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MOSSPEC, a Programme for Resolving Mössbauer Spectra

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Abstract

The programme fits a sum of Lorentzian lines to a given Mössbauer spectrum by means of the Gauss non-linear regression procedure with a facility for constraining any set of parameters or linear combinations of parameters. The results are presented as a table of the fitted parameters, a typewriter plot of the residual deviations with an indication of the goodness of the fit and a plot of the measured points and the fitted lines; if desired the results of each iteration can also be printed out.

The present report describe a modified version of the programme described in Risø-M-1348, February 1971.

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Abstract to

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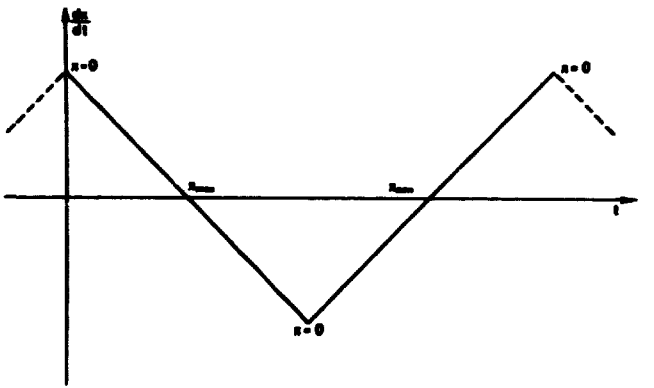
INTRODUCTION

The present report describes a "Mössbauer-fitting-programme" written in FORTRAN for the Burroughs B 6700 computer at Risø. In its present form it can handle up to six hundred channels and fit up to eight lines. If necessary, the capacity can be increased according to instructions given in the programme. Except for the plotting procedure this programme is a modified version of the programme AJS571/GCNLR. MS/2. 2 developed by A. J. Stone for the TITAN-computer in Cambridge, England.

In the Mössbauer spectrometers used at Risø the source is moved with a constant acceleration the direction of which is periodically reversed. If x is the position of the source, then its velocity, $\frac{dx}{dt}$, as a function of time, t, has the well-known form



The pulses from the detector are registered as a function of the source velocity in a multi-channel analyser; this is, for different spectrometers, done in different ways and requires different treatments of the data. Suppose the analyser has 2C channels, then

(1) the pulses registered in the half period (x = 0, x = max, x = 0) are stored in the first C channels, and the pulses in the second half period

(x = 0, x = min, x = 0) are stored in the last C channels; therefore the Mössbauer spectrum is recorded twice, and the two spectra should in principle be the mirror image of each other.

(2) The two half periods are not distinguished from each other, and the pulses are only sorted according to the velocity. In this case only one spectrum is obtained.

(3) The two half periods are distinguished from each other, but the spectrum corresponding to the second half period is stored "backwards" in the last C channels. As in the first case two spectra are obtained; they are, however, not symmetrical, but shifted C channels.

The data are delivered from the multi-channel analysers on tape. In its present form the programme accept data in 'GIER'-code and 'Nuclear Data'-code.

The analysers have a limited capacity (10^5 or 10^6 counts/channel), and if they are overloaded, the first digits in each count number are lost. In this case the correct count numbers may be reconstructed if the count rate and the counting time have been recorded. If the overflow is stored in separate channels, the correct count numbers are constructed by adding the two sets of data.

Conventional Mössbauer experiments result in spectra containing absorption dips, whereas scattering experiments or experiments with resonance detectors result in spectra with peaks. Both types of spectra can be treated.

DESCRIPTION OF THE FITTING PROGRAMME

In the following a brief description of the programme is given. Its practical use is described in the next section (pp. 6 - 8) where also the commands, referred to by number, are treated in detail.

Spectrum Data

If channel numbers are included in the data, the counts can occur in any order, provided that each count is preceded by its channel number, and provided that all counts from initial to final channel are present. If channel numbers are absent, the counts must occur in order from initial channel to final channel (see also the TURN command (3)). Spurious counts, which frequently occur near the beginning and end of a spectrum and are occasionally found elsewhere, can be dealt with in various ways. If a count is read which is less than or equal to zero, this channel is ignored in the fitting

process. Consequently a count is effectively deleted by punching a minus sign before the number, or by editing the data and replacing spurious counts by zeros. Alternatively, the LOSE command (4) may be used.

Function

It is assumed that the lines are 'Lorentzian' and the function fitted is

$$f(x) = [1 + B(3)\sin(\frac{x-B(2)}{C}) + B(4)(x - B(2))](B(1) - \sum_L f(L))$$

with the individual lines of index L:

$$f(L) = \frac{2B(3L+4)}{\pi E(3L+3)(1 + 4(\frac{x' - B(3L+2)}{B(3L+3)})^2)}$$

$x' = x$ if $x < B(2) + C$

$x' = 2(B(2) + C) - x$, if $x > B(2) + C$

B(1) is the baseline,

B(2) is a parameter which is used if the spectrometer has a symmetrical scan, so that channels B(2) to B(2) + C contain the spectrum, and channels B(2) + C to B(2) + 2C contain a mirror image if 2C is the number of channels in the analyser. B(2) should in principle be zero, but for instrumental reasons it often is not. If the two spectra are not mirrored, but translated, the spectrum in channels B(2) + C to B(2) + 2C is turned by means of the command TURN (3). If there is only one spectrum, C must be set to the full width of the spectrum, and B(2) must be constrained to zero (or to the lowest channel number if that is not zero).

B(3) is the fractional sine wave in the baseline,

B(4) is the fractional baseline drift per channel,

B(3L + 2) is the position (in channels) of line L,

B(3L + 3) is the width at half-height (in channels) of line L,

B(3L + 4) is the intensity (in channels x counts) of line L.

Fitting

The fitting of the parameters, B(k), is based on the Gauss non-linear regression procedure with a facility for constraining any set of parameters

or linear combinations of parameters. The success of such a method depends greatly on the sensible use of constraints. With all but the simplest spectra, the procedure will commonly diverge if an attempt is made to fit a spectrum without constraints. The constraints may only be needed in the early stage, where they effectively increase the radius of convergence, and they can often be removed for the later stages. The choice of the most suitable constraints depends very much on the spectrum, but is largely a matter of common sense. The constraints are often dictated by physical considerations, and this is usually the best criterion; for example, one may expect a particular line in a complicated spectrum to have a certain isomer shift because it is thought to arise from a known chemical species.

Constraints

The constraints are of two types:

(a) $B(k) = \text{const.}$

(b) $A(1)B(1) + A(2)B(2) + \ldots + A(3N + 4)B(3N + 4) = \text{const.}$

The value of the 'const.' is implied by the initial values of the parameters.

Of course (a) is only a special case of (b), but it is convenient to specify (a) separately. These constraints are listed on one card by giving the parameter numbers, k (cf. (11/a) in the next section).

Each constraint of type (b) will in practice involve either positions only, widths only, or intensities (areas) only; these constraints are specified on separate cards as POSN, WDTH or AREA followed by the appropriate coefficients. It may for example be required that the intensities of the two first lines should be equal (a quadrupole doublet), i.e.: AREA (1) = AREA (2); then the constraint required is:

$$1 \cdot B(7) + (-1) \cdot B(10) + \ldots + 0 \cdot B(3N + 4) = 0,$$

which is specified as (cf. (11/b) in the next section):

AREA 1. -1. .. 0.

If a centre shift should be kept constant, i.e. POSN(1) + POSN(2) = const., the constraint is:

$$1 \cdot B(5) + 1 \cdot B(8) + \ldots + 0 \cdot B(3N + 2) = \text{const.}$$

which is specified as:

POSN 1. 1. .. 0.

The constraints need not be normalized or orthogonal, but they must be linearly independent.

Convergence

The programme is taken to have converged when

$$\text{TEST VALUE} = \sum_k \frac{\text{DELTA}(k)^2}{\text{COV}(k,k)} < \varepsilon,$$

where DELTA(k) is the last correction to parameter k, and COV(k, k) is an estimate of its variance. The value of ε can be reset if required by means of 'd' in the FIX command (11), but the standard value of 10^{-6} should be quite adequate. This criterion is simply that the computational error in each parameter is at most 10^{-3} of the estimated statistical error. At this stage chi squared usually differs from the minimum value in about the 8th - 10th decimal place.

Divergence

If the process is found to be diverging, the programme automatically enters a simple damping procedure. This will usually force the process to converge, but convergence may be slow and inefficient. The need for damping can usually be avoided by means of addition of extra constraints in the initial stages or use of more accurate estimates of the parameter values, if that is possible.

Results

The information given in the results appears from the example pp. 47-59.

Note that if quantities such as quadrupole splittings or area ratios are derived from the basic parameters, the calculation of their errors involves the covariances as well as the variances. Note also that if a parameter or combination of parameters is constrained, its variance and covariances are all taken to be zero since the programme cannot estimate them. Since they will certainly be non-zero, and may be quite large, some allowance should be made when quoting confidence limits for the unconstrained parameters. The chi squared percentage points are given because they are not usually tabulated for so many degrees of freedom; instrumental deficiencies or

minor impurities may push the chi squared value above the 5-per cent point quite easily, but values above the 0.1-per cent point should be regarded with great suspicion. One spurious count can lead to a very bad chi squared; such counts are listed if they occur, and can be discarded. Note that it is assumed that the number of the counts follows the Poisson-distribution; if this is not the case, the chi squared values are unreliable, and so are the calculated variance and covariances.

Preparation of the Data Set

The data can consist of any number of data sets, one for each spectrum. A data set starts with a 'title card' (1) which is followed by a series of commands, each consisting of one card with a keyword in cols 1-4 and possibly some numerical data in F 10.0 format; some commands must be followed by further data cards. If convenient, the inherent constants in commands nos. 3, 7, 9, 11 and 12 can be changed in the programme. Any or all of the commands can be present in any logical order and are executed in that order. The FIX command starts the fitting on the last-read spectrum data; several sets of estimates and numbers of lines can thus be used successively for the same spectrum data.

If more than one data-set is wanted to the same fit they may be placed immediately after each other. The DATA - command (2) and the following card (2/a) must, however, precede each data-set. The counts of the channels with the same channel number are added. If one of the counts is less than or equal to zero the channel is deleted.

List of Commands etc.

(1) A card containing a title in cols 1 - 80.

(2) DATA a b
(Read the spectrum data from channel 'a' to channel 'b').

(2/a) Two values read with format 2I2.
If the first parameter = 0 then the papertape must be punched in 'Gier' code and if it is 1 the papertape must be punched in "Nuclear Data" code. The second parameter = 2 means overflow and a value NEQ 2 no overflow.

(2/b) The papertape containing the spectrum data

(3) TURN a
(Turn the spectrum data from channel 'a').
If 'a' is zero or absent, a value of 256 is assumed. This is used for analysers of type 3, (see introduction). If this command is used, be careful with the channel numbers in the commands LOSE and SKIP.

(4) LOSE a b
(Throw away channels 'a' through 'b' irretrievably).
Any number of LOSE commands may occur.

(5) SKIP a b
(Give temporarily zero weight to channels 'a' through 'b')
Thus they are ignored in the first following fitting and are restored after the next FIX command. Any number of SKIP commands may occur.

(6) ADD a
(Add 'a' to each count in the spectrum data).
This is used if the multi-channel analyser has been overloaded, and the data should be reconstructed.

(7) JUMP a
(Correct the spectrum data if there is a discontinuity of 'a' counts).
This may appear in the case of overloading. The first point used in the fitting is assumed to be correct. If 'a' is zero or absent, a value of 10^5 is assumed.

(8) PLOL a b
(Plot the spectrum data on line printer from channel 'a' to channel 'b').
If 'b' is zero or absent, the whole spectrum is plotted. This plot can be used for estimates of parameters.

(9) SCAN a
(Set the spectrum scan width C to the value 'a').
A value of 256 is assumed if no SCAN command occurs.

(10) ESTM a b
(Read the initial estimates of the parameters for 'a' lines).
'b' = 1 if spectrum with negative intensity (or dip) is wanted.
Otherwise 'b' = 0 (or absent).

(10/b) Parameters B(1) - B(4) on one card in F10.0 format. B(2), B(3), and B(4) can usually be set to zero initially and left unconstrained.

(10/b) One card for each line, L, with three parameters, B(3L+2), B(3L+3), B(3L+4) on each (F10.0 format). Instead of the intensity B(3L+4) one may insert the dip in counts, preceded by a minus; the programme will then calculate the intensity.

(11) FIX a b c d
(Read the constraints specification with 'a' constraint).

Allow 'b' iterations to reach convergence (i.e. TEST VALUE < 'd').
Print the results according to 'c'.

c = 0: Print the results and the variance-covariance matrix.

c = 1: Print full details of the changes to parameters etc. at last iteration.

c = 2: Print no results at all.

c = 3: Print full details of the changes to parameters etc. at each iteration.

c = 4: Print as for c = 3 and c = 0).

If 'b' is zero or absent, a value of 10 is assumed. If 'd' is zero or absent, a value of 10^{-6} is assumed.

(11/a) A card with all constraints of type (a), cf. 'description', given as a list of parameter numbers in F3.0 format. If there are no (a) constraints, but some (b) constraints, a blank card must be put in.

(11/b) One card for each constraint type (b); specified as POSN, WIDTH or AREA, followed by the appropriate coefficients in F6.0 format, one coefficient for each line the spectrum

(12) PLOT a b c d

(Plot the spectrum from channel 'a' to channel 'b' with 'c' millimetres per channel and 'd' millimetres for the largest amplitude).

If 'b' is zero or absent, the whole spectrum is plotted.
If 'c' is zero or absent, a value of 1 is assumed. If 'd' is zero or absent, a value of 80 is assumed.

(12/a) A card with the number 0 or 1 in column 2. If 0 is punched the plot is drawn without standard deviation. If 1 is punched the plot will contain standard deviation.

(13) CONC a

(Add the counts of 'a' successive channels to form a new channel where

new ch(0) = ch(0) + ch(1) + ... + ch(a-1)
new ch(1) = ch(a) + ch(a+1) + ... + ch(2a-1)
etc., where ch(x) means the count of channel number x.

If one of the 'a' channels is deleted the new channel will be deleted. The parameters in the commands TURN (3), SCAN (9) and ESTM(10) are adjusted automatically.

(14) EXIT

(Reset the scan width C to 256 and read a new title card).

Appendix 1. Programme pp. 47-59

The programme is shown in the version for the B 6700 computer and the plotter-routines that are used at Risø.

In order to run the programme which is stored on the disk you must have the following control cards

```
^ JOB MOSSPEC ; CLASS=2; CHARGE=130102    %FENGER
^ PROCESSTIME=100  ; IOTIME=100  ; PRINTLIMIT=2500 ;
^ BEGIN RUN      OBJECT/MOSSPEC
^ FILE FILE10(TITLE=PLOTFIL/23 , KIND=DISK, MYUSE=OUT, MAXRECSIZE=15, -
BLOCKSIZE=30, AREASIZE=20, AREAS=402, PROTECTION=PROTECTED)
^ FILE FILE9(KIND=DISK, MAXRECSIZE=14, AREASIZE=1,  AREAS=1)
^ DATA MOSSPEC
```

Data as illustrated at pp. 47-49

```
^ END    JOB
```

Appendix 2. Example of Run pp. 47-59

As a demonstration of the operation of the programme the analysis of a spectrum containing two doublets is shown. One of the doublets is composed of two lines of equal intensity and width, the other doublet is composed of two lines which have equal intensity, but different widths. The spectrum was recorded on a spectrometer of type 2 (cf. 'Introduction'); therefore the 'scan reverse' is constrained throughout the calculations (cf. 'Function'). The data, shown on p. 49, were punched in 'GIER'-code.

First the 'base line drift' the 'sine wave component' and all the positions of all four lines are constrained. In the second stage only the positions of one set of doublet lines are constrained. In the third and last stage all positions are left free. Only results of the last stage computations are printed out.

```
$SET INSTALLATION
FILE  5 = MOSSPEC
C     RES*                                                              MAIN   1
C                                                                       MAIN   2
C                                                                       MAIN   3
C                              M O S S P E C                            MAIN   4
C                              *************                            MAIN   5
C                                                                       MAIN   6
C            A PROGRAMME FOR RESOLVING MOESSBAUER SPECTRA               MAIN   7
C                                                                       MAIN   8
C                                                                       MAIN   9
C     ------------------------------------------------------------------MAIN  10
C     ------------------------------------------------------------------MAIN  11
C                                                                       MAIN  12
C                              PROGRAM  CAPACITY                        MAIN  13
C                              -----------------                        MAIN  14
C                                                                       MAIN  15
C     THE PROGRAM CAPACITY CAN BE CHANGED                               MAIN  16
C     BY THE FOLLOWING "DIMENSIONS" :                                   MAIN  17
C                                                                       MAIN  18
C     1)  XX(L) ,       L = MAXIMUM NUMBER OF CHANNELS                  MAIN  19
      DIMENSION         Y(600),Z(600),W(600)                            MAIN  20
C                                                                       MAIN  21
C                                                                       MAIN  22
C     2)  XX(L) ,       L = 4 + 3 * (MAXIMUM NUMBER OF LINES)           MAIN  23
      DIMENSION         A(28),B(28),C(28,28),COV(28,28),                MAIN  24
     *                  D(28),DELTA(28),R(28),T(28,28)                  MAIN  25
C                                                                       MAIN  26
C     ALL SUBROUTINES MUST BE CHANGED TOO)                              MAIN  27
C                                                                       MAIN  28
C     ------------------------------------------------------------------MAIN  29
C                                                                       MAIN  30
C                              INHERENT  CONSTANTS                      MAIN  31
C                              -------------------                      MAIN  32
C                                                                       MAIN  33
C     THE PROGRAM ASSUMES THE FOLLOWING VALUES IF THEY ARE NOT CHANGED  MAIN  34
C     IN THE DATA CARDS  (SE  "PREPARATION OF THE DATA SET"  IN THE     MAIN  35
C     PROGRAM DESCRIPTION),                                             MAIN  36
C                                                                       MAIN  37
```



```
C     TURNA = THE CHANNEL NUMBER FROM WHICH THE SPECTRUM IS TURNED      MAIN  38
C     JUMPA = THE DISCONTINUITY (IN COUNTS) OF THE SPECTRUM             MAIN  39
C     SCANA = THE SPECTRUM SCAN WIDTH (IN CHANNELS)                     MAIN  40
C     FIXB  = MAXIMUM NUMBER OF ITERATIONS                              MAIN  41
C     FIXD  = EPSILON USED FOR THE CONVERGENCE-CRITERION                MAIN  42
C     PLOTC = NUMBER OF MILLIMETRES PER CHANNEL IN THE PLOT             MAIN  43
C     PLOTD = NUMBER OF MILLIMETRES FOR THE LARGEST AMPLITUDE IN PLOT   MAIN  44
C     TEST=0 THE PAPER TAPE IS IN GIER CODE,TEST=1 THE PAPER TAPE IS IN MAIN  45
C     FERGER CODE                                                       MAIN 451
C     TEST2=2 OVERFLOW,TEST2 NEQ 2 NO OVERFLOW
C     PDIV=0. NO STANDARD DEVIATION IN THE PLOT
C     PDIV .NE. 0 STANDARD DEVIATION IS DRAWN IN THE PLOT
C                                                                       MAIN  45
C                                                                       MAIN  46
      TURNA = 256.                                                      MAIN  47
      JUMPA = 1.E5                                                      MAIN  48
      SCANA = 256.                                                      MAIN  49
      FIXB  = 10.                                                       MAIN  50
      FIXD  = 1.E-6                                                     MAIN  51
      PLOTC = 1.                                                        MAIN  52
      PLOTD = 80.                                                       MAIN  53
C                                                                       MAIN  54
C     ------------------------------------------------------------------MAIN  55
C     ------------------------------------------------------------------MAIN  56
C                                                                       MAIN  57
C                                                                       MAIN  58
      DIMENSION         DFL(4),FMT(20),TITLE(20),XSQ(4)                 MAIN  59
C                                                                       MAIN  60
C                                                                       MAIN  61
C                                                                       MAIN  62
      REAL              LOSE                                            MAIN  63
      INTEGER ADDN,CONSTR,P,PO,Q,R,STREAM,STAGE,SW,V,V1,TEST,TEST2,PDIV
      LOGICAL           LN, LM3                                         MAIN  65
      COMMON            CHISQ,PI,CONSTR,IA,P,PO,V,V1                    MAIN  66
      COMMON            /XXX/ C,COV,T,Z                                 MAIN  67
      DATA              ADD,AREA,DATA,ESTM,EXIT,FIX,HUPP,LOSE,PLOTH,    MAIN  68
     *                  PLOTL,POSN,SCANN,SKIP,TURN,WOTH,CONC            MAIN  69
     *                  /4HADD ,4HAREA,4HDATA,4HESTM,4HEXIT,4HFIX ,     MAIN  70
     *                  4HJUMP,4HLOSE,4HPLOT,4HPLOL,4HPOSN,4HSCAN,4HSKIPMAIN  71
```

```
     *                    ,4HTURN,4HNOTH,4HCONC/                          MAIN  72
C                                                                         MAIN  73
      PI=3.1415926535897                                                  MAIN  74
      EPSILO=1.E-6                                                        MAIN  75
      IDATA=0                                                             MAIN  76
      JPLOT=0                                                             MAIN  77
      IPLOT=0                                                             MAIN  78
    1 SCAN=SCANA                                                          MAIN  79
C     -----------------                                                   MAIN  80
C     READ TITLE                                                          MAIN  81
C     -----------------                                                   MAIN  82
      READ (5,281,END=248) TITLE                                          MAIN  83
  281 FORMAT (20A4)                                                       MAIN  84
      WRITE (6,800) TITLE                                                 MAIN  85
C     -----------------                                                   MAIN  86
C     READ COMMAND CARDS                                                  MAIN  87
C     -----------------                                                   MAIN  88
  500 SW=-1                                                               MAIN  89
      ASSIGN 82 TO MESS1                                                  MAIN  90
      READ (5,581,END=248) FF,AA,BB,CC,DD                                 MAIN  91
  581 FORMAT (A4,4F10.0)                                                  MAIN  92
      IF (FF.EQ. DATA) GO TO 201                                          MAIN  93
  520 IF (FF.EQ. TURN) GO TO 230                                          MAIN  94
      IF (FF.EQ. LOSE) GO TO 540                                          MAIN  95
      IF (FF.EQ. SKIP) GO TO 540                                          MAIN  96
      IF (FF.EQ. ADD) GO TO 210                                           MAIN  97
      IF (FF.EQ. HOPP) GO TO 240                                          MAIN  98
      IF (FF.EQ. PLOTL) GO TO 241                                         MAIN  99
      IF (FF.EQ. SCANH) GO TO 243                                         MAIN 100
      IF (FF.EQ. CONC) GO TO 244                                          MAIN 101
      IF (FF.EQ. ESTM) GO TO 212                                          MAIN 102
      IF (FF.EQ. FIX) GO TO 545                                           MAIN 103
      IF (FF.EQ. PLOTM) GO TO 245                                         MAIN 104
      IF (FF.EQ. EXIT) GO TO 247                                          MAIN 105
      WRITE (6,49) FF                                                     MAIN 106
      GO TO 500                                                           MAIN 107
  248 IF (IPLOT .EQ. 1) CALL PTERM                                        MAIN 108
      I=TIME(2)/60.                                                       MAIN 109
      WRITE (6,701) I                                                     MAIN 110
```



```
  701 FORMAT (15H1PROCESS TIME =,I6)                                      MAIN 111
      STOP                                                                MAIN 112
C     -----------------                                                   MAIN 113
  240 IF (AA .EQ. 0.) AA=JUMPA                                            MAIN 114
      WRITE (6,801) FF,AA                                                 MAIN 115
      CALL JUMPP(Y,W,P,AA,PO)                                             MAIN 116
      GO TO 500                                                           MAIN 117
  201 IF (BB .NE. 0.) GO TO 242                                           MAIN 118
      AA=IA                                                               MAIN 119
      BB=IB                                                               MAIN 120
  242 WRITE (6,801) FF,AA,BB                                              MAIN 121
      CALL PLOTUL(Y,P,IA,AA,BB,TITLE)                                     MAIN 122
      WRITE (6,812)                                                       MAIN 123
      GO TO 500                                                           MAIN 124
  243 SCAN=AA                                                             MAIN 125
      WRITE (6,801) FF,AA                                                 MAIN 126
      GO TO 500                                                           MAIN 127
  244 WRITE (6,801) FF,AA                                                 MAIN 128
      NUMM=AA                                                             MAIN 129
      CALL CONCX(Y,W,P,IA,IB,PO,NUMM)                                     MAIN 130
      SCAN=SCAN/NUMM                                                      MAIN 131
      B(1)=B(1)*NUMM                                                      MAIN 132
      B(2)=B(2)/NUMM                                                      MAIN 133
      B(4)=B(4)*NUMM                                                      MAIN 134
      DO 249 I=5,V,3                                                      MAIN 135
      B(I)=B(I)/NUMM                                                      MAIN 136
  249 B(I+1)=B(I+1)/NUMM                                                  MAIN 137
      GO TO 500                                                           MAIN 138
  245 IF (BB .NE. 0.) GO TO 246                                           MAIN 139
      AA=IA                                                               MAIN 140
      BB=IB                                                               MAIN 141
  246 IF (CC .EQ. 0.) CC=PLOTC                                            MAIN 142
      IF (DD .EQ. 0.) DD=PLOTD                                            MAIN 143
      WRITE (6,803) FF,AA,BB,CC,DD                                        MAIN 144
      READ(5,111) PDIV                                                    
111   FORMAT(I2)                                                          
      IF (JPLOT .EQ. 0) CALL PINIT                                        MAIN 145
      JPLOT=1                                                             MAIN 146
      CALL PLOTP(H,V,SCAN,Y,W,P,IA,AA,BB,CC,DD,TITLE,PDIV)
```

```
      IPLOT=1                                                          MAIN 148
      GO TO 500                                                        MAIN 149
  247 WRITE (5,801) FF                                                 MAIN 150
      GO TO 1                                                          MAIN 151
C     -----------------                                                MAIN 152
C     READ SPECTRUM                                                    MAIN 153
C     -----------------                                                MAIN 154
  201 IA=AA                                                            MAIN 155
      IB=BB                                                            MAIN 156
      ADDR=CC                                                          MAIN 157
      IF (DD .EQ. 0.) DD=5.                                            MAIN 158
      STREAM=DD                                                        MAIN 159
      WRITE (6,801) FF,AA,BB,CC,DD                                     MAIN 160
      STAGE=0                                                          MAIN 161
C                                                                      MAIN 162
C     READ TEST,TEST2                                                  
C                                                                      MAIN 164
      READ(5,202) TEST,TEST2                                           
202   FORMAT(2I2)                                                      
      WRITE(6,802) TEST,TEST2                                          
      P=IB-IA+1                                                        MAIN 168
C                                                                      MAIN 169
C     READ SPECTRUM, WITH OR WITHOUT CHANNEL NUMBERS ACCORDING AS      MAIN 170
C     ADDR = 1 OR 0                                                    MAIN 171
C     WITH INPUT FROM PAPER TAPE ADDR MUST BE 0                        MAIN 172
C                                                                      MAIN 172
  213 IF (ADDR) 208,202,208                                            MAIN 173
  208 READ (STREAM, FMT) (Z(J), W(J), J=1,P)                           MAIN 174
      DO 209 J=1,P                                                     MAIN 175
  209 Y(J)=0.                                                          MAIN 176
      DO 205 J=1,P                                                     MAIN 177
      I=Z(J)-IA+1                                                      MAIN 178
  205 Y(I)=W(J)                                                        MAIN 179
      GO TO 214                                                        MAIN 180
202   CALL LAES(Y,P,TEST,TEST2)                                        MAIN 181
  214 READ (5,581) FF,AA,BB,CC,DD                                      MAIN 182
      IF (FF .EQ. DATA) GO TO 215                                      MAIN 183
      IF (IDATA .EQ. 1) GO TO 215                                      MAIN 184
      GO TO 203                                                        MAIN 185
```



```
  215 CALL OASU(Y,Z,P,FF,AA,IA,IB,IDATA)                               MAIN 186
      IF (IDATA .EQ. 1) GO TO 201                                      MAIN 187
C     -----------------                                                MAIN 188
C     REJECT COUNTS Y UNDER 1  , CALCULATE WEIGHTS W                   MAIN 189
C     -----------------                                                MAIN 190
  203 P0=0                                                             MAIN 191
      DO 206 J=1,P                                                     MAIN 192
      IF (Y(J)) 207,207,206                                            MAIN 193
  207 Y(J)=0.                                                          MAIN 194
      W(J)=0.                                                          MAIN 195
      P0=P0+1                                                          MAIN 196
      GO TO 206                                                        MAIN 197
  206 W(J)=1./ SQRT(Y(J))                                              MAIN 198
  206 CONTINUE                                                         MAIN 199
      IF (STAGE .EQ. 0) GO TO 520                                      MAIN 200
      IF (FF.EQ. EXIT) GO TO 1                                         MAIN 201
      GO TO 500                                                        MAIN 202
C     -----------------                                                MAIN 203
C     TURN SPECTRUM FROM CHANNEL AA                                    MAIN 204
C     -----------------                                                MAIN 205
  230 IF (AA .EQ. 0.) AA=TURNA                                         MAIN 206
      WRITE (6,801) FF,AA                                              MAIN 207
      ITURN=AA                                                         MAIN 208
      ISCAN=SCAN                                                       MAIN 209
      IF (IB=ITURN+1 .EQ. ISCAN) GO TO 232                             MAIN 210
      IP=P+1                                                           MAIN 211
      IB=ISCAN+ITURN-1                                                 MAIN 212
      P=IB-IA+1                                                        MAIN 213
      DO 231 I=IP,P                                                    MAIN 214
      Y(I)=0.                                                          MAIN 215
  231 W(I)=0.                                                          MAIN 216
  232 CONTINUE                                                         MAIN 217
      K=ITURN-IA+1                                                     MAIN 218
      KK=1                                                             MAIN 219
      DO 250 I=K,P                                                     MAIN 220
      Z(KK)=Y(I)                                                       MAIN 221
      KK=KK+1                                                          MAIN 222
      Z(KK)=W(I)                                                       MAIN 223
  250 KK=KK+1                                                          MAIN 224
```

```
      DO 251 I=K,P                                                    MAIN 225
      KK=KK+1                                                         MAIN 226
      W(I)=Z(KK)                                                      MAIN 227
      KK=KK+1                                                         MAIN 228
  251 Y(I)=Z(KK)                                                      MAIN 229
      GO TO 500                                                       MAIN 230
C     -----------------                                               MAIN 231
C     GIVE ZERO WEIGHT TO SPECIFIED CHANNELS                          MAIN 232
C     -----------------                                               MAIN 233
  540 I=AA                                                            MAIN 234
      J=BB                                                            MAIN 235
      WRITE (6,801) FF,AA,BB                                          MAIN 236
      I=I-IA+1                                                        MAIN 237
      J=J-IA+1                                                        MAIN 238
      DO 571 K=I,J                                                    MAIN 239
      IF (W(K)) 572,573,572                                           MAIN 240
  572 W(K)=0.                                                         MAIN 241
      PO=PO+1                                                         MAIN 242
  573 IF (FF.EQ. SKIP) GO TO 571                                      MAIN 243
      Y(K)=0.                                                         MAIN 244
  571 CONTINUE                                                        MAIN 245
      GO TO 500                                                       MAIN 246
C     -----------------                                               MAIN 247
C     ADD AA TO SPECTRUM                                              MAIN 248
C     -----------------                                               MAIN 249
  210 DO 211 I=1,P                                                    MAIN 250
      IF (Y(I) .EQ. 0.) GO TO 211                                     MAIN 251
      Y(I)=Y(I)+AA                                                    MAIN 252
      IF (W(I) .EQ. 0.) GO TO 211                                     MAIN 253
      W(I)=1./ SQRT(Y(I))                                             MAIN 254
  211 CONTINUE                                                        MAIN 255
      WRITE (6,801) FF,AA                                             MAIN 256
      GO TO 500                                                       MAIN 257
C     -----------------                                               MAIN 258
C     READ PARAMETER ESTIMATES                                        MAIN 259
C     -----------------                                               MAIN 260
  212 N=AA                                                            MAIN 261
      V=4+3*N                                                         MAIN 262
      V1=5                                                            MAIN 263
```



```
      READ (5,283) (B(I), I=1,V)                                      MAIN 264
  283 FORMAT (F10.0 , (3F10.0))                                       MAIN 265
      WRITE (6,801) FF,AA,BB                                          MAIN 266
      WRITE (6,804) (B(I),I=1,V)                                      MAIN 267
      DO 284 I=7,V,3                                                  MAIN 268
  284 IF (B(I) .LT. 0.) B(I)=-B(I-1)+B(I)*PI/2.                       MAIN 269
      IF (BB .EQ. 0.) GO TO 500                                       MAIN 270
      DO 285 I=7,V,3                                                  MAIN 271
  285 B(I)=-B(I)                                                      MAIN 272
      GO TO 500                                                       MAIN 273
C     -----------------                                               MAIN 274
C     READ CONSTRAINT SPECIFICATION AND SET UP MATRIX T               MAIN 275
C     -----------------                                               MAIN 276
  545 IF (BB .EQ. 0.) BB=FIXB                                         MAIN 277
      IF (DD .EQ. 0.) DD=FIXD                                         MAIN 278
      WRITE (6,805) FF,AA,BB,CC,DD                                    MAIN 279
      STAGE=STAGE+1                                                   MAIN 280
      CONSTR=AA                                                       MAIN 281
      NIT=BB                                                          MAIN 282
      ICC=CC                                                          MAIN 283
      IF (ICC .EQ. 0) ICC=4                                           MAIN 284
      TRACE=0.                                                        MAIN 285
      IF (CC .GE. 3.) TRACE=1.                                        MAIN 286
      CRIT=DD                                                         MAIN 287
      DF=1.                                                           MAIN 288
      ASSIGN 88 TO MESS2                                              MAIN 289
      Q=V-CONSTR                                                      MAIN 290
  505 DO 502 I=1,V                                                    MAIN 291
  502 R(I)=0                                                          MAIN 292
      IF (CONSTR) 99,3,501                                            MAIN 293
  501 IF (Q .LE. 0.) GO TO 99                                         MAIN 294
C                                                                     MAIN 295
C     READ CONSTRAINED PARAMETERS.  ZERO OR BLANK IMPLIES THAT A LINEAMAIN 296
C     COMBINATION FOLLOWS.                                            MAIN 297
C                                                                     MAIN 298
      READ (5,582)  (A(I), I=1,CONSTR)                                MAIN 299
  582 FORMAT (22F3.0)                                                 MAIN 300
      LC=0                                                            MAIN 301
      DO 504 I=1,CONSTR                                               MAIN 302
```

```
      ASSIGN 87 TO MESS2                                              MAIN 303
      IF (A(I))  99,505,541                                           MAIN 304
  541 M=A(I)                                                          MAIN 305
      IF (V-M) 99,542,542                                             MAIN 306
  542 ASSIGN 86 TO MESS2                                              MAIN 307
      IF (R(M) .EQ. 1) GO TO 99                                       MAIN 308
C                                                                     MAIN 309
C     R(I) IS 1 IF PARAMETER I IS FULLY CONSTRAINED                   MAIN 310
C                                                                     MAIN 311
      R(M)=1                                                          MAIN 312
      GO TO 504                                                       MAIN 313
  505 LC=LC+1                                                         MAIN 314
  504 CONTINUE                                                        MAIN 315
      ICO=CONSTR=LC                                                   MAIN 316
      IF (ICO .EQ. 0) WRITE (6,810)                                   MAIN 317
      IF (ICO .GT. 0) WRITE (6,810) (A(I),I=1,ICO)                    MAIN 318
C                                                                     MAIN 319
C     SET UP T WITH CONSTRAINTS IN BOTTOM ROWS                        MAIN 320
C                                                                     MAIN 321
      L=V                                                             MAIN 322
      DO 511 M=1,V                                                    MAIN 323
      IF (R(M))511,511,524                                            MAIN 324
  524 DO 512 I=1,V                                                    MAIN 325
  512 T(L,I)=0.                                                       MAIN 326
      T(L,M)=1.                                                       MAIN 327
      L=L-1                                                           MAIN 328
  511 CONTINUE                                                        MAIN 329
C                                                                     MAIN 330
C     READ THE LC CONSTRAINTS WHICH ARE SPECIFIED AS LINEAR           MAIN 331
C     COMBINATIONS AND STORE THEM IN T, AFTER NORMALISING             MAIN 332
C                                                                     MAIN 333
      IF (LC) 530, 530, 532                                           MAIN 334
  532 ASSIGN 88 TO MESS2                                              MAIN 335
      DO 507 LCI=1,LC                                                 MAIN 336
      READ (5,583)AAA, (D(M), M=1,N)                                  MAIN 337
  583 FORMAT (A4, 10F6.0 / (4X, 10F6.0))                              MAIN 338
      WRITE (6,811) AAA,(D(M),M=1,N)                                  MAIN 339
      F=0.                                                            MAIN 340
      DO 531 I=1,N                                                    MAIN 341
```



```
  531 F=F+D(I)*D(I)                                                   MAIN 342
      F=1.00/ SQRT(F)                                                 MAIN 343
      LCQ=0                                                           MAIN 344
      IF (AAA.EQ. POSN) LCQ=V1                                        MAIN 345
      IF (AAA.EQ. WDTH) LCQ=V1+1                                      MAIN 346
      IF (AAA.EQ. AREA) LCQ=V1+2                                      MAIN 347
      IF (LCQ) 99,99,534                                              MAIN 348
  534 DO 535 I=1,V                                                    MAIN 349
  535 T(L,I)=0.                                                       MAIN 350
      J=1                                                             MAIN 351
      DO 536 I=LCQ,V,3                                                MAIN 352
      T(L,I)=F*D(J)                                                   MAIN 353
  536 J=J+1                                                           MAIN 354
  507 L=L-1                                                           MAIN 355
C     -----------------                                               MAIN 356
C     ORTHOGONALISE, AND THEN ADD ONE UNCONSTRAINED ROW AT A TIME AND MAIN 357
C     ORTHOGONALISE TO CONSTRAINTS AND OTHER UNCONSTRAINED VARIABLES  MAIN 358
C     -----------------                                               MAIN 359
  530 ASSIGN 86 TO MESS2                                              MAIN 360
      M=V+1                                                           MAIN 361
      L1=V+LC+1                                                       MAIN 362
      LCI=L1-1                                                        MAIN 363
      DO 515 J=1,LCI                                                  MAIN 364
      L1=L1-1                                                         MAIN 365
  537 K=L1+1                                                          MAIN 366
      IF (L1-V) 527, 527, 510                                         MAIN 367
  527 M=M-1                                                           MAIN 368
      IF (R(M)) 528, 528, 527                                         MAIN 369
  528 DO 529 I=1,V                                                    MAIN 370
  529 T(L1,I)=0.                                                      MAIN 371
      T(L1,M)=1.                                                      MAIN 372
C                                                                     MAIN 373
C     IF THERE ARE NO LINEAR COMBINATIONS, ORTHOGONALISATION          MAIN 374
C     IS UNNECESSARY                                                  MAIN 375
C                                                                     MAIN 376
      IF (LC) 515,515,510                                             MAIN 377
  510 IF (K .GT. V) GO TO 515                                         MAIN 378
      DO 514 L2=K,V                                                   MAIN 379
      G=0.                                                            MAIN 380
```

```
      DO 516 I=1,V                                                      MAIN 381
  516 G=G+T(L1,I)*T(L2,I)                                               MAIN 382
      IF ( ABS(G)-EPSILO) 514,514,517                                   MAIN 383
  517 IF (1.00-EPSILO - ABS(G)) 518, 526, 526                           MAIN 384
C                                                                       MAIN 385
C     IF G=1. AND L1 .GT. Q, THEN THE CONSTRAINTS ARE NOT INDEPENDENT.  MAIN 386
C     IF G=1. AND L1 .LE. Q THEN THE CURRENT ROW MUST BE REPLACED       MAIN 387
C                                                                       MAIN 388
  518 IF (L1-Q) 537,537,99                                              MAIN 389
  526 H=1.00/ SQRT(1.00-G*G)                                            MAIN 390
      DO 538 I=1,V                                                      MAIN 391
  538 T(L1,I)=H*(T(L1,I)-G*T(L2,I))                                     MAIN 392
  514 CONTINUE                                                          MAIN 393
  515 CONTINUE                                                          MAIN 394
C     ------------------                                                MAIN 395
C     CACULATE MATRIX COV OF DERIVATIVE PRODUCTS                        MAIN 396
C     AND VECTOR D OF DERIVATIVES * DEVIATIONS                          MAIN 397
C     ------------------                                                MAIN 398
    3 S=0                                                               MAIN 399
      IT=1                                                              MAIN 400
  300 CHISQ=0.                                                          MAIN 401
      DO 302 I=1,V                                                      MAIN 402
      DO 303 L=1,V                                                      MAIN 403
  303 COV(I,L)=0.                                                       MAIN 404
  302 D(I)=0.                                                           MAIN 405
      AA=2.00*SCAN                                                      MAIN 406
      U=0.                                                              MAIN 407
      LH3 = (H(3) .EQ.0.) .AND. (R(3) .EQ. 1)                           MAIN 408
      LN = (N .EQ. 0)                                                   MAIN 409
      X=1A                                                              MAIN 410
      M=1                                                               MAIN 411
  309 IF (W(M)) 301,304,301                                             MAIN 412
  301 GO TO 350                                                         MAIN 413
  306 Z(M)=W(M)*(Y(M)-F)                                                MAIN 414
      CHISQ=CHISQ+Z(M)*Z(M)                                             MAIN 415
      DO 305 K=1,V                                                      MAIN 416
      IF (H(K) .EQ. 1) GO TO 305                                        MAIN 417
      DO 307 L=1,K                                                      MAIN 418
  307 COV(K,L)=COV(K,L)+A(K)*A(L)                                       MAIN 419
```



```
      D(K)=D(K)+Z(M)*A(K)                                               MAIN 420
  305 CONTINUE                                                          MAIN 421
  304 X=X+1.                                                            MAIN 422
      IF (M .EQ. P) GO TO 400                                           MAIN 423
      M=M+1                                                             MAIN 424
      GO TO 309                                                         MAIN 425
C     ------------------                                                MAIN 426
C     CALCULATE FUNCTION AND DERIVATIVES                                MAIN 427
C     ------------------                                                MAIN 428
  350 XM=X                                                              MAIN 429
      H=1.                                                              MAIN 430
  361 E=XM-B(2)                                                         MAIN 431
  352 IF (XM-B(2)) 353,351,354                                          MAIN 432
  353 XM=XM+AA                                                          MAIN 433
      GO TO 352                                                         MAIN 434
  354 IF (XM-AA-B(2)) 351,351,355                                       MAIN 435
  355 XM=XM-AA                                                          MAIN 436
      GO TO 354                                                         MAIN 437
C                                                                       MAIN 438
  351 IF (XM-B(2)-SCAN) 362,362,363                                     MAIN 439
  363 XM=B(2)+AA-E                                                      MAIN 440
      H=-H                                                              MAIN 441
  362 IF (LH3) GO TO 365                                                MAIN 442
  364 G=PI*E/SCAN                                                       MAIN 443
      U= SIN(G)                                                         MAIN 444
  365 HB=(1.00+B(3)*U+B(4)*E)                                           MAIN 445
C                                                                       MAIN 446
  357 A(2)=0.                                                           MAIN 447
      F=B(1)                                                            MAIN 448
      IF (LN) GO TO 360                                                 MAIN 449
      DO 358 I=V1,V,3                                                   MAIN 450
      C1=2.00*(XM-B(I))/B(I+1)                                          MAIN 451
      C2=-2.00/(1.00+C1*C1)                                             MAIN 452
      C3=C2/(PI*B(I+1))                                                 MAIN 453
      A(I+2)=H*(M)*C3*HB                                                MAIN 454
      C4=-2.00*A(I+2)*B(I+2)/B(I+1)                                     MAIN 455
      A(I)=C1*C2*C4                                                     MAIN 456
      A(I+1)=0.500*(C1*A(I)+C4)                                         MAIN 457
      F=F+C3*H(I+2)                                                     MAIN 458
```

```
      IF (4) 359,358,358                                                MAIN 459
  359 A(2)=A(2)-2.00*A(1)                                               MAIN 460
  358 CONTINUE                                                          MAIN 461
  360 C1=B(K)*F                                                         MAIN 462
      A(1)=A(1)*BB                                                      MAIN 463
      A(2)=A(2)-C1*B(4)                                                 MAIN 464
      IF (B(3)) 366, 367, 366                                           MAIN 465
  366 A(2)=A(2)-C1*PI*B(3)* COS(G)/SCAN                                 MAIN 466
  367 A(3)= C1*U                                                        MAIN 467
      A(4)= C1*E                                                        MAIN 468
      F=F*BB                                                            MAIN 469
      GO TO 306                                                         MAIN 470
C                                                                       MAIN 471
  400 IF(IT .EQ. 1) GO TO 424                                           MAIN 472
C     -----------------                                                 MAIN 473
C     IF ID .NE. 1 RETURN TO DAMPING PROCEDURE                          MAIN 474
C     -----------------                                                 MAIN 475
      GO TO (454,452,453), ID                                           MAIN 476
C                                                                       MAIN 477
C     -----------------                                                 MAIN 478
C     TEST FOR DIVERGENCE                                               MAIN 479
C     DIVERGING, ENTER DAMPING PROCEDURE                                MAIN 480
C     -----------------                                                 MAIN 481
  454 IF (XSQ(1)-CHISQ) 451, 451, 421                                   MAIN 482
C                                                                       MAIN 483
  451 DFL(1)=0.                                                         MAIN 484
      DFL(3)=DF                                                         MAIN 485
      XSQ(3)=CHISQ                                                      MAIN 486
      DFL(2)= DF/3.00                                                   MAIN 487
      ID=2                                                              MAIN 488
      AA= DFL(2)-DF                                                     MAIN 489
  455 DO 447 I=1,V                                                      MAIN 490
  447 H(I)=B(I)+AA*DELTA(I)                                             MAIN 491
      GO TO 300                                                         MAIN 492
C                                                                       MAIN 493
  452 XSQ(2)=CHISQ                                                      MAIN 494
      ID=3                                                              MAIN 495
C     -----------------                                                 MAIN 496
C     ESTIMATE VALUE OF DF TO MINIMIZE CHISQ                            MAIN 497
```



```
C     -----------------                                                 MAIN 498
      C1=XSQ(3)-XSQ(2)                                                  MAIN 499
      C2=XSQ(2)-XSQ(1)                                                  MAIN 500
      DFL(4)=DFL(2)*(C1-8.00*C2)/(2.00*(C1-2.00*C2))                    MAIN 501
      AA=DFL(4)-DFL(2)                                                  MAIN 502
      GO TO 459                                                         MAIN 503
C     -----------------                                                 MAIN 504
C     FIND DF WHICH GIVES BEST CHISQ                                    MAIN 505
C     -----------------                                                 MAIN 506
  453 AA=CHISQ                                                          MAIN 507
      K=4                                                               MAIN 508
      XSQ(K)=CHISQ                                                      MAIN 509
      DO 455 I=1,3                                                      MAIN 510
      IF (AA-XSQ(I)) 455,455,456                                        MAIN 511
  456 AA=XSQ(I)                                                         MAIN 512
      K=I                                                               MAIN 513
  455 CONTINUE                                                          MAIN 514
      IF (TRACE) 458,457,458                                            MAIN 515
  458 WRITE (6,481)  (DFL(I), XSQ(I), I=1,4)                            MAIN 516
  481 FORMAT (32HODAMPING FACTOR       CHI SQUARED */                   MAIN 517
     *(1H , 0PF11.4, 7X, 1PE16.8))                                      MAIN 518
  457 GO TO (412,462,462,461), K                                        MAIN 519
C     -----------------                                                 MAIN 520
C     K=1, CHI SQUARED CANNOT BE IMPROVED, EXIT                         MAIN 521
C     K=2 OR 3, RECOMPUTE MATRIX (WHICH HAS BEEN OVERWRITEN)            MAIN 522
C     AND CONTINUE                                                      MAIN 523
C     K=4, LAST VALUE OF DF WAS BEST, CONTINUE IF IT IS POSITIVE        MAIN 524
C     -----------------                                                 MAIN 525
  412 SW=3                                                              MAIN 526
      GO TO 32                                                          MAIN 527
  461 DF=DFL(4)                                                         MAIN 528
      IF (DF) 412, 412, 423                                             MAIN 529
  462 ID=1                                                              MAIN 530
      AA=DFL(K)-DFL(4)                                                  MAIN 531
      DF=DFL(K)/3.00                                                    MAIN 532
      GO TO 459                                                         MAIN 533
C     -----------------                                                 MAIN 534
C     CONVERGING                                                        MAIN 535
C     -----------------                                                 MAIN 536
```

```
  421 DF=3.00*DF                                                        MAIN 537
      IF (DF-1.) 423,423,424                                            MAIN 538
  424 DF=1.                                                             MAIN 539
  423 ID=1                                                              MAIN 540
      KSQ(I)=CHISQ                                                      MAIN 541
C     -----------------                                                 MAIN 542
C     OBTAIN UPPER HALF OF COV FROM LOWER                               MAIN 543
C     -----------------                                                 MAIN 544
  401 DO 402 I=1,V                                                      MAIN 545
      DO 402 J=1,I                                                      MAIN 546
  402 COV(J,I)=COV(I,J)                                                 MAIN 547
C     -----------------                                                 MAIN 548
C     TRANSFORM MATRIX COV INTO VECTOR SPACE OF UNCONSTRAINED PARAMETERSMAIN 549
C     -----------------                                                 MAIN 550
      IF (CONSTR) 403,403,404                                           MAIN 551
  404 DO 405 J=1,V                                                      MAIN 552
      DO 405 L=1,Q                                                      MAIN 553
      AA=0.                                                             MAIN 554
      DO 431 K=1,V                                                      MAIN 555
  431 AA=AA+COV(J,K)*T(L,K)                                             MAIN 556
  405 C(J,L)=AA                                                         MAIN 557
C                                                                       MAIN 558
      DO 406 I=1,Q                                                      MAIN 559
      DO 406 L=1,I                                                      MAIN 560
      AA=0.                                                             MAIN 561
      DO 432 J=1,V                                                      MAIN 562
  432 AA=AA+T(I,J)*C(J,L)                                               MAIN 563
      COV(I,L)=AA                                                       MAIN 564
  406 COV(L,I)=AA                                                       MAIN 565
C     -----------------                                                 MAIN 566
C     INVERT COV TO GET VARIANCE-COVARIANCE MATRIX                      MAIN 567
C     -----------------                                                 MAIN 568
  403 CALL MB01B (COV,Q,SW)                                             MAIN 569
      IF (SW) 437,436,437                                               MAIN 570
  437 ASSIGN 83 TO MESS1                                                MAIN 571
      GO TO 99                                                          MAIN 572
C     -----------------                                                 MAIN 573
C     TRANSFORM BACK TO GET COVARIANCE MATRIX W.R.T. ORIGINAL PARAMETERSMAIN 574
C     -----------------                                                 MAIN 575
```



```
  436 IF (CONSTR) 407,407,408                                           MAIN 576
  408 DO 409 J=1,Q                                                      MAIN 577
      DO 409 L=1,V                                                      MAIN 578
      AA=0.                                                             MAIN 579
      DO 433 K=1,Q                                                      MAIN 580
  433 AA=AA+COV(J,K)*T(K,L)                                             MAIN 581
  409 C(J,L)=AA                                                         MAIN 582
C                                                                       MAIN 583
      DO 410 I=1,V                                                      MAIN 584
      DO 410 L=1,I                                                      MAIN 585
      AA=0.                                                             MAIN 586
      DO 434 J=1,Q                                                      MAIN 587
  434 AA=AA+T(J,I)*C(J,L)                                               MAIN 588
      COV(L,I)=AA                                                       MAIN 589
  410 COV(I,L)=AA                                                       MAIN 590
C     -----------------                                                 MAIN 591
C     OBTAIN DELTA = COV * D                                            MAIN 592
C     -----------------                                                 MAIN 593
  407 DO 411 I=1,V                                                      MAIN 594
      DELTA(I)=0.                                                       MAIN 595
      DO 435 J=1,V                                                      MAIN 596
  435 DELTA(I)=DELTA(I)+COV(I,J)*D(J)                                   MAIN 597
  411 CONTINUE                                                          MAIN 598
C     -----------------                                                 MAIN 599
C     TEST FOR CONVERGENCE                                              MAIN 600
C     -----------------                                                 MAIN 601
  413 TEST=0.                                                           MAIN 602
      DO 414 I=1,V                                                      MAIN 603
      IF (DELTA(I)) 415,414,415                                         MAIN 604
  415 TEST=TEST+DELTA(I)*DELTA(I)/ ABS(COV(I,I))                        MAIN 605
  414 CONTINUE                                                          MAIN 606
      SW=0                                                              MAIN 607
      IF (TEST .LT. CRIT) SW=1                                          MAIN 608
C     -----------------                                                 MAIN 609
C     TRACE PROGRESS OF CONVERGENCE                                     MAIN 610
C     -----------------                                                 MAIN 611
      IF (TRACE) 418,419,418                                            MAIN 612
  418 IF (IT-1) 417,440,417                                             MAIN 613
  440 WRITE (6,80) TITLE, STAGE                                         MAIN 614
```

```
  417 WRITE (6,480) IT,CHISQ,TEST, F,(I, B(I), DELTA(I), I=1,V)          MAIN 615
  480 FORMAT (// 12H   ITERATION, I3  /                                  MAIN 616
     *16H  CHI SQUARED = , 1PE16.8 ,16H    TEST VALUE =, E16.8 ,       MAIN 617
     *21H     DAMPING FACTOR =, 0PF7.4, /                               MAIN 618
     *3(4UH  PARAMETER  VALUE         CORRECTION     ),                 MAIN 619
     */5X, I3, F12.3,F15.3 / 5X,   I3, F12.6, F15.6,                    MAIN 620
     *2(10X,I3,F12.9,F15.9)/(5X,2(I3,F12.6,F15.6,10X),I3,F12.0,F15.1))  MAIN 621
      IF (TRACE .EQ. 0.) GO TO 981                                      MAIN 622
C     -----------------                                                 MAIN 623
C     ADJUST PARAMETERS                                                 MAIN 624
C     -----------------                                                 MAIN 625
  419 DO 425 I=1,V                                                      MAIN 626
  425 B(I)=B(I)+DF*DELTA(I)                                             MAIN 627
C     -----------------                                                 MAIN 628
C     VALUES OF SW  0 NORMAL 1 CONVERGED, 2 FAILED                      MAIN 629
C     TO CONVERGE, 3 DIVERGING, OR OVERFLOW IN MATRIX INVERSION         MAIN 630
C     -----------------                                                 MAIN 631
   32 IF (SW) 5,4,5                                                     MAIN 632
    4 IF (IT-NIT) 6,7,7                                                 MAIN 633
    6 IT=IT+1                                                           MAIN 634
      GO TO 300                                                         MAIN 635
    7 SW=2                                                              MAIN 636
C     -----------------                                                 MAIN 637
C     PRINT RESULTS                                                     MAIN 638
C     -----------------                                                 MAIN 639
    5 GO TO (984,983,981,985),ICC                                       MAIN 640
  983 IF (SW .EQ. 3) GO TO 985                                          MAIN 641
  984 WRITE (6,980) STAGE                                               MAIN 642
  980 FORMAT (1H0,5HSTAGE,I2)                                           MAIN 643
      IF (ICC .EQ. 1) GO TO 417                                         MAIN 644
  981 GO TO (986,987,985),SW                                            MAIN 645
  986 WRITE (6,61)                                                      MAIN 646
      GO TO 988                                                         MAIN 647
  987 WRITE (6,62)                                                      MAIN 648
  988 IF (ICC .NE. 2) GO TO 990                                         MAIN 649
      WRITE (6,64) IT,CONSTR,TEST                                       MAIN 650
  990 WRITE (6,813)                                                     MAIN 651
      GO TO 203                                                         MAIN 652
  985 WRITE (6,80) TITLE, STAGE                                         MAIN 653
```



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      GO TO (53,54,55),SW                                               MAIN 654
   53 WRITE (6,61)                                                      MAIN 655
      GO TO 56                                                          MAIN 656
   54 WRITE (6,62)                                                      MAIN 657
      GO TO 56                                                          MAIN 658
   55 WRITE (6,63)                                                      MAIN 659
   56 WRITE (6,64) IT,CONSTR,TEST                                       MAIN 660
      GO TO (52,52,79), SW                                              MAIN 661
   52 WRITE (6,999) SCAN                                                MAIN 662
  999 FORMAT(1H0,7HSCAN  =,F7.2//)                                      MAIN 663
      CALL RESULT(A,B,C,COV,N,Z)                                        MAIN 664
      WRITE (6,812)                                                     MAIN 665
      GO TO 203                                                         MAIN 666
C     -----------------                                                 MAIN 667
C     ERROR MESSAGES                                                    MAIN 668
C     -----------------                                                 MAIN 669
   99 WRITE (6,80) TITLE, STAGE                                         MAIN 670
   80 FORMAT (1HI, 20A4 / 6HOSTAGE, I2)                                 MAIN 671
      GO TO MESS1, (82,83)                                              MAIN 672
   82 WRITE (6,42)                                                      MAIN 673
      GO TO MESS2, (84,86,87,88)                                        MAIN 674
   83 WRITE(6,43)                                                       MAIN 675
      GO TO 79                                                          MAIN 676
   84 WRITE (6,44)                                                      MAIN 677
      GO TO 79                                                          MAIN 678
   86 WRITE (6,46)                                                      MAIN 679
      GO TO 79                                                          MAIN 680
   87 WRITE (6,47)                                                      MAIN 681
      GO TO 79                                                          MAIN 682
   88 WRITE (6,48) AAA                                                  MAIN 683
   79 WRITE (6,85)                                                      MAIN 684
   85 FORMAT (19HOSPECTRUM ABANDONED)                                   MAIN 685
C     -----------------                                                 MAIN 686
C     ABANDONED SPECTRA - SEE WHETHER ANY MORE SPECTRA REMAIN           MAIN 687
C     -----------------                                                 MAIN 688
      WRITE (6,50)                                                      MAIN 689
   75 READ (5,501,END=208,ERR=75) FF,AA,BB                              MAIN 690
   75 IF (FF .EQ. ESTM) GO TO 212                                       MAIN 691
      WRITE (6,801) FF                                                  MAIN 692
```

```
      IF (FF .EQ. EXIT) GO TO 203                                        MAIN 693
      GO TO 78                                                           MAIN 694
C     ----------------                                                   MAIN 695
   61 FORMAT (22HOPROCESS HAS CONVERGED)                                 MAIN 696
   62 FORMAT (31HOPROCESS HAS FAILED TO CONVERGE)                        MAIN 697
   63 FORMAT (21HOPROCESS IS DIVERGING)                                  MAIN 698
   64 FORMAT (6H AFTER,I3,16H ITERATIONS WITH,I3,12H CONSTRAINTS,        MAIN 699
     *14X,12HTEST VALUE =,E16.6)                                         MAIN 700
   42 FORMAT (34HOERROR IN CONSTRAINT SPECIFICATION)                     MAIN 701
   43 FORMAT (29HOOVERFLOW IN MATRIX INVERSION /                         MAIN 702
     *36H DRASTIC DIVERGENCE OR PROGRAM ERROR)                          MAIN 703
   44 FORMAT (47H NUMBER OF CONSTRAINTS IS NEGATIVE OR TOO LARGE)        MAIN 704
   46 FORMAT (32H CONSTRAINTS ARE NOT INDEPENDENT)                       MAIN 705
   47 FORMAT (33H PARAMETER NUMBER IS OUT OF RANGE)                      MAIN 706
   48 FORMAT (17H CONSTRAINT NAME , A4, 15H NOT RECOGNIZED)              MAIN 707
   49 FORMAT (28HOCOMMAND CARD BEGINNING WITH,3X,A4,32H   NOT RECOGNIZEDMAIN 708
     *, CARD IGNORED      )                                            MAIN 709
   50 FORMAT (1HO////                                                    MAIN 710
     *50H SEE WHETHER ANY MORE ESTIMATES OR SPECTRA REMAIN  /)           MAIN 711
  800 FORMAT (7H1***    ,20A4)                                           MAIN 712
  801 FORMAT (7H ***    ,A4,4F10.0)                                      MAIN 713
802   FORMAT(7H ***    ,5HTEST=,I4,6HTEST2=,14)
  803 FORMAT (7H ***    ,A4,2F10.0,F10.1,F10.0)                          MAIN 715
  805 FORMAT (7H ***    ,A4,3F10.0,1PE10.1)                              MAIN 716
  808 FORMAT (7H ***    ,F10.0,F10.2,2F10.6/(7H ***    ,2F10.2,F10.0))  MAIN 717
  809 FORMAT (7H ***    ,20A4)                                           MAIN 718
  810 FORMAT (7H ***    ,22F3.0)                                         MAIN 719
  811 FORMAT (7H ***    ,A4,10F6.2/(4H ***,7X,10F6.2))                   MAIN 720
  812 FORMAT (1HO////)                                                   MAIN 721
  813 FORMAT (1HO)                                                       MAIN 722
C                                                                        MAIN 723
C                                                                        MAIN 724
      END                                                                MAIN 725
      SUBROUTINE DASU(Y,Z,P,FF,AA,IA,IB,IDATA)                           DASU   1
C                                                                        DASU   2
C     1)  XX(L) ,       L = MAXIMUM NUMBER OF CHANNELS                 DASU   3
      DIMENSION         Y(600),Z(600)                                    DASU   4
C     ----------------                                                   DASU   5
C                                                                        DASU   6
```



```
C                                                                        DASU   7
      INTEGER           P                                                DASU   8
      DATA              DATA /4HDATA/                                    DASU   9
C                                                                        DASU  10
      IF (IDATA .EQ. 0) GO TO 10                                         DASU  11
      IF (P .GT. IP) P=IP                                                DASU  12
      IF (FF .EQ. DATA) GO TO 70                                         DASU  13
      GO TO 90                                                           DASU  14
   10 DO 20 I=1,P                                                        DASU  15
   20 Z(I)=Y(I)                                                          DASU  16
      IIA=IA                                                             DASU  17
   30 K=AA=IIA                                                           DASU  18
      IF (K) 40,50,50                                                    DASU  19
   40 L=-K                                                               DASU  20
      K=0                                                                DASU  21
      GO TO 60                                                           DASU  22
   50 L=0                                                                DASU  23
   60 IIA=IIA+K                                                          DASU  24
      IP=P                                                               DASU  25
      IDATA=1                                                            DASU  26
      RETURN                                                             DASU  27
   70 DO 80 I=1,P                                                        DASU  28
      IF (Z(I+K) .LE. 0.) Y(I+L)=0.                                      DASU  29
      IF (Y(I+L) .LE. 0.) Z(I+K)=0.                                      DASU  30
   80 Z(I)=Z(I+K)+Y(I+L)                                                 DASU  31
      GO TO 30                                                           DASU  32
   90 DO 100 I=1,P                                                       DASU  33
      IF (Z(I+K) .LE. 0.) Y(I+L)=0.                                      DASU  34
      IF (Y(I+L) .LE. 0.) Z(I+K)=0.                                      DASU  35
  100 Y(I)=Z(I+K)+Y(I+L)                                                 DASU  36
      IA=IIA                                                             DASU  37
      IB=IA+P-1                                                          DASU  38
      IDATA=0                                                            DASU  39
      RETURN                                                             DASU  40
      END                                                                DASU  41
      SUBROUTINE JUMPP(Y,W,P,HOP,PO)                                     JUMP   1
C                                                                        JUMP   2
C     1)  XX(L) ,       L = MAXIMUM NUMBER OF CHANNELS                 JUMP   3
      DIMENSION         Y(600),W(600)                                    JUMP   4
```

```
C     ******************                                          JUMP   5
C                                                                 JUMP   6
C                                                                 JUMP   7
      INTEGER           P,P0                                      JUMP   8
C                                                                 JUMP   9
      DO 10 J=1,P                                               JUMP  10
      IF (Y(J) .EQ. 0.) GO TO 10                                JUMP  11
      I=J+1                                                     JUMP  12
      ALAST=Y(J)                                                JUMP  13
      GO TO 1                                                   JUMP  14
   10 CONTINUE                                                  JUMP  15
    1 DO 2 J=I,P                                                JUMP  16
      IF (Y(J) .EQ. 0.) GO TO 2                                 JUMP  17
      IF ( ABS(Y(J)-ALAST)+2. .LT. HOP) GO TO 3                 JUMP  18
      IF (Y(J)-ALAST) 4,4,5                                     JUMP  19
    4 Y(J)=Y(J)+HOP                                             JUMP  20
      IF ((ALAST-Y(J))+2.,GT. HOP) GO TO 6                      JUMP  21
    7 IF (W(J) .EQ. 0.) GO TO 3                                 JUMP  22
      W(J)=1./ SQRT(Y(J))                                       JUMP  23
      GO TO 3                                                   JUMP  24
    5 Y(J)=Y(J)-HOP                                             JUMP  25
      IF ((Y(J)-ALAST)+2.,GT. HOP) GO TO 6                      JUMP  26
      GO TO 7                                                   JUMP  27
    6 Y(J)=0.                                                   JUMP  28
      W(J)=0.                                                   JUMP  29
      P0=P0+1                                                   JUMP  30
      GO TO 2                                                   JUMP  31
    3 ALAST=Y(J)                                                JUMP  32
    2 CONTINUE                                                  JUMP  33
      RETURN                                                    JUMP  34
      END                                                       JUMP  35
      SUBROUTINE PLOTOL(Y,P,IA,AA,BB,TITLE)                     PLOL   1
C                                                               PLOL   2
C     1)  XX(L) .         L = MAXIMUM NUMBER OF CHANNELS        PLOL   3
      DIMENSION           Y(600)                                PLOL   4
C     ******************                                        PLOL   5
C                                                               PLOL   6
C                                                               PLOL   7
      REAL                TITLE(20),Y1(150)                     PLOL   8
```



```
      INTEGER             P                                     PLOL   9
      DATA                SYMBOL,BLANK /1H*,1H /                PLOL  10
C                                                               PLOL  11
   90 AIA=IA                                                    PLOL  12
      I1=AA-AIA+1.                                              PLOL  13
      I2=BB-AIA+1.                                              PLOL  14
C     ------------------                                        PLOL  15
C     FIND MAX AND MIN                                          PLOL  16
C     ------------------                                        PLOL  17
      YMAX=0.                                                   PLOL  18
      YMIN=1.E10                                                PLOL  19
      DO 110 I=I1,I2                                            PLOL  20
      IF (Y(I) .EQ. 0.) GO TO 110                               PLOL  21
      IF (Y(I) .GT. YMAX) YMAX=Y(I)                             PLOL  22
      IF (Y(I) .LT. YMIN) YMIN=Y(I)                             PLOL  23
  110 CONTINUE                                                  PLOL  24
C     ------------------                                        PLOL  25
C     WRITE TITLE                                               PLOL  26
C     ------------------                                        PLOL  27
      WRITE (6,1) TITLE                                         PLOL  28
    1 FORMAT (1H1,20A4/1H0,113X,11HCHAN COUNTS)                 PLOL  29
C     ------------------                                        PLOL  30
C     PLOT POINTS ON LINE                                       PLOL  31
C     ------------------                                        PLOL  32
      DO 120 I=1,150                                            PLOL  33
  120 Y1(I)=BLANK                                               PLOL  34
      KN=AA                                                     PLOL  35
      X=110./(YMAX-YMIN)                                        PLOL  36
      DO 130 I=I1,I2                                            PLOL  37
      KCN=Y(I)                                                  PLOL  38
      IX=(Y(I)-YMIN)*X+1.                                       PLOL  39
      IF (IX .GT. 0) GO TO 125                                  PLOL  40
      WRITE (6,4) (Y1(J),J=1,112),KN,KCN                        PLOL  41
    4 FORMAT (1X,1H(,112A1,I3,I8)                               PLOL  42
      GO TO 130                                                 PLOL  43
  125 IY=112-IX                                                 PLOL  44
      WRITE (6,3) (Y1(J),J=1,IX),SYMBOL,(Y1(K),K=1,IY),KN,KCN   PLOL  45
    3 FORMAT (1X,113A1,I3,I8)                                   PLOL  46
  130 KN=KN+1                                                   PLOL  47
```

```
C                                                                       PLOL  48
      RETURN                                                            PLOL  49
      END                                                               PLOL  50
      SUBROUTINE CONCX(Y,W,P,IA,IB,PO,NUMM)                             CONC   1
C                                                                       CONC   2
C     I)  XX(L) =         L = MAXIMUM NUMBER OF CHANNELS                CONC   3
      DIMENSION           Y(600),W(600)                                 CONC   4
C     ****************                                                  CONC   5
C                                                                       CONC   6
C                                                                       CONC   7
      INTEGER             P,PO                                          CONC   8
C                                                                       CONC   9
      MM=1                                                              CONC  10
      K=1                                                               CONC  11
      PO=0                                                              CONC  12
      NUM=NUMM-1                                                        CONC  13
      KK=IA+P                                                           CONC  14
      DO 3 I=0,KK,NUMM                                                  CONC  15
      IF (I .GE. IA) GO TO 4                                            CONC  16
    3 CONTINUE                                                          CONC  17
    4 KK=I-IA+1                                                         CONC  18
      IF (KK .NE. 1) Y(1)=0.                                            CONC  19
      Y(1)=Y(1)/2.                                                      CONC  20
      IA=I/NUMM                                                         CONC  21
      DO 40 I=KK,P,NUMM                                                 CONC  22
      DO 20 J=0,NUM                                                     CONC  23
      IF (I+J .GT. P) GO TO 50                                          CONC  24
      IF (Y(I+J) .NE. 0.) GO TO 10                                      CONC  25
      Y(K)=0.                                                           CONC  26
      W(K)=0.                                                           CONC  27
      PO=PO+1                                                           CONC  28
      GO TO 30                                                          CONC  29
   10 Y(K)=Y(K)+Y(I+J)                                                  CONC  30
      IF (MM .EQ. 0) GO TO 20                                           CONC  31
      IF (W(I+J) .NE. 0.) GO TO 20                                      CONC  32
      MM=0                                                              CONC  33
      W(K)=0.                                                           CONC  34
      PO=PO+1                                                           CONC  35
   20 CONTINUE                                                          CONC  36
```



```
      IF (MM .NE. 0) W(K)=1./ SQRT(Y(K))                                CONC  37
   30 MM=1                                                              CONC  38
      K=K+1                                                             CONC  39
   40 Y(K)=0.                                                           CONC  40
   50 P=K-1                                                             CONC  41
      IB=IA+P-1                                                         CONC  42
      RETURN                                                            CONC  43
      END                                                               CONC  44
      SUBROUTINE MB01B(A,M,SW)                                          MB01   1
C                                                                       MB01   2
C     I)  XX(L) =         L = A + 3 * (MAXIMUM NUMBER OF LINES)         MB01   3
      DIMENSION           A(28,28),IND(28),C(28)                        MB01   4
C     ****************                                                  MB01   5
C                                                                       MB01   6
C                                                                       MB01   7
      INTEGER             SW                                            MB01   8
C                                                                       MB01   9
      SW=0                                                              MB01  10
      M1=M-1                                                            MB01  11
      AMAX=0.                                                           MB01  12
      DO 32 I=1,M                                                       MB01  13
      IND(I)=I                                                          MB01  14
      IF ( ABS(A(I,1))- ABS(AMAX)) 32,32,31                             MB01  15
   31 AMAX=A(I,1)                                                       MB01  16
      IMAX=I                                                            MB01  17
   32 CONTINUE                                                          MB01  18
      ASSIGN 38 TO JUMP                                                 MB01  19
      DO 41 J=1,M1                                                      MB01  20
      IF (IMAX-J)35,35,33                                               MB01  21
   33 IW=IND(IMAX)                                                      MB01  22
      IND(IMAX)=IND(J)                                                  MB01  23
      IND(J)=IW                                                         MB01  24
      DO 34 K=1,M                                                       MB01  25
      W=A(IMAX,K)                                                       MB01  26
      A(IMAX,K)=A(J,K)                                                  MB01  27
      A(J,K)=W                                                          MB01  28
   34 CONTINUE                                                          MB01  29
   35 J1=J+1                                                            MB01  30
      GO TO JUMP,(36,38)                                                MB01  31
```

```
   36 J2=J+1                                                    MAIN  32
      DO 37 I=J1,M                                              MAIN  33
      DO 45 K=1,J2                                              MAIN  34
   45 A(J,I)=A(J,I)-A(J,K)*A(K,I)                               MAIN  35
   37 CONTINUE                                                  MAIN  36
   38 DIV=AMAX                                                  MAIN  37
      AMAX=0.                                                   MAIN  38
      ASSIGN 38 TO JUMP                                         MAIN  39
      IF (DIV) 60,61,60                                         MAIN  40
   60 DO 40 I=J1,M                                              MAIN  41
      A(I,J)=A(I,J)/DIV                                         MAIN  42
      DO 42 K=1,J                                               MAIN  43
   42 A(I,J+1)=A(I,J+1)-A(I,K)*A(K,J+1)                         MAIN  44
      IF ( ABS(A(I,J1))- ABS(AMAX)) 40,40,39                    MAIN  45
   39 AMAX=A(I,J1)                                              MAIN  46
      IMAX=I                                                    MAIN  47
   40 CONTINUE                                                  MAIN  48
   41 CONTINUE                                                  MAIN  49
      DO 13 I1=1,M1                                             MAIN  50
      I=M+1-I1                                                  MAIN  51
      I2=I-1                                                    MAIN  52
      DO 11 J1=1,I2                                             MAIN  53
      J=I2+1-J1                                                 MAIN  54
      J2=J+1                                                    MAIN  55
      W1=-A(I,J)                                                MAIN  56
      IF (I2-J2)10,9,9                                          MAIN  57
    9 DO 43 K=J2,I2                                             MAIN  58
   43 W1=W1-A(K,J)*C(K)                                         MAIN  59
   10 C(J)=W1                                                   MAIN  60
   11 CONTINUE                                                  MAIN  61
      DO 12 K=1,I2                                              MAIN  62
      A(I,K)=C(K)                                               MAIN  63
   12 CONTINUE                                                  MAIN  64
   13 CONTINUE                                                  MAIN  65
      DO 22 I1=1,M                                              MAIN  66
      I=M+1-I1                                                  MAIN  67
      I2=I+1                                                    MAIN  68
      W=A(I,I)                                                  MAIN  69
      DO 20 J=1,M                                               MAIN  70
```



```
      IF (I-J)14,15,16                                          MAIN  71
   14 W1=0                                                      MAIN  72
      GO TO 17                                                  MAIN  73
   15 W1=1.0                                                    MAIN  74
      GO TO 17                                                  MAIN  75
   16 W1=A(I,J)                                                 MAIN  76
   17 IF (I1-1)19,19,18                                         MAIN  77
   18 DO 44 K=I2,M                                              MAIN  78
   44 W1=W1-A(I,K)*A(K,J)                                       MAIN  79
   19 C(J)=W1                                                   MAIN  80
   20 CONTINUE                                                  MAIN  81
      IF (W) 62,61,62                                           MAIN  82
   62 DO 21 J=1,M                                               MAIN  83
      A(I,J)=C(J)/W                                             MAIN  84
   21 CONTINUE                                                  MAIN  85
   22 CONTINUE                                                  MAIN  86
      DO 26 I=1,M                                               MAIN  87
   23 IF (IND(I)-I)24,26,24                                     MAIN  88
   24 J=IND(I)                                                  MAIN  89
      DO 25 K=1,M                                               MAIN  90
      STO=A(K,I)                                                MAIN  91
      A(K,I)=A(K,J)                                             MAIN  92
      A(K,J)=STO                                                MAIN  93
   25 CONTINUE                                                  MAIN  94
      ISTO=IND(J)                                               MAIN  95
      IND(J)=J                                                  MAIN  96
      IND(I)=ISTO                                               MAIN  97
      GO TO 23                                                  MAIN  98
   26 CONTINUE                                                  MAIN  99
   99 RETURN                                                    MAIN 100
   61 SW=3                                                      MAIN 101
      RETURN                                                    MAIN 102
      END                                                       MAIN 103
      SUBROUTINE RESULT(A,B,C,COV,N,Z)                          RESU   1
C                                                               RESU   2
C     1)  XX(L) ,       L = MAXIMUM NUMBER OF CHANNELS          RESU   3
      DIMENSION         A(600),Z(600)                           RESU   4
C                                                               RESU   5
C     2)  XX(L) ,       L = 6 + 3 * (MAXIMUM NUMBER OF LINES)   RESU   6
```

```
      DIMENSION          A(28),B(28),COV(28,28)                          RESU   7
C     ==================                                                 RESU   8
C                                                                        RESU   9
      DIMENSION          C(200),CHAR(10)                                 RESU  10
C                                                                        RESU  11
      REAL               MINUS                                           RESU  12
      INTEGER            CONSTR,P,PO,Q,V,V1                              RESU  13
      COMMON             CHISQ,PI,CONSTR,IA,P,PO,V,V1                    RESU  14
      DATA               CHAR(1),CHAR(2),CHAR(3),CHAR(4),CHAR(5),CHAR(6),RESU  15
     *                   CHAR(7),CHAR(8),CHAR(9),CHAR(10),MINUS,PLUS     RESU  16
     *                   SPACE                  /1H1,1H2,1H3,1H4,1H5,1H6,RESU  17
     *                   1H7,1H8,1H9,1H0,1H-,1H+,1H /                    RESU  18
C                                                                        RESU  19
C     ------------------                                                 RESU  20
C     WRITE PARAMETERS M.M.                                              RESU  21
C     ------------------                                                 RESU  22
  904 DO 902 I=1,V                                                       RESU  23
  902 A(I)= SQRT(COV(I,I))                                               RESU  24
      WRITE (6,964)  (B(I), A(I), I=1,4)                                 RESU  25
  964 FORMAT (11HOBASELINE =,F9.0,36X,18HSTANDARD DEVIATION, F8.2 /      RESU  26
     *25HOSCAN REVERSES AT CHANNEL, F8.3,23X,18HSTANDARD DEVIATION,      RESU  27
     *F8.3, / 31HOBASELINE SINE-WAVE COMPONENT =, 2PF6.3,                RESU  28
     *37H PER CENT           STANDARD DEVIATION, F8.3,                   RESU  29
     */17HOBASELINE DRIFT =, 6PF7.2, 19H P.P.M. PER CHANNEL,             RESU  30
     *13X,18HSTANDARD DEVIATION, F8.2 /)                                 RESU  31
      WRITE (6,982)                                                      RESU  32
  982 FORMAT (45HOLINE      POSITION        S.D.          WIDTH  ,       RESU  33
     *37H      S.D.       INTENSITY          S.D.        ,               RESU  34
     *40H            *          REL.INT.       AMPL.)                   RESU  35
      SUM=0.                                                             RESU  36
      DO 901 I=V1,V,3                                                    RESU  37
  901 SUM=SUM+B(I+2)                                                     RESU  38
      L=0                                                                RESU  39
      DO 906 I=V1,V,3                                                    RESU  40
      L=L+1                                                              RESU  41
      K=I+2                                                              RESU  42
      RELINT=100.*B(K)/SUM                                               RESU  43
      AMPL=(2./PI)*B(K)/B(I+1)                                           RESU  44
  906 WRITE (6,965) L,(B(J),A(J),J=I,K),RELINT,AMPL                      RESU  45
```



```
  965 FORMAT(1HO,I3,2(F14.3,F11.3),F15.0,F13.0,10X,1H*,F15.1,2H %,F12.0)RESU  46
C     ------------------                                                 RESU  47
C     OBTAIN CHI SQUARED PERCENTAGE POINTS                               RESU  48
C     ------------------                                                 RESU  49
  269 L=(P-PO-V+CONSTR)                                                  RESU  50
      IF (L-100) 910,910,911                                             RESU  51
  911 G=L                                                                RESU  52
      F=SQRT(G)                                                          RESU  53
      C(1)=G+2.326*F+0.853                                               RESU  54
      C(2)=G+3.289*F+2.205                                               RESU  55
      C(3)=G+4.37*F+4.15                                                 RESU  56
      WRITE (6,968)      CHISQ, L, C(1), C(2), C(3)                      RESU  57
  968 FORMAT (14HOCHI SQUARED =, F8.2, 5H WITH, I4,12H DEGREES OF ,      RESU  58
     *7HFREEDOM       / 33H 5, 1 AND 0.1 PER CENT POINTS ARE,            RESU  59
     *F7.1, 1H,, F7.1, 5H AND , F7.1, 13H RESPECTIVELY)                  RESU  60
      GO TO 912                                                          RESU  61
  910 WRITE (6,969) CHISQ, L                                             RESU  62
  969 FORMAT (14HOCHI SQUARED =, F8.2, 5H WITH, I4, 12H DEGREES OF ,     RESU  63
     *6HFREEDOM           (REFER TO STATISTICAL TABLES))                 RESU  64
C     ------------------                                                 RESU  65
C     FIND POINTS WHICH DEVIATE SIGNIFICANTLY FROM CURVE                 RESU  66
C     ------------------                                                 RESU  67
  912 J=0                                                                RESU  68
      DO 913 I=1,P                                                       RESU  69
      IF (A(I)) 919,913,919                                              RESU  70
  919 IF (3.6* ABS(Z(I))) 914,913,913                                    RESU  71
  914 J=J+2                                                              RESU  72
      C(J-1)=I+IA-1                                                      RESU  73
      C(J)=Z(I)                                                          RESU  74
      IF (J-200) 913,916,916                                             RESU  75
  913 CONTINUE                                                           RESU  76
      IF (J) 915,915,916                                                 RESU  77
  915 WRITE (6,971)                                                      RESU  78
  971 FORMAT (47HONO POINTS DEVIATE SIGNIFICANTLY FROM THE CURVE)        RESU  79
      GO TO 917                                                          RESU  80
  916 WRITE (6,972) (C(I), I=1,J)                                        RESU  81
  972 FORMAT  (47HOTHE COUNTS FOR THE FOLLOWING CHANNELS DEVIATE ,       RESU  82
     *28HSIGNIFICANTLY FROM THE CURVE //                                 RESU  83
     *(2H  ,5(1H(,F4.0,1H=,F6.2,4H)   )))                               RESU  84
```

```
      IF (J-200) 917,918,918                                          RESU  85
  918 WRITE (6,976)                                                   RESU  86
  976 FORMAT (9HOETCETERA )                                           RESU  87
C     ------------------                                              RESU  88
C     PLOT RESIDUAL DEVIATIONS ON LINE PRINTER                        RESU  89
C     ------------------                                              RESU  90
  917 WRITE (6,980)                                                   RESU  91
  980 FORMAT (1H1)                                                    RESU  92
      AA=P                                                            RESU  93
      H=100./AA                                                       RESU  94
      F=3.5                                                           RESU  95
      DO 923 I=1,P                                                    RESU  96
      IF (A(I)) 921,923,921                                           RESU  97
  921 IF (F- ABS(Z(I))) 922,923,923                                   RESU  98
  922 F= ABS(Z(I))                                                    RESU  99
  923 CONTINUE                                                        RESU 100
C                                                                     RESU 101
C     ROUND OF F                                                      RESU 102
C                                                                     RESU 103
      F=0.1*AINT(10.*F+1.)                                            RESU 104
      G=0.04*F                                                        RESU 105
      U=F+0.5*G                                                       RESU 106
      UU=-U-U                                                         RESU 107
      Q=(75./F)+0.5                                                   RESU 108
C                                                                     RESU 109
C     THE FOLLOWING LOOP PRINTS ONE LINE OF THE PLOT AT A TIME        RESU 110
C                                                                     RESU 111
      DO 925 LL=1,51                                                  RESU 112
      L=LL-26                                                         RESU 113
      U=U-G                                                           RESU 114
      SYM=SPACE                                                       RESU 115
      ZZ=0                                                            RESU 116
      IF (IABS(L)-25)  926,927,926                                    RESU 117
  927 SYM=PLUS                                                        RESU 118
      ZZ=U+0.5*G                                                      RESU 119
  926 IF (IABS(L)-Q)  928,929,928                                     RESU 120
  929 SYM=MINUS                                                       RESU 121
      ZZ=SIGN(3.,U)                                                   RESU 122
C                                                                     RESU 123
```



```
C     SET UP A LINE OF CHARACTERS SYM.   IFZ(I) LIES BETWEEN U AND UU,  RESU 124
C     OVERWRITE WITH THE LAST DIGIT OF I+IA-1.                          RESU 125
C                                                                       RESU 126
  928 C(1)=PLUS                                                         RESU 127
      C(101)=PLUS                                                       RESU 128
      DO930 I=2,100                                                     RESU 129
  930 C(I)=SYM                                                          RESU 130
      X=0.                                                              RESU 131
      DO 932 I=1,P                                                      RESU 132
      X=X+1.                                                            RESU 133
      IF (A(I)) 931,932,931                                             RESU 134
  931 IF (Z(I)-U) 932,935,935                                           RESU 135
  935 K=X*H+1.5                                                         RESU 136
      J=MOD((IABS(I+IA-1)+9),10)+1                                      RESU 137
      C(K)=CHAR(J)                                                      RESU 138
      Z(I)=UU                                                           RESU 139
  932 CONTINUE                                                          RESU 140
C                                                                       RESU 141
C     PRINT LINE                                                        RESU 142
C                                                                       RESU 143
      IF (SYM .EQ. SPACE .AND. L .NE. 0) GO TO 936                      RESU 144
      WRITE (6,973)ZZ, (C(K), K=1,101)                                  RESU 145
  973 FORMAT (1H , F7.1, 2X, 101A1)                                     RESU 146
      GO TO 925                                                         RESU 147
  936 WRITE (6,974)(C(K), K=1,101)                                      RESU 148
  974 FORMAT (10X, 101A1)                                               RESU 149
  925 CONTINUE                                                          RESU 150
C     ------------------                                                RESU 151
C     PRINT CAPTION                                                     RESU 152
C     ------------------                                                RESU 153
      WRITE (6,975)                                                     RESU 154
  975 FORMAT (1H0,22X,39HPLOT OF RESIDUAL DEVIATION (IN STANDARD,       RESU 155
     *36H DEVIATION UNITS) VS. CHANNEL NUMBER / 28X,                    RESU 156
     *45HSMALL BUT ONE OR TWO POINTS SHOULD LIE BETWEEN ,               RESU 157
     *20HHALF HORIZONTAL LINES )                                        RESU 158
C     ------------------                                                RESU 159
C     PRINT  VARIANCE-COVARIANCE MATRIX                                 RESU 160
C     ------------------                                                RESU 161
      WRITE (6,966)                                                     RESU 162
```

```
 966 FORMAT (27H1VARIANCE-COVARIANCE MATRIX)                          RESU 163
     DO 908 J=1,V                                                    RESU 164
 908 WRITE (6,967)  (CO/(I,J), I=1,J)                                RESU 165
 967 FORMAT (1H0, 1P10E12.3/ (1H , 1P10E12.3))                       RESU 166
C                                                                    RESU 167
     RETURN                                                          RESU 168
     END                                                             RESU 169
     SUBROUTINE PLOTP(B,V,SCAN,Y,N,P,IA,AA,BB,CC,DD,TITLE,PDIV)
C                                                                    PLOT   2
C    1)  XX(L) ,        L = MAXIMUM NUMBER OF CHANNELS               PLOT   3
     DIMENSION          B(600),Y(600)                                PLOT   4
C                                                                    PLOT   5
C    2)  XX(L) ,        L = 5 * (MAXIMUM NUMBER OF CHANNELS)         PLOT   6
     DIMENSION          S(3000)                                      PLOT   7
C                                                                    PLOT   8
C    3)  XX(L) ,        L = 4 + 3 * (MAXIMUM NUMBER OF LINES)        PLOT   9
     DIMENSION          H(28)                                        PLOT  10
C                                                                    PLOT  11
C    4)  XX(L) ,        L = 2 * (MAXIMUM NUMBER OF CHANNELS)         PLOT  12
     DIMENSION          F(1200)                                      PLOT  13
C    ******************                                            PLOT  14
C                                                                    PLOT  15
     DIMENSION          TITLE(20)                                    PLOT  16
     INTEGER V,P,ABSP(3),PDIV
     COMMON             /XXX/ SPLOT                                  PLOT  18
     EQUIVALENCE        (SPLOT,S)                                    PLOT  19
     DATA               BLANCK /4H    /                              PLOT  20
C                                                                    PLOT  22
C    -----------------                                             PLOT  23
C    CALCULATE DIMENSIONS                                          PLOT  24
C    -----------------                                             PLOT  25
   5 IF (DD .GT. 125) DD=125.                                        PLOT  26
     AXL=(BB-AA+5.)*0.1*CC                                           PLOT  27
     DYK=0.1*DD                                                      PLOT  28
     PAL=AXL+DYK*0.46                                                PLOT  29
     PAH=1.98*DYK                                                    PLOT  30
     XAF=DYK*0.45                                                    PLOT  31
     AMAX=B(1)                                                       PLOT  32
     AMIN=1.E10                                                      PLOT  33
```



```
     I1=AA-FLOAT(IA)+1.                                              PLOT  34
     I2=BB-AA+FLOAT(I1)                                              PLOT  35
     DO 200 I=I1,I2                                                  PLOT  36
     IF (Y(I) .EQ. 0.) GO TO 200                                     PLOT  37
     IF (Y(I) .LT. AMIN) AMIN=Y(I)                                   PLOT  38
     IF (Y(I) .GT. AMAX) AMAX=Y(I)                                   PLOT  39
 200 CONTINUE                                                        PLOT  40
     YDYK=AMAX-AMIN                                                  PLOT  41
     XMAAL=CC/10.                                                    PLOT  42
     YMAAL=DYK/YDYK                                                  PLOT  43
     AXAF=-((AMAX-B(I))*YMAAL+DYK*0.1)                               PLOT  44
     BDYK=-AXAF+DYK*0.387                                            PLOT  45
     XM=AA                                                           PLOT  46
C    -----------------                                             PLOT  47
C    MOVE CO-ORDINATE SYSTEM                                       PLOT  48
C    -----------------                                             PLOT  49
     CALL PSTART                                                     PLOT  50
C                                                                    PLOT  51
C    -----------------                                             PLOT  73
C    MOVE CO-ORDINATE SYSTEM                                       PLOT  74
C    -----------------                                             PLOT  75
     CALL PORIGO (BDYK,XAF)                                          PLOT  76
C                                                                    PLOT  77
C    -----------------                                             PLOT  78
C    DRAW AXIS                                                     PLOT  79
C    -----------------                                             PLOT  80
     H=DYK/50.                                                       PLOT  81
     XX=AXAF-H*5.                                                    PLOT  82
     X1=AXAF-H/4.                                                    PLOT  83
     X2=X1+H/2.                                                      PLOT  84
     YY=0.                                                           PLOT  85
     INT=AA                                                          PLOT  86
 103 Y1=YY-H/2.                                                      PLOT  87
     CALL PLOT (x1,YY,1)                                             PLOT  89
     CALL PLOT (x2,YY,0)                                             PLOT  90
     IF (YY .GE. AXL-0.5*CC) GO TO 105                               PLOT  91
     CALL PLOT (AXAF,YY,0)                                           PLOT  92
     YY=YY+CC                                                        PLOT  93
     CALL PLOT (AXAF,YY,0)                                           PLOT  94
```

```
      INT=INT+10                                                        PLOT  95
      GO TO 103                                                         PLOT  96
  105 XF=-100./(YMAAL*H(1))                                             PLOT  97
      XN=6.5                                                            PLOT  98
  110 XN=2.*XN                                                          PLOT  99
      XNF=-XN/XF                                                        PLOT 100
      IF (XNF .LT. DYK/5.) GO TO 110                                    PLOT 101
      IXN=XN                                                            PLOT 102
      AXX=0.                                                            PLOT 103
  120 AXX=AXX+XNF                                                       PLOT 104
      IF (AXX .LT. DYK) GO TO 120                                       PLOT 105
      IF (AXX .GT. PAH-BDYK) AXX=AXX-XNF                                PLOT 106
      H=DYK*0.03                                                        PLOT 107
      XX=0.                                                             PLOT 108
      Y3=-DYK/15                                                        PLOT 109
      YY=Y3-H*2.                                                        PLOT 110
      Y1=Y3-H/3.                                                        PLOT 111
      Y2=Y3+H/3.                                                        PLOT 112
      INT=0                                                             PLOT 113
  106 X1=XX-H*1.9                                                       PLOT 114
      CALL PINT (INT,3,X1,YY,H)                                         PLOT 115
      CALL PLOT (XX,Y1,1)                                               PLOT 116
      CALL PLOT (XX,Y2,0)                                               PLOT 117
      CALL PLOT (XX,Y3,0)                                               PLOT 118
      XX=XX+XNF                                                         PLOT 119
      IF (XX .GT. AXX) GO TO 108                                        PLOT 120
      CALL PLOT (XX,Y3,0)                                               PLOT 121
      INT=INT+IXN                                                       PLOT 122
      GO TO 106                                                         PLOT 123
  108 CONTINUE                                                          PLOT 124
C     -----------------                                                 PLOT 125
C     WRITE TEXT                                                        PLOT 126
C     -----------------                                                 PLOT 127
      YY=YY-H*2.                                                        PLOT 128
      H=DYK*0.04                                                        PLOT 129
      XX=DYK*0.1-BDYK                                                   PLOT 131
      YY=DYK*0.1-XAF                                                    PLOT 132
      H=DYK*0.049                                                       PLOT 133
      K=21                                                              PLOT 134
```



```
  130 K=K-1                                                             PLOT 135
      IF (TITLE(K) .EQ. BLANCK) GO TO 130                               PLOT 136
      N=K+4                                                             PLOT 137
      IF (FLOAT(N)*H .LT. PAH*0.9) GO TO 135                            PLOT 138
      H=PAH*0.9/FLOAT(N)                                                PLOT 139
  135 DO 140 I=1,K                                                      PLOT 140
      CALL PSTRNG(TITLE(I),4,XX,YY,H)                                   PLOT 141
  140 XX=XX+4.*H                                                        PLOT 142
C     -----------------                                                 PLOT 143
C     DRAW BASELINE                                                     PLOT 144
C     -----------------                                                 PLOT 145
      CALL PLOT (0.,0.,1)                                               PLOT 146
      RMAAL=(HH-AA)*CC/10.                                              PLOT 147
      CALL PLOT (0.,RMAAL,0)                                            PLOT 148
C     -----------------                                                 PLOT 149
C     CALCULATE AND DRAW CURVES                                         PLOT 150
C     -----------------                                                 PLOT 151
      J1=0                                                              PLOT 152
      J3=0                                                              PLOT 153
      J4=(HH-AA)*5.+1.                                                  PLOT 154
      IF (AA .GT. SCAN+B(2)) GO TO 220                                  PLOT 155
      J1=1                                                              PLOT 156
      IF (HH .GT. SCAN+B(2)) GO TO 210                                  PLOT 157
      J2=J4                                                             PLOT 158
      GO TO 230                                                         PLOT 159
  210 J2=(SCAN+B(2)-AA)*5.+1.                                           PLOT 160
      J3=J2+1                                                           PLOT 161
      GO TO 230                                                         PLOT 162
  220 J3=1                                                              PLOT 163
  230 DO 235 I=1,J4                                                     PLOT 164
  235 S(I)=0.                                                           PLOT 165
      FFF=0.02*YDYK                                                     PLOT 166
      DO 270 L=5,V,3                                                    PLOT 167
      FAL=-2.*B(L+2)/(3.141592*B(L+1))                                  PLOT 168
      N=0                                                               PLOT 169
      IX=0                                                              PLOT 170
      IF (J1 .EQ. 0) GO TO 250                                          PLOT 171
      DO 240 I=J1,J2                                                    PLOT 172
      XX=AA+0.2*FLOAT(I-1)                                              PLOT 173
```

```
      FF=FAC/(1.+4.*((XX-B(L))/B(L+1))**2)                              PLOT 174
      IF (ABS(FF) .LT. FFF) GO TO 240                                   PLOT 175
      IF (N .GT. 1000) GO TO 240                                        PLOT 176
      N=N+1                                                             PLOT 177
      F(N)=FF                                                           PLOT 178
      IF (IX .EQ. 1) GO TO 240                                          PLOT 179
      X=XX                                                              PLOT 180
      IX=1                                                              PLOT 181
  240 S(I)=S(I)+FF                                                      PLOT 182
      IF (N .EQ. 0) GO TO 245                                           PLOT 183
      CALL KURVE(X,F,N,1,XMAAL,YMAAL,XM,0.,-1,0,0.)                     PLOT 184
  245 N=0                                                               PLOT 185
      IF (J3 .EQ. 0) GO TO 270                                          PLOT 186
      IX=0                                                              PLOT 187
  250 DO 260 I=J3,J4                                                    PLOT 188
      XX=XH+0.2*FLOAT(I-1)                                              PLOT 189
      FF=FAC/(1.+4.*((2.*(B(2)+SCAN)-XX-B(L))/B(L+1))**2)               PLOT 190
      IF (ABS(FF) .LT. FFF) GO TO 260                                   PLOT 191
      IF (N .LT. 1000) GO TO 260                                        PLOT 192
      N=N+1                                                             PLOT 193
      F(N)=FF                                                           PLOT 194
      IF (IX .EQ. 1) GO TO 260                                          PLOT 195
      X=XX                                                              PLOT 196
      IX=1                                                              PLOT 197
  260 S(I)=S(I)+FF                                                      PLOT 198
      IF (N .EQ. 0) GO TO 270                                           PLOT 199
      CALL KURVE(X,F,N,1,XMAAL,YMAAL,XM,0.,-1,0,0.)                     PLOT 200
  270 CONTINUE                                                          PLOT 201
      X=XH                                                              PLOT 202
      CALL KURVE(X,S,J4,1,XMAAL,YMAAL,XM,0.,-1,0,0.)                    PLOT 203
C     -----------------                                                 PLOT 204
C     CALCULATE POINTS                                                  PLOT 205
C     -----------------                                                 PLOT 206
      K=1                                                               PLOT 207
      KK=1                                                              PLOT 208
      KKK=1                                                             PLOT 209
      DO 330 I=I1,I2                                                    PLOT 210
      S(KKK)=S(K)                                                       PLOT 211
      F(KK)=1.E10                                                       PLOT 212
```



```
      IF (Y(I) .EQ. 0.) GO TO 310                                       PLOT 213
      XX=XM+FLOAT(I-1)                                                  PLOT 214
      SCANH=SCAN                                                        PLOT 215
      FAK=XX-H(2)                                                       PLOT 216
      FAK=1.+B(3)*SIN(3.141592*FAK/SCANH)*B(4)*FAK                      PLOT 217
      DIF=Y(I)-FAK*(B(1)+S(K))                                          PLOT 218
      F(KK)=DIF+S(K)                                                    PLOT 219
      IF (W(I) .EQ. 0.) GO TO 310                                       PLOT 220
      S(KKK)=F(KK)                                                      PLOT 221
  310 KK=KK+1                                                           PLOT 222
  320 KKK=KKK+1                                                         PLOT 223
  330 K=K+5                                                             PLOT 224
C     -----------------                                                 PLOT 225
C     DRAW POINTS                                                       PLOT 226
C     -----------------                                                 PLOT 227
      X=XH                                                              PLOT 228
      N=KK-1                                                            PLOT 229
      SD=B(1)                                                           PLOT 230
      IF (PDIV .EQ. 0) GO TO 500
      CALL KURVE(X,F,N,1,XMAAL,YMAAL,XM,0.,0,13,SD)                     PLOT 231
C                                                                       PLOT 233
500   RETURN
      END                                                               PLOT 235
      SUBROUTINE KURVE (X,Y,N,K,XMAAL,YMAAL,XNULP,YNULP,LITYPE,NRSYMB,HJ)KURV   1
C                                                                       KURV   2
C     1)  XX(L) ,        L = 5 * (MAXIMUM NUMBER OF CHANNELS)           KURV   3
      DIMENSION          Y(3000)                                        KURV   4
C     -----------------                                                 KURV   5
C                                                                       KURV   6
      INTEGER            T(1)                                           KURV   7
      DATA               T/'X'/                                         KURV   8
C                                                                       KURV   9
      YY=(X-XNULP)*XMAAL                                                KURV  10
      IF (LITYPE) 10,30,30                                              KURV  11
C                                                                       KURV  12
   10 XX=-Y(1)*YMAAL                                                    KURV  13
      CALL PLOT (XX,YY,1)                                               KURV  14
      DO 20 I=2,N                                                       KURV  15
      XX=-Y(I)*YMAAL                                                    KURV  16
```

```
      YY=YY+0.2*XMAAL
   20 CALL PLOT (XX,YY,0)
      RETURN
C
   30 IF (NRSYMB .EQ. 13) GO TO 50
      YY=YY-H/2.
      DO 40 I=1,N
      XX=-Y(I)*YMAAL-H*2./5.
      CALL PSTRNG (T,1,XX,YY,H)
   40 YY=YY+XMAAL
      RETURN
C
   50 DO 60 I=1,N
      IF (Y(I) .EQ. 1.E10) GO TO 60
      IF (H+Y(I) .LE. 0.) GO TO 60
      H1=SQRT(H+Y(I))*YMAAL*2.
      XX=-Y(I)*YMAAL-H1/2.
      CALL PLOT (XX,YY,1)
      XX=XX+H1
      CALL PLOT (XX,YY,0)
   60 YY=YY+XMAAL
      RETURN
C
      END
$INCLUDE 'SF/150'
```


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MOSSPEC 7-12-73 PAGE 1 OF 1

FORTRAN STATEMENT

```
039 LAF
DATA        0          255          0         0
 0 0
ADD     400000
ASTN        4            0
     435000
        96          33      -4900
       153          33      -4900
       118          23      -6500
       140          23      -6500
FIX         10          10          2     1.0E-6
 2  3  4  5  8 11 14
AREA     1      -1      0      0
AREA     0       0      1     -1
WATH     0       0      1     -1
FIX          6                      2
 2 11 14
AREA     1      -1      0      0
AREA     0       0      1     -1
WATH     0       0      1     -1
FIX          4                      4
 2
AREA     1      -1      0      0
AREA     0       0      1     -1
```

IBM

FORTRAN Coding Form

GX28 7327-6 U/M030
Printed in Denmark

HOSSPEC

7-12-73

2 1

FORTRAN STATEMENT

WIDTH	0	0	1	-1	
PLOT					
3					
EXIT					

33065,34262,33170,33922,35220,35211,33997,33650,34290,33257,33224,34634,34049,34091,34107,34257,20
32275,33749,34487,34441,34345,33228,35312,33349,33000,34410,33074,32945,34347,33362,33140,34421,21
33234,32766,32152,33954,33700,32183,33692,31118,32405,32756,31765,32377,32000,31361,32983,32213,22
32922,32714,33068,31953,32847,31869,31470,31128,32732,32211,31778,32099,30907,30937,31477,31251,23
31765,30622,31425,30784,32372,30982,31545,30342,31419,31471,30368,30870,31876,30474,30286,30047,24
30277,30568,29379,29384,29851,28311,28745,29741,28486,28248,28190,28415,27345,27450,27256,27370,25
25457,28145,25956,26900,25133,26503,26253,25812,25668,25977,25860,26365,25349,25494,24916,24927,26
23960,23518,23555,24262,23827,24170,23476,23329,23236,23724,24363,24492,23725,24370,24697,25242,27
25112,23252,22860,24540,24114,23350,22696,22410,23535,21849,20922,21754,21466,21410,22174,20941,30
22928,23074,22807,23635,22933,24518,24711,24676,25122,24969,24399,24781,26290,26252,25823,26297,31
27460,26901,25366,26753,28372,29672,28568,28462,30601,28831,30146,30587,30705,30796,31123,31061,32
31935,30885,31403,33179,31876,32238,31100,32371,32641,32537,33126,33263,33419,33104,33610,32506,33
32254,33899,33505,33483,32492,33645,33996,33178,33960,33562,33930,32827,32925,33434,33808,33330,34
33332,34673,32541,33928,34092,33501,34104,34085,33704,34511,34007,34748,33456,33506,33465,33509,35
33860,32119,34722,34467,33904,33350,33366,33486,34346,33016,34346,34494,34217,33518,35194,34260,36
34069,34047,34572,33159,33990,32978,34251,34039,33392,34679,34127,33472,34557,33767,33835,34345,37

```
?????/********************************* ********* WORK FLOW STATEMENTS FOR JOB 6409 **********************????????????????????????
      ?JOB MOSSPEC $CLASS=2;CHANGE=130102     $FENGER
      ?PROCESS(TIME=100  $IOTIME=100  $PRINTLIMIT=2500 )
      ?BEGIN RUN      OBJECT/MOSSPEC
      ?FILE FILE10(TITLE=PLOTFIL/24 ,KIND=DISK,MYUSE=OUT,MAXRECSIZE=45,-
      BLOCKSIZE=10,AMLASIZE  0,AREAS=400,PROTECTION=PROTECTED)
      ?FILE FILE*(KIND=DISK,  ,RECSIZE=10,AREASIZE=1,AREAS=1)
      ?DATA MOSSPEC
      ?END JOB
```

```
MM       MM   OOOOOOOO     SSSSSSS     SSSSSSS   PPPPPPPPP   EEEEEEEEEEE    CCCCCCC
MMM     MMM  OOOOOOOOOO   SSSSSSSSS   SSSSSSSSS  PPPPPPPPPP  EEEEEEEEEEE  CCCCCCCCC
MMMM   MMMM OOO      OOO SSS     SSS SSS     SSS PPP     PPP EEE         CCC      CCC
MMMMM MMMMM OOO      OOO SSS         SSS         PPP     PPP EEE         CCC      CCC
MMMMMMMMMMM OOO      OOO  SSSSSSSSS   SSSSSSSSS  PPPPPPPPPP  EEEEEE      CCC
MMM MMM MMM OOO      OOO   SSSSSSSSS   SSSSSSSSS  PPPPPPPPP   EEEEEE      CCC
MMM  M  MMM OOO      OOO         SSS         SSS PPP         EEE         CCC      CCC
MMM     MMM OOO      OOO SSS     SSS SSS     SSS PPP         EEE         CCC      CCC
MMM     MMM  OOOOOOOOOO   SSSSSSSSS   SSSSSSSSS  PPP         EEEEEEEEEEE  CCCCCCCCC  **
MMM     MMM   OOOOOOOO     SSSSSSS     SSSSSSS   PPP         EEEEEEEEEEE   CCCCCCC   **
```

```
BEGINNING OF JOB 6409 MOSSPEC.    JAN 15, 1974   15:25:57.023 HRS.
                    QUEUE: 2  PRIORITY: 50  ORIGINATING UNIT: 10
                        CHANGECODE = 130102.

BEGINNING OF TASK  6411 OBJECT/MOSSPEC. (CONTINUE)    JAN 15, 1974   15:25:57.415 HRS.
                    QUEUE: 2  PRIORITY: 50  ORIGINATING UNIT: 10
                        CHANGECODE = 130102.

MESSAGE (6411) 15:26:00.382 HRS.:6411  NO FILE TAPEIN


END OF TASK  6411 OBJECT/MOSSPEC.  JAN 15, 1974   15:27:10.382 HRS.
      PROC TIME= 46.565 SECS.     IO TIME= 7.294 SECS.
      28 CARDS READ     0 CARDS PUNCHED     241 LINES PRINTED
      MEMORY INTEGRALS(KILO-WORDS-SEC) CODE= 168.658 DATA= 284.592


END OF JOB  6409 MOSSPEC.  JAN 15, 1974   15:27:11.132 HRS.
      PROC TIME= 0.090 SECS.     IO TIME= 0.193 SECS.
      0 CARDS READ     0 CARDS PUNCHED     0 LINES PRINTED
      MEMORY INTEGRALS(KILO-WORDS-SEC) CODE= 6.157 DATA= 0.240
      ELAPSED TIME =  0 HRS 01 MIN 14.109 SECS.


VOL1000000                    652020501                                        1
HDRIFILE6                  0000001000000 74015 74015 0000000000000 B8500
HDR2V0002200022011000000000000000002880          00
```

```
***   039 LAF
***   DATA        0.      255.        0.        9.
***   TEST=   DTEST2=   0
```

33865	34262	33170	33922	35220	35211	33997	33650	34290	33257
33224	34634	34049	34091	34107	34237	32275	33749	34467	34441
34345	33220	35312	33349	33000	34410	33074	32945	34347	33362
33140	34421	33234	32766	32152	33954	33700	32183	33692	31118
32405	32756	31765	32377	32000	31361	32983	32213	32922	32714
33060	31953	32947	31569	31470	31128	32732	32211	31778	32049
30917	30937	31477	31251	31765	33622	31425	30784	32372	30962
31545	30342	31419	31471	30368	30870	31876	30474	30286	30047
33277	30565	29379	29384	29851	28311	28745	29741	29406	28240
28193	28415	27345	27450	27256	27370	25457	28185	25956	26900
25133	26593	25453	25012	25668	25977	25860	26365	25349	25494
24916	24927	23960	23513	23555	24262	23827	24170	23476	23329
23235	23724	24351	24492	23725	24370	24697	25242	25112	23252
22563	24540	24114	23350	22696	22410	23535	21849	23922	21754
21465	21410	22174	20941	22928	23074	22607	23635	22933	24510
24711	24676	25122	24959	24399	24741	26290	26252	25823	26297
27460	26901	25366	25753	26372	29672	28566	28462	30601	28831
30146	30547	30765	30796	31123	31061	31935	30665	31403	33179
31876	32239	31100	32371	32681	32517	33126	33263	33419	33104
33610	32506	32254	33599	33505	33403	32492	33645	33996	33170
33960	33502	33930	32627	32925	33434	33806	33330	33332	34673
32543	33924	34092	33501	34104	34045	33704	34511	34007	34740
33456	33506	33465	33509	33860	32119	34722	34467	33904	33350
33366	33496	34346	33316	34366	34494	34217	33516	35194	34260
34064	34097	34572	33159	33990	32978	34251	34039	35392	34679
34127	33472	34557	33767	33335	34345	0	0	0	0
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0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0


```
***   ADD      400000.
***   LSTM           4.            0.
***      435000.        0.00  0.000000  0.000000
***         96.00      33.00     -4900.
***        155.00      33.00     -4900.
***        118.00      21.00     -6500.
***        140.00      23.00     -6500.
***   FIX            10.           10.          2.    1.0E-06
***    2. 3. 4. 5. 8.11.14.
***   AREA  1.00 -1.00  0.00  0.00
***   AREA  0.00  0.00  1.00 -1.00
***   AUTH  0.00  0.00  1.00 -1.00
```

STAGE 1

PROCESS HAS CONVERGED
AFTER 2 ITERATIONS WITH 10 CONSTRAINTS   TEST VALUE = 0.

```
***   FIX             6.           10.          2.    1.0E-06
***    2.11.14.
***   AREA  1.00 -1.00  0.00  0.00
***   AREA  0.00  0.00  1.00 -1.00
***   AUTH  0.00  0.00  1.00 -1.00
```

STAGE 2

PROCESS HAS CONVERGED
AFTER 4 ITERATIONS WITH 6 CONSTRAINTS   TEST VALUE = 0.

```
***   FIX             4.           13.          4.    1.0E-06
***    2.
***   AREA  1.00 -1.00  0.00  0.00
***   AREA  0.00  0.00  1.00 -1.00
***   AUTH  0.00  0.00  1.00 -1.00
```

```
OSV LAP

STAGE 3

 ITERATION  1
CHI SQUARED =  2.0355420218+02    TEST VALUE =  1.000000000E+00     DAMPING FACTOR = 1.0000
PARAMETER  VALUE        CORRECTION        PARAMETER  VALUE        CORRECTION        PARAMETER  VALUE        CORRECTION
    1   134773.419          *33.193          3  0.001261938   *0.000358173          4  0.000004111   0.000000105
    2     0.000000            0.000          6    80.300000    *2.395701           7      6.0051/.    *5.1668E-4
    5   102.6862479         *1.339556          9    45.063943    *1.807083          10      6.0051/.    *5.1668E-4
   11   116.0000000         *0.352174         12    13.247/67    2.747016          13      53444.      24.356E+1
   14   140.0000000         *1.710956         15    13.247/857   2.747016          16      53444.      24.356E+1


 ITERATION  2
CHI SQUARED =  2.0297548081+02    TEST VALUE =  2.000000000E+00     DAMPING FACTOR = 1.0000
PARAMETER  VALUE        CORRECTION        PARAMETER  VALUE        CORRECTION        PARAMETER  VALUE        CORRECTION
    1   134818.819          *36.491          3  0.001603765   *0.000836851          4  0.000004216   0.000000134
    2     0.000000            0.000          6    57.904329    *4.470836           7      5/8430.     *113405.4
    5   101.4531353         *2.956945          9    43.816900    *3.931957          10      5/8830.     *113405.4
    8   146.5808434          2.266853         12    10.3446/3    3.769778          13      77800.      55054.4
   11   117.4478631         *0.108306         15    10.3446/3    3.769778          16      77800.      55054.4

DAMPING FACTOR      CHI SQUARED
     0.0000         2.0297548081E+02
     0.3333         2.0209826421E+02
     1.0000         2.0352777AE+02
     0.4431         2.0197272??E+02


 ITERATION  3
CHI SQUARED =  2.0197272999E+02    TEST VALUE =  0.          DAMPING FACTOR = 0.4431
PARAMETER  VALUE        CORRECTION        PARAMETER  VALUE        CORRECTION        PARAMETER  VALUE        CORRECTION
    1   134375.490          *34.564          3  0.001654133   *0.000571123          4  0.000004276   0.000000186
    2     0.000000            0.000          6    55.701479    *3.243054           7      5/8585.     *6682U.3
    5   100.1412/5         *1.582606          9    42.074909    *3.006079          10      5/8585.     *6682U.3
    8   147.5806605          1.306646         12    17.7148/0    1.149927          13      102192.     30884.4
   11   117.3399845         *0.219693         15    17.7148/0    1.149927          16      102192.     30884.4
   14   134.0092859         *0.27A867


OSV LAP

STAGE 3

PROCESS HAS CONVERGED
AFTER  3 ITERATIONS WITH  8 CONSTRAINTS          TEST VALUE =  0.

SCAN  = 258.03


BASELINE =  4345.0                                STANDARD DEVIATION  103.46

SCAN REVERSES AT CHANNEL   0.000                  STANDARD DEVIATION    0.000

BASELINE SINE-WAVE COMPONENT = 0.027 PER CENT     STANDARD DEVIATION    0.130

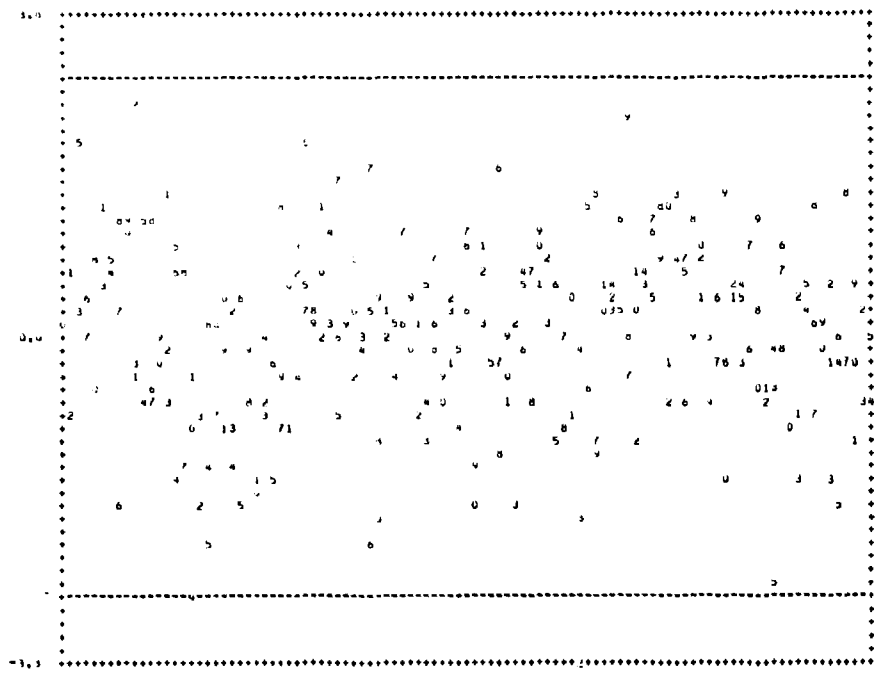
BASELINE DRIFT =   4.36 P.P.M. PER CHANNEL        STANDARD DEVIATION    1.55

LINE      POSITION        S.D.        WIDTH        S.D.        INTENSITY        S.D.          *   REL.INT.    AMPL.
  1        96.440         2.939        34.265        5.009        498980.        107395.       *   40.6 %      3054.
  2       140.164         2.019        40.783        4.587        498980.        107395.       *   40.6 %      7797.
  3       117.313         0.862        18.224        3.762        115778.        51760.        *    9.4 %      4084.
  4       137.970         1.083        18.224        3.762        115778.        51760.        *    9.4 %      4084.

CHI SQUARED =  201.97  WITH 244 DEGREES OF FREEDOM
SO 1 AND 0.1 PER CENT POINTS ARE  201.2-  247.6 AND   316.4 RESPECTIVELY

THE COUNTS FOR THE FOLLOWING CHANNELS DEVIATE SIGNIFICANTLY FROM THE CURVE

(162.+ *3.78)   (
```



PLOT OF RESIDUAL DEVIATION (IN STANDARD DEVIATION UNITS) VS. CHANNEL NUMBER
ALL BUT ONE OR TWO POINTS SHOULD LIE BETWEEN THE HORIZONTAL LINES

VARIANCE-COVARIANCE MATRIX

2.072E+06										
0.	0.									
0.	0.	1.691E+06								
-1.443E+04	0.	-5.787E-10	2.411E-12							
1.385E+02	0.	1.385E-03	6.424E-07	0.000E+00						
5.732E+02	0.	0.482E+04	-2.183E-06	1.051E+01	4.811E+01					
0.000E+00	0.	1.117E+02	-2.817E-02	2.405E+05	5.042E+05	1.153E+10				
-1.727E+02	0.	-1.294E+03	3.433E-07	-3.240E+00	-9.349E+00	-1.697E+05	0.000E+00			
3.444E+02	0.	0.442E-01	-1.682E-04	2.437E+00	2.556E+01	0.197E+05	-0.460E+00	2.104E+01		
0.000E+00	0.	1.117E+02	-2.817E-02	2.405E+05	5.042E+05	1.153E+10	-1.697E+05	0.197E+05	1.153E+10	
-2.557E+01	0.	-1.449E+00	3.121E-07	5.581E-01	-1.379E+00	-0.001E+02	-5.722E+02	-0.034E+01	-0.001E+02	
7.462E+01										
-1.899E+02	0.	-1.723E+03	-2.247E-07	-9.427E+00	-1.119E+01	-3.011E+05	5.787E+00	-7.913E+00	-3.011E+05	
-8.708E+01	1.413E+01									
-3.670E+04	0.	-3.423E+01	3.397E-04	-1.441E+05	-2.102E+05	-4.936E+04	9.753E+04	-1.512E+05	-4.936E+04	
-7.735E+03	1.779E+03	2.687E+04								
4.101E+01	0.	-4.008E+04	-1.787E-07	2.624E-01	2.808E+00	3.636E+04	-2.112E+01	2.852E+00	3.636E+04	
2.995E+02	3.743E+01	-3.243E+03	1.173E+00							
-1.899E+02	0.	-1.723E+01	-2.247E-07	-9.427E+00	-1.119E+01	-3.011E+05	5.787E+00	-7.913E+00	-3.011E+05	
-8.708E+01	1.413E+01	1.779E+03	1.749E+01	1.441E+01						
-1.670E+06	0.	-1.223E+01	3.397E-08	-1.441E+05	-2.102E+05	-4.936E+04	9.753E+04	-1.512E+05	-4.936E+04	
-7.735E+03	1.779E+03	2.687E+04	-3.243E+03	1.779E+03	2.687E+04					

*** PLOT 3* 255. 1.0 63.
*** EXIT

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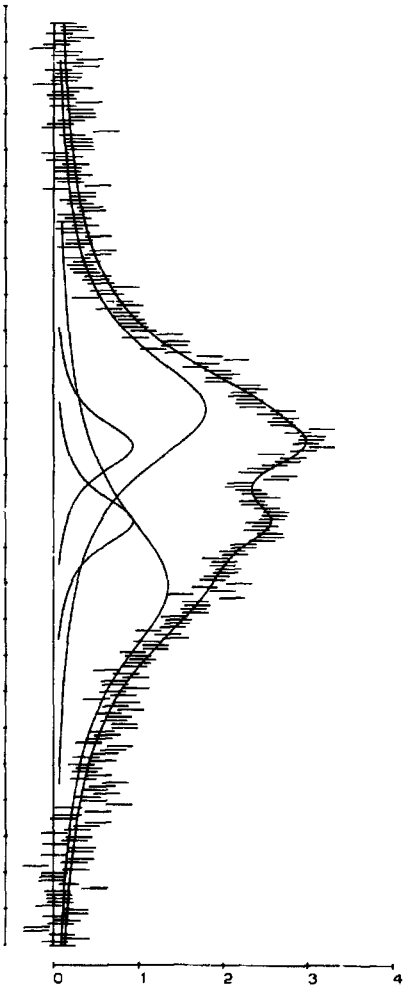

039 LAF