CONVERSATIONAL HIGH-RESOLUTION
MASS SPECTROGRAPHIC DATA REDUCTION

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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 programming 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 necessary 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).

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

\[
ln\ y = ln\ y_{\text{max}} - \frac{5.545(x - x_{\text{max}})^2}{2w^2}
\]

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

\[
y \quad \text{intensity at position } x
\]

\[
y_{\text{max}} \quad \text{intensity at the maximum}
\]

\[
x_{\text{max}} \quad \text{position of the maximum}
\]

\[
w \quad \text{half-width}
\]

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 spectrometry 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
## APPENDIX A

### SAMPLE OF STANDARD MASS ACCURACY

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<th>DIFFERENCE IN PP M</th>
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APPENDIX B
PROGRAM LISTING

I AMERICAN HIGH RESOLUTION DATA TAPE INTO A
DISK FILE WHICH CAN BE ACCESSED BY THE MAIN DATA REDUCTION PROGRAM.

THE DATA ON THE TAPE IS ENCODED IN SEVEN TRACK BCD FORMAT; IT IS CONVERTED INTO EBCDIC
BY AN AMES LIBRARY SUBROUTINE ALBYTES. THE DATA IS CONVERTED TO INTEGER FORMAT BY AN
ASSEMBLY SUBROUTINE TAPERD. THE RAW DATA IN INTEGER FORMAT IS WRITTEN INTO A DISK FILE.

VARIABLES

IBYTES - THE NUMBER OF BCD CHARACTERS FOUND IN ONE TAPE RECORD BY SUBROUTINE
ALBYTES
I HOLD(300) - THE STRING OF CHARACTERS FOUND BY ALBYTES PACKED FOUR TO A WORD IN
ZONE DECIMAL FORMAT
INTTAB(400) - TABLE OF INTEGER INTENSITY VALUES RETURNED BY SUBROUTINE TAPERD
PNTPER(40) - TABLE OF THE NUMBER OF INTENSITY READINGS PER PEAK IN THE INTTAB
DISTAB(40) - TABLE OF DISTANCE VALUES. ONE VALUE FOR EACH PEAK IN PNTPER
PEKNUM - TOTAL NUMBER OF PEAKS IN THE TAPE RECORD
TOTP - TOTAL NUMBER OF INTENSITY READINGS IN THE TAPE RECORD
ERR - AN ERROR FLAG RETURNED BY SUBROUTINE TAPERD. ERR=0 NORMAL RETURN
ERR=1 FOR TAPE FORMAT ERROR
RAWINT(25000) - TABLE OF INTENSITY VALUES FOR THE ENTIRE TAPE FILE
NUMINT(1000) - TABLE OF THE NUMBER OF INTENSITY READINGS PER PEAK IN THE ENTIRE
TAPE FILE
RAWDIS(1000) - TABLE OF DISTANCE READINGS. ONE FOR EACH PEAK IN NUMINT
PNTPERJ40) - TABLE OF THE NUMBER OF PEAKS IN THE INTTAB LIST
PNTPER - Pointer to next variable in the INTTAB array
PNTPER - Pointer to next variable in the NUMINT and RAWDIS arrays
NOLIST - LOGICAL VARIABLE TO OPT FOR RAW DATA LISTING. TRUE FOR NO LISTING
- AND FALSE FOR A LISTING

LOGICAL NOLIST
INTEGER DISTAB,PNTPER,PEKNUM,TOTP,ERR
INTEGER RAWINT,NUMINT,RAWDIS
COMM/A/AMESTP/ IBYTES,I HOLD(300)
COMMON/MASPEC/ INTTAB(400),PNTPER(40),DISTAB(40),PEKNUM,TOTP,ERR
COMMON/FILE/RAWINT(25000),NUMINT(1000),RAWDIS(1000)

CLEAR ALL COMMON AREAS
DO 500 N=1,25000
500 RAWINT(N)=0
DO 501 N=1,1000
501 RAWDIS(N)=0

NOLIST IS THE LOGICAL VARIABLE TO OPT FOR A PRINTER LISTING OF THE
TAPE FILE
READ(5,50) NOLIST
NEXINT=1
NEXDIS=1
DO 1000 1=1,300
1000 HOLD(I)=0

BYTES IS AN AMES LIBRARY SUBROUTINE THAT READS ONE RECORD OF A TAPE
FILE AT A TIME INTO THE I HOLD ARRAY IN ZONE DECIMAL FORMAT. ERR IS
AN ERROR FLAG: 0= NORMAL RETURN; 1= END OF FILE; 2=1/O ERROR
CALL BYTES(I HOLD,IBYTES,ERR)
IF(ERR.EQ.1) GO TO 100
IF(ERFR.EQ.2) GO TO 1000

TAPERD IS AN ASSEMBLY SUBROUTINE TO UNBLOCK THE DATA TAPE FORMAT
AND CONVERT THE ZONE DECIMAL NUMBERS TO INTEGER. ERR=0 FOR NORMAL
RETURN; ERR=1 FOR TAPE FORMAT ERROR
1 CALL TAPERD
IF(ERFR.EQ.1) GO TO 1000
2 IF(.NOT.NOLIST) GO TO 300
3 IF(PENXUN.EQ.0) GO TO 4
LIMIT=MAXINT+TOTP-1
LIMIT2=MAXDIS+PEKNUM-1
KOUNT1=0
DO 4001 I=1,MAXINT,LIMIT1
4001 KOUNT1=KOUNT1+1
DO 4002 I=1,MAXDIS,LIMIT2
4002 KOUNT2=KOUNT2+1
NUMINT(K)=INTTAB(KOUNT1)
NEXINT=NEXINT+1
MAXINT=MAXINT+1
MAXDIS=MAXDIS+1
GO TO 1000

UPON READING AN END OF FILE, THE CONTENTS OF THE RAW DATA COMMON
BLOCK ARE READ OUT INTO A DISK FILE NAMED IN THE DDEF STATEMENT
4 NEXINT=NEXINT+1
NEXDIS=NEXDIS+1
C JANUARY 9, 1973
C
WRITE(7) NEXINT,(RAWINT(I),I=1,NEXINT),NEXDIS,(NUMINT(I),RANGDIS(I),I=1,NEXDIS)
STOP
C IF AN END OF FILE HAS BEEN READ THE VARIABLE PENUM IS SET TO ZERO
100 PENUM=0
GO TO 2
C THIS SECTION WILL PRINT THE CONTENTS OF THE AMES DATA TAPE IF
C REQUESTED BY SETTING NLIST EQUAL TO FALSE
300 IF(PENUM.EQ.0) GO TO 4
   LENGTH=IBYTES/4+1
   INTLN=IBYTES/3
   WRITE(6,10) IBYTES
   WRITE(6,11) (IHOLD(J),J=1,LENGTH)
   WRITE(6,12) (INTTAB(J),J=1,INTLN)
   WRITE(6,13) PNTPER
   WRITE(6,14) DISTAB
   WRITE(6,15) PENUM
   GO TO 3
10 FORMAT(I0)
11 FORMAT(1X,30A4)
12 FORMAT(' ', ' INTENSITIES',301)
13 FORMAT(IX, 'PNTPER',201)
14 FORMAT(IX, 'DISTAB',101)
15 FORMAT(IX, 'PEKNUM',14)
16 FORMAT(I0)
17 FORMAT(1X)
50 FORMAT(L5)
END
THIS SUBROUTINE WILL CONVERT AN AMES HIGH RESOLUTION TAPE RECORD IN EBCDIC FORMAT TO INTEGER FORMAT FOR THE MAIN DATA REDUCTION PROGRAM TO USE.

* xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
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'00000000'
L 7,#F'00000000'
CLEAR ST 7,0(5)
A 5,#F'1'
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'1'
* INITIALIZE 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 INITIALLY 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'00000000'
* LOAD REGISTER EIGHT AS OPTICAL DENSITY PER PEAK COUNTER
L 8,#F'00000000'
* LOAD REGISTER NINE WITH THE ADDRESS OF PNTPER
LR 9,4
A 9,#F'16000000'
* LOAD REG 10 WITH THE ADDRESS OF DISTAB
LR 10,3
A 10,#F'16000000'
* LOAD REG 11 WITH THE ADDRESS OF PEKNUM
LR 11,10
A 11,#F'16000000'
* INITIALIZE REG 12 AS DISTANCE READING COUNTER
L 12,#F'00000000'
* WE BEGIN TO PROCESS THE TAPE RECORD
* END OF RECORD TEST
* TESEND C 5,#F'1'
BNH EXIT
* WE NOW ENTER THE TAPE READ LOGIC
* TESTCH TM 0(3),X'FO'
BNO DISTCE
TM 2(3),X'FO'
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 NEGATIVE WE HAVE A TAPE FORMAT ERROR
CP DBL,#F'00000000'
BNH ERROR
CVB 7,08BL
ST 7,0(0,4)
* INCREMENT THE COUNTERS AND DATA BASE REGISTERS
A 3,#F'1'
A 4,#F'1'
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'DO'
BNO ERROR
PACK DBL,0(6,3)

* CONVERT THE DISTANCE READING TO A LEGITIMATE POSITIVE NUMBER
  DI 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'11'
  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 INITIALIZE THE INTENSITY NUMBER COUNTER
  L 8,=F'0'
  B TESEND

* IF TAPE FORMAT IS INCORRECT GO TO ERROR EXIT

EXIT
TM 0(3),X'FD0'
BD ERROR
TM 5(3),X'FD0'
BD ERROR

* FOR CORRECT TAPE FORMAT TAKE NORMAL EXIT

* STORE FINAL DISTANCE READING IN DISTAB
  PACK DBL,0(6,3)
  DI DBL+7,X'0F'
  CVB 7, DBL
  ST 7,0(0,10)

* INCREMENT DISTANCE READING COUNTER
  A 12,=F'11'

* 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
  A 11,=F'8'

* THIS IS AN ABNORMAL EXIT STORE ONE IN THE ERROR FLAG
  L 4,=F'11'
  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
OCTOBER 10, 1972

MICHAEL ROMIEZ

THIS IS THE PROGRAM WHICH CALLS THE VARIOUS SUBROUTINES TO REDUCE THE HIGH RESOLUTION MASS SPECTRAL DATA.

CALL PARLST
CALL PKLIST
CALL STDFIT
CALL ELELST
STOP
END
THIS SUBROUTINE IS A GENERAL POLYNOMIAL FITTING ALGORITHM. IT WILL FIT UP TO 200 DATA POINTS TO A POLYNOMIAL FROM FIRST TO TENTH DEGREE POLYNOMIAL. THE POLYNOMIAL IS BEST FIT IN THE LEAST SQUARES SENSE.

**VARIABLES**

- **X(200)** - UP TO 200 ABCISSA VALUES
- **Y(200)** - UP TO 200 ORDINATE VALUES
- **C(11)** - UP TO 11 COEFFICIENTS CALCULATED BY THIS SUBROUTINE
- **N** - THE NUMBER OF DATA POINTS IN THE X AND Y ARRAYS
- **IDEG** - THE DEGREE OF THE POLYNOMIAL
- **SUMX(20)** - THE UP TO TWENTY VALUES OF THE SUMMATIONS OF X RAISED TO THE POWERS OF ONE THROUGH IDEG INCLUSIVE.
- **SUMXY(IO)** - THE UP TO TENTH VALUES OF THE SUMMATIONS OF Y TIMES X RAISED TO THE POWERS OF ONE THROUGH IDEG INCLUSIVE.
- **SUMY** - THE SUMMATION OF THE Y VALUES
- **A(I1,11)** - THE IDEG+1 BY IDEG+1 SQUARE MATRIX OF SUMMATION VALUES FROM THE NORMAL EQUATIONS OF THE LEAST SQUARE SYSTEM OF EQUATIONS
- **B(I1)** - THE UP TO ELEVEN CONSTANT TERMS OF THE NORMAL EQUATIONS
- **DM(I1)** - TEMP STORAGE

**SUBROUTINE POLYFT**

```fortran
DOUBLE PRECISION B(11), A(11,11), C(11), DM(11)
DOUBLE PRECISION SUMX(20), SUMXY(IO), SUMY, X(200), Y(200)
COMMON/FIT/X, Y, N, IDEG, C

C CLEAR VARIABLES
DO 1000 J=1,10
  SUMXY(J)=0.
DO 1001 J=1,11
  B(J)=0.
  DM(J)=0.
  C(J)=0.
DO 1002 J=1,20
  SUMX(J)=0.
DO 1003 K=1,11
  A(J,K)=0.
SUMY=0.
C CALCULATE THE SUMMATION VALUES
DO 2000 M=1,IDEG
  SUMXY(M)=SUMXY(M)+Y(K)*X(K)**M
  SUMY=SUMY+Y(M)
  N2=IDEG*2
  DO 2002 M=1,N2
    SUMX(M)=SUMX(M)+X(K)**M
C THIS SECTION ASSIGNS THE SUMMATION VALUES TO THE PROPER MATRIX ELEMENTS
LIMIT=IDEG+1
DO 3001 J=1,LIMIT
  DO 3000 K=1,LIMIT
    DM(K)=A(K+1, J)/A(J, J)
    A(K+1, L)=A(K+1, L)-DM(K)*A(J, L)
    B(K+1)=B(K+1)-DM(K)*B(J)
  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 4000 K=1,NN
    A(K+1, L)=A(K+1, L)-DM(K)*A(J, L)
    B(K+1)=B(K+1)-DM(K)*B(J)
  CONTINUE
A(1,1)=N
B(1)=SUMY
C THIS SECTION CALCULATES THE ELEMENTS OF THE TRIANGULAR MATRIX FROM THE TRIANGULAR MATRIX
MN=LIMIT+1
DO 5001 K=1, LIMIT
  DM(I)=0
  IROW=M-K
  ICOL=IROW
  DO 4000 I=IROW,ICOL
    DM(I)=DM(I)+A(I,J)*B(J)
  CONTINUE
A(1,1)=N
B(1)=SUMY
```

MICHAEL ROMIŽE

JANUARY 30, 1973
C JANUARY 30, 1973

C IF (ICOL .GT. LIMIT) GO TO 5001
DM(1) = DM(1) - A(1ROW,ICOL) * C(ICOL)
GO TO 5000

5001 C(1ROW) = (B(1ROW) + DM(1)) / A(1ROW,1ROW)
RETURN
END
THIS MODULE SETS ALL THE VARIABLE PARAMETERS USED BY THE DECONVOLUTION, PEAK CENTER DETERMINATION, AND DISTANCE TO MASS CONVERSION ROUTINES.

THE VARIABLES HAVE DEFAULT VALUES GIVEN AT COMPIILATION, BUT THEY MAY BE REVIEWED AND CHANGED AT EXECUTION TIME.

VARIABLES

DERDEG - THE DEGREE OF THE FIRST DERIVATIVE POLYNOMIAL
DERNUM - THE NUMBER OF DATA POINTS USED BY THE FIRST DERIVATIVE POLYNOMIAL
SMNUM - THE NUMBER OF DATA POINTS USED BY THE SMOOTHING POLYNOMIAL
SMDEG - THE DEGREE OF THE SMOOTHING POLYNOMIAL
CONNUM - THE NUMBER OF POINTS USED BY THE DISTANCE TO MASS CONVERSION POLYNOMIAL
CONDEG - THE DEGREE OF THE DISTANCE TO MASS CONVERSION POLYNOMIAL
CUTOFF - IF THE TOTAL NUMBER OF DATA POINTS IN THE PEAK PROFILE IS LESS THAN OR EQUAL THIS NUMBER, THE PEAK IS TREATED AS A SINGLE PEAK WITH NO DECONVOLUTION ANALYSIS
INTMIN - IF THE PEAK PROFILE CONTAINS NO INTENSITY READINGS ABOVE THIS VALUE, THE PEAK IS IGNORED. THIS ABILITY IS USEFUL IN DISCRIMINATION AGAINST SUCH ARTIFACTS AS SCRATCHES ON THE PHOTOPLATE
TOLFAC - THIS IS A FACTOR USED BY THE STANDARD MASS SEARCHING ROUTINE TO CALCULATE THE TOLERANCE WITHIN WHICH IT WILL ACCEPT A PEAK AS A STANDARD MASS.
EXPTOL - LOWER LIMIT OF THE NUMBER OF INTENSITY VALUES CONSIDERED AN OVEREXPOSURE.

SUBROUTINE PARLST
INTEGER DERDEG,DERNUM,SMNUM,SMDEG,CUTOFF,CONNUM,CONDEG,TOLFAC,EXPTOL
COMMON/PAR/DERDEG,DERNUM,SMNUM,SMDEG,CUTOFF,CONNUM,CONDEG,TOLFAC,EXPTOL
DERDEG=3
DERNUM=5
SMNUM=25
SMDEG=3
CONNUM=1
CONDEG=2
CUTOFF=30
INTMIN=90
TOLFAC=7
EXPTOL=80
WRITE(6,100)
100 FORMAT(1X'DO YOU WANT TO REVIEW THE PEAK POSITION PARAMETERS?')
READ(6,101) I
101 FORMAT(1X)
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(6,106) CONNUM
106 FORMAT(1X,'THE NUMBER OF MASSES USED BY THE MASS CALCULATION POLYNOMIAL IS',13)
CALL INTGER(M)
IF(M.NE.0) CONNUM=M
WRITE(6,107) CONDEG
107 FORMAT(1X,'THE DEGREE OF THE MASS CALCULATION POLYNOMIAL IS',13)
CALL INTGER(M)
IF(M.NE.0) CONDEG=M
WRITE(6,108) CUTOFF
108 FORMAT(1X,'THE CUTOFF VALUE FOR A SINGLE PEAK IS',14)
CALL INTGER(M)
IF(M.NE.0) CUTOFF=M
WRITE(6,109) INTMIN
109 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
WRITE(6,111) EXPTOL
FORMAT(1X,'THE NUMBER OF INTENSITY VALUES ABOVE WHICH A PEAK WILL BE EDITED IS',I5)
CALL INTEGER(M)
IF(M.NE.0) EXPTOL=M
RETURN
END
THE SUBROUTINE SENDS RAW PEAK PROFILES TO SUBROUTINE PEAK WHICH IN TURN CONTROLS
THE SMOOTHING, DECONVOLUTION, AND PEAK CENTER CALCULATION ROUTINES. THIS MODULE
Sends up to 100 data points to subroutine peak and is returned up to ten peak centers
and maximum intensity values. These centers and intensities are stored for the rest
of the data reduction routines.

VARIABLES

RAWINT(25000) - Table of intensity values for the entire raw data file
NUMINT(1000) - Table of the number of intensity readings per peak in the entire
RAWDIS(1000) - Table of distance readings, one for each peak in NUMINT
CENTER(1500) - Distance of peak centers from the left edge of the photoplate
- in millimeters
HEIGHT(1500) - Maximum intensity value of each peak
NUMPK - Number of peaks in the peak list table
LIST(400) - Holding table to pass one peak profile between modules
NUM - Either the number of intensity values in the peak profile or the
DIS - The distance in half-microns of the last intensity reading in the
CENT(10) - Up to 10 peak centers returned by subroutine peak
HGT(IO) - Up to ten maximum intensity values, one for each peak in CENT
LSTPAR(IO) - List of parameters from the PARLIST module
PTINT - Points to next intensity reading in RAWINT
PTDIS - Points to next position in the RAWDIS and NUMINT arrays
PTCENT - Points to next position in the CENTER and HEIGHT arrays
INTHMIN - All intensity readings in a profile must be above this value
- or the peak is ignored. This is useful in discriminating against
- scratches on the photoplate
IEDIT - Lower limit of the number of intensity readings for editing

SUBROUTINE PKLIST
DOUBLE PRECISION CENTER,CENT(IO)
INTEGER RAWINT(25000),NUMINT(1000),RAWDIS(IOOO)
INTEGER PTINT,PTDIS,LIST(400),PTCENT,DIS
INTEGER YES,'Y'
DIMENSION HGT(IO)
COMMON/PKLIST/ CENTER(ISOO),HEIGHT(I500),NUMPK
COMMON/PK/L1ST,NUM,DIS,CENT,HGT
COMMON/PAR/LSTPAR(10)

SET THE INTMIN VALUE AS GIVEN BY THE PARAMETER LIST MODULE
INTMIN=LSTPAR(6)
SET THE LOWER LIMIT OF THE NUMBER OF INTENSITY READINGS FOR PROFILE EDITING
IEDIT=LSTPAR(10)

CLEAR VARIABLES
DO 100 M=1,1500
CENTER(M)=0.
100 HIGHT(M)=0.
DO 150 M=1,25000
RAWINT(M)=0.
DO 151 M=1,1000
RAWDIS(M)=0.
151 NUMINT(M)=0.

READ 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.
RETURN IF THERE ARE NO MORE PROFILES IN THE RAW DATA FILE
IF(NUMINT(PTDIS).EQ.0) GO TO 9999
IF(NUMINT(PTDIS).GT.400) GO TO 200
IF(NUMINT(PTDIS).GT.10) GO TO 200
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

READ PEAK PROFILE AND DISTANCE INTO DATA PASSING ARRAYS
200 NUM=NUMINT(PTDIS)
DO 225 I=1,NUM
225 LIST(I)=0
DO 250 J=1,NUM
PTINT=PTINT+1
250 LIST(J)=RAWINT(PTINT)
DIS=RAWDIS(PTDIS)

18
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.90) GO TO 100
   PTDIS=PTDIS+1
GO TO 10
100 WRITE(6,1)
   1 FORMAT('0,'THE PEAK LIST WAS TRUNCATED AT',16,'VALUES')
9999 NUMPK=PTCENT
RETURN
END
THIS SUBROUTINE CONTROLS DATA SMOOTHING, PEAK DECONVOLUTION, AND PEAK CENTER CALCULATION

VARIABLES

LIST(400) - HOLDING TABLE TO PASS ONE PEAK PROFILE BETWEEN MODULES
NUM - EITHER THE NUMBER OF INTENSITY VALUES IN THE PEAK PROFILE OR THE
      NUMBER OF PEAK CENTERS RETURNED BY SUBROUTINE ANAL
DIS - THE DISTANCE IN HALF-MICRONS OF THE LAST INTENSITY READING IN THE
      PROFILE
CENT(10) - UP TO 10 PEAK CENTERS RETURNED TO THIS SUBROUTINE FOR EACH PEAK
HGT(10) - UP TO TEN MAXIMUM INTENSITY VALUES, ONE FOR EACH PEAK IN CENT
LSTPAR(10) - LIST OF PARAMETERS FROM THE PARLIST MODULE
CUTOFF - MINIMUM NUMBER OF POINTS FOR A PROFILE TO BE ANALYZED FOR
         MORE THAN ONE PEAK. PROFILES WITH LESS THAN CUTOFF DATA
         POINTS WILL BE TREATED AS A SINGLE PEAK
NUMSM - NUMBER OF POINTS USED BY THE SMOOTHING ROUTINE
         PROFILES WITH LESS THAN CUTOFF DATA POINTS WILL BE TREATED AS A SINGLE PEAK

SUBROUTINE PEAK
DOUBLE PRECISION CENT(IO)
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)
c= 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+1)) GO TO 150
CALL ONEPK
RETURN
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)
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 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
This routine calls a general least square polynomial fitting routine to smooth the profile data. It returns num less (numsm-1) smoothed data points. The degree of the polynomial and the number of data points used for smoothing is selected in the parameter selecting subroutine parlist.

**Variables**

- LIST(400) - Holding table to pass one peak profile between modules
- NUM - The number of intensity values in the peak profile
- DIS - The distance in half-microns of the last intensity reading in the peak profile
- CENT(IO) - Up to 10 peak centers
- HGT(IO) - Up to 10 maximum intensity values, one for each peak in cent
- LSTPAR(IO) - List of parameters from the parlist module
- X(200) - Up to 200 abscissa values to be passed to the polynomial fitting routine
- Y(200) - Up to 200 ordinate values to be passed to the polynomial fitting routine
- N - Number of X and Y values passed
- IDEG - Degree of the polynomial (up to tenth possible)
- C(11) - Up to 11 coefficients returned by the polynomial routine
- DEGSM - Degree of the smoothing polynomial, supplied by the parlist module
- NUMSM - Number of data points used by the smoothing polynomial
- HOLD(400) - Temporary storage used by this module

**Subroutine Smooth**

```fortran
DOUBLE PRECISION X(200), Y(200), C(11), CENT(IO)
DIMENSION LIST(IO), HGT(IO)
INTEGER DIS, DEGSM, HOLD(400)
COMMON/PAR/LSTPAR(IO)
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
  HOLD(M)=0
LIMIT=NUMSM-1
M=NUM-LIMIT
C LOAD RAW DATA POINTS INTO X AND Y ARRAYS
DO 200 I=2, NUMSM
  Y(I)=DFLOAT(LIST(I))
DO 250 L=I, NUMSM
  X(L)=DFLOAT(LIST(I))
DO 200 L=1, DEGSM
  LL=L+1
C THIS DO LOOP (DOWN TO STMT 200) CONTROLS THE SENDING OF NUMSM RAW DATA POINTS TO THE POLYNOMIAL ROUTINE TO OBTAIN THE SMOOTHED DATA POINTS. ALL NUMSM DATA POINTS ARE USED TO CALCULATE ONE SMOOTH DATA POINT. THE LOWEST RAW DATA POINT IS DISCARDED AND THE REMAINING POINTS ARE MOVED DOWN ONE POSITION. A NEW HIGH DATA POINT IS READ IN FROM THE PROFILE DATA AND THE NEXT SMOOTHED DATA POINT IS CALCULATED. THE PROCESS IS REPEATED UNTIL WE HAVE NUM-(NUMSM-1) SMOOTHED DATA POINTS.
DO 200
  INDEX1=I-LIMIT
  INDEX2=LIMIT/2+1
  HOLD(INDEX1)=C(1)
  DO 200 L=1, DEGSM
    200 HOLD(INDEX1)=HOLD(INDEX1)+C(LL)*FLOAT(INDEX2)**L
  NUM=NUM-LIMIT
C THE LAST TWO DO LOOPS MOVE THE SMOOTHED DATA POINTS FROM TEMP STORAGE BACK TO THE PROFILE PASSING ARRAY
DO 300 K=ISTRT, ISTOP
  LIST(K)=0
LIST(K)=HOLD(K)
ISTRT=N+1
ISTOP=N+NUMSM
DO 301 K=ISTRT, ISTOP
  LIST(K)=0
RETURN
END
```
C THIS MODULE CALLS THE GENERAL LEAST SQUARE FITTING ROUTINE TO CALCULATE A FIRST DERIVATIVE OF THE SMOOTHED PEAK PROFILE. THE FIRST DERIVATIVE IS FOUND BY OVERLAPPING POLYNOMIALS IN THE SAME MANNER AS THE SMOOTHING ALGORITHM.

VARIABLES

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 OF PEAKS FOUND BY THIS MODULE
C DIS - THE DISTANCE IN HALF-MICRONS OF THE LAST INTENSITY READING IN THE PEAK PROFILE MEASURED FROM THE LEFT END OF THE PHOTOPLATE
C CENT(IO) - UP TO 10 PEAK CENTERS
C HGT(IO) - UP TO TEN MAXIMUM INTENSITY VALUES, ONE FOR EACH PEAK IN CENT
C LSTPAR(IO) - LIST OF PARAMETERS FROM THE PARLIST MODULE
C X(200) - UP TO 200 ABCISSA VALUES TO BE PASSED TO THE POLYNOMIAL FITTING ROUTINE
C Y(200) - UP TO 200 ORDINATE VALUES TO BE PASSED TO THE POLYNOMIAL FITTING ROUTINE
C N - NUMBER OF X AND Y VALUES PASSED
C IDEG - DEGREE OF THE POLYNOMIAL (UP TO TENTH POSSIBLE)
C C(I1) - UP TO 11 COEFFICIENTS RETURNED BY THE POLYNOMIAL ROUTINE
C XUMFT - DEGREE OF THE 1ST DERIVATIVE POLYNOMIAL, SUPPLIED BY THE PARLIST MODULE
C NUMFT - NUMBER OF DATA POINTS USED BY THE 1ST DERIVATIVE POLYNOMIAL, SUPPLIED BY THE PARLIST MODULE
C FSTDER(IO) - 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

DOUBLE PRECISION CENT(IO),C(I1),X(200),Y(200)
0 IMENSI ON L IST (1)00) , HGT (10) , FSTDER (<lOO)
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=1,100
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+LIMIT
DO 150 K=1,LIMIT
150 X(L)=X(L)
10 Y(I)=DFLOAT(LIST(J))
DO 150 L=2,DEGFT
LL=L-1
150 FSTDER(INDEXI)=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 HEIGHT OF UP TO TEN PEAKS CONTAINED IN EACH PEAK PROFILE. IN THIS SECTION J IS THE CENT AND HGT ARRAY POINTER AND M IS THE FSTDER ARRAY POINTER.
C JANUARY 16, 1973
M. ROMIEZ

C

J=1
M=0
1 IF(M.GT.INDEX3-1) GO TO 99

C UPSLOPE LOGIC
2 M=M+1
3 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
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.IO) 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
80 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
This subroutine will determine the center and height of a single peak. It fits the peak profile to a Gaussian distribution curve.

**Variables**

- `X(200)` - Up to 200 points that are used by the polynomial fitting routine for the best least squares Gaussian fit
- `Y(200)` - One ordinate value for each X value
- `N` - Number of X and Y values
- `IDEG` - In this case `IDEG=2`. It is the degree of the polynomial used for fitting
- `C(11)` - The first three values of the array contain the coefficients of the second degree polynomial
- `LIST(400)` - Holding table to pass peak profiles between modules
- `NUM` - Either the number of intensities in the peak profile or `NUM-1` to indicate the number of peaks found by this module
- `DIS` - The distance in half-microns of the last intensity reading in the profile as measured from the left end of the photographic plate
- `CENT(IO)` - The center calculated by this module is put in `CENT(I)`
- `HGT(IO)` - The height calculated by this module is put in `HGT(I)`

```fortran
SUBROUTINE ONEPK
DOUBLE PRECISION CENT(IO),C(11),X(200),Y(200)
INTEGER DIS
DIMENSION HGT(IO),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 ORDNATE 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(I)=(-C(2)/C(3))/2.
  HGT(I)=(CENT(I))/SQRT(-(1./C(3)))**2
  HGT(I)=EXP(HGT(I))
  CENT(I)=DIS-(NUM-CENT(I))
  NUM=1
99 RETURN
END
```
THIS MODULE WILL ALLOW EDITING OF THE RAW PEAK PROFILE. PART OF THE PROFILE MAY BE DELETED AND SELECTED INTENSITY READINGS MAY BE CHANGED.

VARIABLES

LIST(I00) - HOLDING TABLE TO PASS ONE PEAK PROFILE BETWEEN MODULES
NUM - THE NUMBER OF INTENSITY VALUES IN THE PEAK PROFILE
DIS - THE DISTANCE IN HALF-MICRONS OF THE LAST INTENSITY READING IN THE PROFILE
CENT(IO) - UP TO 10 PEAK CENTERS
HGT(IO) - UP TO TEN MAXIMUM INTENSITY VALUES, ONE FOR EACH PEAK IN CENT

SUBROUTINE EDIT
DOUBLE PRECISION CENT(IO)
INTEGER LIST(l00),NUM,DIS
DIMENSION HGT(IO)
COMMON/PK/L1ST,NUM,DIS,CENT,HGT
DATA YES/'Y'/
C THIS SECTION LISTS THE RAW PEAK PROFILE
WRITE(6,100)
100 FORMAT('OPEAK 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 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 INTEGER(LOW)
IF(LOW.GT.NUM) GO TO 400
IF (.EQ.1) GO TO 200
LIMIT=NUM-(LOW-I)
DO 150 J=LOW,J+1
INDEX=LOW-1+J
150 LIST(J)=LIST(INDEX)
200 WRITE(6,103)
103 FORMAT('0,ENTER NEW ENDING SUBSCRIPT')
C IF NOTHING IS ENTERED FOR THE ENDING SUBSCRIPT, THE OLD VALUE IS KEPT.
CALL INTEGER(IHIGH)
IF(IHIGH.EQ.0) IHIGH=NUM
IF (.EQ.NUM) GO TO 300
ISTRAT=IHIGH+1
D250 J=ISTRAT,NUM
250 LIST(J)=0
DIST=DIS-(NUM-IHIGH)
300 NUM=NUM-(NUM-IHIGH)-(LOW-1)
C THIS SECTION WILL ACCEPT INTENSITY VALUE CHANGES
WRITE(6,104)
104 FORMAT('0,ENTER NEW INTENSITY')
CALL INTEGER(M)
IF(M.EQ.0) RETURN
WRITE(6,105)
105 FORMAT('0,ANY INTENSITY EDITING?')
READ(5,106)
106 FORMAT(A1)
IF(.NE.YES) RETURN
WRITE(6,107)(LIST(I),I=1,NUM)
405 WRITE(6,107)
107 FORMAT('0,ENTER SUBSCRIPT')
CALL INTEGER(N)
IF(N.EQ.0) RETURN
WRITE(6,108)
108 FORMAT('0,ENTER INTENSITY')
CALL INTEGER(N)
LIST(N)=N
GO TO 450
END
This subroutine controls the standard mass search and listing routines.

Variables:

- **CENTER(1500)**: Distance of peak centers from the left edge of the photoplate in millimeters.
- **HEIGHT(1500)**: Maximum intensity value of each peak.
- **NUMPK**: Number of peaks in the peak list table.
- **STDDIS(160)**: The distance values of peak centers identified as standard masses.
- **STDMAS(160)**: The square root of the mass value of identified standard masses.
- **NUMSTD**: The number of identified standard masses.
- **REFMAS(160)**: A table of the most intense lines in the marker compound spectrum, these are the masses searched for by the standard mass identification routine.

Subroutine `STDFIT`:

```fortran
SUBROUTINE STDFIT
DOUBLE PRECISION CENTER,STDDIS,STDMAS,REFMAS
INTEGER YES/'Y'
COMMON/PKLST/ CENTER(1500),HEIGHT(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) 1=40
WRITE(6,1) !
1 FORMAT(IX,'THESE ARE THE FIRST ',13,'DISTANCE VALUES')
WRITE(6,2)(CENTER(J),J=1,I)
2 FORMAT(IX,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(IX,10,'ENTER SUBSCRIPT')
CALL INTGER(I)
IF(I.EQ.0) GO TO 66
WRITE(6,5)
5 FORMAT(IX,10,'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(IX,10,'ANY ADDITIONS?')
READ(5,8) I
8 FORMAT(A10)
IF(I.EQ.YES) GO TO 500
GO TO 600
C CALL THE STANDARD MASS FINDER SUBROUTINE
200 CALL STDFNT
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(IX,10,'ANY CHANGES?')
READ(5,8) I
IF(I.EQ.YES) GO TO 500
450 WRITE(6,10)
10 FORMAT(IX,10,'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.EQ.YES) RETURN
GO TO 600
500 CALL CHANGE
GO TO 450
600 CALL ADD
GO TO 200
END
```
THIS MODULE WILL SEARCH FOR THE MAKER COMPOUND PEAKS IN ARRAY CENTER

VARIABLES

CENTER(1500) - DISTANCE OF PEAK CENTERS FROM THE LEFT EDGE OF THE PHOTOPLATE
- IN MILLIMETERS
HEIGHT(1500) - MAXIMUM INTENSITY VALUE OF EACH PEAK
NUPK - NUMBER OF PEAKS IN THE PEAK LIST TABLE
STDDIS(160) - THE DISTANCE VALUES OF PEAK CENTERS IDENTIFIED AS STANDARD MASSES
STDMAS(160) - THE SQUARE ROOT OF THE MASS VALUE OF IDENTIFIED STANDARD MASSES
NUMSTD - THE NUMBER OF IDENTIFIED STANDARD MASSES
REFMAS(160) - A TABLE OF THE MOST INTENSE LINES IN THE MARKER COMPOUND SPECTRUM.
- THESE ARE THE MASSES SEARCHED FOR BY THE STANDARD MASS IDENTIFICATION ROUTINE
- ROUTINE
LSTPAR(IO) - PARAMETER LIST FROM PARAMETER LIST MODULE
X(200) - UP TO 200 POINTS THAT ARE USED FOR POLYNOMIAL FITTING
Y(200) - ONE ORIGINATE VALUE FOR EACH X VALUE
N - NUMBER OF X AND Y VALUES
IDEG - IT IS THE DEGREE OF THE POLYNOMIAL USED FOR FITTING
C(I) - UP TO ELEVEN COEFFICIENTS OF THE POLYNOMIAL CALCULATED
ITOL - THIS IS A FACTOR USED BY THE STANDARD MASS SEARCHING ROUTINE TO CALCULATE THE TOLERANCE WITHIN WHICH IT WILL ACCEPT A PEAK AS A STANDARD MASS. A SMALL VALUE MEANS A SMALL TOLERANCE
K - THE REFMAS ARRAY POINTER
M - THE CENTER ARRAY POINTER
MSTRT - LOWER LIMIT FOR VALUES OF M
MSTOP - UPPER LIMIT FOR VALUES OF M
KSTOP - UPPER LIMIT FOR VALUES OF K
TEMP - THE DISTANCE WHERE THE NEXT STANDARD MASS IS EXPECTED
- TO BE FOUND
ITOL=LSTPAR(9)
CLEAR VARIABLES
DO 100 M=1,200
X(M)=0.
100 Y(M)=0.
WE WANT TO USE A QUADRATIC SEARCH ROUTINE FOR WHICH WE NEED THREE PEAKS. THE FIRST TIME WE ENTER THIS SUBROUTINE WE MAY ONLY HAVE TWO IDENTIFIED STANDARD MASSES. A LINEAR SEARCH SECTION IS PROVIDED FOR THIS CASE
IF(NUMSTD.GT.2) GO TO 200
DO 150 M=1,12
X(M)=STDDIS(M)
150 Y(M)=STDMAS(M)
NUM=2
IDEG=1
CALL POLYFT
GO TO 275
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
THIS IS THE SEARCHING SECTION
275 K=0
M=1
KSTOP=160
MSTOP=NUMP
301 K=K+1
IF WE HAVE LOOKED FOR ALL THE REFMAS ENTRIES, RETURN
IF(K.GT.KSTOP) RETURN
IF(NUMSTD.LT.3) GO TO 350
THIS IS THE SECTION WHERE THE EXPECTED DISTANCE VALUE FOR THE NEXT ENTRY 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)
WE MUST SPECIFY A TOLERANCE WITHIN WHICH WE WILL ACCEPT A DISTANCE VALUE AS THE SEARCHED FOR STANDARD MASS. WE HAVE A
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=I,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).GT.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 ASCENDING ORDER.
600 LIMIT=NUMSTD
   DO 625 J=I,LIMIT
      IF(CENTER(M).GT.STDDIS(J)) GO TO 625
      ITP=160-J
      DO 650 LL=1,ITOP
         JJ=160-LL
         JJJ=JJ+1
         STDDIS(JJJ)=STDDIS(JJ)
         STDMAS(JJJ)=STDMAS(JJ)
         STDDIS(J)=CENTER(M)
         STDMAS(J)=REFMAS(K)
      650 STDMAS(J)=STDMAS(J)
      NUMSTD=NUMSTD+1
   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
THIS MODULE WILL ACCEPT CHANGES AND/OR DELETIONS TO THE STANDARD MASS LIST

VARIABLES

STDDIS(I60) - THE DISTANCE VALUES OF PEAK CENTERS IDENTIFIED AS STANDARD MASSES
STDMAS(I60) - THE SQUARE ROOT OF THE MASS VALUE OF IDENTIFIED STANDARD MASSES
NUMSTD - THE NUMBER OF IDENTIFIED STANDARD MASSES
REFMAS(I60) - A TABLE OF THE MOST INTENSE LINES IN THE MARKER COMPOUND SPECTRUM
- THESE ARE THE MASSES SEARCHED FOR BY THE STANDARD MASS IDENTIFICATION ROUTINE

SUBROUTINE CHANGE
DOUBLE PRECISION STDDIS(160), STDMAS(160), REFMAS(160)
COMMON/PFKLST/ STDDIS, STDMAS, REFMAS, NUMSTD

5000 WRITE(6,1)
1 FORMAT('ENTER SUBSCRIPT')
CALL INTEGER(MM)
IF(MM.EQ.O) GO TO 5001
WRITE(6,3)
3 FORMAT('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 MM=M+1
5003 IF(STDMAS(M).NE.O.) GO TO 5002
DO 5005 J=M,NUMSTD
   IF(STDMAS(J).NE.O.) 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
THIS MODULE WILL DISPLAY AREAS OF THE CENTER LIST AND ADD ENTERIES TO THE STANDARD MASS LIST

VARIABLES

CENTER(1500) - DISTANCE OF PEAK CENTERS FROM THE LEFT EDGE OF THE PHOTOPLATE
- IN MILLIMETERS
HEIGHT(1500) - MAXIMUM INTENSITY VALUE OF EACH PEAK
NUMPK - NUMBER OF PEAKS IN THE PEAK LIST TABLE
STDDIS(160) - THE DISTANCE VALUES OF PEAK CENTERS IDENTIFIED AS STANDARD MASSES
STDMAS(160) - THE SQUARE ROOT OF THE MASS VALUE OF IDENTIFIED STANDARD MASSES
NUMSTD - THE NUMBER OF IDENTIFIED STANDARD MASSES
REFMAS(160) - A TABLE OF THE MOST INTENSE LINES IN THE MARKER COMPOUND SPECTRUM.
- THESE ARE THE MASSES SEARCHED FOR BY THE STANDARD MASS IDENTIFICATION ROUTINE
TEMP - TEMPORARY STORAGE

SUBROUTINE ADD
DOUBLE PRECISION STDDIS(160),STDMAS(160),REFMAS(160),TEMP
DOUBLE PRECISION CENTER
COMMON/PFKLST/STDDIS,STDMAS,REFMAS,NUMSTD
COMMON/PKLST/CENTER(1500),HEIGHT(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 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 11
M=0
I M=M+1
IF(CENTER(M).EQ.O.) 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
40 WRITE(6,33) J,CENTER(J),HEIGHT(J)
WRITE(6,34)
34 FORMAT('0', 'ENTER SUBSCRIPT')
CALL INTEGER(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
DO 7777 1=1,NN
IF(TEMP.GT.STDMAS(1)) TO TO 7777
LTOP=160-I
DO 8000 J=1,LTOP
8000 STDDIS(J)=STDDIS(J-1)
STDMAS(J)=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(N-1)
37 FORMAT('0', 'THE LARGEST DISTANCE VALUE IN THE FILE IS',F10.5)
GO TO 2
999 RETURN
THIS MODULE WILL LIST THE STANDARD MASSES FOUND BY THE SEARCHING ROUTINE

VARIABLES

STDDIS(160) - THE DISTANCE VALUES OF PEAK CENTERS IDENTIFIED AS STANDARD MASSES
STDMAS(I60) - THE SQUARE ROOT OF THE MASS VALUE OF IDENTIFIED STANDARD MASSES
NUMSTD - THE NUMBER OF IDENTIFIED STANDARD MASSES
REFMAS(I60) - A TABLE OF THE MOST INTENSE LINES IN THE MARKER COMPOUND SPECTRUM.
STDMAS(I60) - THESE ARE THE MASSES SEARCHED FOR BY THE STANDARD MASS IDENTIFICATION ROUTINE
X(200) - UP TO 200 ABCISSA VALUES TO BE PASSED TO THE POLYNOMIAL FITTING ROUTINE
Y(200) - UP TO 200 ORDEINATE VALUES TO BE PASSED TO THE POLYNOMIAL FITTING ROUTINE
NUMSTD - THE NUMBER OF IDENTIFIED STANDARD MASSES
IDEG - DEGREE OF THE POLYNOMIAL (UP TO TENTH POSSIBLE)
C(I1) - UP TO 11 COEFFICIENTS RETURNED BY THE POLYNOMIAL ROUTINE
PFKMAS(I60) - THE MASSES OF IDENTIFIED STANDARD MASSES CALCULATED BY USING THE SURROUNDING INUM STANDARD MASSES
STDMAS(I60) - THE DIFFERENCE IN MILLIMASS UNITS BETWEEN THE EXACT MASS AND THE CALCULATED MASS OF EACH IDENTIFIED STANDARD LINE
PPM(I60) - THE DIFFERENCE IN PARTS PER MILLION BETWEEN THE EXACT MASS AND THE CALCULATED MASS OF EACH IDENTIFIED STANDARD LINE
CC(I60,11) - THE UP TO 160 SETS OF COEFFICIENTS CALCULATED BY THIS MODULE FOR EACH SET OF INUM STANDARD MASSES USED IN THE DISTANCE TO MASS CALCULATION
INUM - THE NUMBER OF STANDARD MASSES USED FOR EACH SUCCESSIVE POLYNOMIAL FIT
INDEX - POINTER TO THE CC ARRAY
INDEX - THE TOTAL NUMBER OF SETS OF COEFFICIENTS
IORDER - THE NUMBER OF COEFFICIENTS RETURNED BY THE POLYNOMIAL FITTING ROUTINE
ISTRT - POINTER TO THE LOWEST OF THE INUM VALUES TO BE TRANSFERED TO THE POLYNOMIAL FITTING ROUTINE
ITOP - POINTER TO THE HIGHEST OF THE INUM VALUES TO BE TRANSFERED TO THE POLYNOMIAL FITTING ROUTINE
M - THE STDDIS AND STDMAS ARRAY POINTER

SUBROUTINE STDLST

DOUBLE PRECISION X(200),Y(200),C(I1)
DOUBLE PRECISION STDMAS(I60),STDDIS(I60),PFKMAS(I60)
DOUBLE PRECISION PPKMAS(I60),STD(I60),DIFF(I60),CC(I60,11)
COMMON/PFKLST/STDDIS,STDMAS,REFMAS,NUMSTD
COMMON/FIT/X,Y,N,IDEG,C
COMMON/OUTLST/PPKMAS,STD,DIFF,PPM,CC
COMMON/PAR/LSTPAR(10)
WRITE(6,II)

C SET THE NUMBER OF STANDARD MASSES USED, AND THE DEGREE OF THE CONVERSION POLYNOMIAL
INUM=STPAR(7)
LIMDEG=STPAR(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
LIMDEG=NUMSTD-2
DO 500 M=1,NUMSTD
X(M)=STDDIS(M)
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
501 CC(I, M) = C(M)
INDEX = I
M = 1
GO TO 3000
C THIS SECTION IS FOR MORE THAN JNUM IDENTIFIED STANDARD MASSES
1000 INDEX = I
1001 ISTART = I
1002 IF (TOP = ISTART + JNUM) GO TO 2000
M = 0
C ALL THE STANDARD MASSES ARE SENT TO THE POLYNOMIAL FITTING ROUTINE IN GROUPS OF JNUM.
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 = JNUM
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
INDEX = NUMSTD - JNUM
M = 1
DO 3000 IF (M .LT. KNUM) GO TO 5000
3000 IF (INDEX .LT. INDEX + 1) INDEX = INDEX + 1
IF (INDEX .LT. INDEX + 1) INDEX = INDEX + 1
PFKMAS(M) = CC(INDEX, 1)
DO 4000 K = 1, 10
4000 PFKMAS(M) = PFKMAS(M) + CC(INDEX, K + I) * STDDIS(M)**K
INDEX = INDEX + 1
GO TO 3000
5000 DO 4500 K = 1, NUMSTD
4500 PFKMAS(K) = PFKMAS(K) + PFKMAS(K)
STD(K) = STDMAS(K)**2
DIFF(K) = (PFKMAS(K) - STD(K))**2
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 (11)
202 FORMAT (' 10', 10X, 'MASS', 35X, 'IN MUN', 14X, 'IN PPM')
203 FORMAT (1)
204 FORMAT (3X, 13, 3X, 8.4, 3X, 10.5, 10X, 13X, 15X, F5.2)
END
THIS MODULE ACCEPTS ADDITIONS TO THE ELEMENT LIST USED FOR FITTING COMPOSITIONS
TO THE UNKNOWN PEAKS. IT ALSO WILL ACCEPT A CHANGE IN THE ELEMENT FITTING TOLERANCE
SUPPLIED BY THE PARAMETER SETTING MODULE. IT WILL, AT THE USERS OPTION, WRITE ALL THE DATA
OBTAINED SO FAR INTO A DISK FILE OR WILL CALL THE MODULES TO DO THE ELEMENT FITTING FOR
LISTING ON THE CONVERSATIONAL TERMINAL.

VARIABLES

CENTER(ISOO) - DISTANCE OF PEAK CENTERS FROM THE LEFT EDGE OF THE PHOTOPLATE
- IN MILLIMETERS
HIGHT(ISOO) - MAXIMUM INTENSITY VALUE OF EACH PEAK
NUMPK - NUMBER OF PEAKS IN THE PEAK LIST TABLE
STDDIS(160) - THE DISTANCE VALUES OF PEAK CENTERS IDENTIFIED AS STANDARD MASSES
STDMAS(160) - THE SQUARE ROOT OF THE MASS VALUE OF IDENTIFIED STANDARD MASSES
NUMSTD - THE NUMBER OF IDENTIFIED STANDARD MASSES
REFMAS(160) - A TABLE OF THE MOST INTENSE LINES IN THE MARKER COMPOUND SPECTRUM.
- THESE ARE THE MASSES SEARCHED FOR BY THE STANDARD MASS IDENTIFICATION
- ROUTINE
LSTPAR(IO) - LIST OF PARAMETERS FROM THE PARLIST MODULE
PFKMAS(160) - THE MASSES OF IDENTIFIED STANDARD MASSES CALCULATED BY USING THE
- SURROUNDING STANDARD MASSES
STD(160) - THE KNOWN EXACT MASS OF EACH IDENTIFIED STANDARD MASS
DIFF(160) - THE DIFFERENCE IN MILLIMASS UNITS BETWEEN THE EXACT MASS AND THE
- CALCULATED MASS OF EACH IDENTIFIED STANDARD LINE
PPM(160) - THE DIFFERENCE IN PARTS PER MILLION BETWEEN THE EXACT MASS AND THE
- CALCULATED MASS OF EACH IDENTIFIED STANDARD LINE
CC(160,11) - THE UP TO 160 SETS OF COEFFICIENTS CALCULATED FOR EACH SET OF
- STANDARD MASSES USED IN THE DISTANCE TO MASS CALCULATION
MASS(12) - UP TO TWELVE MASSES OF ELEMENTS USED FOR ELEMENT FITTING
NAME(12) - A FOUR CHARACTER NAME FOR UP TO TWELVE ELEMENTS
NUMBER(12) - THE MAXIMUM NUMBER OF EACH ELEMENT USED IN ELEMENT FITTING
NTOL - THE TOLERANCE IN MILLIMASS UNITS USED FOR ELEMENT FITTING
NUM - THE NUMBER OF ELEMENTS IN THE MASS ARRAY

SUBROUTINE ELELST
DOUBLE PRECISION CENTER,STDMAS(160),STDDIS(160),PFKMAS(160),PPM(160),REFMAS(160)
DOUBLE PRECISION PFKMAS(160),STD(160),DIFF(160),CC(160,11),MASS(12)
INTEGER NUMPK,NUMSTD
COMMON/PFKLST/STDDIS,STDMAS,PFKMAS,NUMSTD
COMMON/PAR/LSTPAR(IO)
COMMON/OUTLST/PFKMAS,STD,DIFF,PPM,CC
COMMON/PKLST/CENTER(1500),HIGHT(1500),NUMPK
COMMON/ELEM/MASS(12),NAME(12),NUMBER(12),NTOL,NUM
DATA MAS/1.0078246,12.,13.0033554,14.0030732,15.9949141,70/
DATA NAME/H ','C12 ','C13',<ti, ','016 ',70/
DATA NUMBER/2*0,2,3,7*0/
DATA YES,IBLK/ 'Y', 'I' /
DO 50 M=1,12
MASS(M)=MAS(M)
NAME(M)=NAME(M)
50 NUMBER(M)=NUMBER(M)
I=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 INTEGER(II)
IF(II.NE.O) 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.1BLK) GO TO 1999
WRITE(6,104)
READ(5,53) MASS(I)
WRITE(6,105)
CALL INTEGER(NUMBER(I))
GO TO 1
1999 NAME(I)=0.
2000 NUMPK=1
2001 WRITE(6,103)
READ(5,57) IFLAG
IF(IFLAG.EQ.1YES) 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,PFKMAS,NUMSTD,-
XSTPAR,PFKMAS,STD,DIFF,PPM,CC,MASS,NAME,NUMBER,NTOL,NUM
STOP
CALL THE ELEMENT FITTING ROUTINE FOR CALCULATION AND DISPLAY ON THE CONVERSATIONAL TERMINAL

3000 CALL ELEMFT

RETURN

100 FORMAT('O', 'DO YOU WISH TO REVIEW ELEMENT FITTING PARAMETERS?')
102 FORMAT('O', 'ENTER ISOTOPE NAME')
103 FORMAT('O', 'IS THIS TERMINAL OUTPUT?')
104 FORMAT(' ', 'ENTER MASS')
105 FORMAT(' ', 'NUMBER FOR THIS ISOTOPE')
106 FORMAT('X', 'THE TOLERANCE FOR ELEMENT FITTING IS', 'MMU')
51 FORMAT(A1)
52 FORMAT(A4)
53 FORMAT(F10.0)

END
This module will calculate an exact mass for each unknown peak in the peak list. It will also determine all elemental compositions that are within a specified tolerance of the exact mass from the given list of elements.

Variables

- CENTER(1500) - distance of peak centers from the left edge of the photoplate in millimeters
- HIGHT(1500) - maximum intensity value of each peak
- NUMPK - number of peaks in the peak list table
- STD DIS(160) - the distance values of peak centers identified as standard masses
- STDMAS(160) - the square root of the mass value of identified standard masses
- NUMSTD - the number of identified standard masses
- REF MAS(160) - a table of the most intense lines in the marker compound spectrum. These are the masses searched for by the standard mass identification routine
- LSTPAR(10) - list of parameters from the PARLIST module
- TRKMAS(160) - the masses of identified standard masses calculated by using the surrounding standard masses
- STO(160) - the known exact mass of each identified standard mass
- DIFF(160) - the difference in millimass units between the exact mass and the calculated mass of each identified standard line
- PPM(16) - the difference in parts per million between the exact mass and the calculated mass of each identified standard line
- CC(160,11) - the up to 160 sets of coefficients calculated for each set of standard masses used in the distance to mass calculation
- MASS(12) - up to twelve masses of elements
- NAME(12) - a four character name for up to twelve elements
- NUMER(12) - the maximum number of each element used in element fitting
- NTOL - the tolerance in millimass units used for element fitting
- CALMA S(391) - a list of the masses of the peaks in the marker compound that will be removed from the CLCMAS table if found
- CLCMAS(1500) - a calculated mass for each peak in array CENTER
- ATNUM(12) - the number of atoms of each element that fits a particular elemental composition
- COUNT1 - a counter that controls the output listing
- COUNT2 - the number of elemental compositions found so far for the particular CLCMAS value under consideration

Subroutine ELEMFT

DOUBLE PRECISION CENTER, STDMAS(160), STDDIS(160), PPM(160), REF MAS(160)
DOUBLE PRECISION TRKMAS(160), STO(160), DIFF(160), CC(160,11)
DOUBLE PRECISION CLCMAS(1500), DIF, NTOL, CALMAS(391), MASS
INTEGER COUNT1, COUNT2, ATNUM(12)

REAL MAX

COMMON/PFKLST/STDDIS, STDMAS, REF MAS, 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, MAS

CLEAR CLCMAS ARRAY
DO 50 J=1,1500
C 0 CLCMAS(J)=0.
C SET THE NUMBER OF STANDARD MASSES USED FOR POLYNOMIAL FITTING IN MODULE STDLST
INUM=LSTPAR(7)
C CALL THE MARKER COMPOUND LISTING MODULE
CALL STDLST
C INITIALIZE THE COUNTER THAT CONTROLS THE OUTPUT FORMAT
COUNT=1
C CALCULATE THE EXACT MASS OF EACH PEAK USING THE PROPER SET OF POLYNOMIAL COEFFICIENTS FROM MODULE STDLST. INDEX IS THE CC ARRAY POINTER, INDEX IS THE POINTER TO THE LAST SET OF COEFFICIENTS IN THE CC ARRAY.

1012 INDEX=1
INDEX=NUMSTD-INUM+1
IF(INDEX.LT.1) INDEX=1
H=1
1 DO 1000 J=1,NUMSTD
IF(STDDIS(J).LT.CENTER(M)) GO TO 1000
GO TO 1001
1000 CONTINUE
1001 INDEX=INDEX+(INUM/2)
IF(J.LT.1) INDEX=INDEX+1
IF(INDEX.GT.INUM) INDEX=INDEX
CLCMAS(1)=CC(INDEX,1)
DO 1005 KL=1,10
K=K+1
1005 CLCMAS(1)=CLCMAS(1)+CC(INDEX,K)*CENTER(K)**K

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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)**2
C READ IN MASSES TO BE STRIPPED 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.O.) 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.O.) GOTO 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.O) RETURN
C CALCULATE NEW NUMPK VALUE
2700 DO 2800 L=1,NUMPK
IF (CLCMAS(L).NE.O.) 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.O) 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)-H
NUM7=NUMBER(7)+1
NUM8=NUMBER(8)+1
NUM9=NUMBER(9)+1
NUM10=NUMBER(10)-H
NUM11=NUMBER(11)-H
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 I=1,NUM1
4050 ATNUM(I)=I
DO 4050 1=1,NUM2
110 ATNUM(1)=I
DO 4050 I=1,NUM9
119 ATNUM(1)=I
4050 CONTINUE
COUNT2=COUNT2+1
DO 4050 I=1,NUM8
4050 CONTINUE
COUNT2=COUNT2+1
DO 4050 I=1,NUM7
4050 CONTINUE
COUNT2=COUNT2+1
DO 4050 I=1,NUM6
4050 CONTINUE
C FEBRUARY 1, 1973
M. ROMIEZ

ATNUM(8)=118
DO 4050 I7=1,NUM7
117=17-1
ATNUM(7)=117
DO 4050 I6=1,NUM6
116=16-1
ATNUM(6)=116
DO 4050 I5=1,NUM5
115=15-1
ATNUM(5)=115
DO 4050 I4=1,NUM4
114=14-1
ATNUM(4)=114
DO 4050 I3=1,NUM3
113=13-1
ATNUM(3)=113
DO 4050 I2=1,NUM2
112=12-1
ATNUM(2)=112
SUM=0.
DO 4100 I=2,NUM
4100 SUM=SUM+ATNUM(I)*MASS(I)
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.ZERO) GO TO 4050
IF(ITEST) 4050,4051,4051
14051 ATNUM(I)=ITEST
SUM=SUM-MASS(I)*ATNUM(I)
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(I)
ATNUM(I)=ATNUM(I)+1
4053 IF(SUM.GT.HTOL) GO TO 4050
IF(SUM.LT.LTOL) GO TO 4052
COUNT2=COUNT2+1
DIF=(CLCMAS(M)-SUM)/TOL.
IMAS=IMAS
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=IMAS
IF(COUNT2.EQ.ZERO) CALL OUTPUT
4000 CONTINUE
RETURN
END
THIS MODULE LISTS ELEMENTAL COMPOSITIONS FOUND BY THE ELEMENT FITTING ROUTINE

VARIABLES

CENTER(ISOO) - DISTANCE OF PEAK CENTERS FROM THE LEFT EDGE OF THE PHOTOPLATE
HIGHT(1500) - MAXIMUM INTENSITY VALUE OF EACH PEAK
NUMPK - NUMBER OF PEAKS IN THE PEAK LIST TABLE
NAME(12) - UP TO TWELVE MASSES OF ELEMENTS
NUMBER(12) - A FOUR CHARACTER NAME FOR UP TO TWELVE ELEMENTS
MASS(12) - THE MAXIMUM NUMBER OF EACH ELEMENT USED IN ELEMENT FITTING
NTOL - THE NUMBER OF ELEMENTS IN THE MASS ARRAY
NUM - THE NUMBER OF ELEMENTS IN THE MASS ARRAY
ATNUM(12) - THE NUMBER OF ATOMS OF EACH ELEMENT THAT FITS A PARTICULAR - ELEMEN\nCOUNT1 - A COUNTER THAT CONTROLS THE OUTPUT LISTING
COUNT2 - THE NUMBER OF ELEMENTAL COMPOSITIONS FOUND SO FAR FOR THE - COMPO\n
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,D1,F1,IMAS

C TEST NEED FOR A NEW PAGE HEADING
IF(COUNT1.GE.^S) GO TO 1002

C IF COUNT2 IS ZERO, THERE HAVE BEEN NO ELEMENTAL FITS FOR THIS MASS
500 IF(COUNT2.EQ.O) 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(1MAS),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('I')
100 FORMAT('I')
300 FORMAT('6X,'DISTANCE',6X,'RELATIVE',7X,'MASS',7X,'DIFFERENCE')
301 FORMAT('20X,'INTENSITY',15X,'IN MMU',5X,12AS)
302 FORMAT('I')
303 FORMAT('6X,8.4,7X,5.1,5X,F10.8,8X,F5.2,3X,12AS')
304 FORMAT('0',5X,F8.4,7X,F5.1,5X,F10.8,10X,'NO ELEMENTAL COMPOSITIONS FOUND WITHIN',13,' MMU')
END
REFERENCES


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—National Aeronautics and Space Act of 1958

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