALCULATE ONE SMOOTH DATA POINT. THE LOWEST RAW DATA POINT IS DISCARDED AND THE
C REMAINING POINTS ARE MOVED DOWN ONE POSITION. A NEW HIGH DATA POINT IS READ IN FROM THE
C PROFILE DATA AND THE NEXT SMOOTHED DATA POINT IS CALCULATED. THE PROCESS IS REPEATED
C UNTIL WE HAVE NUM-(NUMSM-1) SMOOTHED DATA POINTS.
      DO 200 I=1,M
      J=I+LIMIT
      DO 11 K=1,LIMIT
      KA=K+1
   11 Y(K)=Y(KA)
      Y(NUMSM)=DFLOAT(LIST(J))
      CALL POLYFT
      INDEX1=J-LIMIT
      INDEX2=LIMIT/2+1
      HOLD(INDEX1)=C(1)
      DO 200 L=1,DEGSM
      LL=L+1
C PUT THE CALCULATED SMOOTH DATA POINT INTO ARRAY HOLD FOR TEMP STORAGE
  200 HOLD(INDEX1)=HOLD(INDEX1)+C(LL)*FLOAT(INDEX2)**L
C CHANGE THE VALUE OF NUM TO THE NEW NUMBER OF DATA POINTS IN THE PROFILE AFTER
C SMOOTHING
      NUM=NUM-LIMIT
C THE LAST TWO DO LOOPS MOVE THE SMOOTH DATA POINTS FROM TEMP STORAGE BACK TO THE
C PROFILE PASSING ARRAY
      DO 300 L=1,NUM
  300 LIST(L)=HOLD(L)
      ISTRT=NUM+1
      ISTOP=NUM+NUMSM
      DO 301 K=ISTRT,ISTOP
  301 LIST(K)=0
      RETURN
      END
```

```
C     JANUARY 16,1973                                              MICHAEL ROMIEZ
C
C     THIS MODULE CALLS THE GENERAL LEAST SQUARE FITTING ROUTINE TO CALCULATE A FIRST DERIVATIVE
C     OF THE SMOOTHED PEAK PROFILE. THE FIRST DERIVATIVE IS FOUND BY OVERLAPPING POLYNOMIALS
C     IN THE SAME MANNER AS THE SMOOTHING ALGORITHM.
C
C                                                                    VARIABLES
C
C     LIST(400)          - HOLDING TABLE TO PASS ONE PEAK PROFILE BETWEEN MODULES
C     NUM                - THE NUMBER OF INTENSITY VALUES IN THE PEAK PROFILE OR THE NUMBER
C                        - OF PEAKS FOUND BY THIS MODULE
C     DIS                - THE DISTANCE IN HALF-MICRONS OF THE LAST INTENSITY READING IN THE
C                        - PEAK PROFILE MEASURED FROM THE LEFT END OF THE PHOTOPLATE
C     CENT(10)           - UP TO 10 PEAK CENTERS
C     HGT(10)            - UP TO TEN MAXIMUM INTENSITY VALUES, ONE FOR EACH PEAK IN CENT
C     LSTPAR(10)         - LIST OF PARAMETERS FROM THE PARLIST MODULE
C     X(200)             - UP TO 200 ABCISSA VALUES TO BE PASSED TO THE POLYNOMIAL FITTING
C                        - ROUTINE
C     Y(200)             - UP TO 200 ORDINATE VALUES TO BE PASSED TO THE POLYNOMIAL FITTING
C                        - ROUTINE
C     N                  - NUMBER OF  X AND Y  VALUES PASSED
C     IDEG               - DEGREE OF THE POLYNOMIAL (UP TO TENTH POSSIBLE)
C     C(11)              - UP TO 11 COEFFICIENTS RETURNED BY THE POLYNOMIAL ROUTINE
C     DEGFT              - DEGREE OF THE 1ST DERIVATIVE POLYNOMIAL,SUPPLIED BY THE PARLST MODULE
C     NUMFT              - NUMBER OF DATA POINTS USED BY THE 1ST DERIVATIVE POLYNOMIAL, SUPPLIED
C                        - BY THE PARLST MODULE
C     FSTDER(400)        - TABLE OF FIRST DERIVATIVE POINTS AS CALCULATED BY THIS MODULE
C     INDEX1             - POINTER FOR THE FSTDER ARRAY
C     INDEX2             - POINTS TO THE CENTER OF THE NUMFT POINTS USED BY THE POLYNOMIAL
C     INDEX3             - POINTS TO THE LAST USED POSITION IN THE FSTDER ARRAY
C
C     XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      SUBROUTINE ANAL
      DOUBLE PRECISION CENT(10),C(11),X(200),Y(200)
      DIMENSION LIST(400),HGT(10),FSTDER(400)
      INTEGER DIS,DEGFT,HOLD(400)
      COMMON/FIT/X,Y,N,IDEG,C
      COMMON/PAR/LSTPAR(10)
      COMMON/PK/LIST,NUM,DIS,CENT,HGT
C SET THE DEGREE AND NUMBER OF POINTS USED BY THE 1ST DERIVATIVE POLYNOMIAL
      DEGFT=LSTPAR(1)
      NUMFT=LSTPAR(2)
C CLEAR VARIABLES
      DO 100 M=1,400
  100 FSTDER(M)=0.
      DO 110 M=1,200
      X(M)=0.
  110 Y(M)=0.
      IDEG=DEGFT
      N=NUMFT
      LIMIT=NUMFT-1
      M=NUM-LIMIT
C LOAD DATA POINTS INTO  X AND Y  ARRAYS
      DO 10 I=2,NUMFT
      J=I-1
   10 Y(I)=DFLOAT(LIST(J))
      DO 150 L=1,NUMFT
  150 X(L)=DFLOAT(L)
C THIS DO LOOP (DOWN TO STMT 200) CONTROLS THE SENDING OF NUMFT DATA POINTS TO THE
C POLYNOMIAL ROUTINE TO OBTAIN THE 1ST DERIVATIVE CURVE. ALL NUMSM DATA POINTS ARE USED
C TO CALCULATE ONE 1ST DERIVATIVE DATA POINT. THE LOWEST DATA POINT IS DISCARDED AND THE
C REMAINING POINTS ARE MOVED DOWN ONE POSITION. A NEW HIGH DATA POINT IS READ IN FROM THE
C PROFILE DATA AND THE NEXT 1ST DERIVATIVE POINT IS CALCULATED. THE PROCESS IS REPEATED
C UNTIL WE HAVE NUM-(NUMFT-1) 1ST DERIVATIVE POINTS.
      DO 200 I=1,M
      J=I+LIMIT
      DO 11 K=1,LIMIT
      KA=K+1
   11 Y(K)=Y(KA)
      Y(NUMFT)=DFLOAT(LIST(J))
      CALL POLYFT
      INDEX1-J-LIMIT
      INDEX2=LIMIT/2+1
      FSTDER(INDEX1)=C(2)
      DO 200 L=2,DEGFT
      LL=L+1
      LLL=L-1
  200 FSTDER(INDEX1)=FSTDER(INDEX1)+DFLOAT(L)*C(LL)*DEFLOAT(INDEX2)**LLL
      INDEX3=NUM-LIMIT
C THIS SECTION SEARCHES THROUGH THE FIRST DERIVATIVE CURVE TO LOCATE THE CENTER OF AND
C HEIGHT OF UP TO TEN PEAKS CONTAINED IN EACH PEAK PROFILE. IN THIS SECTION  J  IS THE CENT
C AND HGT ARRAY POINTER AND  M  IS THE FSTDER ARRAY POINTER.
```

```
C    JANUARY 16,1973                                    MICHAEL ROMIEZ
C
       J=1
       M=0
     1 M=M+1
       IF(M.GT.INDEX3-1) GO TO 99
C UPSLOPE LOGIC
       IF(FSTDER(M+1)-FSTDER(M))3,1,1
     2 M=M+1
       IF (M.GT.INDEX3) GO TO 99
C WE HAVE JUST STARTED DOWN THE SIDE OF THE FIRST DERIVATIVE CURVE. WE CONTINUE DOWN
C UNTIL WE GO THROUGH THE X-AXIS. THE POINT AT WHICH THE FIRST DERIVATIVE CURVE PASSES
C THROUGH THE X-AXIS GOING FROM POSITIVE TO NEGATIVE, IS THE CENTER OF A PEAK.
     3 IF(FSTDER(M).GT.0.) GO TO 2
C THE NEXT SIX STATEMENTS CALCULATE THE CENTER AND HEIGHT OF THE JUST FOUND PEAK
       DHIGH=FSTDER(M-1)
       DLOW=ABS(FSTDER(M))
       CENT(J)=FLOAT(M-1)+DHIGH/DHIGH+DLOW)
       CENT(J)=CENT(J)+LIMIT/2
       K-M+LIMIT/2
       HGT(J)=LIST(K)
C IF THIS MODULE HAS ALREADY FOUND TEN PEAKS, STOP LOOKING
       J=J+1
       IF(J.GT.10) GO TO 99
C THIS LOOP TESTS IF THE FIRST DERIVATIVE CURVE GOES BACK ABOVE THE X-AXIS. IF IT
C DOES IT CAUSES A BRANCH TO THE UPSLOPE LOGIC SECTION
       DO 80 K=M,INDEX3
       IF(FSTDER(K).LT.0.) GO TO 80
       GO TO 101
    80 CONTINUE
       GO TO 99
   101 M=K-1
       GO TO 1
    99 NN=J-1
C THE CENTER OF EACH PEAK FOUND BY THIS MODULE IS CALCULATED IN TERMS OF THE DISTANCE
C IN HALF-MICRONS FROM THE LEFT EDGE OF THE PHOTO PLATE.
       DO 89 K=1,NN
    89 CENT(K)=DIS-(NUM-CENT(K))
C NUM IS SET TO THE NUMBER OF PEAKS FOUND
       NUM=NN
       RETURN
       END
```

```
C     JANUARY 17,1973                                     MICHAEL ROMIEZ
C
C     THIS SUBROUTINE WILL DETERMINE THE CENTER AND HIGHT OF A SINGLE PEAK. IT FITS
C     THE PEAK PROFILE TO A GAUSSIAN DISTRIBUTION CURVE.
C
C                                                         VARIABLES
C
C     X(200)           - UP TO 200 POINTS THAT ARE USED BY THE POLYNOMIAL FITTING
C                      - ROUTINE FOR THE BEST LEAST SQUARES GAUSSIAN FIT
C     Y(200)           - ONE ORDINATE VALUE FOR EACH X VALUE
C     N                - NUMBER OF  X AND Y  VALUES
C     IDEG             - IN THIS CASE IDEG=2. IT IS THE DEGREE OF THE POLYNOMIAL USED
C                      - FOR FITTING
C     C(11)            - THE FIRST THREE VALUES OF THE ARRAY CONTAIN THE COEFFICIENTS OF
C                      - THE SECOND DEGREE POLYNOMIAL
C     LIST(400)        - HOLDING TABLE TO PASS PEAK PROFILES BETWEEN MODULES
C     NUM              - EITHER THE NUMBER OF INTENSITIES IN THE PEAK PROFILE OR NUM=1
C                      - TO INDICATE THE NUMBER OF PEAKS FOUND BY THIS MODULE
C     DIS              - THE DISTANCE IN HALF-MICRONS OF THE LAST INTENSITY READING IN
C                      - THE PROFILE AS MEASURED FROM THE LEFT END OF THE PHOTOGRAPHIC
C                      - PLATE
C     CENT(10)         - THE CENTER CALCULATED BY THIS MODULE IS PUT IN CENT(1)
C     HGT(10)          - THE HEIGHT CALCULATED BY THIS MODULE IS PUT IN HGT(1)
C
C     XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      SUBROUTINE ONEPK
      DOUBLE PRECISION CENT(10),C(11),X(200),Y(200)
      INTEGER DIS
      DIMENSION HGT(10),LIST(400)
      COMMON/FIT/X,Y,N,IDEG,C
      COMMON/PK/LIST,NUM,DIS,CENT,HGT
      IF(NUM.GT.200) RETURN
      N=NUM
      IDEG=2
C PUT THE LOG OF THE INTENSITY VALUE IN THE ORDINATE LIST
      DO 50 J=1,NUM
      X(J)=DFLOAT(J)
   50 Y(J)=DLOG(DFLOAT(LIST(J)))
C CALL THE POLYNOMIAL FITTING ROUTINE
      CALL POLYFT
      IF(C(3).GT.0.) GO TO 99
C CALCULATE THE CENTER AND HEIGHT OF THE PEAK FROM THE COEFFICIENTS OF THE POLYNOMIAL
      CENT(1)=(-C(2)/C(3))/2.
      HGT(1)=C(1)+(CENT(1)/SQRT(-1./C(3)))**2
      HGT(1)=EXP(HGT(1))
      CENT(1)=DIS-(NUM-CENT(1))
      NUM=1
   99 RETURN
      END
```

```
C    FEBRUARY 3,1973                                    MICHAEL ROMIEZ
C
C    THIS MODULE WILL ALLOW EDITING OF THE RAW PEAK PROFILE. PART OF THE PROFILE MAY BE
C    DELETED AND SELECTED INTENSITY READINGS MAY BE CHANGED.
C
C                                                       VARIABLES
C
C    LIST(400)          - HOLDING TABLE TO PASS ONE PEAK PROFILE BETWEEN MODULES
C    NUM                - THE NUMBER OF INTENSITY VALUES IN THE PEAK PROFILE
C    DIS                - THE DISTANCE IN HALF-MICRONS OF THE LAST INTENSITY READING IN THE
C                       - PEAK PROFILE MEASURED FROM THE LEFT END OF THE PHOTOPLATE
C    CENT(10)           - UP TO 10 PEAK CENTERS
C    HGT(10)            - UP TO TEN MAXIMUM INTENSITY VALUES, ONE FOR EACH PEAK IN CENT
C
C    XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      SUBROUTINE EDIT
      DOUBLE PRECISION CENT(10)
      INTEGER LIST(400),DIS
      DIMENSION HGT(10)
      COMMON/PK/LIST,NUM,DIS,CENT,HGT
      DATA IYES/'Y'/
C THIS SECTION LISTS THE RAW PEAK PROFILE
      WRITE(6,100)
  100 FORMAT('0','PEAK PROFILE')
      WRITE(6,101)(LIST(I),I=1,NUM)
  101 FORMAT(5X,2015)
C THIS SECTION WILL DELETE PART OF THE PEAK PROFILE. IT WILL ACCEPT A LOW AND HIGH
C SUBSCRIPT AND ADJUST THE INTENSITY READINGS IN ARRAY LIST TO THESE NEW VALUES.
C IF THE NEW LOW SUBSCRIPT ENTERED IS GREATER THAN NUM, THIS SECTION WILL BE SKIPPED.
      WRITE(6,102)
  102 FORMAT('0','ENTER A NEW STARTING INTENSITY')
      CALL INTGER(LOW)
      IF(LOW.GT.NUM) GO TO 400
      IF (I.EQ.1) GO TO 200
      LIMIT=NUM-(LOW-1)
      DO 150 J=1,LIMIT
      INDEX=LOW-1+J
  150 LIST(J)=LIST(INDEX)
  200 WRITE(6,104)
  104 FORMAT('0','ENTER NEW ENDING SUBSCRIPT')
C IF NOTHING IS ENTERED FOR THE ENDING SUBSCRIPT, THE OLD VALUE IS KEPT.
      CALL INTGER(IHIGH)
      IF(IHIGH.EQ.0) IHIGH=NUM
      IF(IHIGH.EQ.NUM) GO TO 300
      ISTRT=IHIGH+1
      DO 250 J=ISTRT,NUM
  250 LIST(J)=0
      DIST=DIS-(NUM-IHIGH)
  300 NUM=NUM-(NUM-IHIGH)-(LOW-1)
C THIS SECTION WILL ACCEPT INTENSITY VALUE CHANGES
  400 WRITE(6,105)
  105 FORMAT('0','ANY INTENSITY EDITING?')
      READ(5,106) I
  106 FORMAT(A1)
      IF(I.NE.IYES) RETURN
      WRITE(6,101)(LIST(I),I=1,NUM)
  405 WRITE(6,107)
  107 FORMAT(1X,'ENTER SUBSCRIPT')
      CALL INTGER(M)
      IF(M.EQ.0) RETURN
      WRITE(6,108)
  108 FORMAT(1X,'ENTER INTENSITY')
      CALL INTGER(N)
      LIST(M)=N
      GO TO 450
      END
```

```
C    JANUARY 26,1973                                    MICHAEL ROMIEZ
C
C    THIS SUBROUTINE CONTROLS THE STANDARD MASS SEARCH AND LISTING ROUTINES
C
C                                                         VARIABLES
C
C    CENTER(1500)       - DISTANCE OF PEAK CENTERS FROM THE LEFT EDGE OF THE PHOTOPLATE
C                       - IN MILLIMETERS
C    HIGHT(1500)        - MAXIMUM INTENSITY VALUE OF EACH PEAK
C    NUMPK              - NUMBER OF PEAKS IN THE PEAK LIST TABLE
C    STDDIS(160)        - THE DISTANCE VALUES OF PEAK CENTERS IDENTIFIED AS STANDARD MASSES
C    STDMAS(160)        - THE SQUARE ROOT OF THE MASS VALUE OF IDENTIFIED STANDARD MASSES
C    NUMSTD             - THE NUMBER OF IDENTIFIED STANDARD MASSES
C    REFMAS(160)        - A TABLE OF THE MOST INTENSE LINES IN THE MARKER COMPOUND SPECTRUM.
C                       - THESE ARE THE MASSES SEARCHED FOR BY THE STANDARD MASS IDENTIFICATION
C                       - ROUTINE
C
C    XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
       SUBROUTINE STDFIT
       DOUBLE PRECISION CENTER,STDDIS(160),STDMAS(160),REFMAS(160)
       INTEGER YES/'Y'/
       COMMON/PKLST/ CENTER(1500),HIGHT(1500),NUMPK
       COMMON/PFKLST/ STDDIS,STDMAS,REFMAS,NUMSTD
C CLEAR VARIABLES
       DO 99 M=1,160
       STDDIS(M)=0.
    99 STDMAS(M)=0.
C READ IN THE STANDARD MASSES AND GET THEIR SQUARE ROOT
       READ(7) REFMAS
       DO 100 M=1,160
   100 REFMAS(M)=DSQRT(REFMAS(M))
C LIST UP TO THE FIRST FORTY DISTANCE VALUES IN ARRAY CENTER ON THE OUTPUT TERMINAL
       I=NUMPK
       IF(I.GT.40) I=40
       WRITE(6,1) I
     1 FORMAT('0','THESE ARE THE FIRST',I3,'DISTANCE VALUES')
       WRITE(6,2)(CENTER(J),J=1,I)
     2 FORMAT(1X,10F12.5)
       NUMSTD=0
     3 NUMSTD=NUMSTD+1
C THE PROGRAM USER MUST ENTER A KNOWN MASS VALUE FOR AT LEAST TWO OF THE MASS VALUES
C IN ARRAY CENTER.
       WRITE(6,4)
     4 FORMAT(1X,'ENTER SUBSCRIPT')
       CALL INTGER(I)
       IF(I.EQ.0) GO TO 66
       WRITE(6,5)
     5 FORMAT(1X,'ENTER MASS')
       READ(5,6) STDMAS(NUMSTD)
     6 FORMAT(F10.0)
       STDDIS(NUMSTD)=CENTER(I)
       STDMAS(NUMSTD)=DSQRT(STDMAS(NUMSTD))
       GO TO 3
    66 NUMSTD=NUMSTD-1
C AT THIS POINT THE USER CAN TRANSFER CONTROL TO THE STANDARD MASS MANUAL ADDITION MODULE
C SO THAT HE CAN USE THE LIST EDITING CAPABILITIES OF THAT MODULE.
       WRITE(6,7)
     7 FORMAT('0','ANY ADDITIONS?')
       READ(5,8) I
     8 FORMAT(A1)
       IF(I.NE.YES) GO TO 200
       GO TO 600
C CALL THE STANDARD MASS FINDER SUBROUTINE
   200 CALL STDHNT
C LIST THE CURRENT STANDARD MASSES IDENTIFIED BY THE LAST PASS OF THE FINDER ROUTINE
   300 CALL STDLST
C AT THIS POINT THE USER MAY EDIT THE STANDARD MASS LIST
   400 WRITE(6,9)
     9 FORMAT('0','ANY CHANGES?')
       READ(5,8) I
       KEY=I
       IF(I.EQ.YES) GO TO 500
   450 WRITE(6,10)
    10 FORMAT('0','ANY ADDITIONS?')
       READ(5,8) I
       IF(I.EQ.YES) GO TO 600
C IF THERE ARE NO CHANGES OR ADDITIONS, THE CURRENT LIST OF STANDARD MASSES IS USED
C BY THE DISTANCE TO MASS CONVERSION POLYNOMIAL FOR LEAST SQUARE POLYNOMIAL FITTING.
       IF(KEY.NE.YES) RETURN
       GO TO 200
   500 CALL CHANGE
       GO TO 450
   600 CALL ADD
       GO TO 200
       END
```

```
C     JANUARY 26,1973                                    MICHAEL ROMIEZ
C
C     THIS MODULE WILL SEARCH FOR THE MAKER COMPOUND PEAKS IN ARRAY CENTER
C
C                                                        VARIABLES
C
C     CENTER(1500)        - DISTANCE OF PEAK CENTERS FROM THE LEFT EDGE OF THE PHOTOPLATE
C                         - IN MILLIMETERS
C     HIGHT(1500)         - MAXIMUM INTENSITY VALUE OF EACH PEAK
C     NUMPK               - NUMBER OF PEAKS IN THE PEAK LIST TABLE
C     STDDIS(160)         - THE DISTANCE VALUES OF PEAK CENTERS IDENTIFIED AS STANDARD MASSES
C     STDMAS(160)         - THE SQUARE ROOT OF THE MASS VALUE OF IDENTIFIED STANDARD MASSES
C     NUMSTD              - THE NUMBER OF IDENTIFIED STANDARD MASSES
C     REFMAS(160)         - A TABLE OF THE MOST INTENSE LINES IN THE MARKER COMPOUND SPECTRUM.
C                         - THESE ARE THE MASSES SEARCHED FOR BY THE STANDARD MASS IDENTIFICATION
C                         - ROUTINE
C     LSTPAR(10)          - PARAMETER LIST FROM PARAMETER LIST MODULE
C     X(200)              - UP TO 200 POINTS THAT ARE USED FOR POLYNOMIAL FITTING
C     Y(200)              - ONE ORDINATE VALUE FOR EACH X VALUE
C     N                   - NUMBER OF  X  AND  Y  VALUES
C     IDEG                - IT IS THE DEGREE OF THE POLYNOMIAL USED FOR FITTING
C     C(11)               - UP TO ELEVEN COEFFICIENTS OF THE POLYNOMIAL CALCULATED
C     ITOL                - THIS IS A FACTOR USED BY THE STANDARD MASS SEARCHING ROUTINE TO CALCULATE
C                         - THE TOLERANCE WITHIN WHICH IT WILL ACCEPT A PEAK AS A STANDARD MASS. A SMALL
C                         - VALUE MEANS A SMALL TOLERANCE
C     K                   - THE REFMAS ARRAY POINTER
C     M                   - THE CENTER ARRAY POINTER
C     MSTRT               - LOWER LIMIT FOR VALUES OF M
C     MSTOP               - UPPER LIMIT FOR VALUES OF M
C     KSTOP               - UPPER LIMIT FOR VALUES OF K
C     TEMP                - THE DISTANCE WHERE THE NEXT STANDARD MASS IS EXPECTED
C                         - TO BE FOUND
C
C     XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
        SUBROUTINE STDHNT
        DOUBLE PRECISION CENTER,STDDIS(160),STDMAS(160),REFMAS(160)
        DOUBLE PRECISION X(200),Y(200),C(11),TEMP,HTOL,LTOL
        COMMON/PKLST/ CENTER(1500),HIGHT(1500),NUMPK
        COMMON/PFKLST/ STDDIS,STDMAS,REFMAS,NUMSTD
        COMMON/FIT/ X,Y,NUM,IDEG,C
        COMMON/PAR/LSTPAR(10)
C SET THE SLIDING TOLERANCE FACTOR
        ITOL=LSTPAR(9)
C CLEAR VARIABLES
        DO 100 M=1,200
        X(M)=0.
  100   Y(M)=0.
C WE WANT TO USE A QUADRATIC SEARCH ROUTINE FOR WHICH WE NEED
C THREE PEAKS.  THE FIRST TIME WE ENTER THIS SUBROUTINE WE MAY
C ONLY HAVE TWO IDENTIFIED STANDARD MASSES. A LINAER SEARCH SECTION
C IS PROVIDED FOR THIS CASE
        IF(NUMSTD.GT.2) GO TO 200
        DO 150 M=1,2
        X(M)=STDDIS(M)
  150   Y(M)=STDMAS(M)
        NUM=2
        IDEG=1
        CALL POLYFT
        GO TO 275
C THIS IS THE QUADRATIC SEARCH SECTION
  200   DO 250 M=1,3
        X(M)=STDDIS(M)
  250   Y(M)=STDMAS(M)
        NUM=3
        IDEG=2
        CALL POLYFT
C THIS IS THE SEARCHING SECTION
  275   K=0
        M=1
        KSTOP=160
        MSTOP=NUMPK
  301   K=K+1
C IF WE HAVE LOOKED FOR ALL THE REFMAS ENTRIES, RETURN
        IF(K.GT.KSTOP) RETURN
        IF(NUMSTD.LT.3) GO TO 350
C THIS IS THE SECTION WHERE THE EXPECTED DISTANCE VALUE FOR THE NEXT ENTERY
C IN THE REFMAS ARRAY IS CALCULATED.
        TEMP=(-C(2)+DSQRT(C(2)**2-4*C(3)*(C(1)-REFMAS(K))))/(2*C(3))
        GO TO 351
  350   TEMP=(REFMAS(K)-C(1))/C(2)
C WE MUST SPECIFY A TOLERANCE WITHIN WHICH WE WILL ACCEPT A
C DISTANCE VALUE AS THE SEARCHED FOR STANDARD MASS. WE HAVE A
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C    JANUARY 26,1973                                    MICHAEL ROMIEZ
C
C FORMULA WHICH ALLOWS A HIGHER TOLERANCE AT THE HIGH MASS END. IT
C USES A FACTOR (ITOL) WHICH IS SUPPLIED BY THE PARAMETER
C SETTING MODULE.
  351  TOL=(FLOAT(ITOL)*.001/(TEMP/350.)
       HTOL=TEMP+TOL
       LTOL=TEMP-TOL
       GO TO 402
  401  M=M+1
C SEARCH ONLY WITHIN THE SUBLIST SPECIFIED BY MSTRT AND MSTOP.
  402  IF(M.GT.MSTOP) RETURN
       IF(CENTER(M).LT.LTOL) GO TO 401
       IF(CENTER(M).GT.HTOL) GO TO 301
C WE REACH THIS POINT ONLY IF WE HAVE A HIT.
C IF THE IDENTIFIED STANDARD MASS IS ALREADY IN THE FILE IGNORE
C THIS FIND.
       DO 450 J=1,NUMSTD
       IF(CENTER(M).EQ.STDDIS(J)) GO TO 800
       IF(STDMAS(J).EQ.REFMAS(K)) GO TO 800
  450  CONTINUE
C IF THE NEW STANDARD MASS IS LARGER THAN THE LARGEST MASS ALREADY
C IN THE FILE THEN WE CAN ADD IT TO THE END OF THE LIST.
  500  IF(CENTER(M).LT.STDDIS(NUMSTD)) GO TO 600
       NUMSTD=NUMSTD+1
       STDMAS(NUMSTD)=REFMAS(K)
       STDDIS(NUMSTD)=CENTER(M)
       J=NUMSTD
       GO TO 800
C THIS SECTION WILL INSERT AN IDENTIFIED STANDARD MASS WITHIN THE
C STANDARD MASS LIST IN THE PROPER PLACE. THE MASSES MUST BE STORED IN
C ASENDING ORDER.
  600  LIMIT=NUMSTD
       DO 625 J=1,LIMIT
       IF(CENTER(M).GT.STDDIS(J)) GO TO 625
       ITOP=160-J
       DO 650 LL=1,ITOP
       JJ=160-LL
       JJJ=JJ+1
       STDDIS(JJJ)=STDDIS(JJ)
  650  STDMAS(JJJ)=STDMAS(JJ)
       STDDIS(J)=CENTER(M)
       STDMAS(J)=REFMAS(K)
       NUMSTD=NUMSTD+1
       GO TO 800
  625  CONTINUE
C THIS SECTION CHOOSES THE STANDARD MASSES THAT WILL BE USED TO
C CALCULATE A NEW SET OF COEFFICIENTS. NOTE THAT VARIABLE J
C POINTS TO WHERE IN THE STDDIS LIST THE LAST STANDARD MASS
C WAS INSERTED OR ALREADY FOUND.
  800  IF(NUMSTD.EQ.2) GO TO 401
       IF(STDDIS(J+1).NE.0.) J=J+1
       IF(J.LT.3) J=3
       DO 850 NEW=1,3
       INDEX=J-3+NEW
       X(NEW)=STDDIS(INDEX)
  850  Y(NEW)=STDMAS(INDEX)
       NUM=3
       IDEG=2
       CALL POLYFT
       GO TO 301
       END
```

```
C    JANUARY 29,1973                                    MICHAEL ROMIEZ
C
C    THIS MODULE WILL ACCEPT CHANGES AND/OR DELETIONS TO THE STANDARD MASS LIST
C
C                                                       VARIABLES
C
C    STDDIS(160)         - THE DISTANCE VALUES OF PEAK CENTERS IDENTIFIED AS STANDARD MASSES
C    STDMAS(160)         - THE SQUARE ROOT OF THE MASS VALUE OF IDENTIFIED STANDARD MASSES
C    NUMSTD              - THE NUMBER OF IDENTIFIED STANDARD MASSES
C    REFMAS(160)         - A TABLE OF THE MOST INTENSE LINES IN THE MARKER COMPOUND SPECTRUM
C                         - THESE ARE THE MASSES SEARCHED FOR BY THE STANDARD MASS IDENTIFICATION
C                         - ROUTINE
C
C    XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
        SUBROUTINE CHANGE
        DOUBLE PRECISION STDDIS(160),STDMAS(160),REFMAS(160)
        COMMON/PFKLST/ STDDIS,STOMAS,REFMAS, NUMSTD
   5000 WRITE(6,1)
      1 FORMAT('0','ENTER SUBSCRIPT')
        CALL INTGER(MM)
        IF(MM.EQ.0) GO TO 5001
        WRITE(6,3)
      3 FORMAT(1X,'ENTER NEW MASS VALUE')
C IF IT IS DESIRED TO DELETE A PEAK, ENTER ZERO FOR THE MASS VALUE
        READ(5,2) STDMAS(MM)
      2 FORMAT(F10.0)
        STDMAS(MM)=DSQRT(STDMAS(MM))
        GO TO 5000
C AFTER ALL CHANGES AND DELETIONS HAVE BEEN MADE, THE STANDARD MASS LIST MUST BE COMPRESSED.
   5001 M=0
   5002 M=M+1
   5003 IF(STDMAS(M).NE.0.) GO TO 5002
        DO 5005 J=M,NUMSTD
        IF(STDMAS(J).NE.0.) GO TO 5008
   5005 CONTINUE
        NUMSTD=M-1
        RETURN
   5008 DO 5010 J=M,NUMSTD
        STDDIS(J)=STDDIS(J+1)
   5010 STDMAS(J)=STDMAS(J+1)
        GO TO 5003
        END
```

```
C    JANUARY 29,1973                                    MICHAEL ROMIEZ
C
C    THIS MODULE WILL DISPLAY AREAS OF THE CENTER LIST AND ADD ENTERIES TO THE STANDARD
C    MASS LIST
C
C                                                       VARIABLES
C
C    CENTER(1500)       - DISTANCE OF PEAK CENTERS FROM THE LEFT EDGE OF THE PHOTOPLATE
C                       - IN MILLIMETERS
C    HEIGHT(1500)       - MAXIMUM INTENSITY VALUE OF EACH PEAK
C    NUMPK              - NUMBER OF PEAKS IN THE PEAK LIST TABLE
C    STDDIS(160)        - THE DISTANCE VALUES OF PEAK CENTERS IDENTIFIED AS STANDARD MASSES
C    STDMAS(160)        - THE SQUARE ROOT OF THE MASS VALUE OF IDENTIFIED STANDARD MASSES
C    NUMSTD             - THE NUMBER OF IDENTIFIED STANDARD MASSES
C    REFMAS(160)        - A TABLE OF THE MOST INTENSE LINES IN THE MARKER COMPOUND SPECTRUM.
C                       - THESE ARE THE MASSES SEARCHED FOR BY THE STANDARD MASS IDENTIFICATION
C                       - ROUTINE
C    TEMP               - TEMPORARY STORAGE
C
C    XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
       SUBROUTINE ADD
       DOUBLE PRECISION STDDIS(160),STDMAS(160),REFMAS(160),TEMP
       DOUBLE PRECISION CENTER
       COMMON/PFKLST/STDDIS,STDMAS,REFMAS,NUMSTD
       COMMON/PKLST/CENTER(1500),HIGHT(1500),NUMPK
     2 WRITE(6,30)
    30 FORMAT('0','ENTER DISTANCE AREA FOR DISPLAY')
C ENTER ZERO TO RETURN TO THE CALLING MODULE. ENTER A VALUE LESS THAN 1. TO SKIP THE
C DISPLAY SECTION AND GO DIRECTLY TO THE PEAK INPUT SECTION.
       READ(5,31) TEMP
    31 FORMAT(F10.7)
       IF(TEMP.EQ.0.) GO TO 999
       IF(TEMP.LT.1.) GO TO 41
       M=0
     1 M=M+1
       IF(CENTER(M).EQ.0.) GO TO 1000
       IF(CENTER(M).LT.TEMP) GO TO 1
       M=M-3
       K=M+6
       WRITE(6,32)
C LIST THE RAW PEAK DATA IN THE VACINITY OF THE DESIRED PEAK
    32 FORMAT('0',10X,'DISTANCE',10X,'RAW INTENSITY')
       IF(M.LT.1) M=1
       DO 40 J=M,K
       IF(CENTER(J).EQ.0.) GO TO 41
    40 WRITE(6,33) J,CENTER(J),HIGHT(J)
    33 FORMAT(4X,I3,4X,F8.4,12X,F7.1)
    41 WRITE(6,34)
    34 FORMAT('0','ENTER SUBSCRIPT')
       CALL INTGER(L)
       IF(L.EQ.0) GO TO 2
       WRITE(6,35)
    35 FORMAT(1X,'ENTER MASS')
       READ(5,36) TEMP
    36 FORMAT(F10.0)
       TEMP=DSQRT(TEMP)
       NN=NUMSTD
C PLACE THE ADDED PEAK IN THE PROPER PLACE IN THE STANDARD MASS LIST
       DO 7777 I=1,NN
       IF(TEMP.GT.STDMAS(I)) TO TO 7777
       LTOP=160-I
       DO 8000 J=1,LTOP
       MM=160-J
       MMM=MM+1
       STDDIS(MMM)=STDDIS(MM)
  8000 STDMAS(MMM)=STDMAS(MM)
       STDDIS(MM)=CENTER(L)
       STDMAS(MM)=TEMP
       NUMSTD=NUMSTD+1
       GO TO 2
  7777 CONTINUE
C IF THE NEW PEAK IS LARGER THAN THE OTHER ENTERIES, ADD IT TO THE END OF THE LIST.
       NUMSTD=NUMSTD+1
       STDDIS(NUMSTD)=CENTER(L)
       STDMAS(NUMSTD)=TEMP
       GO TO 2
  1000 WRITE(6,37) CENTER(M-1)
    37 FORMAT('0','THE LARGEST DISTANCE VALUE IN THE FILE IS',F10.5)
       GO TO 2
   999 RETURN
       END
```

```
C     JANUARY 26,1973                                        MICHAEL ROMIEZ
C
C     THIS MODULE WILL LIST THE STANDARD MASSES FOUND BY THE SEARCHING ROUTINE
C
C                                                              VARIABLES
C
C     STDDIS(160)          - THE DISTANCE VALUES OF PEAK CENTERS IDENTIFIED AS STANDARD MASSES
C     STDMAS(160)          - THE SQUARE ROOT OF THE MASS VALUE OF IDENTIFIED STANDARD MASSES
C     NUMSTD               - THE NUMBER OF IDENTIFIED STANDARD MASSES
C     REFMAS(160)          - A TABLE OF THE MOST INTENSE LINES IN THE MARKER COMPOUND SPECTRUM.
C                          - THESE ARE THE MASSES SEARCHED FOR BY THE STANDARD MASS IDENTIFICATION
C                          - ROUTINE
C     X(200)               - UP TO 200 ABCISSA VALUES TO BE PASSED TO THE POLYNOMIAL FITTING
C                          - ROUTINE
C     Y(200)               - UP TO 200 ORDINATE VALUES TO BE PASSED TO THE POLYNOMIAL FITTING
C                          - ROUTINE
C     N                    - NUMBER OF  X  AND  Y  VALUES PASSED
C     IDEG                 - DEGREE OF THE POLYNOMIAL (UP TO TENTH POSSIBLE)
C     C(11)                - UP TO 11 COEFFICIENTS RETURNED BY THE POLYNOMIAL ROUTINE
C     LSTPAR(10)           - LIST OF PARAMETERS FROM THE PARLIST MODULE
C     PFKMAS(160)          - THE MASSES OF IDENTIFIED STANDARD MASSES CALCULATED BY USING THE
C                          - SURROUNDING INUM STANDARD MASSES
C     STD(160)             - THE KNOWN EXACT MASS OF EACH IDENTIFIED STANDARD MASS
C     DIFF(160)            - THE DIFFERENCE IN MILLIMASS UNITS BETWEEN THE EXACT MASS AND THE
C                          - CALCULATED MASS OF EACH IDENTIFIED STANDARD LINE
C     PPM(16)              - THE DIFFERENCE IN PARTS PER MILLION BETWEEN THE EXACT MASS AND THE
C                          - CALCULATED MASS OF EACH IDENTIFIED STANDARD LINE
C     CC(160,11)           - THE UP TO 160 SETS OF COEFFICIENTS CALCULATED BY THIS MODULE FOR
C                          - EACH SET OF INUM STANDARD MASSES USED IN THE DISTANCE TO MASS
C                          - CALCULATION
C     INUM                 - THE NUMBER OF STANDARD MASSES USED FOR EACH SUCCESSIVE
C                          - POLYNOMIAL FIT
C     INDEX                - POINTER TO THE CC ARRAY
C     IHDEX                - THE TOTAL NUMBER OF SETS OF COEFFICIENTS
C     IORDER               - THE NUMBER OF COEFFICIENTS RETURNED BY THE POLYNOMIAL FITTING
C                          - ROUTINE
C     ISTRT                - POINTER TO THE LOWEST OF THE INUM VALUES TO BE TRANSFERED TO
C                          - THE POLYNOMIAL FITTING ROUTINE
C     ITOP                 - POINTER TO THE HIGHEST OF THE INUM VALUES TO BE TRANSFERED TO
C                          - THE POLYNOMIAL FITTING ROUTINE
C     M                    - THE STDDIS AND STDMAS ARRAY POINTER
C
C     XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      SUBROUTINE STDLST
      DOUBLE PRECISION X(200),Y(200),C(11)
      DOUBLE PRECISION STDMAS(160),STDDIS(160),PPM(160),REFMAS(160)
      DOUBLE PRECISION PFKMAS(160),STD(160),DIFF(160),CC(160,11)
      COMMON/PFKLST/STDDIS,STDMAS,REFMAS, NUMSTD
      COMMON/FIT/X,Y,N,IDEG,C
      COMMON/OUTLST/ PFKMAS,STD,DIFF,PPM,CC
      COMMON/PAR/LSTPAR(10)
      WRITE(6,11)
C SET THE NUMBER OF STANDARD MASSES USED, AND THE DEGREE OF THE CONVERSION POLYNOMIAL
      INUM=LSTPAR(7)
      LIMDEG=LSTPAR(8)
C CLEAR VARIABLES
      DO 100 M=1,160
      PFKMAS(M)=0.
      STD(M)=0.
      PPM(M)=0.
      DIFF(M)=0.
      DO 100 J=1,11
      C(J)=0.
  100 CC(M,J)=0.
C INUM IS THE NUMBER OF POINTS USED BY THE DISTANCE TO MASS CONVERSION POLYNOMIAL
C JNUM IS ONE LESS THAN INUM, AND KNUM IS ONE HALF INUM.
      JNUM=INUM-1
      KNUM=INUM/2
C THIS SECTION IS FOR LESS THAN INUM IDENTIFIED STANDARD MASSES
      IF(NUMSTD.GT.INUM) GO TO 1000
C IF THERE ARE LESS THAN INUM IDENTIFIED STANDARD MASSES, SEND THEM ALL TO CALCULATE
C A POLYNOMIAL OF DEGREE NUMSTD-2; PROVIDED THAT THE DEGREE DOES NOT EXCEED LIMDEG
      N=NUMSTD
      DO 500 M=1,NUMSTD
      X(M)=STDDIS(M)
  500 Y(M)=STDMAS(M)
      IDEG=NUMSTD-2
      IF(IDEG.GT.LIMDEG)IDEG=LIMDEG
      CALL POLYFT
      IORDER=IDEG+1
C STORE THE RETURNED SET OF COEFFICIENTS IN THE CC ARRAY, IN THIS CASE THERE WILL BE
C ONLY ONE SET.
      DO 501 M=1,IORDER
```

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C    JANUARY 26,1973                                    MICHAEL ROMIEZ
C
  501 CC(1,M)=C(M)
      IHDEX=1
      M=1
      GO TO 3000
C THIS SECTION IS FOR MORE THAN INUM IDENTIFIED STANDARD MASSES
 1000 INDEX=1
      ISTART=1
 1001 ITOP=ISTART+JNUM
      IF(LTOP.GT.NUMSTD) GO TO 2000
      MM=0
C ALL THE STANDARD MASSES ARE SENT TO THE POLYNOMIAL FITTING ROUTINE IN GROUPS OF INUM.
C AFTER ALL THE MASSES HAVE BEEN USED FOR POLYNOMIAL CALCULATION IN THIS MANNER, THERE
C WILL BE NUMSTD-JNUM SETS OF COEFFICIENTS STORED IN THE CC ARRAY. THESE SETS OF COEFFICIENTS
C REPRESENT THE BEST POLYNOMIAL FITS FOR DISTANCE TO MASS CONVERSIONS IN THE NUMSTD-JNUM
C OVERLAPPING AREAS OF THE STANDARD MASS LIST.
      DO 300 M=ISTART,ITOP
      MM=MM+1
      X(MM)=STDDIS(M)
  300 Y(MM)=STDMAS(M)
      N=INUM
      IDEG=LIMDEG
C STORE COEFFICIENTS IN THE PROPER PLACE IN THE CC ARRAY
      CALL POLYFT
      DO 350 M=1,11
  350 CC(INDEX,M)=C(M)
      INDEX=INDEX+1
      ISTART=ISTART+1
      GO TO 1001
C AFTER ALL SETS OF COEFFICIENTS HAVE BEEN CALCULATED, USE THEM TO DETERMINE THE ERROR
C IN THE DISTANCE TO MASS CONVERSION. LIST THE DIFFERENCE BETWEEN THE KNOWN MASSES OF
C THE REFERENCE PEAKS AND THE MASSES CALCULATED FOR THESE REFERENCE LINES USING THE SAME
C METHOD OF CALCULATION AS FOR UNKNOWN LINES.
 2000 INDEX=1
      IHDEX=NUMSTD-JNUM
      M=1
 3000 IF(M.GT.NUMSTD) GO TO 5000
      IF(M.LT.KNUM) INDEX=1
      IF(INDEX.GT.IHDEX) INDEX=IHDEX
      PFKMAS(M)=CC(INDEX,1)
      DO 4000 K=1,10
      KK=K+1
 4000 PFKMAS(M)=PFKMAS(M)+CC(INDEX,KK)*STDDIS(M)**K
      M=M+1
      INDEX=INDEX+1
      GO TO 3000
 5000 DO 4500 K=1,NUMSTD
      PFKMAS(K)=PFKMAS(K)*PFKMAS(K)
      STD(K)=STDMAS(K)*STDMAS(K)
      DIFF(K)=(PFKMAS(K)-STD(K))*1000.
 4500 PPM(K)=DABS((DIFF(K)/STD(K))*1000.)
C THIS IS THE LISTING SECTION
      WRITE(6,201)
      WRITE(6,202)
      WRITE(6,203)
      DO 4001 M=1,NUMSTD
 4001 WRITE(6,204) M,STDDIS(M),PFKMAS(M),STD(M),DIFF(M),PPM(M)
      RETURN
    1 FORMAT('1')
  201 FORMAT('0',10X,'DISTANCE',10X,'CALCULATED',10X,'EXACT MASS',10X,'DIFFERENCE',10X,'DIFFERENCE')
  202 FORMAT(' ',31X,'MASS',35X,'IN MMU',14X,'IN PPM')
  203 FORMAT(' ')
  204 FORMAT(3X,I3,5X,F8.4,9X,F10.5,10X,F10.5,13X,F5.2,15X,F5.2)
      END
```

```
C     JANUARY 30,1973                                              MICHAEL ROMIEZ
C
C     THIS MODULE ACCEPTS ADDITIONS TO THE ELEMENT LIST USED FOR FITTING COMPOSITIONS
C     TO THE UNKNOWN PEAKS. IT ALSO WILL ACCEPT A CHANGE IN THE ELEMENT FITTING TOLERANCE
C     SUPPLIED BY THE PARAMETER SETTING MODULE. IT WILL, AT THE USERS OPTION, WRITE ALL THE DATA
C     OBTAINED SO FAR INTO A DISK FILE OR WILL CALL THE MODULES TO DO THE ELEMENT FITTING FOR
C     LISTING ON THE CONVERSATIONAL TERMINAL.
C
C                                                                       VARIABLES
C
C     CENTER(1500)          - DISTANCE OF PEAK CENTERS FROM THE LEFT EDGE OF THE PHOTOPLATE
C                           - IN MILLIMETERS
C     HIGHT(1500)           - MAXIMUM INTENSITY VALUE OF EACH PEAK
C     NUMPK                 - NUMBER OF PEAKS IN THE PEAK LIST TABLE
C     STDDIS(160)           - THE DISTANCE VALUES OF PEAK CENTERS IDENTIFIED AS STANDARD MASSES
C     STDMAS(160)           - THE SQUARE ROOT OF THE MASS VALUE OF IDENTIFIED STANDARD MASSES
C     NUMSTD                - THE NUMBER OF IDENTIFIED STANDARD MASSES
C     REFMAS(160)           - A TABLE OF THE MOST INTENSE LINES IN THE MARKER COMPOUND SPECTRUM.
C                           - THESE ARE THE MASSES SEARCHED FOR BY THE STANDARD MASS IDENTIFICATION
C                           - ROUTINE
C     LSTPAR(10)            - LIST OF PARAMETERS FROM THE PARLIST MODULE
C     PFKMAS(160)           - THE MASSES OF IDENTIFIED STANDARD MASSES CALCULATED BY USING THE
C                           - SURROUNDING STANDARD MASSES
C     STD(160)              - THE KNOWN EXACT MASS OF EACH IDENTIFIED STANDARD MASS
C     DIFF(160)             - THE DIFFERENCE IN MILLIMASS UNITS BETWEEN THE EXACT MASS AND THE
C                           - CALCULATED MASS OF EACH IDENTIFIED STANDARD LINE
C     PPM(160)              - THE DIFFERENCE IN PARTS PER MILLION BETWEEN THE EXACT MASS AND THE
C                           - CALCULATED MASS OF EACH IDENTIFIED STANDARD LINE
C     CC(160,11)            - THE UP TO 160 SETS OF COEFFICIENTS CALCULATED FOR EACH SET OF
C                           - STANDARD MASSES USED IN THE DISTANCE TO MASS CALCULATION
C     MASS(12)              - UP TO TWELVE MASSES OF ELEMENTS USED FOR FITTING
C     NAME(12)              - A FOUR CHARACTER NAME FOR UP TO TWELVE ELEMENTS
C     NUMBER(12)            - THE MAXIMUM NUMBER OF EACH ELEMENT USED IN ELEMENT FITTING
C     NTOL                  - THE TOLERANCE IN MILLIMASS UNITS USED FOR ELEMENT FITTING
C     NUM                   - THE NUMBER OF ELEMENTS IN THE MASS ARRAY
C
C     XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      SUBROUTINE ELELST
      DOUBLE PRECISION CENTER,STDMAS(160),STDDIS(160),PPM(160),REFMAS(160)
      DOUBLE PRECISION PFKMAS(160),STD(160),DIFF(160),CC(160,11),MASS,MAS(12)
      INTEGER NAM(12),NUMB(12)
      COMMON/PFKLST/STDDIS,STDMAS,REFMAS,NUMSTD
      COMMON/PAR/ LSTPAR(10)
      COMMON/OUTLST/ PFKMAS,STD,DIFF,PPM,CC
      COMMON/PKLST/ CENTER(1500),HEIGHT(1500),NUMPK
      COMMON/ELEM/ MASS(12),NAME(12),NUMBER(12),NTOL,NUM
      DATA MAS/1.0078246,12.,13.0033554,14.0030732,15.9949141,7*0/
      DATA NAM/' H  ','C12 ','C13 ','N14 ','O16 ',7*0/
      DATA NUMB/2*0,2,3,4,7*0/
      DATA IYES,IBLK/'Y','    '/
      DO 50 M=1,12
      MASS(M)=MAS(M)
      NAME(M)=NAM(M)
   50 NUMBER(M)=NUMB(M)
      I=5
      NUM=5
      NTOL=5
      WRITE(6,100)
      READ(5,51) J
      IF(J.NE.IYES) GO TO 2001
C ENTER NEW VALUE FOR ELEMENT FITTING TOLERANCE OR ENTER ZERO TO RETAIN OLD VALUE
      WRITE(6,106) NTOL
      CALL INTGER(II)
      IF(II.NE.0) NTOL=II
C ENTER ADDITIONAL ELEMENTS USED FOR FITTING
    1 I=I+1
      IF(I.EQ.13) GO TO 2000
      WRITE(6,102)
      READ(5,52) NAME(I)
      IF(NAME(I).EQ.IBLK) GO TO 1999
      WRITE(6,104)
      READ(5,53) MASS(I)
      WRITE(6,105)
      CALL INTGER(NUMBER(I))
      GO TO 1
 1999 NAME(I)=0.
 2000 NUM=I-1
 2001 WRITE(6,103)
      READ(5,51) IFLAG
      IF(IFLAG.EQ.IYES) GO TO 3000
C WRITE ALL DATA INTO DISK FILE FOR ACCESS BY THE BATCH ELEMENT FITTING ROUTINE
      WRITE(3) NUMPK,(CENTER(I),HIGHT(I),I=1,NUMPK),STDDIS,STDMAS,REFMAS,NUMSTD,-
     XLSTPAR,PFKMAS,STD,DIFF,PPM,CC,MASS,NAME,NUMBER,NTOL,NUM
      STOP
```

```
C    JANUARY 30,1973                                    MICHAEL ROMIEZ
C
C CALL THE ELEMENT FITTING ROUTINE FOR CALCULATION AND DISPLAY ON THE CONVERSATIONAL
C TERMINAL
  3000 CALL ELEMFT
       RETURN
   100 FORMAT('0','DO YOU WISH TO REVIEW ELEMENT FITTING PARAMETERS?')
   102 FORMAT('0','ENTER ISOTOPE NAME')
   103 FORMAT('0','IS THIS TERMINAL OUTPUT ?')
   104 FORMAT(' ','ENTER MASS')
   105 FORMAT(' ','NUMBER FOR THIS ISOTOPE')
   106 FORMAT(1X,'THE TOLERANCE FOR ELEMENT FITTING IS',I3,' MMU')
    51 FORMAT(A1)
    52 FORMAT(A4)
    53 FORMAT(F10.0)
       END
```

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C     FEBRUARY 1, 1973                              MICHAEL ROMIEZ
C
C     THIS MODULE WILL CALCULATE AN EXACT MASS FOR EACH UNKNOWN PEAK IN THE PEAK LIST.  IT
C     WILL ALSO DETERMINE ALL ELEMENTAL COMPOSITIONS THAT ARE WITHIN A SPECIFIED TOLERANCE
C     OF THE EXACT MASS FROM THE GIVEN LIST OF ELEMENTS.
C
C                                                      VARIABLES
C
C     CENTER(1500)        - DISTANCE OF PEAK CENTERS FROM THE LEFT EDGE OF THE PHOTOPLATE
C                         - IN MILLIMETERS
C     HIGHT(1500)         - MAXIMUM INTENSITY VALUE OF EACH PEAK
C     NUMPK               - NUMBER OF PEAKS IN THE PEAK LIST TABLE
C     STDDIS(160)         - THE DISTANCE VALUES OF PEAK CENTERS IDENTIFIED AS STANDARD MASSES
C     STDMAS(160)         - THE SQUARE ROOT OF THE MASS VALUE OF IDENTIFIED STANDARD MASSES
C     NUMSTD              - THE NUMBER OF IDENTIFIED STANDARD MASSES
C     REFMAS(160)         - A TABLE OF THE MOST INTENSE LINES IN THE MARKER COMPOUND SPECTRUM.
C                         - THESE ARE THE MASSES SEARCHED FOR BY THE STANDARD MASS IDENTIFICATION
C                         - ROUTINE
C     LSTPAR(10)          - LIST OF PARAMETERS FROM THE PARLIST MODULE
C     PEKMAS(160)         - THE MASSES OF IDENTIFIED STANDARD MASSES CALCULATED BY USING THE
C                         - SURROUNDING STANDARD MASSES
C     STD(160)            - THE KNOWN EXACT MASS OF EACH IDENTIFIED STANDARD MASS
C     DIFF(160)           - THE DIFFERENCE IN MILLIMASS UNITS BETWEEN THE EXACT MASS AND THE
C                         - CALCULATED MASS OF EACH IDENTIFIED STANDARD LINE
C     PPM(16)             - THE DIFFERENCE IN PARTS PER MILLION BETWEEN THE EXACT MASS AND THE
C                         - CALCULATED MASS OF EACH IDENTIFIED STANDARD LINE
C     CC(160,11)          - THE UP TO 160 SETS OF COEFFICIENTS CALCULATED FOR EACH SET OF
C                         - STANDARD MASSES USED IN THE DISTANCE TO MASS CALCULATION
C     MASS(12)            - UP TO TWELVE MASSES OF ELEMENTS
C     NAME(12)            - A FOUR CHARACTER NAME FOR UP TO TWELVE ELEMENTS
C     NUMBER(12)          - THE MAXIMUM NUMBER OF EACH ELEMENT USED IN ELEMENT FITTING
C     NTOL                - THE TOLERANCE IN MILLIMASS UNITS USED FOR ELEMENT FITTING
C     NUM                 - THE NUMBER OF ELEMENTS IN THE MASS ARRAY
C     CALMAS(391)         - A LIST OF THE MASSES OF THE PEAKS IN THE MARKER COMPOUND THAT
C                         - WILL BE REMOVED FROM THE CLCMAS TABLE IF FOUND
C     CLCMAS(1500)        - A CALCULATED MASS FOR EACH PEAK IN ARRAY CENTER
C     ATNUM(12)           - THE NUMBER OF ATOMS OF EACH ELEMENT THAT FITS A PARTICULAR
C                         - ELEMENTAL COMPOSITION
C     COUNT1              - A COUNTER THAT CONTROLS THE OUTPUT LISTING
C     COUNT2              - THE NUMBER OF ELEMENTAL COMPOSITIONS FOUND SO FAR FOR THE
C                         - THE PARTICULAR CLCMAS VALUE UNDER CONSIDERATION
C
C     XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX

      SUBROUTINE ELEMFT
      DOUBLE PRECISION CENTER,STDMAS(160),STDDIS(160),PPM(160),REFMAS(160)
      DOUBLE PRECISION PFKMAS(160),STD(160),DIFF(160),CC(160,11)
      DOUBLE PRECISION CLCMAS(1500),DIF,HTOL,LTOL,CALMAS(391),MASS
      INTEGER COUNT1,COUNT2,ATNUM(12)
      REAL MAX
      COMMON/PFKLST/STDDIS,STDMAS,REFMAS,NUMSTD
      COMMON/PAR/ LSTPAR(10)
      COMMON/OUTLST/ PFKMAS,STD,DIFF,PPM,CC
      COMMON/PKLST/ CENTER(1500),HIGHT(1500),NUMPK
      COMMON/ELEM/ MASS(12),NAME(12),NUMBER(12),NTOL,NUM
      COMMON/COMP/CLCMAS,ATNUM,COUNT1,COUNT2,DIF,IMAS
C CLEAR CLCMAS ARRAY
      DO 50 I=1,1500
   50 CLCMAS(I)=0.
C SET THE NUMBER OF STANDARD MASSES USED FOR POLNOMIAL FITTING IN MODULE STDLST
      INUM=LSTPAR(7)
C CALL THE MARKER COMPOUND LISTING MODULE
      CALL STDLST
C INITALIZE THE COUNTER THAT CONTROLS THE OUTPUT FORMAT
      COUNT1=45
C CALCULATE THE EXACT MASS OF EACH PEAK USING THE PROPER SET OF POLYNOMIAL COEFFICIENTS
C FROM MODULE STDLST. INDEX IS THE CC ARAY POINTER, IHDEX IS THE POINTER TO THE LAST
C SET OF COEFFICIENTS IN THE CC ARRAY.
 1012 INDEX=1
      IHDEX=NUMSTD-INUM+1
      IF(IHDEX.LT.1) IHDEX=1
      M=1
    1 DO 1000 J=1,NUMSTD
      IF(STDDIS(J).LT.CENTER(M)) GO TO 1000
      GO TO 1001
 1000 CONTINUE
 1001 INDEX=J-(INUM/2)
      IF(J.LE.INUM/2) INDEX=1
      IF(INDEX.GT.IHDEX) INDEX=IHDEX
      CLCMAS(M)=CC(INDEX,1)
      DO 1005 K=1,10
      KK=K+1
 1005 CLCMAS(M)=CLCMAS(M)+CC(INDEX,KK)*CENTER(M)**K
```

```
C    FEBRUARY 1, 1973                                    MICHAEL ROMIEZ
C
       M=M+1
       IF(M.GT.NUMPK) GO TO 2000
       GO TO 1
  2000 DO 1010 M=1,NUMPK
  1010 CLCMAS(M)=CLCMAS(M)*CLCMAS(M)
C  READ IN MASSES TO BE STRIPED OUT
       READ(4) CALMAS
C STRIP OUT BACKGROUND AND MARKER COMPOUND PEAKS
       TOL=FLOAT(NTOL)*.001
       J=0
    10 J=J+1
       IF(J.GT.NUMKP) GO TO 2500
       DO 2001 M=1,391
       HTOL=CALMAS(M)+TOL
       LTOL=CALMAS(M)-TOL
       IF(CLCMAS(J).LT.LTOL) GO TO 10
       IF(CLCMAS(J).GT.HTOL) GO TO 2001
       CLCMAS(J)=0.
       GO TO 10
  2001 CONTINUE
       GO TO 10
C COMPRESS CLCMAS ARRAY
 2500 M=0
  100 M=M+1
  170 IF(CLCMAS(M).NE.0.) GO TO 100
       DO 150 J=M,NUMPK
       CLCMAS(J)=CLCMAS(J+1)
       CENTER(J)=CENTER(J+1)
  150  HIGHT(J)=HIGHT(J+1)
       DO 167 K=M,NUMPK
       IF(CLCMAS(K).EQ.0.) GO TO 167
       GO TO 170
  167  CONTINUE
C IF THERE ARE NO PEAKS IN THE MASS SPECTRUM, RETURN TO THE CALLING MODULE
       IF(CLCMAS(1).EQ.0) RETURN
C CALCULATE NEW NUMPK VALUE
 2700  DO 2800 L=1,NUMPK
       IF(CLCMAS(L).NE.0.) GO TO 2800
       LL=L-1
       TO TO 2900
 2800  CONTINUE
 2900  NUMPK=LL
C NORMALIZE INTENSITY VALUES
       MAX=HIGHT(1)
       DO 4950 J=2,NUMPK
       IF(HIGHT(J).GT.MAX) MAX=HIGHT(J)
 4950  CONTINUE
       IF(MAX.EQ.0) GO TO 3005
       DO 4951 J=1,NUMPK
 4951  HIGHT(J)=(HIGHT(J)/MAX)*100.
C CALCULATE ELEMENTAL COMPOSITIONS
 3005  NUM3=NUMBER(3)
       NUM4=NUMBER(4)
       NUM5=NUMBER(5)
       NUM6=NUMBER(6)+1
       NUM7=NUMBER(7)+1
       NUM8=NUMBER(8)+1
       NUM9=NUMBER(9)+1
       NUM10=NUMBER(10)+1
       NUM11=NUMBER(11)+1
       NUM12=NUMBER(12)+1
       DO 4000 M=1,NUMPK
       HTOL=CLCMAS(M)+TOL
       LTOL=CLCMAS(M)-TOL
       COUNT2=0
       NUM2=IDINT(HTOL/12.)+1
       NUM1=NUM2*2+8
       DO 4050 I12=1,NUM12
       I112=I12-1
       ATNUM(12)=I112
       DO 4050 I11=1,NUM11
       I111=I11-1
       ATNUM(11)=I111
       DO 4050 I10=1,NUM10
       I110=I10-1
       ATNUM(10)=I110
       DO 4050 I9=1,NUM9
       I19=I9-1
       ATNUM(9)=I19
       DO 4050 I8=1,NUM8
       I18=I8-1
```

```
C    FEBRUARY 1, 1973                                    MICHAEL ROMIEZ
C
       ATNUM(8)=I18
       DO 4050 I7=1,NUM7
       I17=I7-1
       ATNUM(7)=I17
       DO 4050 I6=1,NUM6
       I16=I6-1
       ATNUM(6)=I16
       DO 4050 I5=1,NUM5
       I15=I5-1
       ATNUM(5)=I15
       DO 4050 I4=1,NUM4
       I14=I4-1
       ATNUM(4)=I14
       DO 4050 I3=1,NUM3
       I13=I3-1
       ATNUM(3)=I13
       DO 4050 I2=1,NUM2
       I12=I2-1
       ATNUM(2)=I12
       SUM=0.
       DO 4100 I1=2,NUM
 4100 SUM=SUM+ATNUM(I1)*MASS(I1)
C ITEST IS AN INTEGER VALUE WHICH IS USED TO FIT THE ELEMENT HYDROGEN INTO THE
C ELEMENTAL COMPOSITIONS. IF ITEST IS LESS THAN ZERO THIS MEANS THAT SUM
C IS GREATER THAN CLCMAS(M) PLUS THE TOLERANCE AND WE WILL DISMISS THIS COMPOSITION.
C WHEN ITEST IS ZERO OR POSITIVE WE HAVE A POSSIBLE COMPOSITION AND WE MAKE FURTHER
C TESTS
       ITEST=IDINT(HTOL-SUM)
       IF(ITEST.GT.NUM1) GO TO 4050
       IF(ITEST) 4050,4051,4051
 4051  ATNUM(1)=ITEST
       SUM=SUM+MASS(1)*ATNUM(1)
       GO TO 4053
C WE CONTINUE TO ADD HYDROGEN ATOMS TO THE COMBINATIONS OF OTHER ELEMENTS UNTIL WE HAVE
C A FIT OR WE HAVE TOO HIGH OF A TOTAL MASS FOR A FIT.
 4052  SUM=SUM+MASS(1)
       ATNUM(1)=ATNUM(1)+1
 4053  IF(SUM.GT.HTOL) GO TO 4050
       IF SUM.LT.LTOL) GO TO 4052
       COUNT2=COUNT2+1
       DIF=(CLCMAS(M)-SUM)*1000.
       IMAS=M
       CALL OUTPUT
 4050  CONTINUE
C IF THERE WERE NO ELEMENTAL COMPOSITIONS FOUND FOR THIS MASS, LIST THIS INFORMATION
C AS PART OF THE OUTPUT.
       IMAS=M
       IF(COUNT2.EQ.0) CALL OUTPUT
 4000  CONTINUE
       RETURN
       END
```

```
C     FEBRUARY 1,1973                                        MICHAEL ROMIEZ
C
C     THIS MODULE LISTS ELEMENTAL COMPOSITIONS FOUND BY THE ELEMENT FITTING ROUTINE
C
C                                                            VARIABLES
C
C     CENTER(1500)         - DISTANCE OF PEAK CENTERS FROM THE LEFT EDGE OF THE PHOTOPLATE
C                          - IN MILLIMETERS
C     HIGHT(1500)          - MAXIMUM INTENSITY VALUE OF EACH PEAK
C     NUMPK                - NUMBER OF PEAKS IN THE PEAK LIST TABLE
C     MASS(12)             - UP TO TWELVE MASSES OF ELEMENTS
C     NAME(12)             - A FOUR CHARACTER NAME FOR UP TO TWELVE ELEMENTS
C     NUMBER(12)           - THE MAXIMUM NUMBER OF EACH ELEMENT USED IN ELEMENT FITTING
C     NTOL                 - THE TOLERANCE IN MILLIMASS UNITS USED FOR ELEMENT FITTING
C     NUM                  - THE NUMBER OF ELEMENTS IN THE MASS ARRAY
C     ATNUM(12)            - THE NUMBER OF ATOMS OF EACH ELEMENT THAT FITS A PARTICULAR
C                          - ELEMENTAL COMPOSITION
C     COUNT1               - A COUNTER THAT CONTROLS THE OUTPUT LISTING
C     COUNT2               - THE NUMBER OF ELEMENTAL COMPOSITIONS FOUND SO FAR FOR THE
C                          - THE PARTICULAR CLCMAS VALUE UNDER CONSIDERATION
C
C     XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      SUBROUTINE OUTPUT
      DOUBLE PRECISION CENTER,MASS,CLCMAS(1500),DIFF
      INTEGER ATNUM(12),COUNT1,COUNT2
      COMMON/ELEM/MASS(12),NAME(12),NUMBER(12),NTOL,NUM
      COMMON/PKLST/ CENTER(1500),HIGHT(1500),NUMPK
      COMMON/COMP/CLCMAS,ATNUM,COUNT1,COUNT2,DIFF,IMAS
C TEST NEED FOR A NEW PAGE HEADING
      IF(COUNT1.GE.45) GO TO 1002
C IF COUNT2 IS ZERO, THERE HAVE BEEN NO ELEMENTAL FITS FOR THIS MASS
  500 IF(COUNT2.EQ.0) GO TO 1001
C IF THIS IS A NEW MASS WE SKIP A SPACE
      IF(COUNT2.EQ.1) GO TO 1003
 1000 WRITE(6,303) CENTER(IMAS),HIGHT(IMAS),CLCMAS(IMAS),DIFF,(ATNUM(M),M=1,NUM)
      COUNT1=COUNT1+1
      RETURN
 1001 WRITE(6,304) CENTER(IMAS),HIGHT(IMAS),CLCMAS(IMAS),NTOL
      COUNT1=COUNT1+2
      RETURN
 1002 WRITE(6,100)
      WRITE(6,300)
      WRITE(6,301)(NAME(M),M=1,NUM)
      WRITE(6,302)
      COUNT1=5
      GO TO 500
 1003 WRITE(6,203)
      COUNT1=COUNT1+1
      GO TO 1000
  203 FORMAT(' ')
  100 FORMAT('1')
  300 FORMAT(6X,'DISTANCE',6X,'RELATIVE',7X,'MASS',7X,'DIFFERENCE')
  301 FORMAT(20X,'INTENSITY',19X,'IN MMU',5X,12A5)
  302 FORMAT('0')
  303 FORMAT(6X,F8.4,7X,F5.1,5X,F10.5,8X,F5.2,3X,12I5)
  304 FORMAT('0',5X,F8.4,7X,F5.1,5X,F10.5,10X,'NO ELEMENTAL COMPOSITIONS FOUND WITHIN',I3,' MMU')
      END
```

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