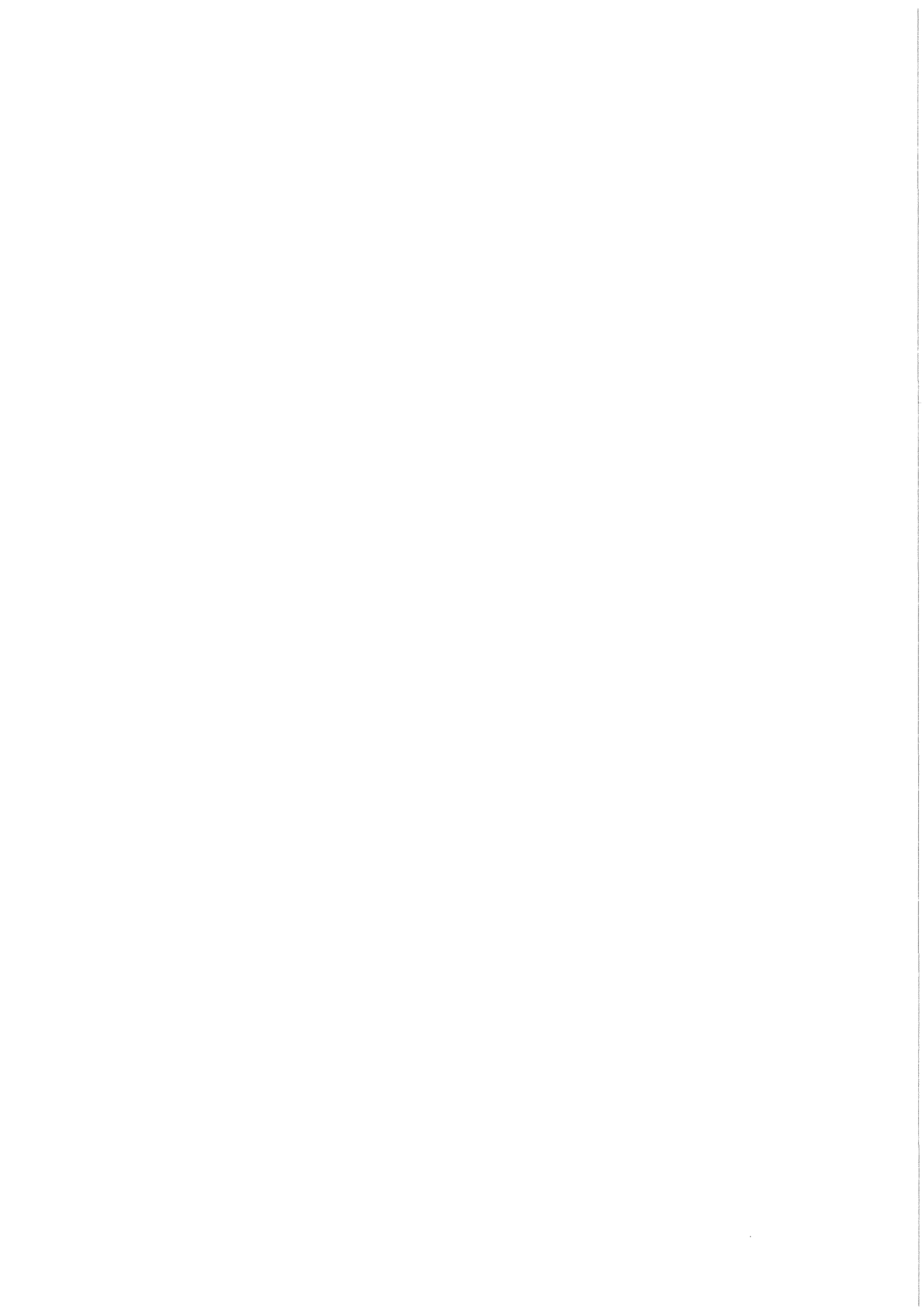


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Computer Code FIT

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Abstract:

This is a description of the computer code FIT, written in FORTRAN-77 for a PDP 11/34. FIT is an interactive program to deduce position, width and intensity of lines of X-ray spectra (max. length of 4K channels). The lines (max. 30 lines per fit) may have Gauss- or Voigt-profile, as well as exponential tails. Spectrum and fit can be displayed on a Tektronix terminal.

Zusammenfassung:

Es wird der Computer Code FIT beschrieben, der in FORTRAN-77 für eine PDP 11/34 geschrieben wurde. FIT ist ein interaktives Programm zur Bestimmung der Position, Breite und Intensität der Linien von X-ray Spektren (max. 4K Kanäle lang). Die zu bestimmenden Linien (max. 30 Linien pro Durchlauf) können Gauss- oder Voigt-Profil haben, sowie exponentielle Füße besitzen. Spektrum und Fit können auf einem Tektronix Terminal angesehen werden.

Contents

1.	INTRODUCTION	1
2.	PROGRAM STRUCTURE	3
2.1	Flow chart	3
2.2	F77-Compiler file (FITF77.COMD)	4
2.3	Task-builder files	4
2.3.1	TKB command-file (FIT.COMD)	4
2.3.2	TKB overlay-description-file (FIT.ODL)	5
3.	DESCRIPTION OF PARAMETERS AND COMMON-BLOCKS (FIT.COM)	5
3.1	PARAMETERS	5
3.2	FILES - Byte arrays	6
3.3	COMMON-blocks	6
4.	SHORT DESCRIPTION OF THE FUNCTIONS AND SUBROUTINES	9
4.1	CALVAL - Calibration of peak-parameters	9
4.2	FIT - Main program	10
4.3	FITBAC - Contribution of background to fit	11
4.4	FITCUR - Peak parameters via crosshair cursor	12
4.5	FITDIS - Display spectrum (and fit)	13
4.6	FITEND - Terminate program	14
4.7	FITENE - Read energy table	15
4.8	FITFIT - Fit the spectrum	16
4.9	FITIJ - Look up the values of the inverse matrix	18
4.10	FITIO - I/O of spectrum and parameter file	19
4.11	FITMEN - Master menu of program FIT	20
4.12	FITOUT - Output of results	21
4.13	FITPAR - Prepare data for fit	22
4.14	FITPEA - Contribution of peaks to fit	23
4.15	FITPFL - Read/write fit-parameter file	24
4.16	FITPRT - Write output to print-output file	25
4.17	FITROU - Route print-output file to spooler	26
4.18	FITSET - Submenu for fit (option -F- of main-menu)	27
4.19	FITSFP - Write output to plotter-output file	29
4.20	FITSPR - Read spectrum file	30
4.21	FITST1 - Peak parameters via menu	31
4.22	FITST2 - Global flag definition	32
4.23	MARKER - Mark the cursor position on screen	33
4.24	PEKDEF - Set default values for peak	34
4.25	SETUP - Set up program parameters	35
5.	GENERAL ASPECTS OF INPUT/OUTPUT FILES USED BY FIT	36
5.1	Spectrum file SPESPC	36
5.2	Fit-parameter file PARSPC	36
5.3	Calibration file CALSPC	36
5.4	Print-output file FILPRT	37
5.5	Energy table file ENESPC	37
5.6	Plotter-output file SAVFIL	37
6.	MATHEMATICS OF THE FIT	38
6.1	Pure Gaussian peak	38
6.2	Gaussian peak with exponential tail(s)	38
6.3	Lorentzian peak folded with Gaussian energy resolution	39

7. FITSPY – A SPY TO THE FITTING PROCEDURE	41
References	41
Appendix A: Example	42
Appendix B: Program listings	44

Figures

1. Fit to the 4→3 region of \bar{p}-atomic ^{17}O.	42
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1. Introduction

FIT is an interactive spectrum fit program. It was – in its present form – built up for a LSI and/or a PDP computer on the basis of EVAL (and later FITOS) during the years 1983/84 by D.Rohmann and Th.Köhler.

The program-language is FORTRAN-77 except for some library-routines written in MACRO. The program is menu driven (MNPACK in RSXLIB [1]). FIT needs a Tektronix 4010 (or compatible) terminal to display spectra and fits.

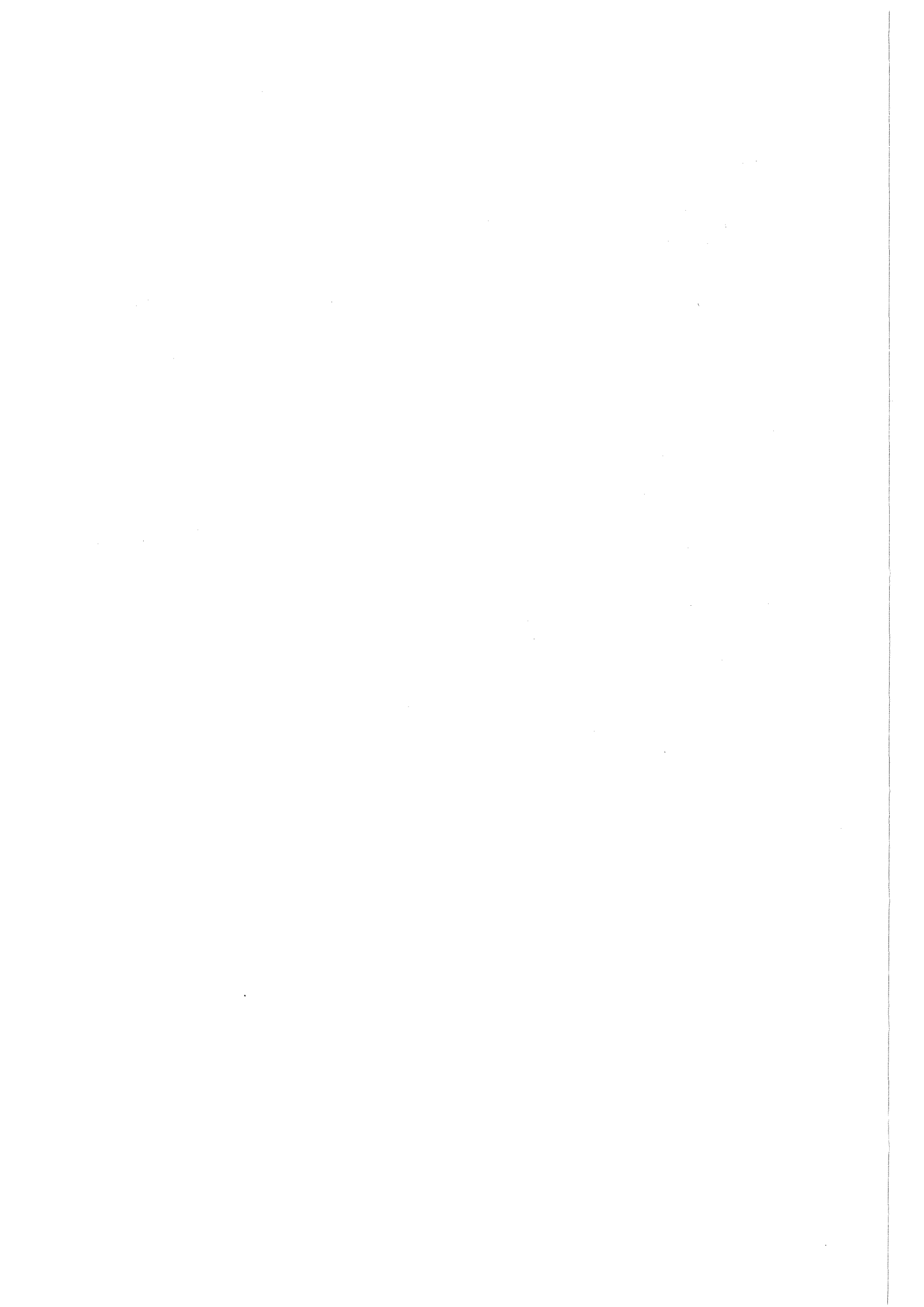
The major part of the program is either handling Input/Output (routines FITIO, FITPFL, FITSPR, FITENE, FITOUT, FITCUR, FITST1, FITST2, FITPRT, FITSFP, FITROU) or controlling the various possibilities of the code (routines FITMEN, FITDIS, FITSET) in a dialogue. The fitting itself is done in the routines FITFIT, FITBAC, and FITPEA. The routines FITPAR and PEKDEF do some preparation for the fit procedure. The main control is handled by the main program FIT. (The routines SETUP and FITEND are subroutines only because of memory space problems. Logically they are part of the main program FIT.) A detailed description of the single program-parts is given in chapter 4.

The high segmentation of the FIT-program (see chapter 2) is not only due to modularity but because of the relatively small address space of 64 kbytes of a LSI/PDP computer with 16 bit addressing.

The FIT-program can handle a maximum of 30 peaks in a time. (This limit is given only by the space restrictions mentioned above.) The peaks can either have pure Gaussian form or be the convolution of a Lorentzian curve with a detector resolution (Gaussian line shape), or a pure Gaussian with an exponential low or high tail. For the mathematical formalism see chapter 6 and for the description of the control of these possibilities see chapter 4.

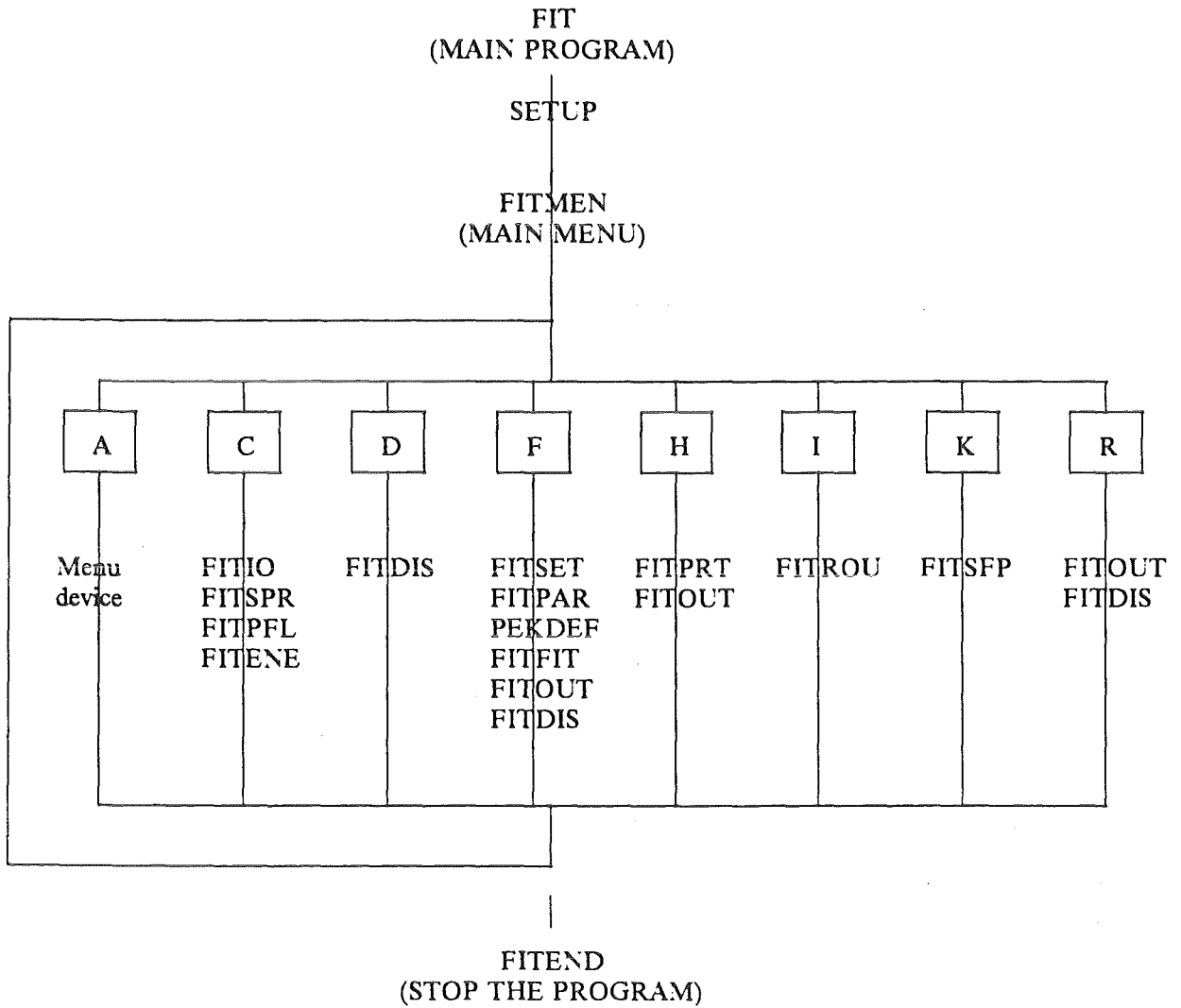
In chapter 5 the different Input/Output files of FIT are described.

Chapter 7 describes other tasks which deal with the FIT. Such as FITSPY, a task which reads in a temporary parameter file written by FITFIT before each iteration, and prints the peak-parameters on the line-printer. This is very useful to have a look to the development of the fit.



2. Program structure

2.1 Flow chart



2.2 F77-Compiler file (FITF77.CMD)

This file is used to compile all modules of FIT.

```
FIT,FIT = FIT
SETUP,SETUP = SETUP
FITMEN,FITMEN = FITMEN
FITIO,FITIO = FITIO
FITDIS,FITDIS = FITDIS
FITROU,FITROU = FITROU
FITBAC,FITBAC = FITBAC
FITPEA,FITPEA = FITPEA
FITSET,FITSET = FITSET
FITCUR,FITCUR = FITCUR
FITST1,FITST1 = FITST1
FITST2,FITST2 = FITST2
FITPAR,FITPAR = FITPAR
PEKDEF,PEKDEF = PEKDEF
FITFIT,FITFIT = FITFIT
FITOUT,FITOUT = FITOUT
FITPRT,FITPRT = FITPRT
FITEND,FITEND = FITEND
FITSFP,FITSFP = FITSFP
```

Some routines of the program not shown here are in the following program libraries:

```
GENLIB.OLB (modules of general interest)
DISLIB.OLB (modules concerning the display)
RSXLIB.OLB (system modules, written at CERN)
```

or they are standard FORTRAN run time modules.

2.3 Task-builder files

The program FIT is so large that it can only be run by segmentating the various program parts. Therefore the task is overlayed. The following describes the two task-builder files needed for this overlay.

2.3.1 TKB command-file (FIT.CMD)

The following TKB command-file is used to build the task FIT :

```
FIT/FP,FIT = FIT/MP
TASK = FIT
ASG = TI:6
//
```

2.3.2 TKB overlay-description-file (FIT.ODL)

The TKB overlay-description-file looks like the following :

```

.PSECT PARFIC
MNPACK: .FCTR LB:[1,1]RSXLIB.OLB/LB:MNPACK:MNEXPK
LIBR: .FCTR GLIB-DLIB-RLIB-FLIB
  GLIB: .FCTR US1:[374,101]GENLIB.OLB/LB
  DLIB: .FCTR US1:[374,101]DISLIB.OLB/LB
  RLIB: .FCTR LB:[1,1]RSXLIB.OLB.LB
  FLIB: .FCTR US1:[1,1]F77DSKIO.OLB/LB
SEG1: .FCTR SETUP-FITMEN-FITEND-FITROU-FITSFP-LIBR
SEG2: .FCTR FITIO-LIBR-*(SEG21,SEG22,SEG23)
  SEG21: .FCTR FITPFL-LIBR
  SEG22: .FCTR FITSPR-LIBR
  SEG23: .FCTR FITENE-LIBR
SEG3: .FCTR FITDIS-FITBAC-FITPEA-LIBR
SEG4: .FCTR FITSET-LIBR-*(SEG41,SEG42,SEG43,SEG44)
  SEG41: .FCTR FITCUR-LIBR
  SEG42: .FCTR FITST1-LIBR
  SEG43: .FCTR FITST2-LIBR
  SEG44: .FCTR FITPAR-FITBAC-PEKDEF-LIBR
SEG5: .FCTR FITFIT-RLIB-FLIB-*(SEG51,SEG52)
  SEG51: .FCTR FITPEA-FITBAC-LIBR
  SEG52: .FCTR GLIB:SPXINV:BEEP:VDZERO-LIBR
SEG6: .FCTR FITOUT-FITPRT-LIBR
      .END

```

3. Description of PARAMETERS and COMMON-blocks (FIT.COM)

In general all REAL-variables are REAL*8 (Double Precision) variables : (IMPLICIT REAL*8 (A-H,O-Z)).

3.1 PARAMETERS

LUNSPE = 1	Logical unit used for spectrum input
LUNCAL = 2	Logical unit used for calibration input or energy table
LUNPRT = 3	Logical unit used for printer
LUNPAR = 4	Logical unit used for parameter file (PARFIL)
LUNTRM = 5	Logical unit used for terminal I/O (incl. DLPACK and MNPACK)
MAXCHN = 4096	Maximum number of channels in spectrum
MAXPK = 30	Maximum number of peaks possible
MAXCO = 6	Maximum number of coefficients for the background polynomial
MAXREG = 7	Maximum number of fit regions
MAXPAR = 40	Maximum dimension of Matrix
NPPARM = 6	Number of peak-parameters
MXCALF = 3	Maximum nr.of coeff. for the calib. polynomial
MPOINT = 500	Number of points for display-buffer
MXLINK = 20	Maximum number of linked peak-parameters

3.2 FILES – Byte arrays

SPESPC(30)	Spectrum file name
PARSPC(30)	Parameter file name
CALSPC(30)	Calibration file name
FILPRT(30)	Print-output file name
ENESPC(30)	Energy table file name
SAVFIL(30)	Plotter-output file name

3.3 COMMON-blocks

/SPECTR/ JCOUNT(MAXCHN)

JCOUNT() [I*4] Spectrum buffer (maximum dimension MAXCHN)

/SPDESC/ NXCHAN, NYCHAN, IDATIM(9), NRUN, ISPILL, ITARG, ITEXT(18), LABEL

NXCHAN	[I*2] Number of X-channels
NYCHAN	[I*2] Number of Y-channels
IDATIM()	[I*2] Date of data saving (FORMAT : dd-mmm-yy_hh:mm:ss)
NRUN	[I*2] Run number
ISPILL	[I*2] Spill number
ITARG	[I*2] Target number
ITEXT()	[I*2] Text (comment)
LABEL	[I*2] Label number (i.e. detector number)

/OPPARS/ MDEV, SPESPC, PARSPC, MXITER, LBFIX, INREG, LIXLO, LIXHI, LIYLO, LIYHI, IYPWR, LIFLO, LIFHI, IPEAK, LBACK, LPEAK, LPEBA, NCOEFF, COEFF(MAXCO), ITERA, NFREE, PEAK(NPPARM,MAXPK), IFLAG(NPPARM,MAXPK), INDEX(NPPARM,MAXPK), ISELEC, IGNOR(MAXPK), NREG, KREGLO(MAXREG), KREGHI(MAXREG), IMODE, INTCOR, NCALF, CALFAC(MXCALF), SIGMA(MAXPK), GAMMA(MAXPK), CALSPC, FILPRT, ENESPC

MDEV	[I*2] Menu device type
SPESPC()	[L*1] Spectrum file name
PARSPC()	[L*1] Parameter file name
MXITER	[I*2] Maximum number of iterations
LBFIX	[I*2] Flag controlling the fitting of the background
INREG	[I*2] Index of fit region
LIXLO	[I*2] Lower X limit for display
LIXHI	[I*2] Higher X limit for display
LIYLO	[I*2] Lower Y limit for display
LIYHI	[I*2] Higher Y limit for display
IYPWR	[I*2] Power of 10 for Y display
LIFLO	[I*2] Lower X limit for fit region
LIFHI	[I*2] Higher X limit for fit region
IPEAK	[I*2] Peak index
LBACK	[I*2] Flag controlling the display of the background
LPEAK	[I*2] Flag controlling the display of the peak
LPEBA	[I*2] Flag controlling the display of the fit
NCOEFF	[I*2] Number of background coeff.

COEFF() [R*8] Background coefficients
 ITERA [I*2] Number of iterations
 NFREE [I*2] Number of degrees of freedom
 PEAK(,) [R*8] Peak parameters
 IFLAG(,) [I*2] Flags for peak-parameters
 INDEX(,) [I*2] Peak indices (flags)
 ISELEC [I*2] Selected spectrum
 IGNOR(,) [I*2] Ignore-flags
 NREG [I*2] Number of fit regions
 KREGLO(,) [I*2] Low end of fit regions
 KREGHI(,) [I*2] High end of fit regions
 IMODE [I*2] Display mode
 INTCOR [I*2] Status of internal start-value correction
 NCALF [I*2] Number of calibration coefficients
 CALFAC(,) [R*8] Calibration coefficients
 SIGMA(,) [R*8] Internal Gaussian widths
 GAMMA(,) [R*8] Internal Lorentzian widths
 CALSPC(,) [L*1] Calibration file name
 FILPRT(,) [L*1] Print-output file name
 ENESPC(,) [L*1] Energy table file name

/OPPART/ IOPARS

IOPARS [I*2] Dummy variable

/RESULT/ CHINEW, CHIOLD, FVBACK, FVPEAK

CHINEW [R*8] χ^2 of fit
 CHIOLD [R*8] χ^2_{old} of previous iteration
 FVBACK [R*8] Contribution of background
 FVPEAK [R*8] Contribution of peaks

/ERRCOM/ IERROR

IERROR [I*2] RSXLIB error codes

/PARAM/ ILINK(NPPARM,MAXPK), NPAR, NDIMM, KUSE, KSKIP, TOLO(6), TOHI(6)

ILINK(,) [I*2] Flags for linked parameters
 NPAR [I*2] Number of fit-parameters
 NDIMM [I*2] Dimension of matrix
 KUSE [I*2] Number of used parameters
 KSKIP [I*2] Number of skipped parameters
 TOLO(6) [R*8] Lower limits for fit
 TOHI(6) [R*8] Higher limits for fit

/ARRAYS/ VMAT(MAXPAR*(MAXPAR + 1)/2), DERIV(MAXPAR), RVEC(MAXPAR), HDERIV(MAXPAR)

VMAT(,) [R*8] Matrix
 DERIV(,) [R*8] Derivatives
 RVEC(,) [R*8] R-Vector
 HDERIV(,) [R*8] Parameter increments

/CONST/ PICON, EPSILN, SQRTPI, SRLN2

PICON	[R*8] Constant π
EPSILN	[R*8] Radius of convergence for $\chi^2 - \chi^2_{\text{old}} := 1$
SQRTPI	[R*8] $\sqrt{\pi}$
SRLN2	[R*8] $\sqrt{\ln(2)}$

/GLOBAL/ IOP, T0, IFIT, FILOPN

IOP	[I*2] Meun control parameter
T0	[R*4] Start-time of fit
IFIT	[I*2] Fit-status control parameter
FILOPN	[L*2] = .TRUE. : Print-output file is open

4. Short description of the functions and subroutines

In this chapter we introduce the FUNCTIONS and SUBROUTINES in alphabetical order. For each program section a more or less brief description of the function and/or the method of solution is given. The calling sequence is shown and the parameters – if any – are explained. The routines and library-programs called are listed and the library indicated. If the module is menu driven, the menu is shown and explained – if necessary –. In order to give a better overview the "Master"-program(s) are mentioned also.

4.1 CALVAL – Calibration of peak-parameters

Purpose : This function returns the calibrated value of a "channel-value" (if there is any calibration). The function CALVAL is part of the FITOUT.FTN file. The calibration is done via the polynomial :

$$E = a_0 + a_1 \times \text{chn} + a_2 \times \text{chn}^2$$

The calibration coefficients are read in via option -K- of the input-menu of FIT (FITIO).

Calling sequence : Result = CALVAL (DCHAN)

where DCHAN is the channel-value

Subroutines and library-programs needed : – – – none – – –

Menu-description : – – – none – – –

Called from :

FITOUT – Output of results

4.2 FIT - Main program

Purpose : This is the main-program for the interactive fit of spectra. Together with SETUP and FITEND the main-program controls the program-flow.

Calling sequence : - - - none - - -

Subroutines and library-programs needed :

DIINI	- Initialize display (DIPACK in DISLIB)
FITDIS	- Display spectrum (and fit)
FITEND	- Terminate program
FITFIT	- Fit the spectrum
FITIO	- I/O of spectrum and parameter file
FITMEN	- Master menu of program FIT
FITOUT	- Output of results
FITPRT	- Write output to print-output file
FITROU	- Route print-output file to spooler
FITSET	- Submenu for fit (option -F- of main-menu)
FITSFP	- Write output to plotter-output file
SETUP	- Set up program parameters

Menu-description : - - - none - - -

Called from : - - - none - - -

4.3 FITBAC – Contribution of background to fit

Purpose : This subroutines calculates at a given channel –X– the contribution of the background and –if fit processing– its derivative. The background is taken as a polynomial:

$$Y = a_0 + a_1 \times \text{chn}^1 + \dots + a_5 \times \text{chn}^5$$

The background coefficients are either set by option -E- of the fit-menu (FITSET) of program FIT or determined automatically by the program itself (FITPAR).

Calling sequence : CALL FITBAC (X,IBACK)

where X is the actual channel
and IBACK < 0 : Only one peak |IBACK| for display and output
= 0 : All peaks for fit processing
> 0 : All peaks for display and output

Subroutines and library-programs needed : - - - none - - -

Menu-description : - - - none - - -

Called from :

FITDIS – Display spectrum (and fit)
FITFIT – Fit the spectrum
PEKDEF – Set default values for peak

4.4 FITCUR – Peak parameters via crosshair cursor

Purpose : This subroutine handles the option -N- of the fit-menu (FITSET) of program FIT. It sets the fit-parameters in cursor mode.

Before displaying data, all peak-parameters and flags are set to zero, all peaks are disabled, and the fit-region(s) are reset. Thus you have to define the low and the high end(s) of the fit-region(s). With X and Y you have the possibility to change the display region. At the end of FITCUR the option -L- (Start value correction) of the fit-menu (FITSET) is set to YES to determine the start-values for the Gauss-FWHM and the height of each peak as well as to set some background start-parameters (FITPAR, and PEKDEF).

Cursor handling characters :

H	Define high end of fit region
L	Define low end of fit region
P	Define peak position
X	Define new X-display
Y	Define new Y-display
blank	Return to calling program

Each character entered ("H", "L", "P") is displayed on the screen to have a control of positions already marked (MARKER).

Calling sequence : CALL FITCUR

Subroutines and library-programs needed :

DIANU	– Set alpha mode (DIPACK in DISLIB)
DIHOME	– Set alpha mode and clear home (DIPACK in DISLIB)
DIPAGE	– Erase screen, set alpha mode, and clear home (DIPACK in DISLIB)
DIPNT	– Set point mode (DIPACK in DISLIB)
DJCURI	– Display the cursor and wait for response (DISLIB)
DL...	– Terminal I/O routines (DLPACK in RSXLIB)
MARKER	– Mark the cursor position on screen
PREPDI	– Prepare display (DISLIB)
SDISPL	– Display spectrum (DISLIB)

Menu-description : – – – none – – –

Called from :

FITSET – Submenu for fit (option -F- of main-menu)

4.5 FITDIS – Display spectrum (and fit)

Purpose : This subroutine handles the option -D- of the main-menu (FITMEN) of program FIT. It shows the menu for display and displays the spectrum and optionally the contribution of the peaks and/or the background. The setting of the limits in X=channel (options -A- and -B-) and Y = countrate (options -D- and -E-) contains an automatic scaling: If the "lower...limit" is greater than the "higher...limit" the program searches for both the smallest/greatest values and takes these as lower/higher limit. The "power of 10" (option -F-) is needed for a Y higher than $2^{15} - 1 = 32767$ (normal Integer*2 limit). Options -H- (Display of background) and -J- (Display of peak and background) are automatically set to YES after fit. Option -I- (Display of peaks separately) gives the display of each individual peak as well as the background in the display region. The display mode can be changed in option -N-. The display is started by option -R-.

Calling sequence : CALL FITDIS

Subroutines and library-programs needed :

DJDRWA – Draw absolute light vector in user space (DJABS in DISLIB)
 DJMOVA – Draw absolute dark vector in user space (DJABS in DISLIB)
 DJWNDW – Define screen window in user coordinates (DISLIB)
 DL.... – Terminal I/O routines (DLPACK in RSXLIB)
 FITBAC – Contribution of background to fit
 FITPEA – Contribution of peaks to fit
 MN.... – Menu routines (MN:PACK in RSXLIB)
 PREPDI – Prepare display (DISLIB)
 PRTHDR – Display header (GENLIB)
 SDISPL – Display spectrum (DISLIB)

Menu-description :

Display spectrum, peaks and background

A Lower X limit
 B Higher X limit
 D Lower Y-limit
 E Higher Y limit
 F Power of 10 for Y – low, Y – high
 H Display of background
 I Display peaks separately
 J Display of peak + background
 N Display mode: 0 = Histo, 1 = Err, 2 = Spec, 3 = Point
 R Redisplay

Called from :

FIT – Main program

4.6 FITEND - Terminate program

Purpose : This subroutine saves the parameters in COMMON-block /OPPARS/ to US1:[250,2]FIT.LAS and stops the FIT program. Since it often happened that the user didn't really want to stop but hit the "1" or "2" (= stop) in the main-menu by chance, a question was introduced to confirm the exit with the default NO:

— > Do you really want to stop ? [NO]

Calling sequence : CALL FITEND

Subroutines and library-programs needed :

DL.... - Terminal I/O routines (DLPACK in RSXLIB)
MN.... - Menu routines (MNPACK in RSXLIB)
PAR... - Disk I/O routines (PARFIL in RSXLIB)

Menu-description : - - - none - - -

Called from :

FIT - Main program

4.7 FITENE – Read energy table

Purpose : This subroutine handles the option -M- of the input-menu (FITIO) of program FIT. In order to help the user with the setting up of fit-parameters you have the possibility to read an energy table (see chapter 5.5.) containing reference energies in keV. These are calculated into channel-numbers by the program. Thus the positions are set according to the internal calibration.

Calling sequence : CALL FITENE

Subroutines and library-programs needed : - - - none - - -

Menu-description : - - - none - - -

Called from :

FITIO – I/O of spectrum and parameter file

4.8 FITFIT – Fit the spectrum

Purpose : This subroutine handles the option -S- of the fit-menu (FITSET) of program FIT. It fits the spectrum by doing the following for each iteration (maximum MXITER) :

- Set widths to formula-parameters, e.g. the FWHM (PEAK(2/6,ipeak)) is set to :
 Gauss : SIGMA = $\sigma_0 = \text{PEAK}(2,\text{ipeak}) / \text{SRLN2}$
 Lorentz : GAMMA = $\Gamma = \text{PEAK}(6,\text{ipeak}) / 2$.
 Save old fit-parameters for this iteration to a temporary file FIT.TMP. This file is used by FITSPY (see chapter 7.) to print the fit-parameters on the line-printer for each iteration (format like in FITOUT).
- Set up arrays for next iteration. CHIOLD holds old CHI. Reset R and V
- Start the loop over fit regions
- Start the loop over the channels
- Reset YFIT, DERIV. Define COUNT = actual countrate
- Calculate contribution of background (FITBAC)
- Calculate contribution of peak(s) (FITPEA)
- Calculate V and R
- End of loop over channels
- End of loop over fit regions
- Calculate parameter increments H
- Update background coefficients
- Update peak-parameters (Special treatment for linked peak height parameters)
- Reset widths to physics values
- Compare old and new χ^2

If $\chi^2_{\text{old}} - \chi^2_{\text{new}}$ is greater than 1 the next iteration is started, if this difference is less than 1, convergence is reached. Then the fit procedure is stopped and terminal "beep" notifies the user of the end of the procedure.

After each iteration (including the 0. = start-values) a message is given to the screen containing the χ^2/NFREE (NFREE is the number of degrees of freedom) and the elapsed (not CPU) time used so far.

If the update of a peak-parameter would exceed its boundaries (FITPAR) the program gives the message:

— > Parm. n of Peak m out

and skips the update. The parameters are: 1=position, 2=Gauss-FWHM, 3=height, 4=low tail, 5=high tail, 6=Lorentz-FWHM. If the parameter is linked to other peaks the increment is globally determined and updated for all peaks with that linking parameter. Is the Gaussian width of a Lorentzian peak linked to the non-Lorentzian Gauss width(s) the update of the Gaussian width will be done in the same way as the non-Lorentzian Gaussian width(s), but not used for the determination. This is done to change the energy resolution of the Lorentzian peak according to the "fitted" resolution in the neighbourhood from iteration to iteration.

The message

— > *** Bad matrix ***

means that the determinant of the inverse matrix is zero. This (error)-message is mainly caused by a Gauss-FWHM less than 1. Other reasons may be a zero background value.

Calling sequence : CALL FITFIT

Subroutines and library-programs needed :

BEEP - Beep on terminal (GENLIB)
DL.... - Terminal I/O routines (DLPACK in RSXLIB)
FITBAC - Contribution of background to fit
FITPEA - Contribution of peaks to fit
PAR... - Disk I/O routines (PARFIL in RSXLIB)
SPXINV - Matrix - inversion (GENLIB)
VDZERO - Reset R*8 array (GENLIB)

Menu-description : - - - none - - -

Called from :

FIT - Main program

4.9 FITIJ - Look up the values of the inverse matrix

Purpose : This function returns the value of element (I,J) of the packed symmetric matrix V. The function FITIJ is part of the FITOUT.FTN file. It calculates the index in the packed matrix and checks for "Out of range".

Calling sequence : Result = FITIJ (VMAT,NDIMM,I,J)

where VMAT is the packed upper symmetric matrix
NDIMM is the dimension of the matrix
and I and J are the indices of the matrix element

Subroutines and library-programs needed : - - - none - - -

Menu-description : - - - none - - -

Called from :

FITOUT - Output of results

4.10 FITIO – I/O of spectrum and parameter file

Purpose : This subroutine handles the option -C- of the main-menu (FITMEN) of program FIT. It displays the menu for Input/Output. The names of both the spectrum and the fit-parameter files have to be declared (options -A- and -B-) before the reading/writing. The label (i.e. detector) of the spectrum is defined by option -G- and the spectrum read in (FITSPR). The saved fit-parameters (option -E-) (FITPFL) are of no other use than to be read in (option -D-) by FIT again, there is no possibility to handle these files in a different way. Option -I- scans through the spectrum file (given by option -A-) and displays the header information for each label on the screen. At the end of option -I- the spectrum buffer contains the spectrum of the last label. The calibration file name (option -K-) is asked for and the calibration read in. It is absolutely necessary to have the correct label number already declared in option -G- since this number is the control for reading the corresponding calibration (see also chapter 5.3). In order to help the user with the setup of new parameter files, the option -M- (FITENE) allows you to read in a energy table (see also chapter 5.3 myene.).

Calling sequence : CALL FITIO

Subroutines and library-programs needed :

DL.... – Terminal I/O routines (DLPACK in RSXLIB)
FITENE – Read energy table
FITPFL – Read/write fit-parameter file
FITSPR – Read spectrum file
MN.... – Menu routines (MNPACK in RSXLIB)

Menu-description :

Get spectrum / save fit-parameters

A Spectrum file []
B Fit parameter file []
D Save fit-parameters (FITPFL)
E Read fit-parameters (FITPFL)
G Get spectrum from disk (FITSPR) []
I Show spectra available in spectrum file
K Enter calibration polynomial []
M Enter energy table (FITENE) []

Called from :

FIT – Main program

4.11 FITMEN – Master menu of program FIT

Purpose : This subroutine displays the master menu and returns the option number to the calling program.

Calling sequence : CALL FITMEN

Subroutines and library-programs needed :

MN.... – Menu routines (MNPACK in RSXLIB)

Menu-description :

FIT 0.0 – – Interactive fit of spectra

A Menu device: 4 = T2, 6 = NB, 9 = D1 []
C Get spectrum / Save fit-parameters (FITIO).
D Display (FITDIS)
F Fit the spectrum (FITSET and co.)
H Write output to print-output file (FITPRT).
I Route print-output file to spooler (FITROU).
K Save spectrum and fit-parameters for plotting (FITSFP).
R Redisplay results (FITOUT).

Called from :

FIT – Main program

4.12 FITOUT – Output of results

Purpose : This subroutine prints the results on either the terminal screen (LUN=5) or the printer-output file (LUN=3). It calculates the errors for the background parameters and uses the calibration (if any) to print the results not only in channels but also in keV (energies) or eV (Gauss and Lorentzian FWHM). The output contains the background, the calibration polynomial, and the peak-parameters.

Calling sequence : CALL FITOUT (LUN)

where LUN is the logical unit number for the printout
= 3 : printer-output file
= 5 : terminal screen

Subroutines and library-programs needed :

CALVAL – Calibration of peak-parameters
DATE – Get actual date from CPU (GENLIB)
DL.... – Terminal I/O routines (DLPACK in RSXLIB)
FITJ – Look up the values of the inverse matrix
MN.... – Menu routines (MNPACK in RSXLIB)
TIME – Get actual time from CPU (GENLIB)

Menu-description : – – – none – – –

Called from :

FIT – Main program
FITPRT – Write output to print-output file

4.13 FITPAR – Prepare data for fit

Purpose : This subroutine handles the option **-L-** of the fit-menu (FITSET) of program FIT. It defines the boundaries for the fitted quantities, prepares data for fit and determines the number of free parameters. The boundaries are :

position	low end < - > high end
Gauss-FWHM	0 < - > high - low end
height	0 < - > 10^9
low tail	0 < - > 1
high tail	0 < - > 1
Lorentz-FWHM	0 < - > high - low end

If option **-L-** of the fit-menu (FITSET) is set to YES, it defines the fit-parameters HEIGHT (= parameter 3) and FWHM-GAUSS (= parameter 2) and it determines some background start coefficients by putting a straight line through the very low end (average of ± 5 channels) and the very high end (average of ± 5 channels) of the fit-region. If the background is a higher order (> 2) function the following coefficients (> 2) are set like :

$$c(i+1) = -c(i) / (\text{high end})^i$$

just to give it some non zero values (no magic behind!!)The option **-L-** is obligatory for previously done option **-N-** (define peaks by crosshair cursor).

Calling sequence : CALL FITPAR

Subroutines and library-programs needed :

DL....	- Terminal I/O routines (DLPACK in RSXLIB)
MN....	- Menu routines (MNPACK in RSXLIB)
PEKDEF	- Set default values for peak
VIZERO	- Reset I*2 array (GENLIB)

Menu-description : - - - none - - -

Called from :

FITSET	- Submenu for fit (option -F- of main-menu)
--------	--

4.14 FITPEA – Contribution of peaks to fit

Purpose : This subroutines calculate at a given channel – X – the contribution of the peaks and (if fit) their derivatives (for the mathematics see chapter 6.) :

1. Lorentzian peak or
2. Gaussian peak and
 - exponential tail to the left (if any) or
 - exponential tail to the right (if any)

Calling sequence : CALL FITPEA (X,IBACK)

where X is the actual channel
and IBACK < 0 : Only one peak |IBACK| for display and output
= 0 : All peaks for fit processing
> 0 : All peaks for display and output

Subroutines and library-programs needed :

CWERF – Complex error function (GENLIB)

Menu-description : – – – none – – –

Called from :

FITDIS – Display spectrum (and fit)
FITFIT – Fit the spectrum

4.15 FITPFL – Read/write fit-parameter file

Purpose : This subroutine handles the options -D- and -E- of the input-menu (FITIO) of program FIT. It reads or writes the actual fit-parameter file whose name has to be declared (FITIO) before action. The saved fit-parameters are of no other use than to be read in by FIT again, there is no possibility to handle these files in a different way. For instance, to be able to print the fit-parameters on the line-printer you must use option -H- of the main-menu (FITMEN, and FITPRT).

Calling sequence : CALL FITPFL

Subroutines and library-programs needed :

PAR... – Disk I/O routines (PARFIL in RSXLIB)

Menu-description : – – – none – – –

Called from :

FITIO – I/O of spectrum and parameter file

4.16 FITPRT – Write output to print-output file

Purpose : This subroutine handles the option -H- of the main-menu (FITMEN) of program FIT. It opens the print-output file (if not already open) and sends the output of the fit results to the print-output file (see FITOUT). It asks you :

— > Do you want a new output file ? [NO]

so that you have the possibility to send your output to different files.

Calling sequence : CALL FITPRT

Subroutines and library-programs needed :

DL... – Terminal I/O routines (DLPACK in RSXLIB)
FITOUT – Output of results
MN... – Menu routines (MNPACK in RSXLIB)

Menu-description : – – – none – – –

Called from :

FIT – Main program

4.17 FITROU – Route print-output file to spooler

Purpose : This subroutine handles the option -I- of the main-menu (FITMEN) of program FIT. It checks wether a print-output file is open or not. If yes, closes it and opens a new one. It routes the old file to the printer.

This option is not yet implemented.

Calling sequence : CALL FITROU

Subroutines and library-programs needed :

DL.... – Terminal I/O routines (DLPACK in RSXLIB)
MN.... – Menu routines (MNPACK in RSXLIB)

Menu-description : – – – none – – –

Called from :

FIT – Main program

4.18 FITSET – Submenu for fit (option -F- of main-menu)

Purpose : This subroutine handles the option -F- of the main-menu (FITMEN) of program FIT. It displays the menu for the parameter definition. The maximum iteration count (option -A-) is 15. If you need more just start the fit a second time having option -L- set to NO if not already. Then the fit-procedure will continue at the conditions of the previous stop. The background is given by a polynomial of the form:

$$Y = a_0 + a_1 \times \text{chn}^1 + \dots + a_5 \times \text{chn}^5$$

The maximum number of background coefficients (option -C-) that makes sense is 4 (allowed is 6). The higher the order of the background polynomial the greater the risk of fitting to nonsense. For a normal X-ray spectrum a background of the order 2 or 3 is absolutely sufficient. The background can be fixed (option -D-) to what ever values you want. The option -E- (to set the coefficients to some definite values) only shows up if you set the background fixed (YES in option -D-). The maximum number of fit regions (option -F-) is 7. For each fit region (option -G-) you have to define the low (option -H-) and the high end (option -I-). Since 30 peaks are allowed it sometimes is useful to have all peaks globally reset (option -K-). All peak-parameters (parameters 1 to 6, see FITPAR) are set to zero and simultaneously disabled (the peaks are all set to "ignor"). The internal start-value correction (option -L-) is automatically set to YES after the use of the cursor (option -N-) and to NO after the parameter setting (option -O-). For detailed informations concerning option -L- please see FITPAR, PEKDEF. Options -N- (FITCUR), -O- (FITST1), and -Q- (FITST2) give you the possibility to define the peaks. With option -S- you really start the fit. The peak-parameters will be prepared for the fit (FITPAR) and shown on the screen to ask for confirmation. If everything is correct the fit is started (FITFIT and co.), otherwise the setting up of parameters is again made available (FITSET and co.).

Calling sequence : CALL FITSET

Subroutines and library-programs needed :

DIPAGE	– Erase screen, set alpha mode, and clear home (DIPACK in DISLIB)
DL....	– Terminal I/O routines (DLPACK in RSXLIB)
FITCUR	– Peak parameters via crosshair cursor
FITPAR	– Prepare data for fit
FITST1	– Peak parameters via menu
FITST2	– Gobal flag definition
MN....	– Menu routines (MNPACK in RSXLIB)
VDZERO	– Reset R*8 array (GENLIB)
VIZERO	– Reset I*2 array (GENLIB)

Menu-description

Set parameters for fit

- A Maximum iteration count
- C No of background coeffs.
- D Fixed background
- (E Set background coeff. only if D is "YES"
- F No of fit regions
- G Define fit region
- H Lower end of fit region
- I Upper end of fit region
- K Reset peak-parameters and disable peaks
- L Do internal start-value correction
- N Define peak by crosshair cursor
- O Define peaks by setting parameters
- Q Define flags globally
- S Start the fit

Called from :

FIT – Main program

4.19 FITSFP – Write output to plotter-output file

Purpose : This subroutine handles the option -K- of the main-menu (FITMEN) of program FIT. It saves spectrum and parameters for plotting on a main frame computer.

Calling sequence : CALL FITSFP

Subroutines and library-programs needed :

DL.... – Terminal I/O routines (DLPACK in RSXLIB)
MN.... – Menu routines (MNPACK in RSXLIB)

Menu-description : – – – none – – –

Called from :

FIT – Main program

4.20 FITSPR – Read spectrum file

Purpose : This subroutine handles the option -G- of the input-menu (FITIO) of program FIT. It reads in the spectrum. The spectrum file name has to be declared (FITIO) before action. The spectrum buffer will be reset (VJZERO), the label of the spectrum wanted is searched for and read in. A control message is given on the screen.

Calling sequence : CALL FITSPR

Subroutines and library-programs needed :

DL.... – Terminal I/O routines (DLPACK in RSXLIB)
MN.... – Menu routines (MNPACK in RSXLIB)
VJZERO – Reset I*4 array (GENLIB)

Menu-description : – – – none – – –

Called from :

FITIO – I/O of spectrum and parameter file

4.21 FITST1 – Peak parameters via menu

Purpose : This subroutine handles the option -O- of the fit-menu (FITSET) of program FIT. It modifies the fit-parameters if necessary. With option -A- you choose the peak whose parameters and/or flags you want to change or define. Options -C- to -H- give you the actual values of the peak-parameters for control and wait for the new values. If you don't want to enter a new value just give a slash (/). The (link-) flags are set and changes by options -K- to -O-. The maximum group identifier possible is 20. Option -R- tells you whether this peak will be at all taken into account during the fit or not. Thus you have the possibility to turn on and off peaks (for the fit and/or the display). After the end of the setting the option -L- of the fit-menu is set to NO (see FITSET, PEKDEF) since a correction of the values is normally not required.

Calling sequence : CALL FITST1

Subroutines and library-programs needed :

MN.... – Menu routines (MNPACK in RSXLIB)

Menu-description :

Changes to peak-parameters

A	Peak Nr.	
C	Set position	
D	Set Gauss-FWHM	
E	Set height	
F	Set low tail	
G	Set high tail	
H	Set Lorentz-FWHM	
J	Position: - 1 = fix, 0 = fit, > 0 = group-id	<input type="checkbox"/>
K	FWHM-Gauss: - 1 = fix, 0 = fit, > 0 = group-id	<input type="checkbox"/>
L	Height: - 1 = fix, 0 = fit, > 0 = group-id	<input type="checkbox"/>
M	Low tail: - 1 = fix, 0 = fit, > 0 = group-id	<input type="checkbox"/>
N	High tail: - 1 = fix, 0 = fit, > 0 = group-id	<input type="checkbox"/>
O	FWHM-Lorentz: - 1 = fix, 0 = fit, > 0 = group-id	<input type="checkbox"/>
R	Ignore this peak (Do not fit)	<input type="checkbox"/>

Called from :

FITSET – Submenu for fit (option -F- of main-menu)

4.22 FITST2 – Global flag definition

Purpose : This subroutine handles the option -Q- of the fit-menu (FITSET) of program FIT. It globally sets the flags for the parameters (if necessary). Sometimes it is very useful for time- and type-conservation to have this possibility. This subroutine asks you for the flag-number you would like to set or change :

1 Position	- 1 = fix, 0 = fit, > 0 = group-id
2 FWHM-Gauss	- 1 = fix, 0 = fit, > 0 = group-id
3 Height	- 1 = fix, 0 = fit, > 0 = group-id
4 Low tail	- 1 = fix, 0 = fit, > 0 = group-id
5 High tail	- 1 = fix, 0 = fit, > 0 = group-id
6 FWHM-Lorentz	- 1 = fix, 0 = fit, > 0 = group-id
8 Ignor-flag	YES / NO

Which flag do you want to set

(0 = No setting wanting)

and then gives you this flag for each peak (which is not to be ignored) in order to change or confirm it. It will ask you for the flag number again after each global setting. If you want to go back to the fit-menu give it the "flag number" 0.

Calling sequence : CALL FITST2

Subroutines and library-programs needed :

DIPAGE – Erase screen, set alpha mode, and clear home (DIPACK in DISLIB)
DL... – Terminal I/O routines (DLPACK in RSXLIB)

Menu-description : - - - none - - -

Called from :

FITSET – Submenu for fit (option -F- of main-menu)

4.23 *MARKER* – Mark the cursor position on screen

Purpose : This subroutine writes the hitted character when using the cursor to the graphic screen. Thus it gives the user a control, where he did set which mark to the spectrum. The subroutine *MARKER* is part of the *FITCUR.FTN* file.

Calling sequence : CALL *MARKER* (IX,IY,CHAR)

where IX and IY are the coordinates on the screen
and CHAR is the character to be written at position (IX,IY)

Subroutines and library-programs needed :

DIANU – Set alpha mode (DIPACK in DISLIB)
DIDRWA – Draw absolute light vector in screen space (DIABS in DISLIB)
DIMOVA – Draw absolute dark vector in screen space (DIABS in DISLIB)
DIVEC – Set vector mode (DIPACK in DISLIB)

Menu-description : - - - none - - -

Called from :

FITCUR – Peak parameters via crosshair cursor

4.24 PEKDEF – Set default values for peak

Purpose : This subroutine sets default values for a selected peak :

- First do some adjustment of the position (parameter 1). Find out in which fit region the peak is situated. The countrate in the two neighbouring channels is compared with the one of the actual position. The position start-value will be set to the channel with the highest countrate of these three channels unless there is again a peak defined within the range of two channels.
- Then set height (parameter 3). The height is set to the countrate of the position (channel) subtracted by the contribution of the background to this channel.
- Now try to estimate a Gauss-FWHM (parameter 2). If the distance to the nearest peak is less than 1.5 channels the position of the two peaks are set to a distances of 1.5 channels. The Gauss-FWHM is set to the channel difference of the locations where the background subtracted countrate is in the order of half the height of this peak. If within this difference there is another peak the Gauss-FWHM is set to half this value. In the case that this difference cannot be determined because the spectrum has no half-height countrate within the range of 15 channels the Gauss-FWHM is set to 15 channels.

The message

— > Merde n

(where n is the peak number) notifies that the determined Gauss-FWHM was negative and now set to 1.5 channels.

Calling sequence : CALL PEKDEF (IPK)

where IPK is the peak number

Subroutines and library-programs needed :

DL.... – Terminal I/O routines (DLPACK in RSXLIB)
FITBAC – Contribution of background to fit

Menu-description : – – – none – – –

Called from :

FITPAR – Prepare data for fit

4.25 *SETUP* – Set up program parameters

Purpose : This subroutine sets up the fit program.

Calling sequence : CALL SETUP

Subroutines and library-programs needed :

DIWNDW – Define absolute display window of screen (DISLIB)
ERRSET – Check for error 29 : "No such file" (F77LIB)
MN... – Menu routines (MNPACK in RSXLIB)
PAR... – Disk I/O routines (PARFIL in RSXLIB)
VJZERO – Reset I*4 array (GENLIB)

Menu-description : – – – none – – –

Called from :

FIT – Main program

5. General aspects of input/output files used by FIT

5.1 Spectrum file SPESPC

Normally a spectrum file (options -A- and -G- of the input-menu (FITIO) and FITSPR) has the extension .BIN or .SUM. (Of course it can have every other extension.) The general form of the spectrum file is :

1. Label = first detector

FORTRAN record 1 contains the header-information (all INTEGER*2):

NXCHAN, NYCHAN, IDATIM, NRUN, ISPILL, ITARG, ITEXT, LABEL

where	NXCHAN	is the length of the spectrum in x (energy)
	NYCHAN	is the length of the spectrum in y (time)
	IDATIM(9)	contains date and time of data - saving
	NRUN	is the run number
	ISPILL	is the spill number
	ITARG	is the target number
	ITEXT(18)	contains the spectrum description
	LABEL	is the label number (= diode number)

FORTRAN record 2 contains the spectrum-buffer (INTEGER*4):

JBUFF(I), I= 1, NXCHAN

where JBUFF(4096) is the spectrum buffer

2. Label same as 1. Label

The highest label number used so far is 8, i.e. one spectrum file contains the spectra of maximum 8 detectors.

5.2 Fit-parameter file PARSPC

The fit-parameter file (options -B-, -D- and -E- of the input-menu (FITIO) and FITPFL) is read (written) via PARFIL (RSXLIB) with the COMMON-blocks : /OPPARS/ and /OPPART/. This means the whole COMMON-block /OPPARS/ is fetched from (dumped on) disk. The COMMON-block /OPPART/ is only necessary because this procedure is done in a subroutine and not in the main program [1].

5.3 Calibration file CALSPC

The calibration file (option -K- of the input-menu (FITIO)) should have the following format : (It is the same as needed for the calibration file for the LINPRE-program).

n, number of channels, 'text', a₀, a₁, a₂

 - 1/

where "n" gives the label number (detector number). "n" = - 1/ means the end of the file. (Don't forget the slash.)

5.4 Print-output file FILPRT

The print-output file (option -H- of the main-menu (FITMEN)) will contain all the informations that are written on the terminal after the fit was done, except for the picture, of course. It will contain also some printer control characters (such as "1" for "top of form").

The program RESULT takes this print-output file as an input file in order to do some modifications to the output-form or to produce a CALIB input file.

5.5 Energy table file ENESPC

The energy table file (option -M- of the input-menu (FITIO) and FITENE) has the following general structure : (It is the same as needed for the energy table file for the LINPRE-program).

'Z', A, 'trans', E_{weight}, E⁻⁺, E⁺⁺, E⁻⁻

where	'Z'	is the two letter code of the element,
	A	is the atomic weight number,
	'trans'	is the atomic transition for exotic atoms or a description for nuclear γ -lines,
	E _{weight}	is the weighted energy for \bar{p} -atoms or the total energy for single lines,
	E ^{ij}	are the fine structure components for \bar{p} -atomic lines or zero for single lines.

The energy table file will contain in most cases more than one of the above described input lines. The program will identify E_{weight} of the first line with the peak nr. 1 if the E^{ij} are zero or the E^{ij} with peaks nr. 1 (E⁻⁺) to 3 (E⁻⁻) if those are none-zero no matter whether peak nr. 1 is ignored or not (etc.). So you have to be very careful in editing your energy tables.

5.6 Plotter-output file SAVFIL

The plotter-output file (option -K- of the main-menu (FITMEN)) saves some general informations concerning the part of the actual spectrum, the background coefficients, the peak-parameters, and a termination record:

LIXLO, LIXHI, LIYLO, LIYHI, IYPWR, LIFLO, LIFHI, IMODE,	(817,416)
MAXREG, NREG, MAXCO, NCOEFF	(1415)
KREGLO, KREGHI	(4(1PE20.13))
COEFF	(12,6(1X,1PE12.6))
J, (PEAK(K,J),K = 1,NPPARM)	MAXPK times
.....	
- 1/	

6. Mathematics of the fit

This chapter gives you a – brief – description of the mathematical formula used for the fit.

6.1 Pure Gaussian peak

The pure Gaussian peak is fitted by the $F(x)$ [2] as:

$$F(x) = H_0 \exp (- [(x - x_0) / \sigma_0]^2)$$

where : H_0 = Height
 x_0 = Position in channels (center of gravity)
 σ_0 = FWHM / ($2 \sqrt{\ln 2}$)

and the intensity of the line is given by :

$$\text{Area} = \sqrt{\pi} \sigma_0 H_0$$

The parameters x_0 (= parameter 1), FWHM (= parameter 2), and H_0 (= parameter 3) are given to the program either via the cursor (see FITCUR and co.) or by hand (see FITSET and co.).

6.2 Gaussian peak with exponential tail(s)

In addition to the pure Gaussian peak (see there) you have the possibility to modify the peak shape(s) by exponential tail(s). This is done by the definition (only possible in the parameter setting mode (FITSET and co.)) of a characteristic value t_0 whose sign determines the direction of the tail:

negative sign = > low energy tail (parameter 4)
 positive sign = > high energy tail (parameter 5)

The value t_0 itself is the quotient of two parameters (a) and (b) which define the strength and form of the "anomaly". (a) gives the half width of the normal Gaussian peak at $1/e$ of the total height, (b) is the half width of the normal Gaussian peak at the height where the exponential tail should start:

$$t_0 = \pm b / a$$

The total peak is then fitted by $G(x)$ [2] as :

$$G(x) = \begin{cases} H_0 \exp ([t_0 - 2 (x-x_0) / \sigma_0] t_0) & \text{in the region of the tail} \\ H_0 \exp (- [(x-x_0) / \sigma_0]^2) & \text{elsewhere} \end{cases}$$

where : H_0 = Height
 x_0 = Position in channels (center of gravity)
 σ_0 = FWHM / ($2 \sqrt{\ln 2}$)
 t_0 = Exponential tail (including the sign)

and the intensity of the line is given by :

$$\text{Area} = \sqrt{\pi} \sigma_0 H_0$$

The parameter t_0 (= parameter 4 or 5) can only be set by hand (see FITSET and co.). For all other parameters (meanings as described in chapter 6.1) both cursor and manual setting is possible.

6.3 Lorentzian peak folded with Gaussian energy resolution

The problem of fitting a Lorentzian line which has been measured with a detector of a non zero resolution (normally Gaussian line shape) was solved in the old FITOS/EVAL program [2] by a Voigt-formula. This means a folding mechanism using Hermite polynomials for the integration. Unfortunately this method is only valid [3] if the ratio Γ/σ_0 is greater than 0.5. If this ratio is smaller the Voigt-formula will lead to oscillations above the original line shape. These oscillations can be avoided using the complex error function as discussed in [3]:

The shape of a line with a natural width is of Lorentzian form :

$$I_0(E) = \frac{\Gamma}{2\pi} \frac{1}{E^2 + \frac{1}{4}\Gamma^2}$$

be approximately of Gaussian form :

$$D(E) = \exp (- [E/\sigma_0]^2) / (\sigma_0 \sqrt{\pi})$$

Thus the signal will be the folding of the two functions :

$$I(E) = \int_{-\infty}^{\infty} I_0(E') D(E-E') dE'$$

$$= \text{Re } w(z) \times [E/\sigma_0 + i \Gamma/2\sigma_0] / (\sigma_0 \sqrt{\pi})$$

Here $w(z)$ is the complex error function :

$$w(z) = \exp (- z^2) \text{erfc} (-iz)$$

$$\text{erfc}(z) = 1 - \text{erf}(z)$$

$$\operatorname{erf}(z) = 2 / \sqrt{\pi} \times \int_0^z \exp(-t^2) dt$$

Since the first derivations of the complex error function are combinations of the same function and its arguments :

$$\operatorname{Re}\left(\frac{dw(z)}{dy}\right) = -2/\sqrt{\pi} + 2 \times x \times \operatorname{Im} w(z) + 2 \times y \times \operatorname{Re} w(z)$$

$$\operatorname{Re}\left(\frac{dw(z)}{dx}\right) = -2 \times x \times \operatorname{Re} w(z) + 2 \times y \times \operatorname{Im} w(z)$$

with $z = x + iy$

a single calculation of the complex error function not only gives the value of the Voigt integral but also gives its derivations with respect to x and y .

The Lorentzian peak is fitted by the $L(x)$ as :

$$L(x) = H_\ell \operatorname{Re} w(z) \sqrt{\pi} \Gamma / \sigma_0$$

where :

$$w(z) = (x - x_0) / \sigma_0 + i \Gamma / \sigma_0$$

$$H_\ell = \text{Height of the Lorentzian line}$$

$$x_0 = \text{Position in channels (center of gravity)}$$

$$\sigma_0 = \text{Gauss-FWHM} / (2 \sqrt{\ln 2})$$

$$\Gamma = \text{Lorentz-FWHM} / 2$$

and the intensity of the line is given by :

$$\text{Area} = \pi \Gamma H_\ell$$

The parameters x_0 (= parameter 1) and Gauss-FWHM (= parameter 2) can be either set by cursor (see FITCUR and co.) or by hand (see FITSET and co.), the Lorentz-FWHM (= parameter 6) only by hand (see FITSET and co.).

The height of the Lorentzian line H_ℓ (= parameter 3) is connected to the "pure Gaussian height H_0 " :

$$H_\ell = \frac{\sigma_0}{\Gamma \sqrt{\pi}} \times H_0$$

It can be set by cursor, but then it has to be corrected by hand.

7. FITSPY – A spy to the fitting procedure

FITSPY is a separate task which can be started by FIT. It has to be installed to get active. It uses the temporary fit-parameter file FIT.TMP written by FITFIT. This file is read in via PARFIL and printed on the line-printer. Thus the user has the possibility to control each iteration.

Note If the fitting time is smaller than the printing time the FITSPY will print only the parameters saved last.

References

- [1] CERN RSXLIB library manual, Version 1.8 of 11 January 1983.
- [2] R. Guigas, Thesis, Kernforschungszentrum Karlsruhe, KfK 3208, (Appendix), 1981
- [3] C.J. Batty, S.D. Hoath, and B.L. Roberts, Nucl. Instrum. Meth.137 (1976) 179.

APPENDIX A**EXAMPLE**

As an example for the output of FIT we present in figure 1 a part of the \bar{p} ^{17}O spectrum containing the shifted and broadened atomic $4 \rightarrow 3$ transition. A print-output file is given on the next page.

09-Aug-84 20:00, Run 122, Spill1134, Target 13, Label 3
30398 = Sum, 1000 = Maximum 03 0-17 sum

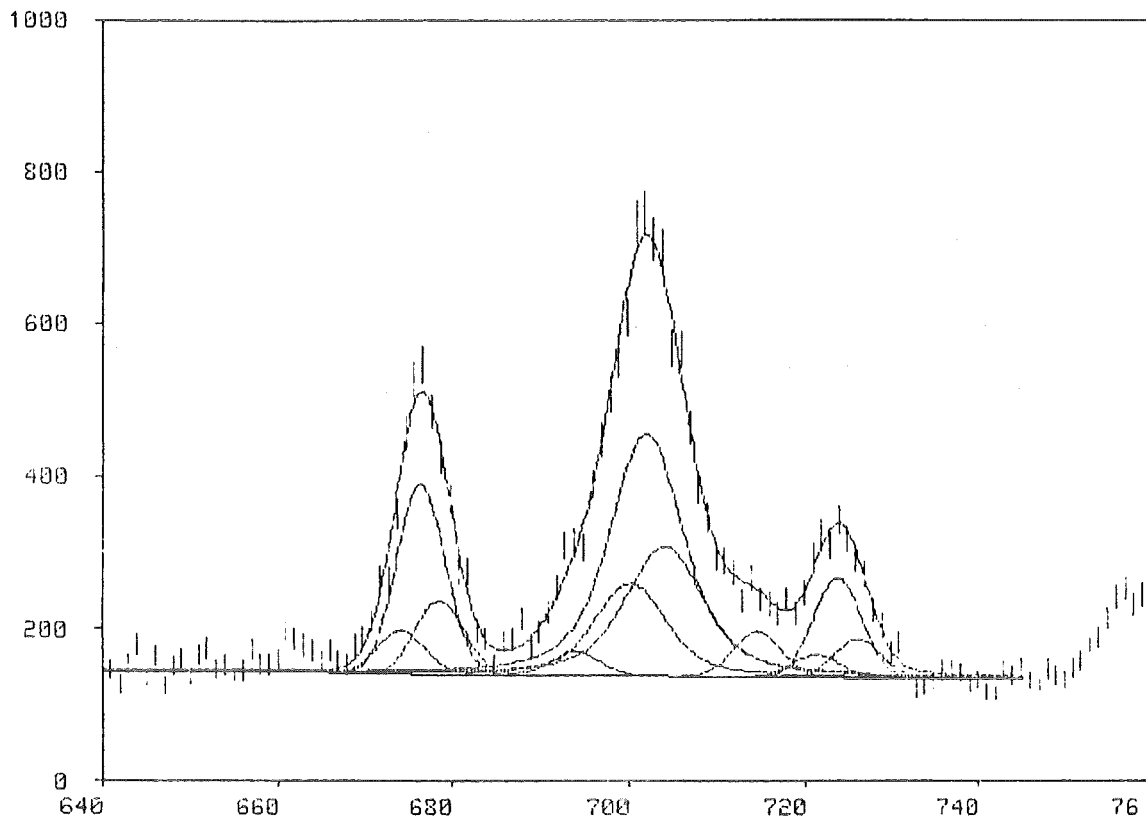


Figure 1: Fit to the $4 \rightarrow 3$ region of \bar{p} -atomic ^{17}O .

Output from 14-AUG-85 22:02:49 DMZ:0312257.017
 08-AUG-84 23:03:41 Run 122, Spill 5, Target 13 Label 3 GE 1 ENERGY
 3. Iteration, CH1=2: 136.0871 NFREE: 119 CH1=2/NFREE: 1.1436

Fit regions used : 620- 745

Background with 2 coefficients:

Coeffs: 3.88319607E+01 -2.54994220E-02
 Errors: 8.91122148E+00 1.33337766E-02

Calibration polynomial:

Coeffs: -2.10750600E-01 1.05227300E-01

Position Gauss-FWHM Height Low-tail High-tail Lorentz-FWHM Intensity

Peak 1 (Flags:-1,-1,4,-2,-2,-2)
 674.113 6.614 0.13 0.000 0.000 0.000 0.92
 0.000 0.000 0.01 0.000 0.000 0.000 0.85
 E: 70.7243(0.0000), G: 696.0(0.0), L: 0.0(0.0)

Peak 2 (Flags:-1,-1,4,-2,-2,-2)
 674.134 6.614 4.57 0.000 0.000 0.000 32.16
 0.000 0.000 0.08 0.000 0.000 0.000 2.14
 E: 70.7265(0.0000), G: 696.0(0.0), L: 0.0(0.0)

Peak 3 (Flags:-1,-1,4,-2,-2,-2)
 674.193 6.614 3.52 0.000 0.000 0.000 24.81
 0.000 0.000 0.23 0.000 0.000 0.000 1.65
 E: 70.7538(0.0000), G: 696.0(0.0), L: 0.0(0.0)

Peak 4 (Flags:-1,-1,4,-2,-2,-2)
 676.478 6.614 0.58 0.000 0.000 0.000 4.07
 0.000 0.000 0.04 0.000 0.000 0.000 0.27
 E: 70.9732(0.0000), G: 696.0(0.0), L: 0.0(0.0)

Position Gauss-FWHM Height Low-tail High-tail Lorentz-FWHM Intensity

Peak 5 (Flags:-1,-1,4,-2,-2,-2)
 676.489 6.614 20.25 0.000 0.000 0.000 142.44
 0.000 0.000 1.35 0.000 0.000 0.000 5.48
 E: 70.9744(0.0000), G: 696.0(0.0), L: 0.0(0.0)

Peak 6 (Flags:-1,-1,4,-2,-2,-2)
 676.750 6.614 15.61 0.000 0.000 0.000 109.83
 0.000 0.000 1.04 0.000 0.000 0.000 7.32
 E: 71.0019(0.0000), G: 696.0(0.0), L: 0.0(0.0)

Peak 7 (Flags:-1,-1,4,-2,-2,-2)
 678.576 6.614 7.83 0.000 0.000 0.000 1.58
 0.000 0.000 0.01 0.000 0.000 0.000 0.12
 E: 71.1939(0.0000), G: 696.0(0.0), L: 0.0(0.0)

Peak 8 (Flags:-1,-1,4,-2,-2,-2)
 678.597 6.614 7.83 0.000 0.000 0.000 55.14
 0.000 0.000 0.57 0.000 0.000 0.000 3.67
 E: 71.1962(0.0000), G: 696.0(0.0), L: 0.0(0.0)

Peak 9 (Flags:-1,-1,4,-2,-2,-2)
 678.859 6.614 6.04 0.000 0.000 0.000 42.53
 0.000 0.000 0.49 0.000 0.000 0.000 2.83
 E: 71.2238(0.0000), G: 696.0(0.0), L: 0.0(0.0)

Peak 10 (Flags:-1,-1,4,-2,-2,-2)
 693.876 6.614 4.57 0.000 0.000 0.000 32.16
 0.000 0.000 0.10 0.000 0.000 0.000 2.14
 E: 72.8040(0.0000), G: 696.0(0.0), L: 0.0(0.0)

Peak 11 (Flags:-1,-1,4,-2,-2,-1)
 699.418 6.614 0.84 0.000 0.000 4.752 6.20
 0.000 0.000 0.05 0.000 0.000 0.000 0.42
 E: 73.3871(0.0000), G: 696.0(0.0), L: 500.0(0.0)

Peak 12 (Flags:-1,-1,4,-2,-2,-1)
 699.699 6.614 16.82 0.000 0.000 4.752 125.52
 0.000 0.000 1.12 0.000 0.000 0.000 8.36
 E: 73.4167(0.0000), G: 696.0(0.0), L: 500.0(0.0)

Peak 13 (Flags:-1,-1,4,-2,-2,-1)
 700.751 6.614 11.77 0.000 0.000 4.752 87.86
 0.000 0.000 0.78 0.000 0.000 0.000 5.85
 E: 73.5274(0.0000), G: 696.0(0.0), L: 500.0(0.0)

Position Gauss-FWHM Height Low-tail High-tail Lorentz-FWHM Intensity

Peak 14 (Flags:-1,-1,7,-2,-2,-1)
 701.211 6.614 2.35 0.000 0.000 4.752 21.21
 0.348 0.000 0.49 0.000 0.000 1.254 5.24
 E: 73.5758(0.0366), G: 696.0(0.0), L: 500.0(111.9)

Peak 15 (Flags:-1,-1,7,-2,-2,-1)
 701.494 6.614 57.25 0.000 0.000 4.752 425.84
 0.348 0.000 3.84 0.000 0.000 1.254 119.45
 E: 73.6055(0.0366), G: 696.0(0.0), L: 500.0(111.9)

Peak 16 (Flags:-1,-1,7,-2,-2,-1)
 702.553 6.614 33.93 0.000 0.000 4.752 298.06
 0.248 0.000 5.89 0.000 0.000 1.254 83.33
 E: 73.7170(0.0366), G: 696.0(0.0), L: 500.0(111.9)

Peak 17 (Flags:-1,-1,4,-2,-2,-1)
 703.295 6.614 1.23 0.000 0.000 6.177 10.81
 0.000 0.000 0.27 0.000 0.000 2.222 0.67
 E: 73.7951(0.0000), G: 696.0(0.0), L: 650.0(2.0)

Peak 18 (Flags:-1,-1,4,-2,-2,-1)
 703.273 6.614 12.84 0.000 0.000 6.177 200.24
 0.000 0.000 1.27 0.000 0.000 2.222 15.33
 E: 73.6249(0.0000), G: 696.0(0.0), L: 650.0(0.0)

Peak 19 (Flags:-1,-1,4,-2,-2,-1)
 704.643 6.614 14.45 0.000 0.000 6.177 140.17
 0.000 0.000 0.95 0.000 0.000 2.222 9.23
 E: 73.3370(0.0000), G: 696.0(0.0), L: 650.0(0.0)

Peak 20 (Flags:-1,-1,4,-2,-2,-2)
 714.451 6.614 3.62 0.000 0.000 0.000 60.69
 0.000 0.000 0.57 0.000 0.000 0.000 4.04
 E: 74.2690(0.0000), G: 696.0(0.0), L: 0.0(0.0)

Peak 21 (Flags:-1,-1,8,-2,-2,-2)
 721.055 6.614 2.28 0.000 0.000 0.000 0.50
 0.000 0.000 0.21 0.000 0.000 0.000 0.06
 E: 75.6640(0.0000), G: 696.0(0.0), L: 0.0(0.0)

Peak 22 (Flags:-1,-1,5,-2,-2,-2)
 721.070 6.614 2.28 0.000 0.000 0.000 20.33
 0.000 0.000 0.29 0.000 0.000 0.000 2.01
 E: 75.6655(0.0000), G: 696.0(0.0), L: 0.0(0.0)

Position Gauss-FWHM Height Low-tail High-tail Lorentz-FWHM Intensity

Peak 23 (Flags:-1,-1,8,-2,-2,-2)
 721.235 6.614 2.23 0.000 0.000 0.000 15.60
 0.000 0.000 0.22 0.000 0.000 0.000 1.35
 E: 75.6305(0.0000), G: 696.0(0.0), L: 0.0(0.0)

Peak 24 (Flags:-1,-1,8,-2,-2,-2)
 723.375 6.614 2.37 0.000 0.000 0.000 2.97
 0.000 0.000 0.24 0.000 0.000 0.000 0.25
 E: 75.3291(0.0000), G: 696.0(0.0), L: 0.0(0.0)

Peak 25 (Flags:-1,-1,8,-2,-2,-2)
 723.552 6.614 1.78 0.000 0.000 0.000 90.07
 0.000 0.000 1.02 0.000 0.000 0.000 8.13
 E: 75.3307(0.0000), G: 696.0(0.0), L: 0.0(0.0)

Peak 26 (Flags:-1,-1,5,-2,-2,-2)
 723.852 6.614 5.95 0.000 0.000 0.000 69.44
 0.000 0.000 2.97 0.000 0.000 0.000 5.25
 E: 75.3588(0.0000), G: 696.0(0.0), L: 0.0(0.0)

Peak 27 (Flags:-1,-1,5,-2,-2,-2)
 725.322 6.614 2.14 0.000 0.000 0.000 1.22
 0.000 0.000 0.21 0.000 0.000 0.000 2.04
 E: 75.1664(0.0000), G: 696.0(0.0), L: 0.0(0.0)

Peak 28 (Flags:-1,-1,5,-2,-2,-2)
 725.345 6.614 4.95 0.000 0.000 0.000 34.35
 0.000 0.000 2.43 0.000 0.000 0.000 2.44
 E: 75.1679(0.0000), G: 696.0(0.0), L: 0.0(0.0)

Peak 29 (Flags:-1,-1,5,-2,-2,-2)
 726.114 6.614 3.82 0.000 0.000 0.000 25.58
 0.000 0.000 0.38 0.000 0.000 0.000 2.96
 E: 75.1362(0.0000), G: 696.0(0.0), L: 0.0(0.0)

APPENDIX B
PROGRAM LISTINGS

The following pages give a listing of the FIT program with all its subroutines and functions, of the group-written library routines (GENLIB and DISLIB), and of the FITSPY program.

```

0001 PROGRAM FIT
      *****
      C#
      C# Interactive fit of spectra
      C#
0002 INCLUDE 'FIT.COM'
0003 IMPLICIT REAL*8 (A-H,O-Z)
      C#
      C# Logical unit numbers used:
      C#
      C# LUNSPC: Lun to read spectrum
      C# LUNPAR: Lun for PARFIL
      C# LUNPRT: Lun for print output
      C# LUNCAL: Lun for calibration input, and energy table
      C# LUNTRM: Lun for terminal I/O (Incl. DLPACK, MNPACK)
0004 PARAMETER LUNSPC=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
0005 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
      C# NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
0006 BYTE SPESPC(30),PARSPC(30),CALSPC(30),FILPRT(30),ENESPC(30)
0007 CHARACTER*20 HDGLIN
0008 INTEGER*4 JCOUNT
0009 REAL*4 T0,SECONDS
      C#
0010 COMMON /SPECTR/ JCOUNT(MAXCHN)
0011 COMMON /SPDESC/ NXCHAN,NYCHAN,IDATIM(9),NRUN,ISPILL,ITARG,
      C# ITEXT(18),LABEL
0012 COMMON /OPPARS/ MDEV,SPESPC,PARSPC,MXITER,LBFX,INREG,LIXLO,LIXHI,
      C# LIYLO,LIVHI,IYPWR,LIFLO,LIFHI,IPEAK,LBACK,LPEAK,
      C# LPEBA,NCOEFF,COEFF(MAXCO),ITERA,NFREE,
      C# PEAK(NPPARM,MAXPK),IFLAG(NPPARM,MAXPK),
      C# INDEX(NPPARM,MAXPK),ISELEC,IGNOR(MAXPK),NREG,
      C# KREGLO(MAXREG),KREGHI(MAXREG),IMODE,INTCOR,NCALF,
      C# CALFAC(MXCALF),SIGMA(MAXPK),GAMMA(MAXPK),CALSPC,
      C# FILPRT,ENESPC
0013 COMMON /OPPART/ IOPARS
0014 COMMON /RESULT/ CHINEW,CHIOLD,FVBACK,FVPEAK
0015 COMMON /ERRCOM/ IERROR
0016 COMMON /PARAM/ ILINK(NPPARM,MXLINK),NPAR,NDIMM,KUSE,KSKIP,
      C# TOL0(6),TOL1(6)
0017 COMMON /ARRAYS/ VMAX(MAXPAR*(MAXPAR+1)/2),DERIV(MAXPAR),
      C# RVEC(MAXPAR),HDERIV(MAXPAR)
0018 COMMON /CONST/ PICON,EPSILN,SQRTPI,SRLN2
      C#
0019 LOGICAL FILOPN
0020 COMMON /GLOBAL/ IOP,T0,IFIT,FILOPN
      C#
0021 DATA IOPARS /0/
    
```

```

      C#
      C# Opt D(4) : Display spectrum and fit data
0030 1015 CALL FITDIS
0031 IF (IFIT .EQ. 0)
0032 GOTO 1000
      C#
      C# Opt F(6) : Fit
0033 1020 CALL FITSET
0034 IF (IFIT .EQ. 0) GOTO 1000
0035 IF (IERROR .LT. 0) GOTO 1000
0036 CALL FITFIT
0037 GOTO 1040
      C#
      C# Opt H(8) : Output results to print file
0038 1025 CALL FITPRT
0039 GOTO 1000
      C#
      C# Opt I(9) : Route print file to printer
0040 1030 CALL FITROU
0041 GOTO 1000
      C#
      C# Opt K(11) : Save spectrum and fit parameters for plotting
    
```

```

0042 1035 CALL FITSFP
0043 GOTO 1000
      C#
      C# Opt R(18) : (Re)display results
0044 1040 CALL FITOUT (5)
0045 IF (IFIT .EQ. 1) GOTO 1015
0046 GOTO 1000
      C#
      C# Terminate program
0047 9000 CALL FITEND
0048 IF (IOP .NE. 1) GOTO 1000
0049 STOP
0050 ***
      END
    
```

```

      C#
      C# SQRTPI = sqrt(pi)
      C# SRLN2 = 2. * sqrt(ln2)
0022 DATA EPSILN /30*0./, ENESPC /30*0./, PARSPC /30*0./,
      C# EPSILN /1.00/, PICON /3.14159265400/,
      C# SQRTPI /1.77245385100/, SRLN2 /1.6651092200/,
      C# FILOPN /FALSE./
      C#
      C# Set up program
0023 CALL DIINI (600)
0024 CALL SETUP
      C#
      C# Display master menu and get option
0025 1000 CALL FITMEN
0026 IF (IOP) 9000,1000,1005
      C#
      C# The big option switch
0027 1005 GOTO (1000, 1000, 1010, 1015, 1000, 1020, 1000, 1025,
      C# 1030, 1000, 1035, 1000, 1000, 1000, 1000, 1000,
      C# 1000, 1040), IOP
      C#
      C# Opt C(3) : Store/Restore spectrum
0028 1010 CALL FITIO
0029 GOTO 1000
    
```

```

0001 SUBROUTINE FITBAC (X,IBACK)
      *****
      C*
      C* This subroutine calculates at a given -X- the contribution
      C* of the background
      C*
      C* Ver. 1.0 12-OCT-83 (DR)  !!Original version!!
      C*
0002 INCLUDE 'FIT.COM'
0003 IMPLICIT REAL*8 (A-H,O-Z)
      C*
      C* Logical unit numbers used:
      C*
      C* LUNSPE: Lun to read spectrum
      C* LUNPAR: Lun for PARFIL
      C* LUNPRT: Lun for print output
      C* LUNCAL: Lun for calibration input, and energy table
      C* LUNTRM: Lun for terminal I/O (incl. DLPACK, MNPACK)
0004 PARAMETER LUNSPE=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
      C*
0005 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
      C* NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
      C*
0006 BYTE SPESPC(30),PARSPC(30),CALSPC(30),FILPRT(30),ENESPC(30)
0007 CHARACTER*20 HDGLIN
      C*
0008 INTEGER*4 JCOUNT
      C*
0009 REAL*4 TD,SECNDS
      C*
0010 COMMON /SPECTR/ JCOUNT(MAXCHN)
0011 COMMON /SPDESC/ NXCHAN,NYCHAN, IDATIM(9),NRUN,ISPILL,ITARG,
      C* ITEXT(18),LABEL
0012 COMMON /OPPARS/ MDEV,SPESPC,PARSPC,MXITER,LBFX,INREG,LIXLO,LIXHI,
      C* LIYLO,LIYHI,IYPWR,LIFLO,LIFHI,IPEAK,LBACK,LPEAK,
      C* LPEBA,NCOEFF,COEFF(MAXCO),ITERA,NFREE,
      C* INDEX(NPPARM,MAXPK),ISELEC,IGNOR(MAXPK),NREG,
      C* KREGLO(MAXREG),KREGHI(MAXREG),IMODE,INTCOR,NCALF,
      C* CALFAC(MXCALF),SIGMA(MAXPK),GAMMA(MAXPK),CALSPC,
      C* FILPRT,ENESPC
0013 COMMON /OPPART/ IOPARS
0014 COMMON /RESULT/ CHINEW,CHIOLD,FVBACK,FVPEAK
0015 COMMON /ERRCOM/ IERROR
0016 COMMON /PARAM/ ILINK(NPPARM,MXLINK),NPAR,NDIMM,KUSE,KSKIP,
      C* TOL(6),TOHI(6)
0017 COMMON /ARRAYS/ VMAT(MAXPAR*(MAXPAR+1)/2),DERIV(MAXPAR),
      C* RVEC(MAXPAR),HDERIV(MAXPAR)
0018 COMMON /CONST/ PICON,EPSILN,SQRTPI,SRLN2
      C*
0019 LOGICAL FILOPN
0020 COMMON /GLOBAL/ IOP,TD,IFIT,FILOPN
    
```

```

0021 DATA IOPARS /0/
      C*
      C* Prepare values
      C*
0022 FVBACK = 0.000
      C*
      C* Calculate contribution of background
      C*
0023 XT = 1.000
0024 DO 1000 J=1,NCOEFF,1
0025 FVBACK = FVBACK + (COEFF(J) * XT)
0026 IF (COEFF(J).NE.0.00) THEN
0027 IF ((LBFX+IBACK).EQ.0) DERIV(J) = XT
0028 ENDIF
0029 XT = XT*X
0030 CONTINUE
      C*
      C* Return to calling program
      C*
0031 9000 RETURN
      C* *****
0032 END
    
```

```

0001 SUBROUTINE FITCUR
      *****
      C*
      C* This subroutine sets the fit parameters in cursor mode
      C*
0002 INCLUDE 'FIT.COM'
0003 IMPLICIT REAL*8 (A-H,O-Z)
      C*
      C* Logical unit numbers used:
      C*
      C* LUNSPE: Lun to read spectrum
      C* LUNPAR: Lun for PARFIL
      C* LUNPRT: Lun for print output
      C* LUNCAL: Lun for calibration input, and energy table
      C* LUNTRM: Lun for terminal I/O (incl. DLPACK, MNPACK)
0004 PARAMETER LUNSPE=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
0005 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
      C* NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
      C*
0006 BYTE SPESPC(30),PARSPC(30),CALSPC(30),FILPRT(30),ENESPC(30)
0007 CHARACTER*20 HDGLIN
      C*
0008 INTEGER*4 JCOUNT
0009 REAL*4 TD,SECNDS
      C*
0010 COMMON /SPECTR/ JCOUNT(MAXCHN)
0011 COMMON /SPDESC/ NXCHAN,NYCHAN, IDATIM(9),NRUN,ISPILL,ITARG,
      C* ITEXT(18),LABEL
0012 COMMON /OPPARS/ MDEV,SPESPC,PARSPC,MXITER,LBFX,INREG,LIXLO,LIXHI,
      C* LIYLO,LIYHI,IYPWR,LIFLO,LIFHI,IPEAK,LBACK,LPEAK,
      C* LPEBA,NCOEFF,COEFF(MAXCO),ITERA,NFREE,
      C* INDEX(NPPARM,MAXPK),ISELEC,IGNOR(MAXPK),NREG,
      C* KREGLO(MAXREG),KREGHI(MAXREG),IMODE,INTCOR,NCALF,
      C* CALFAC(MXCALF),SIGMA(MAXPK),GAMMA(MAXPK),CALSPC,
      C* FILPRT,ENESPC
0013 COMMON /OPPART/ IOPARS
0014 COMMON /RESULT/ CHINEW,CHIOLD,FVBACK,FVPEAK
0015 COMMON /ERRCOM/ IERROR
0016 COMMON /PARAM/ ILINK(NPPARM,MXLINK),NPAR,NDIMM,KUSE,KSKIP,
      C* TOL(6),TOHI(6)
0017 COMMON /ARRAYS/ VMAT(MAXPAR*(MAXPAR+1)/2),DERIV(MAXPAR),
      C* RVEC(MAXPAR),HDERIV(MAXPAR)
0018 COMMON /CONST/ PICON,EPSILN,SQRTPI,SRLN2
      C*
0019 LOGICAL FILOPN
0020 COMMON /GLOBAL/ IOP,TD,IFIT,FILOPN
0021 DATA IOPARS /0/
      C*
0022 BYTE JCHAR,XCHAR,YCHAR,LCHAR,HCHAR,PCHAR,BLANK
    
```

```

0023 NLAL*4 YL,YH
0024 INTEGER*4 JMIN,JMAX,JSUM,JY
0025 DATA LCHAR /'L'//, HCHAR /'H'//, PCHAR /'P'//, XCHAR /'X'//,
      C* YCHAR /'Y'//, BLANK /' '//, ICHAR /' '//
0026 EQUIVALENCE (ICHAR,JCHAR)
      C*
0027 IREGL = 0
0028 IREGH = 0
0029 IPEAK = 0
0030 IDISX = 0
0031 IDISY = 0
      C*
      C* If no spectrum present, Go home
      C*
0032 IF (NXCHAN.LE.0) THEN
0033 CALL DIPAGE
0034 CALL DLOUT ('No data to display')
0035 CALL DLKEY
0036 GOTO 9000
0037 ENDIF
    
```

```

Cs
Cs Redisplay spectrum
0038 1000 CALL PREPDI (JCOUNT,LIXLO,LIXHI,LIYLO,LIYHI,IYPWR,JMIN,JMAX,JSUM)
0039 IF (JSUM .LE. 0) THEN
0040 CALL DIPAGE
0041 CALL DLOUT ('0No counts in spectrum')
0042 CALL DLKEY
0043 GOTO 9000
0044 ENDIF
0045 CALL SDISPL (JCOUNT,LIXLO,LIXHI,JMIN,JMAX,IMODE)
0046 CALL DIMOHE
0047 CALL DIANU
0048 WRITE (5,1005)
0049 1005 FORMAT ('+.. Hit P to define peak position',10X,
+ .. blank to finish input',
+ .. X new X-display ',10X,
+ .. Y new Y-display',
+ .. L fit regions (low end) ',10X,
+ .. H (high end)')
Cs
0050 1010 JCHAR = BLANK
0051 CALL DIPNT
0052 CALL DJCUR1 (ICHAR,IX,JY)
0053 IF (JCHAR .EQ. BLANK) GOTO 4000
Cs
Cs Get absolute x and y value for MARKER
0054 KX = 105 + IFIX (FLOAT (IX-LIXLO) / FLOAT (LIXHI-LIXLO) * 918.)
0055 KY = 650

```

PDP-11 FORTRAN-77 VS. 0-0 09:38:51 26-Sep-86 Page 3
FITCUR.FTN,1 /F77/OP/TR:BLOCKS/WR

```

Cs
Cs Hit M : Define high end of fit region
0056 IF (JCHAR .EQ. HCHAR) THEN
0057 IREGH = IREGH + 1
0058 IF (IREGH .NE. IREGL) GOTO 3000
0059 KREGHI(IREGH) = IX
0060 CALL MARKER (KX,KY,HCHAR)
0061 GOTO 1010
0062 ENDIF
Cs
Cs Hit L : Define low end of fit region
0063 IF (JCHAR .EQ. LCHAR) THEN
0064 IREGL = IREGL + 1
0065 IF (IREGL .GT. MAXREG) GOTO 3005
0066 KREGL(IREGL) = IX
0067 CALL MARKER (KX,KY,LCHAR)
0068 GOTO 1010
0069 ENDIF
Cs
Cs Hit P : Define peak positions
0070 IF (JCHAR .EQ. PCHAR) THEN
0071 IPEAK = IPEAK + 1
0072 IF (IPEAK .GT. MAXPK) GOTO 3010
0073 PEAK(1,IPEAK) = DBLC(IX)
0074 PEAK(3,IPEAK) = JCOUNT(INT(PEAK(1,IPEAK)))
0075 IGNOR(IPEAK) = 0
0076 CALL MARKER (KX,KY,PCHAR)
0077 GOTO 1010
0078 ENDIF
Cs
Cs Hit X : Define new X-display
0079 IF (JCHAR .EQ. XCHAR) THEN
0080 IDISX = IDISX + 1
0081 IF (IDISX .EQ. 1) THEN
0082 IF (IX .LT. LIXLO) THEN
0083 LIXLO = 1
0084 ELSE
0085 LIXLO = IX
0086 ENDIF
0087 GOTO 1010
0088 ENDIF
0089 IF (IDISX .EQ. 2) THEN
0090 IF (IX .LT. LIXHI) THEN
0091 LIXHI = IX
0092 LIYHI = LIYLO - 10
0093 ELSE
0094 LIXHI = NXCHAN
0095 ENDIF
0096 IDISX = 0
0097 GOTO 1000
0098 ENDIF

```

PDP-11 FORTRAN-77 VS. 0-0 09:38:51 26-Sep-86 Page 4
FITCUR.FTN,1 /F77/OP/TR:BLOCKS/WR

```

0099 ENDIF
Cs
Cs Hit Y : Define new Y-display
0100 IF (JCHAR .EQ. YCHAR) THEN
0101 IYPWR = 0
0102 IDISY = IDISY + 1
0103 IF (IDISY .EQ. 1) THEN
0104 IF (JY .LT. LIYLO) THEN
0105 LIYLO = 0
0106 ELSE
0107 LIYLO = JY
0108 ENDIF
0109 GOTO 1010
0110 ENDIF
0111 IF (IDISY .EQ. 2) THEN
0112 IF (JY .LT. LIYHI) THEN
0113 LIYHI = JMAX
0114 ELSE
0115 LIYHI = JY
0116 ENDIF
0117 GOTO 1000
0118 ENDOIF
0119 ENDIF
Cs
Cs Error message for wrong character
0120 WRITE (5,2000)
0121 2000 FORMAT ('..Undefined symbol')
0122 GOTO 3100
Cs
Cs Error message for fit region failure
0123 3000 CALL DLOUT ('!Low end of this region is missing')
0124 GOTO 3100
Cs
Cs Error message for max number of fit regions reached
0125 3005 CALL DLOUT ('!Max nr. of fit regions got')
0126 GOTO 3100
Cs
Cs Error message for max peak nr.
0127 3010 CALL DLOUT ('!Max nr. of peaks got')
0128 3100 CALL DLKEY
0129 GOTO 1000
Cs
Cs Define other parameters for fit
0130 4000 IF (IREGL .NE. 0) THEN
0131 NREG = IREGL
0132 INREG = 1
0133 ENDOIF

```

PDP-11 FORTRAN-77 VS. 0-0 09:38:51 26-Sep-86 Page 5
FITCUR.FTN,1 /F77/OP/TR:BLOCKS/WR

```

Cs
Cs Return to calling program
0134 9000 RETURN
0135 *****
END

```

PDP-11 FORTRAN-77 VS. 0-0 09:39:13 26-Sep-86 Page 8
FITCUR.FTN,1 /F77/OP/TR:BLOCKS/WR

```

0001 SUBROUTINE MARKER (IX,IY,CHAR)
Cs
Cs *****
0002 BYTE CHAR
Cs
Cs *****
0003 CALL DIMOVA (IX-15,IY)
0004 CALL DIANU
0005 WRITE (5,1000) CHAR
0006 1000 FORMAT ('X,A1)
0007 CALL DIVIC
0008 CALL DIMOVA (IX,IY-50)
0009 CALL DIURWA (IX,IY-75)
Cs
Cs Return to calling program
0010 RETURN
0011 *****
END

```

```

0001 SUBROUTINE FITDIS
      *****
      C# This subroutine displays the spectrum and optionally the
      C# contribution of the peaks and/or the background
      C#
      C# Ver. 1.0/07-Sep-81(TK) Original version
      C# Ver. 1.1/14-Dec-81(TK) Some enhancements
      C# Ver. 1.2/17-Jan-84(TK) Some enhancements
      C# Ver. 1.3/25-Jan-84(TK) Separated peak display
      C#
0002 INCLUDE 'FIT.COM'
0003 IMPLICIT REAL*8 (A-H,O-Z)
      C#
      C# Logical unit numbers used:
      C#
      C# LUNSP: LUN to read spectrum
      C# LUNPAR: LUN for PARFIL
      C# LUNPRT: LUN for print output
      C# LUNCAL: LUN for calibration input, and energy table
      C# LUNTRM: LUN for terminal i/o (incl. DLPACK, MNPACK)
      C#
0004 PARAMETER LUNSP=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
0005 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
      C# NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
0006 BYTE SPESPC(30), PARSPC(30), CALSPC(30), FILPRT(30), ENESPC(30)
0007 CHARACTER=20 HDGLIN
0008 INTEGER=4 JCOUNT
0009 REAL=4 TO,SECDG
      C#
0010 COMMON /SPECTR/ JCOUNT(MAXCHN)
0011 COMMON /SPDESC/ NXCHAN, NYCHAN, IDATIM(9), NRUN, ISPILL, ITARG,
      C# ITEXT(18), LABEL
0012 COMMON /OPPARS/ MDEV, SPESPC, PARSPC, MXITER, LBFIX, INREG, LIXLO, LIXHI,
      C# LIYLO, LIYHI, IYPWR, LIFLO, LIFHI, IPEAK, LBACK, LPEAK,
      C# LPEBA, NCOEFF, COEFF(MAXCO), ITERA, NFREE,
      C# PEAK(NPPARM, MAXPK), IFLAG(NPPARM, MAXPK),
      C# INDEX(NPPARM, MAXPK), ISELEC, IGNOR(MAXPK), NREG,
      C# KREGLO(MAXREG), KREGHI(MAXREG), IMODE, INTCOR, NCALF
      C# CALFAC(MXCALF), SIGMA(MAXPK), GAMMA(MAXPK), CALSPC,
      C# FILPRT, ENESPC
      C# IOPARS
0013 COMMON /OPPART/ CHINEM, CHIOLD, FVBACK, FVPEAK
0014 COMMON /RESULT/
0015 COMMON /ERRCOM/ IERROR
0016 COMMON /PARAM/ ILINK(NPPARM, MXLINK), NPAR, NOIMM, KUSE, KSKIP,
      C# TOLO(G), TONI(G)
0017 COMMON /ARRAYS/ VMAT(MAXPAR*(MAXPAR+1)/2), DERIV(MAXPAR),
      C# RVCC(MAXPAR), HDERIV(MAXPAR)
0018 COMMON /CONST/ PICON, EPSILN, SQRTPI, SRLN2
  
```

```

0019 LOGICAL FILOPN
0020 COMMON /GLOBAL/ IOP, TO, IFIT, FILOPN
0021 DATA IOPARS /0/
0022 LOGICAL NODRAW
0023 INTEGER=4 JMIN, JMAX, JSUM, JYVAL
0024 COMMON /BUFMEN/ MBUFF(600)
      C#
      C# If no spectrum present: Go home
      C#
0025 IF (NXCHAN.LC.0) THEN
0026 CALL MNERAS
0027 CALL DROUT ('DNo data to display')
0028 CALL DLKEY
0029 GOTO 9000
0030 ENDF
0031 IF (IFIT.EQ.1) GOTO 1010
  
```

```

0032 Display sub menu
0033 CALL MNBUFF (MBUFF,600)
0034 CALL MNHEAD ('Display spectrum, peaks and background')
0035 CALL MNDEC (1, 'Lower X limit', LIXLO, LIXLO, 1, MAXCHN)
0036 CALL MNDEC (2, 'Higher X limit', LIXHI, LIXHI, 1, MAXCHN)
0037 CALL MNDEC (4, 'Lower Y limit', LIYLO, LIYLO, 0)
0038 CALL MNDEC (5, 'Higher Y limit', LIYHI, LIYHI, 1)
0039 CALL MNDEC (6, 'Power of 10 for Y-low, Y-high', IYPWR, IYPWR, 0.35)
0040 CALL MNNOF (8, 'Display of background', LBACK, LBACK)
0041 CALL MNNOF (9, 'Display peaks separately', LPEAK, LPEAK)
0042 CALL MNNOF (10, 'Display of peak+background', LPEBA, LPEBA)
0043 CALL MNDEC (14, 'Display mode: 0=Histo, 1=Err, 2=Spec, 3=Point',
      C# IMODE, IMODE, 0.3)
0044 CALL MNOPT (18, 'Redisplay')
0045 CALL MNDISP
0046 CALL MNIN (IOP)
0047 IF (IOP) 9000, 1000, 1005
      C#
      C# The big option switch
      C#
0048 1005 IF (IOP.NE.18) GOTO 1000
      C#
      C# Option R(18): Redisplay spectrum
      C#
0049 1010 LIXHI = MIN (LIXHI, NXCHAN)
0050 IF (LIXLO.GE.LIXHI) THEN
0051 LIXLO = 1
0052 LIXHI = NXCHAN
0053 ENDF
0054 CALL PREPDI (JCOUNT, LIXLO, LIXHI, LIYLO, LIYHI, IYPWR, JMIN, JMAX, JSUM)
  
```

```

0055 IF (JSUM.LE.0) THEN
0056 CALL MNERAS
0057 CALL DROUT ('DNo counts in spectrum')
0058 CALL DLKEY
0059 GOTO 1000
0060 ENDF
0061 CALL SDISPL (JCOUNT, LIXLO, LIXHI, JMIN, JMAX, IMODE)
      C#
      C# Display fit data (if requested)
      C#
0062 IF ((LPEAK + LBACK + LPEBA).NE.0) THEN
      C#
      C# Find limits for display
      C#
0063 LIFLO = KREGLO(1)
0064 LIFHI = KREGHI(1)
0065 DO 1020 J=2, NREG, 1
0066 LIFLO = MIN (LIFLO, KREGLO(J))
0067 LIFHI = MAX (LIFHI, KREGHI(J))
0068 1020 CONTINUE
0069 LIFLO = MAX (LIFLO, LIXLO)
0070 LIFHI = MIN (LIFHI, LIXHI)
      C#
      C# Prepare new scalings for background and fit
      C#
0071 IF (LIFLO.LT.LIFHI) THEN
0072 IDIV = LIXHI - (LIXLO + 1)
0073 RDIV = DIFDAT(MPOINT) / IDIV
0074 IPHI = IFIX (SNGL(RDIV) + LIXLO + 0.5)
0075 IPHI = IFIX (SNGL(RDIV) + LIXHI + 0.5)
0076 CALL DJWNOV (IPLO, IPHI, JMIN, JMAX)
0077 IPLO = IFIX (SNGL(RDIV) + LIFLO + 0.5)
0078 IPHI = IFIX (SNGL(RDIV) + LIFHI + 0.5)
      C#
      C# Display background (if requested)
      C#
0079 IF (LBACK.NE.0) THEN
0080 NODRAW = .TRUE.
0081 DO 1025 J=IPLO, IPHI, 1
0082 CALL FITBAC (DFLOAT(J)/RDIV, 1)
0083 JYVAL = JDINT(FVBACK+0.5)
0084 JYVAL = MAX(JYVAL, JMIN)
0085 JYVAL = MIN(JYVAL, JMAX)
0086 IF (NODRAW) THEN
0087 CALL DJMOVA (J, JYVAL)
0088 NODRAW = .FALSE.
0089 ELSE
0090 CALL DJDRVA (J, JYVAL)
0091 ENDF
0092 1025 CONTINUE
0093 ENDF
  
```

```

C#
C#      Display peak(s) (if requested)
C#
0094      IF (LPEAK.NE.0) THEN

PDP-11 FORTRAN-77 VS. 0-0      09:37:11      26-Sep-86      Page 4
FITDIS.FTN,1      /F77/OP/TR:BLOCKS/WR

0095      DO 1035 I=1,MAXPK,1
0096      IF (IGNOR(I).EQ.1) GOTO 1035
0097      NODRAW = .TRUE.
0098      DO 1030 J=IPLO,IPHI,1
0099      CALL FITPEA (DFLOAT(J)/RDIV,-I)
0100      IF (FVPEAK.GT.0.400) THEN
0101      CALL FITBAC (DFLOAT(J)/RDIV,1)
0102      FVBPK = FVBACK
0103      JYVAL = JIDINT(FVBPK-FVPEAK*0.5)
0104      JYVAL = MAX(JYVAL,JMIN)
0105      JYVAL = MIN(JYVAL,JMAX)
0106      IF (NODRAW) THEN
0107      CALL DJMOVA (J,JYVAL)
0108      NODRAW = .FALSE.
0109      ELSE
0110      CALL DJDRWA (J,JYVAL)
0111      ENDIF
0112      CONTINUE
0113      CONTINUE
0114      CONTINUE
0115      ENDIF

C#
C#      Display peak(s) and background (if requested)
C#
0116      IF (LPEBA.NE.0) THEN
0117      NODRAW = .TRUE.
0118      DO 1040 J=IPLO,IPHI,1
0119      CALL FITBAC (DFLOAT(J)/RDIV,1)
0120      FVBPK = FVBACK
0121      CALL FITPEA (DFLOAT(J)/RDIV,1)
0122      JYVAL = JIDINT(FVBPK+FVPEAK*0.5)
0123      JYVAL = MAX(JYVAL,JMIN)
0124      JYVAL = MIN(JYVAL,JMAX)
0125      IF (NODRAW) THEN
0126      CALL DJMOVA (J,JYVAL)
0127      NODRAW = .FALSE.
0128      ELSE
0129      CALL DJDRWA (J,JYVAL)
0130      ENDIF
0131      CONTINUE
0132      CONTINUE
0133      ENDIF
0134      ENDIF

C#
C#      Put some headerlines onto the pictures
C#
0135      CALL PRTHDR (JMAX,JSUM)
0136      READ (5,1045) J
0137      FORMAT (A1)
0138      IF (IFIT.EQ.0) GOTO 1000

C#
C#      Return to calling program
C#
0139      9000 RETURN
C#      *****

PDP-11 FORTRAN-77 VS. 0-0      09:37:11      26-Sep-86      Page 5
FITDIS.FTN,1      /F77/OP/TR:BLOCKS/WR

0140      END

```

PDP-11 FORTRAN-77 VS. 0-0 09:42:10 26-Sep-86 Page 1
FITEND.FTN,1 /F77/OP/TR:BLOCKS/WR

```

0001      SUBROUTINE FITEND
C#
C#      *****
C#
C#      This subroutine does some cleanup at the end of
C#      fit program
C#
C#      Ver. 1.0/22-Nov-83(TK) Original version
C#
0002      INCLUDE 'FIT.COM'
0003      IMPLICIT REAL*8 (A-H,O-Z)
C#
C#      Logical unit numbers used:
C#
C#      LUNSPE: Lun to read spectrum
C#      LUNPAR: Lun for PARFIL
C#      LUNPRT: Lun for print output
C#      LUNCAL: Lun for calibration input, and energy table
C#      LUNTRM: Lun for terminal I/O (incl. DLPACK, MNPACK)
C#
0004      PARAMETER LUNSPE=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
0005      PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
C#      NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
0006      BYTE SPESPC(30),PARSPC(30),CALSPC(30),FILPRT(30),ENESPC(30)
0007      CHARACTER*20 HDGLIN
0008      INTEGER*4 JCOUNT
0009      REAL*4 T0,SECNDS
C#
0010      COMMON /SPECTR/ JCOUNT(MAXCHN)
0011      COMMON /SPDESC/ NXCHAN,NYCHAN,IDATIM(9),NRUN,ISPILL,ITARG,
C#      ITEXT(18),LABEL
0012      COMMON /OPPARS/ MDEV,SPESPC,PARSPC,MXITER,LSFIX,INREG,LIXLO,LIXHI,
C#      LYELO,LIVHI,IYPWR,LIFLO,LIFHI,IPEAK,LBACK,LPEAK,
C#      LPEBA,NCOEFF,COEFF(MAXCO),ITERA,NFREE,
C#      PEAK(NPPARM,MAXPK),IFLAG(NPPARM,MAXPK),
C#      INDEX(NPPARM,MAXPK),ISLEEC,IGNOR(MAXPK),NREG,
C#      KREGLO(MAXREG),KREGHI(MAXREG),IMODE,INTCOR,NCALF,
C#      CALFAC(MXCALF),SIGMA(MAXPK),GAMMA(MAXPK),CALSPC,
C#      FILPRT,ENESPC
0013      COMMON /OPPART/ IOPANS
0014      COMMON /RESULT/ CHINW,CHIOLD,FVBACK,FVPEAK
0015      COMMON /ERRCOM/ IERROR
0016      COMMON /PARAM/ ILINK(NPPARM,MXLINK),NPAR,NDIMM,KUSE,KSKIP,
C#      TOLC(S),TOHI(S)
0017      COMMON /ARRAYS/ VWHAT(MAXPAR*(MAXPAR+1)/2),DERIV(MAXPAR),
C#      RVEC(MAXPAR),HDERIV(MAXPAR)
0018      COMMON /CONST/ PICON,EPSILN,SGRPI,SRNLN2
0019      LOGICAL FILOPN
0020      COMMON /GLOBAL/ IOP,T0,IFIT,FILOPN

```

PDP-11 FORTRAN-77 VS. 0-0 09:42:10 26-Sep-86 Page 2
FITEND.FTN,1 /F77/OP/TR:BLOCKS/WR

```

0021      DATA IOPANS /0/
C#
0022      CALL PARWT
0023      CALL MNLAS
0024      CALL DLYCNO ('Do you really want to stop',0,IOP)
C#
C#      Return to calling program
C#
0025      RETURN
C#      *****
0026      END

```



```

0001 SUBROUTINE FITENE
*****
C#
C# This subroutine handles the option -M- of program FITIO
C#
C#
C#
0002 PARAMETER MAXNUC=10
0003 C#
0004 INCLUDE 'FIT.COM'
IMPLICIT REAL*8 (A-H,O-Z)
C#
C# Logical unit numbers used:
C#
C# LUNSPC: Lun to read spectrum
C# LUNPAR: Lun for PARFIL
C# LUNPRT: Lun for print output
C# LUNCAL: Lun for calibration input, and energy table
C# LUNTRM: Lun for terminal I/O (incl. DLPACK, MNPACK)
0005 PARAMETER LUNSPC=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
0006 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
0007 BYTE SPESPC(30), PARSPC(30), CALSPC(30), FILPRT(30), ENESPC(30)
0008 CHARACTER*20 HDGLIN
0009 INTEGER*4 JCOUNT
0010 REAL*4 TO, SECNDS
0011 C#
0012 COMMON /SPECTR/ JCOUNT(MAXCHN)
0013 COMMON /SPDESC/ NXCHAN, NYCHAN, IDATIM(9), NRUN, ISPILL, ITARG,
ITEXT(16), LABEL
+ COMMON /OPPARS/ MDEV, SPESPC, PARSPC, MXITER, LBFIX, INREG, LIXLO, LIXHI,
LIYLO, LIYHI, IYPWR, LIFLO, LIFHI, IPEAK, LBACK, LPEAK,
LPEBA, NCOEFF, COEFF(MAXCO), ITERA, NFREE,
PEAK(NPPARM, MAXPK), IFLAG(NPPARM, MAXPK),
INDEX(NPPARM, MAXPK), ISELEC, IGNOR(MAXPK), NREG,
KREGLO(MAXREG), KREGHI(MAXREG), IMODE, INTCOR, NCALF,
CALFAC(MXCALF), SIGMA(MAXPK), GAMMA(MAXPK), CALSPC,
FILPRT, ENESPC
0014 COMMON /OPPART/ IOPARS
0015 COMMON /RESULT/ CHINEW, CHIOLD, FVBACK, FVPEAK
0016 COMMON /ERRCOM/ IERROR
0017 COMMON /PARAM/ ILINK(NPPARM, MXLINK), NPAR, NDIMM, KUSE, KSKIP,
TOLC(6), TOLH(6)
+ COMMON /ARRAYS/ VMAT(MAXPAR*(MAXPAR+1)/2), DERIV(MAXPAR),
RVEC(MAXPAR), HDGRIV(MAXPAR)
0018 COMMON /CONST/ PICON, EPSILN, SORTPI, SRLN2
0020 LOGICAL FILOPN

```

```

0021 COMMON /GLOBAL/ IOP, TO, IFIT, FILOPN
0022 DATA IOPARS /0/
0023 CHARACTER*4 TRANS
0024 CHARACTER*2 NUCLUS, NUCL(MAXNUC)
0025 REAL*8 ESPLIT(3)
0026 C##
0027 CALL ASSIGN (LUNCAL, ENESPC, LEN)
0028 NPEAK = 0
0029 1000 READ (LUNCAL, *, END=1010) NUCLUS, IAA, TRANS, WTENER, ESPLIT
0030 IF (ESPLIT(1) .EQ. 0.00) THEN
0031 NPEAK = NPEAK + 1
0032 PEAK(1, NPEAK) = (WTENER - CALFAC(1)) / CALFAC(2)
0033 ELSE
0034 DO 1005 I=1, 3, 1
0035 NPEAK = NPEAK + 1
0036 IF (IGNOR(NPEAK) .EQ. 1) GOTO 1005
0037 PLAK(1, NPLAK) = (ESPLIT(I) - CALFAC(1)) / CALFAC(2)
0038 1005 CONTINUE
0039 ENDF
0040 GOTO 1000
0041 CLOSE (UNIT=LUNCAL)
C#
C# Return to calling program
C#
0041 9000 RETURN
*****
0042 END

```

0042

```

0001 SUBROUTINE FITFIT
*****
C#
C# This routine fits a spectrum
C#
C#
C# Ver. 0.0/09-SEP-83(TK) Original version
C# Ver. 1.0/06-OCT-83(DR)
C# Ver. 2.0/31-OCT-83(DR)
C# Ver. 2.1/03-Nov-83(TK) Beep implemented
C#
0002 INCLUDE 'FIT.COM'
0003 IMPLICIT REAL*8 (A-H,O-Z)
C#
C# Logical unit numbers used:
C#
C# LUNSPC: Lun to read spectrum
C# LUNPAR: Lun for PARFIL
C# LUNPRT: Lun for print output
C# LUNCAL: Lun for calibration input, and energy table
C# LUNTRM: Lun for terminal I/O (incl. DLPACK, MNPACK)
0004 PARAMETER LUNSPC=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
0005 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
0006 BYTE SPESPC(30), PARSPC(30), CALSPC(30), FILPRT(30), ENESPC(30)
0007 CHARACTER*20 HDGLIN
0008 INTEGER*4 JCOUNT
0009 REAL*4 TO, SECNDS
0010 C#
0011 COMMON /SPECTR/ JCOUNT(MAXCHN)
0012 COMMON /SPDESC/ NXCHAN, NYCHAN, IDATIM(9), NRUN, ISPILL, ITARG,
ITEXT(16), LABEL
+ COMMON /OPPARS/ MDEV, SPESPC, PARSPC, MXITER, LBFIX, INREG, LIXLO, LIXHI,
LIYLO, LIYHI, IYPWR, LIFLO, LIFHI, IPEAK, LBACK, LPEAK,
LPEBA, NCOEFF, COEFF(MAXCO), ITERA, NFREE,
PEAK(NPPARM, MAXPK), IFLAG(NPPARM, MAXPK),
INDEX(NPPARM, MAXPK), ISELEC, IGNOR(MAXPK), NREG,
KREGLO(MAXREG), KREGHI(MAXREG), IMODE, INTCOR, NCALF,
CALFAC(MXCALF), SIGMA(MAXPK), GAMMA(MAXPK), CALSPC,
FILPRT, ENESPC
0013 COMMON /OPPART/ IOPARS
0014 COMMON /RESULT/ CHINEW, CHIOLD, FVBACK, FVPEAK
0015 COMMON /ERRCOM/ IERROR
0016 COMMON /PARAM/ ILINK(NPPARM, MXLINK), NPAR, NDIMM, KUSE, KSKIP,
TOLC(6), TOLH(6)
+ COMMON /ARRAYS/ VMAT(MAXPAR*(MAXPAR+1)/2), DERIV(MAXPAR),
RVEC(MAXPAR), HDGRIV(MAXPAR)
0017 COMMON /CONST/ PICON, EPSILN, SORTPI, SRLN2
0018

```

```

0019 LOGICAL FILOPN
0020 COMMON /GLOBAL/ IOP, TO, IFIT, FILOPN
0021 DATA IOPARS /0/
0022 LOGICAL NOUPDT
0023 IERROR = 0
0024 CHINEW = 0.000
0025 NOUPDT = .TRUE.
C#
C# Set widths to formula-parameters
C#
0026 DO 1000 I=1, MAXPK, 1
0027 SIGMA(IP) = PEAK(2, IP) / SRLN2
0028 GAMMA(IP) = PEAK(6, IP) / 2.00
0029 1000 CONTINUE
C#
C# Loop up to label 1060 does the iterations
C#
0030 DO 1060 ITERA=0, MXITER, 1
0031 CALL PARDEF
0032 CALL PARWT
0033 CALL PARDEF (VMAT, (MAXPAR*(MAXPAR+1)/2)*8)
0034 CALL PARWT ('IMP')
0035 CALL RVEC (HADUC='FITSPY', .LNEG)

```

0035

```

C*
C* Set up for next iteration. CHIOLD holds old CHINEW
C*
0036 CHIOLD = CHINEW
0037 CHINEW = 0.000
0038 IF (NOUPDT) GOTO 1051

C*
C* Update background coefficients
C*
0039 IF (LSFIX.LE.0) THEN
0040 DO 1035 J=1,NCOEFF,1
0041 COEFF(J) = COEFF(J) + HDERIV(J)
0042 CONTINUE
0043 ENDIF

C*
C* Update peak parameters
C*
0044 DO 1050 IP=1,MAXPK,1
0045 IF (IGNOR(IP).EQ.1) GOTO 1050
0046 DO 1045 IV=1,NPPARM,1
0047 I = INDEX(IV,IP)
0048 IF (I.LE.0) GOTO 1045

C*
C* Special treatment for linked peak height parameters
C*
0049 IF (IV.EQ.3) THEN
0050 IF (IFLAG(3,IP).GT.0) THEN
0051 XX = PEAK(3,IP) * (1.000 + HDERIV(I))

PDP-11 FORTRAN-77 V5.0-0 09:40:41 26-Sep-86 Page 3
FITFIT.FTN;1 /F77/OP/TR:BLOCKS/WR

0052 ELSE
0053 XX = PEAK(3,IP) + HDERIV(I)
0054 ENDIF
0055 ELSE
0056 XX = PEAK(IV,IP) + HDERIV(I)
0057 IF (IV.EQ.2) XX = SRLN2 * (SIGMA(IP) + HDERIV(I))
0058 IF (IV.EQ.6) XX = 2.000 * (GAMMA(IP) + HDERIV(I))
0059 ENDIF

C*
0060 IF (XX.LE.TOLO(IV).OR.XX.GE.TOHI(IV)) THEN
0061 WRITE(5,1040) IV,IP
0062 FORMAT(' Parm. ',I2,' of Peak',I3,' out')
0063 ELSE
0064 PEAK(IV,IP) = XX
0065 ENDIF
0066 CONTINUE
0067 SIGMA(IP) = PEAK(2,IP) / SRLN2
0068 GAMMA(IP) = PEAK(6,IP) / 2.00
0069 CONTINUE

1050 CONTINUE

C*
C* Reset temporary variables
C*
0070 NOUPDT = .FALSE.
0071 CALL VDZERO (RVEC,MAXPAR)
0072 CALL VDZERO (VMAT,(MAXPAR*(MAXPAR+1)/2))

C*
C* Run through the regions
C*
0073 DO 1020 LREG=1,NREG,1

C*
C* Run through the channels
C*
0074 DO 1015 ICHAN=KREGLO(LREG),KREGHI(LREG),1
0075 VFIT = 0.000
0076 CALL VDZERO (DERIV,MAXPAR)
0077 COUNT = JCOUNT(ICHAN)
0078 IF (COUNT.LT.1.000) COUNT = 0.4500

C*
C* Calculate contribution of background
C*
0079 CALL FITBAC (DFLOAT(ICHAN),0)
0080 VFIT = VFIT + FVBACK

C*
C* Calculate contribution of peaks
C*
0081 CALL FITPEA (DFLOAT(ICHAN),0)
0082 VFIT = VFIT + FVPEAK

C*
C* The fit value VFIT is now computed Update CHINEW
C*
0083 VFIT = COUNT - VFIT
0084 IF (DABS(CHINEW).LT.1.0015)
CHINEW = CHINEW + (VFIT * VFIT / COUNT)

C*
C* Calculate:

```

```

PDP-11 FORTRAN-77 V5.0-0 09:40:41 26-Sep-86 Page 4
FITFIT.FTN;1 /F77/OP/TR:BLOCKS/WR

C*
C* T: packed upper triangular normal matrix
C* R: right side of normal equation
C*
0085 IJ = 0
0086 DO 1010 I=1,NPAR,1
0087 XX = DERIV(I)/COUNT
0088 RVEC(I) = RVEC(I) + XX * VFIT
0089 DO 1005 J=I,NPAR,1
0090 IJ = IJ+1
0091 VMAT(IJ) = VMAT(IJ) + (DERIV(J) * XX)
0092 CONTINUE
0093 CONTINUE

C*
0094 1015 CONTINUE
0095 1020 CONTINUE

C*
C* CHISQ2 is calculated Print message.
C*
0096 WRITE(5,1055) ITERA,CHINEW/DOUBLE(NFREE),SECNDS(TD)
0097 FORMAT(' ',I2,' Iteration done. CHISQ2/NFREE ',F12.2,
3X,'(,F6.1,' secs fitting)')

C*
C* If desired accuracy reached, terminate iteration
C*
0098 IF (ABS(CHINEW-CHIOLD).LT.EPSILN) GOTO 1065

C*
C* We ran through all channels. Do a matrix inversion
C*
0099 CALL SPXINV (VMAT,NPAR)
0100 IF (IERROR.LT.0) THEN
0101 CALL DLOUT (' ** Bad matrix **')
0102 GOTO 1065
0103 ENDIF

C*
C* Calculate parameter increments
C*
0104 CALL VDZERO (HDERIV,MAXPAR)
0105 IJ = 0
0106 DO 1030 I=1,NPAR,1
0107 IJ = IJ + 1
0108 DO 1025 J=I,NPAR,1
0109 HDERIV(IJ) = HDERIV(I) + VMAT(IJ) * RVEC(J)
0110 IF (I.NE.J) HDERIV(J) = HDERIV(J) + VMAT(IJ) * RVEC(I)
0111 CONTINUE
0112 CONTINUE
0113 1030 CONTINUE

C*
C* Max. iteration count exhausted
C*
0114 ITERA = ITERA - 1
0115 1065 CALL BEEP
0116 CALL PARDD ('TMP')
0117 CALL PARDEF

PDP-11 FORTRAN-77 V5.0-0 09:40:41 26-Sep-86 Page 5
FITFIT.FTN;1 /F77/OP/TR:BLOCKS/WR

C*
C* Set flags for display
C*
0118 LBACK = 1
0119 LPEGA = 1
0120 LPEAK = 0

C*
C* Wait until user looked at the data
C*
0121 CALL DLKEY

C*
C* Return to calling program
C*
0122 RETURN
0123 *****
END

```

```

0001 SUBROUTINE FITIO
      *****
      C#
      C# This subroutine handles the option -C- of program FIT
      C#
      C# Ver. 1.0 29-Sep-83 (TK) Original version
      C# Ver. 1.1 14-Dec-83 (TK) Clear entire spectrum before reading new one
      C# Ver. 2.0 01-Feb-84 (TK) Implementation of calibration polynomial
      C# Ver. 3.0 28-May-85 (DR) Bug in calibration-read removed
      C# Ver. 4.0 21-Jun-85 (DR) Implementation of energy table
      C#
0002 INCLUDE 'FIT.COM'
0003 IMPLICIT REAL*8 (A-H,O-Z)
      C#
      C# Logical unit numbers used:
      C#
      C# LUNSP: Lun to read spectrum
      C# LUNPAR: Lun for PARFIL
      C# LUNPRT: Lun for print output
      C# LUNCAL: Lun for calibration input, and energy table
      C# LUNTRM: Lun for terminal i/o (incl. DLPACK, MNPACK)
      C#
0004 PARAMETER LUNSP=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
0005 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
      NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
      C#
0006 BYTE SPESPC(30), PARSPC(30), CALSPC(30), FILPRT(30), ENESPC(30)
      C#
0007 CHARACTER*20 HDGLIN
      C#
0008 INTEGER*4 JCOUNT
      C#
0009 REAL*4 T0,SECONDS
      C#
0010 COMMON /SPECTR/ JCOUNT(MAXCHN)
0011 COMMON /SPDESC/ NXCHAN,NYCHAN, IDATIM(9),NRUN,ISPILL,ITARG,
      ITEXT(10),LABEL
0012 COMMON /OPPARS/ MDEV,SPESPC,PARSPC,MXITER,LBFX,INREG,LIXLO,LIXHI,
      LIYLO,LIYHI,IYPWR,LIFLO,LIFHI,IPEAK,LBACK,LPEAK,
      LPEBA,NCOEFF,COEFF(MAXCO),ITERA,NFREE,
      PEAK(NPPARM,MAXPK),IFLAG(NPPARM,MAXPK),
      INDEX(NPPARM,MAXPK),ISELEC,IGNOR(MAXPK),NREG,
      KREGLO(MAXREG),KREGHI(MAXREG),IMODE,INTCOR,NCALF,
      CALFAC(MXCALF),SIGMA(MAXPK),GAMMA(MAXPK),CALSPC,
      FILPRT,ENESPC
0013 COMMON /OPPART/ IOPARS
0014 COMMON /RESULT/ CHINEW,CHIOLD,FVBACK,FVPEAK
0015 COMMON /ERRCOM/ IERROR
0016 COMMON /PARAM/ ILINK(NPPARM,MXLINK),NPAR,NDIMM,KUSE,KSKIP,
      TOLD(6),TOHI(6)
0017 COMMON /ARRAYS/ VMAI(MAXPAR*(MAXPAR+1)/2),DERIV(MAXPAR),
      RVECC(MAXPAR),HDERIV(MAXPAR)
  
```

```

0018 COMMON /CONST/ PICON,EP5ILN,SQRTPI,SRLN2
      C#
0019 LOGICAL FILOPN
0020 COMMON /GLOBAL/ IOP,T0,IFIT,FILOPN
      C#
0021 DATA IOPARS /0/
      C#
0022 COMMON /BUFMEN/ MBUFF(600)
      C#
      C# Display sub menu
      C#
0023 1000 CALL MNCLR
0024 CALL MNBUFF (MBUFF,600)
0025 CALL MNHEAD ('Get spectrum / save fit parameters')
0026 CALL MNTXT (1, 'Spectrum file', SPESPC, SPESPC, 29)
0027 CALL MNTXT (2, 'Fit parameter file', PARSPC, PARSPC, 29)
0028 CALL MNOPT (4, 'Save fit parameters')
0029 CALL MNOPT (5, 'Read fit parameters')
0030 CALL MNDEC (7, 'Get spectrum from disk', ISELEC, ISELEC)
0031 CALL MNOPT (9, 'Show spectra available in spectrum file')
0032 CALL MNTXT (11, 'Enter calibration polynomial', CALSPC, CALSPC, 29)
0033 CALL MNTXT (13, 'Enter energy table', ENESPC, ENESPC, 29)
0034 CALL MNDISP
0035 CALL MJIN (IOP)
0036 IF (IOP) 9000,1000,1005
  
```

```

      C# The big option switch
      C#
0037 1005 GOTO (1000, 1000, 1000, 1010, 1010, 1000, 1020, 1000,
      1040, 1010, 1065, 1000, 1080), IOP
      C#
      C# Option D(4): Save fit parameters
      C# Option E(5): Read fit parameters
      C#
0038 1010 CALL FITPFL
0039 GOTO 1000
      C#
      C# Option G(7): Get spectrum from disk
      C#
0040 1020 CALL FITSPR
0041 GOTO 1000
      C#
      C# Option I(9): Show spectra available
      C#
0042 1040 CALL MNERAS
0043 NXCHAN = 0
0044 CALL ASSIGN (LUNSP, SPESPC)
0045 DO 1055 J=1,6,1
0046 READ (LUNSP, ERR=1060, END=1060) NXCHAN, NYCHAN, IDATIM, NRUN,
      ISPILL, ITARG, ITEXT, LABEL
0047 WRITE (5, 1035) LABEL, IDATIM, NRUN, ISPILL, ITARG, ITEXT, NXCHAN
0048 FORMAT ('0', 'Spectrum with label', I6/
      ' ', '9A2', 'Run', I4, ' ', 'Spill', I4, ' ', 'Target', I3/
      ' ', '18A2.3x', 'No. of channels:', I5)
0049 DO 1050 K=1, NYCHAN, 1
  
```

```

      C#
0050 READ (LUNSP, ERR=1060, END=1060) (JCOUNT(I), I=1, NXCHAN)
0051 1050 CONTINUE
0052 1055 CONTINUE
0053 CALL DLKEY
0054 CALL MNERAS
0055 GOTO 1045
      C#
0056 1060 CLOSE (UNIT=LUNSP)
0057 CALL DLKEY
0058 GOTO 1000
      C#
      C# Option K(11): Input of calibration polynomial
      C#
0059 1065 CALL MNERAS
0060 CALL ASSIGN (LUNCAL, CALSPC)
0061 1070 READ (LUNCAL, *, END=2005) ID, LIMIT, HDGLIN, CALFAC
0062 IF (ID.NE. ISELEC) GOTO 1070
0063 NCALF = 3
0064 CALL DLOUT (' ')
0065 WRITE (5, 1075) CALFAC
0066 1075 FORMAT (' Calibration polynomial : '/' a0 = '.E15.7/
      ' a1 = '.E15.7/' a2 = '.E15.7)
0067 CALL DLKEY
0068 CLOSE (UNIT=LUNCAL)
0069 GOTO 1000
      C#
      C# Option M(13): Input of energy table
      C#
0070 1080 CALL MNERAS
0071 CALL FITENE
0072 GOTO 1000
      C#
      C# Disk i/o error
      C#
0073 2000 CALL DLOUT ('DNo such spectrum')
0074 NXCHAN = 0
0075 CLOSE (UNIT=LUNSP)
0076 CALL DLKEY
0077 GOTO 1000
      C#
0078 2005 CALL DLOUT ('DNo such calibration')
0079 CALL DLKEY
0080 GOTO 1000
      C#
      C# Return to calling program
      C#
0081 9000 RETURN
      C#
0082 END
  
```

```

0001 SUBROUTINE FITMEN
      C* *****
      C* This subroutine displays the master menu and
      C* transmits the option number to the calling program
      C*
      C* VER. 0.0/07-SEP-83(TK) Original version
      C*
0002 INCLUDE 'FIT.COM'
0003 IMPLICIT REAL*8 (A-H,O-Z)
      C*
      C* Logical unit numbers used:
      C*
      C* LUNSPC: Lun to read spectrum
      C* LUNPAR: Lun for PARFIL
      C* LUNPRT: Lun for print output
      C* LUNCAL: Lun for calibration input, and energy table
      C* LUNTRM: Lun for terminal I/O (incl. DLPACK, MNPACK)
      C*
0004 PARAMETER LUNSPC=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
0005 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
      C* NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
0006 BYTE SPESPC(30),PARSPC(30),CALSPC(30),FILPRT(30),ENESPC(30)
      C*
0007 CHARACTER*20 HDGLIN
0008 INTEGER*4 JCOUNT
0009 REAL*4 TD,SECNOS
      C*
0010 COMMON /SPECTR/ JCOUNT(MAXCHN)
0011 COMMON /SPDESC/ NXCHAN,NYCHAN, IDATIM(9),NRUN,ISPILL,ITARG,
      C* ITEXT(18),LABEL
0012 COMMON /OPPARS/ MDEV,SPESPC,PARSPC,MXITER,LBFX,INREG,LIXLO,LIXHI,
      C* LIYLO,LIYHI,IYPWR,LIFLO,LIFHI,IPEAK,LBACK,LPEAK,
      C* LPEBA,NCOEFF,COEFF(MAXCO),ITERA,NFREE,
      C* PEAK(NPPARM,MAXPK),IFLAG(NPPARM,MAXPK),
      C* INDEX(NPPARM,MAXPK),ISELEC,IGNOR(MAXPK),NREG,
      C* KREGLO(MAXREG),KREGHI(MAXREG),IMODE,INTCOR,NCALF,
      C* CALFAC(MXCALF),SIGMA(MAXPK),GAMMA(MAXPK),CALSPC,
      C* FILPRT,ENESPC
0013 COMMON /OPPART/ IOPARS
0014 COMMON /RESULT/ CHINEW,CHIOLD,FVBACK,FVPEAK
0015 COMMON /ERRCOM/ IERROR
0016 COMMON /PARAM/ ILINK(NPPARM,MXLINK),NPAR,NDIMM,KUSE,KSKIP,
      C* TOLO(6),TOHI(6)
0017 COMMON /ARRAYS/ VMAT(MAXPAR*(MAXPAR+1)/2),DERIV(MAXPAR),
      C* RVEC(MAXPAR),HDERIV(MAXPAR)
0018 COMMON /CONST/ PICON,EPSILN,SORTPI,SRLN2
      C*
0019 LOGICAL FILOPN
0020 COMMON /GLOBAL/ IOP,TD,IFIT,FILOPN
      C*

```

```

0021 DATA IOPARS /0/
0022 COMMON /BUFMEN/ MBUFF(600)
      C*
      C* Set up menu
      C*
0023 1000 CALL MNDEV (MDEV)
0024 CALL MNCLR
0025 CALL MNBUFF (MBUFF,600)
      C*
0026 CALL MNHID ('FIT 0.0 -- Interactive fit of spectrum')
0027 CALL MNHID (1,'Menu device: 4=TD, 6=NU, 9=D1,MDEV,MDEV)
0028 CALL MNOPT (3,'Get spectrum / Save fit parameters')
0029 CALL MNOPT (4,'Display')
0030 CALL MNOPT (6,'Fit spectrum')
0031 CALL MNOPT (8,'Output results to print file')
0032 CALL MNOPT (9,'Route print file to printer')
0033 CALL MNOPT (11,'Save spectrum and fit parameters for plotting')
0034 CALL MNOPT (18,'Redisplay results')
0035 CALL MNDISP
0036 CALL MNIN (IOP)
0037 IF (IOP) 9000,1000,1005
      C*
0038 1005 GOTO (1000,1000,9000,9000,1000,1000,9000,1000,9000,
      C* 9000,1000,9000,1000,1000,1000,1000,1000,
      C* 1000,9000), IOP
      C*
      C* Return to calling program
      C*
0039 9000 RETURN
0040 END

```

```

0001 SUBROUTINE FITOUT (LUN)
      C* *****
      C* This routine prints the results (LUN=LUNTRM -> screen)
      C*
      C* Ver. 1.0/09-SEP-83(TK) Original version
      C* Ver. 1.1/11-OCT-83(DR) Error included version
      C* Ver. 1.2/19-JAN-84(TK) Output format slightly changed
      C* Ver. 2.0/02-FEB-84(TK) Output of flags and calibration
      C* Ver. 2.1/10-FEB-84(TK) Output of FIT regions included
      C* Ver. 2.2/10-JAN-85(DR) Output of FIT date and time included
      C*
0002 PARAMETER MAXLIN=6
0003 INCLUDE 'FIT.COM'
0004 IMPLICIT REAL*8 (A-H,O-Z)
      C*
      C* Logical unit numbers used:
      C*
      C* LUNSPC: Lun to read spectrum
      C* LUNPAR: Lun for PARFIL
      C* LUNPRT: Lun for print output
      C* LUNCAL: Lun for calibration input, and energy table
      C* LUNTRM: Lun for terminal I/O (incl. DLPACK, MNPACK)
      C*
0005 PARAMETER LUNSPC=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
0006 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
      C* NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
0007 BYTE SPESPC(30),PARSPC(30),CALSPC(30),FILPRT(30),ENESPC(30)
      C*
0008 CHARACTER*20 HDGLIN
0009 INTEGER*4 JCOUNT
0010 REAL*4 TD,SECNOS
      C*
0011 COMMON /SPECTR/ JCOUNT(MAXCHN)
0012 COMMON /SPDESC/ NXCHAN,NYCHAN, IDATIM(9),NRUN,ISPILL,ITARG,
      C* ITEXT(18),LABEL
0013 COMMON /OPPARS/ MDEV,SPESPC,PARSPC,MXITER,LBFX,INREG,LIXLO,LIXHI,
      C* LIYLO,LIYHI,IYPWR,LIFLO,LIFHI,IPEAK,LBACK,LPEAK,
      C* LPEBA,NCOEFF,COEFF(MAXCO),ITERA,NFREE,
      C* PEAK(NPPARM,MAXPK),IFLAG(NPPARM,MAXPK),
      C* INDEX(NPPARM,MAXPK),ISELEC,IGNOR(MAXPK),NREG,
      C* KREGLO(MAXREG),KREGHI(MAXREG),IMODE,INTCOR,NCALF,
      C* CALFAC(MXCALF),SIGMA(MAXPK),GAMMA(MAXPK),CALSPC,
      C* FILPRT,ENESPC
0014 COMMON /OPPART/ IOPARS
0015 COMMON /RESULT/ CHINEW,CHIOLD,FVBACK,FVPEAK
0016 COMMON /ERRCOM/ IERROR
0017 COMMON /PARAM/ ILINK(NPPARM,MXLINK),NPAR,NDIMM,KUSE,KSKIP,
      C* TOLO(6),TOHI(6)

```

```

0018 COMMON /ARRAYS/ VMAT(MAXPAR*(MAXPAR+1)/2),DERIV(MAXPAR),
      C* RVEC(MAXPAR),HDERIV(MAXPAR)
0019 COMMON /CONST/ PICON,EPSILN,SORTPI,SRLN2
      C*
0020 LOGICAL FILOPN
0021 COMMON /GLOBAL/ IOP,TD,IFIT,FILOPN
      C*
0022 DATA IOPARS /0/
0023 LOGICAL NODLKY
0024 INT IGLR(4),FTDAT(9),KDATE(5),KTIME(4)
0025 REAL*8 DCOLFF(MAXCO),DH(MAXPAR),DPEAK(NPPARM)
0026 DATA DT /1000.00/, FTDAT /9= ' ' /
0027 EQUIVALENCE (DPEAK(1),HDERIV(1)),(DCOLFF(1),HDERIV(NPPARM+1))
      C*
      C* Get actual date and time
      C*
0028 CALL DATE (KDATE)
0029 CALL TIME (KTIME)

```

```

C#
C# Start printout with header lines
0030 IF (LUN .EQ. LUNTRM) THEN
0031 CALL MNERAS
0032 ELSE
0033 WRITE (LUN,1000)
0034 FORMAT ('1')
0035 ENDDIF
0036 WRITE (LUN,1001) KDATE, KTIME, PARSPEC
0037 FORMAT ('1', 'Output from SA2, 4A2, 20X, 30A1)
0038 WRITE (LUN,1005) IDATIM, NRUN, XSPILL, ITARG, ITEXT
0039 FORMAT ('0', 'SA2', 'Run', I4, ' Spill', I3, ' Target', I3, /
+ '18A2)
0040 WRITE (LUN,1010) ITERA, CHINEW, NFREE, CHINEW/DBLE(NFREE),
0041 FORMAT ('0', I2, ' Iteration, CHI**2:', F12.4, ' NFREE:', I5, /
+ 'CHI**2/NFREE:', F9.4)
C#
C# Printout of FIT regions
0042 WRITE (LUN,1015) ((KREGLO(J), KREGHI(J)), J=1, NREG)
0043 FORMAT ('0', 'FIT regions used:', /,
+ '6(I5, ', 'I4)')
C#
C# Calculate error for background
0044 DO 1020 I=1, NPAR, 1
0045 DH(I) = SQRT (ABS (FITIJ (VMAT, NPAR, I, I)))
0046 CONTINUE
C#
C# Store errors for background
1020 CONTINUE
C#

POP-11 FORTRAN-77 VS. 0-0 09:41:11 26-Sep-86 Page 3
FITOUT.FTN;1 /F77/OP/TR:BLOCKS/WR
0047 DO 1025 J=1, NCOEFF, 1
0048 DCOEFF(J) = 0.000
0049 IF (LBFIX .EQ. 0) DCOEFF(J) = DH(J)
0050 CONTINUE
C#
C# Printout of background
0051 WRITE (LUN,1030) NCOEFF
0052 FORMAT ('0', 'Background with', I3, ' coefficients:')
0053 WRITE (LUN,1035) (COEFF(J), J=1, NCOEFF)
0054 FORMAT (' ', 'Coeffs:', 3(IPE16.8)/
+ '3(IPE16.8)')
0055 WRITE (LUN,1040) (DCOEFF(J), J=1, NCOEFF)
0056 FORMAT (' ', 'Errors:', 3(IPE16.8)/
+ '3(IPE16.8)')
C#
C# Printout of calibration polynomial
0057 IF (NCALF .GT. 0) THEN
0058 WRITE (LUN,1045)
0059 FORMAT ('0', 'Calibration polynomial:')
0060 WRITE (LUN,1035) (CALFAC(J), J=1, NCALF)
0061 ENDDIF
C#
C# Finish header page
0062 IF (LUN .NE. LUNTRM) THEN
0063 CALL DROUT (' ')
0064 CALL DLYENO (' Do you want to see the results', 1, IOP)
0065 IF (IOP .NE. 1) GOTO 2000
0066 CALL MNERAS
0067 ENDDIF
0068 NODLKY = .FALSE.
C#
C# Printout of peaks
0069 NPLINE = 0
0070 DO 1080 IPK=1, MAXPK, 1
0071 IF (IGNOR(IPK) .EQ. 1) GOTO 1080
0072 NODLKY = TRUE.
0073 DO 1050 IPARM=1, NPPARM, 1
0074 IN = INDEX(IPARM, IPK)
0075 DPEAK(IPARM) = 0.000
0076 IF (IN .GT. 0) DPEAK(IPARM) = DH(IN)
0077 CONTINUE
C#
C# Convert width to FWHM
0078 IF (IFLAG(3, IPK) .GT. 0) DPEAK(3) = DPEAK(3) * PEAK(3, IPK)
0079 INHIG = INDEX(3, IPK)
C#
C# Gaussian
0080 IPARM = 2
0081 XPI = SORTPI

```

```

0082 WIDTH = SIGMA(IPK)
C#
C# Lorentzian
0083 IF (IFLAG(6, IPK) .NE. -2) THEN
0084 IPARM = 6
0085 XPI = PICON
0086 WIDTH = GAMMA(IPK)
0087 ENDDIF
0088 IWIDTH = INDEX(IPARM, IPK)
0089 DWIDTH = DPEAK(IPARM)
C#
C# Area
0090 AREA = PEAK(3, IPK) * WIDTH
0091 DAREA = (PEAK(3, IPK) * DWIDTH) **2 + (WIDTH * DPEAK(3)) **2
+ DAREA * 2 * AREA * FITIJ(VMAT, NPAR, IWIDTH, INHIG)
0092 DAREA = XPI * SORT (ABS(DAREA))
0093 AREA = XPI * AREA
0094 DPEAK(2) = DPEAK(2) * SRLN2
0095 DPEAK(6) = DPEAK(6) * 2.000
C#
C# Start output
0096 IF (NPLINE .EQ. 0) THEN
0097 WRITE (LUN,1055)
0098 FORMAT (' ')
0099 WRITE (LUN,1060)
0100 FORMAT (' ', 'Position', 2X, 'Gauss-FWHM', 3X, 'Height', 1X, /
+ 'Low-tail', 1X, 'High-tail', 1X, 'Lorentz-FWHM', /
+ '1X, 'Intensity')
0101 ENDDIF
0102 WRITE (LUN,1065) IPK, (IFLAG(I, IPK), I=1, NPPARM)
0103 FORMAT ('0', 'Peak', I3, 10X, '(Flags: ', 5(I2, ', '). I2, ')')
0104 WRITE (LUN,1070) (PEAK(I, IPK), I=1, NPPARM), AREA
0105 FORMAT (' ', F8.3, 1X, F7.3, 1X, F13.2, 2X, DPF7.3, 2X, F7.3, 2X, F7.3, /
+ '1X, F13.2)')
0106 WRITE (LUN,1070) (DPEAK(I), I=1, NPPARM), DAREA
C#
C# Print calibration (if any)
0107 IF (NCALF .GT. 0) THEN
0108 XPI = PEAK(1, IPK)
0109 WIDTH = 0.500 * PEAK(2, IPK)
0110 DWIDTH = 0.500 * PEAK(6, IPK)
0111 DPEAK(1) = 0.500 * DPEAK(1)
0112 DPEAK(2) = 0.500 * DPEAK(2)
0113 DPEAK(6) = 0.500 * DPEAK(6)
0114 WRITE (LUN,1075) CALVAL(XPI), /
+ CALVAL(XPI+DPEAK(1)), -CALVAL(XPI-DPEAK(1)), /
+ DT*(CALVAL(XPI+WIDTH)-CALVAL(XPI-WIDTH)), /
+ DT*(CALVAL(XPI+DPEAK(2))-CALVAL(XPI-DPEAK(2))), /
+ DT*(CALVAL(XPI+DWIDTH)-CALVAL(XPI-DWIDTH)), /
+ DT*(CALVAL(XPI+DPEAK(6))-CALVAL(XPI-DPEAK(6)))
0115 FORMAT (' ', 'E', F9.4, '( ', F8.4, ')', ' ')
C#

```

```

0116 ENDDIF
C#
C# Make a nice paging
0117 NPLINE = NPLINE+1
0118 IF (NPLINE .GE. MAXLIN) THEN
0119 IF (LUN .EQ. LUNTRM) THEN
0120 NPLINE = 0
0121 CALL DROUT (' ')
0122 CALL DLYENO (' Continue', 1, IOP)
0123 IF (IOP .NE. 1) GOTO 2000
0124 CALL MNERAS
0125 NODLKY = .FALSE.
0126 ENDDIF
0127 ENDDIF
0128 CONTINUE
0129 IF I1 = 0
0130 IF (LUN .NE. LUNTRM) GOTO 9000
0131 IF (NODLKY) CALL DLKEY
C#
0132 2000 CALL MNERAS
0133 CALL DLYENO (' Do you want the picture', 1, IFIT)
C#
C# Return to calling program
0134 9000 RETURN
0135 *****
END

```

```

0001      DOUBLE PRECISION FUNCTION FITIJ (VMAT,NDIMM,I,J)
0002      .....
0003      This function returns the value of element (I,J) of
0004      packed symmetric matrix
0005      .....
0006      Ver. 0.0/12-OCT-83 (DR) Original version
0007      REAL*8 VMAT(1)
0008
0009      IF (I .LE. 0 .OR. I .GT. NDIMM) GOTO 1000
0010      IF (J .LE. 0 .OR. J .GT. NDIMM) GOTO 1000
0011
0012      IF (I .LE. J) THEN
0013          Upper triangular matrix
0014
0015          II = I
0016          JJ = J
0017      ELSE
0018          Lower triangular matrix
0019
0020          II = J
0021          JJ = I
0022      ENDIF
0023
0024      Calculate index in packed matrix
0025
0026      IJ = (2 * NDIMM - II) * (II - 1) / 2 + JJ
0027      FITIJ = VMAT(IJ)
0028      GOTO 9000
0029
0030      Out of range return
0031
0032      1000 FITIJ = 0.000
0033
0034      Return to calling program
0035
0036      9000 RETURN
0037      END
    
```

```

0001      DOUBLE PRECISION FUNCTION CALVAL (DCHAN)
0002      .....
0003      This function returns the ...
0004      .....
0005      INCLUDE 'FIT.COM'
0006      IMPLICIT REAL*8 (A-H,O-Z)
0007
0008      Logical unit numbers used:
0009      LUNSPE: Lun to read spectrum
0010      LUNPAR: Lun for PARFIL
0011      LUNPRT: Lun for print output
0012      LUNCAL: Lun for calibration input, and energy table
0013      LUNTRM: Lun for terminal I/O (incl. DLPACK, MNPACK)
0014
0015      PARAMETER LUNSPE=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
0016
0017      PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
0018      NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
0019
0020      BYTE SPESPC(30), PARSPC(30), CALSPC(30), FILPRT(30), ENESPC(30)
0021
0022      CHARACTER*20 HDGLIN
0023
0024      INTEGER*4 JCOUNT
0025
0026      REAL*4 TO, SECNDS
0027
0028      COMMON /SPECTR/ JCOUNT(MAXCHN)
0029      COMMON /SPDESC/ NXCHAN, NYCHAN, IDATIM(9), NRUN, ISPELL, ITARG,
0030      ITEXT(18), LABEL
0031
0032      COMMON /OPPARS/ MDEV, SPESPC, PARSPC, MXITER, LBFIX, INREG, LIXLO, LIXHI,
0033      LIYLO, LIYHI, IYPWR, LIFLO, LIFHI, IPEAK, LBACK, LPEAK,
0034      LPEGA, NCoeff, COEFF(MAXCO), ITERA, NFREE,
0035      PEAK(NPPARM, MAXPK), IFLAG(NPPARM, MAXPK),
0036      INDEX(NPPARM, MAXPK), ISELEC, IGNOR(MAXPK), NREG,
0037      KREGLO(MAXREG), KREGHI(MAXREG), IMODE, INTCOR, NCALF,
0038      CALFAC(MXCALF), SIGMA(MAXPK), GAMMA(MAXPK), CALSPC,
0039      FILPRT, ENESPC
0040
0041      COMMON /OPPART/ IOPARS
0042      COMMON /RESULT/ CHNEW, CHIOLD, FVBACK, FVPEAK
0043      COMMON /ERRCDM/ IERROR
0044      COMMON /PARAM/ ILINK(NPPARM, MXLINK), NPAR, NDIMM, KUSE, KSKIP,
0045      TOL(6), TOHI(6)
0046
0047      COMMON /ARRAYS/ VMAT(MAXPAR*(MAXPAR+1)/2), DERIV(MAXPAR),
0048      RVEC(MAXPAR), HDERIV(MAXPAR)
0049
0050      COMMON /CONST/ PICON, EPSILN, SQRTPI, SRLN2
0051
0052      LOGICAL FILOPN
0053      COMMON /GLOBAL/ IOP, TO, IFIT, FILOPN
0054
0055      DATA IOPARS /0/
    
```

```

0001      Apply calibration (if any)
0002
0003      IF (NCALF .GT. 0) THEN
0004          DTEMP = DCHAN
0005          CALVAL = CALFAC(1)
0006          DO 1000 J=2,NCALF,1
0007              CALVAL = CALVAL*(DTEMP=CALFAC(J))
0008              DTEMP = DTEMP*DTEMP
0009
0010          1000 CONTINUE
0011      ELSE
0012          CALVAL = 0.000
0013      ENDIF
0014
0015      Return to calling program
0016
0017      RETURN
0018      *****
0019      END
    
```

```

0001 SUBROUTINE FITPAR (IANW)
      *****
      C*
      C* This routine defines parameters for fit
      C*
      C* Ver. 0.0/09-SEP-83(TK) Original version
      C* Ver. 1.0/26-SEP-83(DR)
      C* Ver. 1.0/02-DEC-83(DR)
      C*
0002 INCLUDE 'FIT.COM'
0003 IMPLICIT REAL*8 (A-H,O-Z)
      C*
      C* Logical unit numbers used:
      C*
      C* LUNSPC: Lun to read spectrum
      C* LUNPAR: Lun for PARFIL
      C* LUNPRT: Lun for print output
      C* LUNCAL: Lun for calibration input, and energy table
      C* LUNTRM: Lun for terminal i/o (incl. DLPACK, MNPACK)
0004 PARAMETER LUNSPC=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
0005 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
      C* NPPARM=5, MXCALF=3, MPOINT=500, MXLINK=20
0006 BYTE SPESPC(30), PARSPC(30), CALSPC(30), FILPRT(30), ENESPC(30)
0007 CHARACTER*20 HDGLIN
0008 INTEGER*4 JCOUNT
0009 REAL*4 TD,SECONDS
      C*
0010 COMMON /SPECTR/ JCOUNT(MAXCHN)
0011 COMMON /SPDESC/ NXCHAN,NYCHAN,IDATIM(9),NRUN,ISPILL,ITARG,
      C* ITEXT(10),LABEL
0012 COMMON /OPPARS/ MDEV,SPESPC,PARSPC,MXITER,LBFX,INREG,LIXLO,LIXHI,
      C* LIYLO,LIYHI,IYPAR,LIFLO,LIFHI,IPEAK,LBACK,LPEAK,
      C* LPBA,NCOEFF,COEFF(MAXCO),ITERA,NFREE,
      C* PEAK(NPPARM,MAXPK),IFLAG(NPPARM,MAXPK),
      C* INDEX(NPPARM,MAXPK),ISELEC,IGNOR(MAXPK),NREG,
      C* KREGLO(MAXREG),KREGHI(MAXREG),IMODC,INTCOR,NCALF,
      C* CALFAC(MXCALF),SIGMA(MAXPK),GAMMA(MAXPK),CALSPC,
      C* FILPRT,ENESPC
0013 COMMON /OPPART/ IOPARS
0014 COMMON /RESULT/ CHINEW,CHIOLD,FVBACK,FVPEAK
0015 COMMON /ERRCOM/ IERROR
0016 COMMON /PARAM/ ILINK(NPPARM,MXLINK),NPAR,NDIMM,KUSE,KSkip,
      C* TOL0(6),TOHI(6)
0017 COMMON /ARRAYS/ VMAT(MAXPAR*(MAXPAR+1)/2),DERIV(MAXPAR),
      C* RVEC(MAXPAR),HDERIV(MAXPAR)
0018 COMMON /CONST/ PICON,EPSILN,SGRTPI,SRLN2
0019 LOGICAL FILOPN

```

```

0020 COMMON /GLOBAL/ IOP,TD,IFIT,FILOPN
0021 DATA IOPARS /0/
0022 DATA TOL0 /MAXCHN, 0.000, 0.000, 0.000, 0.000, 0.000/
0023 DATA TOHI /0.000, MAXCHN, 1.000, 1.000, 1.000, 0.000/
      C**
      C*
0024 IERROR = 0
      C*
      C* Clear screen
0025 CALL MNIRAS
0026 TU = SCLNDS(0.0)
      C*
      C* Define limits for fitted quantities
      C*
0027 DO 1000 J=1,NREG,1
0028 TOL0(J) = MIN(TOL0(1),DBLE(KREGLO(J)))
0029 TOHI(1) = MAX(TOHI(1),DBLE(KREGHI(J)))
0030 CONTINUE
0031 TOHI(2) = TOHI(1) - TOL0(1)
0032 TOHI(6) = TOHI(2)

```

```

0033 Internal start-value corrections
      C*
      C* IF (INTCOR .NE. 1) GOTO 1015
      C*
      C* Setup start background parameters
0034 IF (LBFX .EQ. 0) THEN
      C*
      C* Determine lower average
      C*
0035 IL = 9999
0036 IM = 0
0037 DO 1005 J=1,NREG,1
0038 IL = MIN(IL,KREGLO(J))
0039 IM = MAX(IM,KREGHI(J))
1005 CONTINUE
0040 IL = MAX(2,IL)
0041 IM = MIN(MXCHAN-1,IM)
0042 SL = (JCOUNT(IL-1) + JCOUNT(IL) + JCOUNT(IL+1)) / 3
0043 SH = (JCOUNT(IM-1) + JCOUNT(IM) + JCOUNT(IM+1)) / 3
      C*
0044 COEFF(2) = (SH - SL) / DBLE(IM-IL)
      C*
0045 IF (COEFF(2) .EQ. 0.00) COEFF(2) = 5.0-5
0046 COEFF(1) = SL - COEFF(2) * IL
0047 DO 1010 I=1,NCOEFF-1,1
0048 COEFF(I) = SIGN(MAX(ABS(COEFF(I)),1.00-15),COEFF(I))
0049 IF (I .GE. 2) COEFF(I-1) = - COEFF(I) / TOHI(1)*#I
0050 CONTINUE
1010 CONTINUE
0051 ENDIF
0052
      C*
      C* Prepare data for fit

```

```

0053 1015 CALL VIZERO (INDEX,MAXPK,NPPARM)
0054 CALL VIZERO (ILINK,MXLINK,NPPARM)
      C*
      C* Run through the fit regions
      C*
0055 KUSE = 0
0056 DO 1020 J=1,NREG,1
0057 KUSE = KUSE + KREGHI(J) - KREGLO(J) + 1
1020 CONTINUE
0058 KSKIP = NXCHAN - KUSE
      C*
      C* Reserve parameters for background
      C*
0059 NPAR = 0
0060 IF (LBFX .EQ. 0) NPAR = NCOEFF
      C*
      C* Run through the peaks
      C*
0061 DO 1030 IPK=1,MAXPK,1
0062 IF (IGNOR(IPK) .EQ. 1) GOTO 1030
0063 IF (INTCOR .EQ. 1) CALL PEKDEF (IPK)
0064
      C*
      C* Set 'forgotten' flags
      C*
0065 IF (PEAK(4,IPK) .EQ. 0.000) IFLAG(4,IPK) = -2
0066 IF (PEAK(5,IPK) .EQ. 0.000) IFLAG(5,IPK) = -2
0067 IF (PEAK(6,IPK) .EQ. 0.000) THEN
0068 IFLAG(6,IPK) = -2
      C*
      C* ELSE
0069 IFLAG(2,IPK) = -1
      C*
      C* ENDIF
      C*
      C* Interpret flags
      C*
0070 DO 1025 IPARM=1,NPPARM,1
      C*
      C* IFLAG = 0: Free parameter
      C*
0071 IF (IFLAG(IPARM,IPK) .EQ. 0) THEN
0072 NPAR = NPAR+1
0073 IF (NPAR .GT. MAXPAR) GOTO 7000
0074 INDEX(IPARM,IPK) = NPAR
0075 ENDOF
      C*
      C* Linked parameter
      C*
0076 IF (IFLAG(IPARM,IPK) .GT. 0) THEN
0077 K = IFLAG(IPARM,IPK)
0078 IF (K .GT. MXLINK) GOTO 7005
0079 IF (ILINK(IPARM,K) .LE. 0) THEN
0080 NPAR = NPAR+1
0081 IF (NPAR .GT. MAXPAR) GOTO 7000
0082 ILINK(IPARM,K) = NPAR
0083 ENDOF

```

```

0084          INDEX(IPARM,IPK) = ILINK(IPARM,K)
0085          ENDIF
0086          1025 CONTINUE
0087          1030 CONTINUE
C*
C* Calculate number of degrees of freedom
C*
0088          NFREE = KUSE - NPAR
0089          NDIM = NPAR * (NPAR+1) / 2
0090          GOTO 9000
C*
C* Error message: Too many parameters
C*
0091          7000 CALL MNERAS
0092          CALL DLOUT ('Too many parameters ==')
0093          CALL DLOUT (' NPAR = ',NPAR)
0094          CALL DLOUT (' KUSE = ',KUSE)
0095          CALL DLOUT (' NDIM = ',NDIM)
0096          GOTO 8000
C*
C* Error message: Linkage flag too big
C*
0097          7005 CALL MNERAS
0098          CALL DLOUT ('Linkage flag too big ==')
0099          CALL DLKEY
0100          IERROR = -1
C*
C* Return to calling program
C*
0101          9000 RETURN
0102          *****
          END

```

```

0001          SUBROUTINE FITPFL
C*
C*
0002          INCLUDE 'FIT COM'
0003          IMPLICIT REAL*8 (A-H,O-Z)
C*
C* Logical unit numbers used:
C*
C* LUNSPE: Lun to read spectrum
C* LUNPAR: Lun for PARFIL
C* LUNPRI: Lun for print output
C* LUNCAL: Lun for calibration input, and energy table
C* LUNTRM: Lun for terminal I/O (incl. DLPACK, MNPACK)
C*
0004          PARAMETER LUNSPE=1, LUNCAL=2, LUNPRI=3, LUNPAR=4, LUNTRM = 5
C*
0005          PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
C*          NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
C*
0006          BYTE SPESPC(30),PARSPC(30),CALSPC(30),FILPRI(30),ENCSPC(30)
C*
0007          CHARACTER*20 HDGLIN
C*
0008          INTEGER*4 JCOUNT
C*
0009          REAL*4 T0,SECNDS
C*
0010          COMMON /SPECTR/ JCOUNT(MAXCHN)
0011          COMMON /SPDESC/ NXCHAN,NYCHAN,IDATIM(9),NRUN,ISPILL,ITARG,
C*          ITEXT(18),LABEL
0012          COMMON /OPPARS/ MDEV,SPESPC,PARSPC,MXITER,LBFI,INREG,LIXLO,LIXHI,
C*          LIYLO,LIYHI,IYPWR,LIFLO,LIFHI,IPEAK,LBACK,LPEAK,
C*          LPEHA,NCOEFF,COEFF(MAXCO),ITERA,NRICE,
C*          PEAK(NPPARM,MAXPK),IFLAG(NPPARM,MAXPK),
C*          INDEX(NPPARM,MAXPK),ISELC,IGNOK(MAXPK),NREG,
C*          KREGLO(MAXREG),KREGHI(MAXREG),IMODE,INTCOR,NCALF,
C*          CALFAC(MXCALF),SIGMA(MAXPK),GAMMA(MAXPK),CALSPC,
C*          FILPRI,ENESPC
0013          COMMON /OPPART/ IOPARS
0014          COMMON /RESULT/ CHINEW,CHIOLD,FVBACK,FVPEAK
0015          COMMON /ERRCOM/ IERROR
0016          COMMON /PARAM/ ILINK(NPPARM,MXLINK),NPAR,NDIMM,KUSE,KSKIP,
C*          TOL0(6),TOL1(6)
0017          COMMON /ARRAYS/ VMAT(MAXPAR*(MAXPAR+1)/2),DERIV(MAXPAR),
C*          RVEC(MAXPAR),HDERIV(MAXPAR)
0018          COMMON /CONST/ PICON,EPSILN,SQRTPI,SRLN2
C*
0019          LOGICAL FILOPN
0020          COMMON /GLOBAL/ IOP,T0,IFIT,FILOPN
C*
0021          DATA IOPARS /0/
C*
C* Option D(4). Save fit parameters
C*

```

```

0022          IF (IOP.EQ.4) THEN
0023              CALL PARLUN (LUNCAL)
0024              CALL PARFIL (PARSPC)
0025              CALL PARWT
0026              GOTO 1000
0027          ENDIF
C*
C* Option E(5): Read fit parameters
C*
0028          IF (IOP.EQ.5) THEN
0029              CALL PARLUN (LUNCAL)
0030              CALL PARFIL (PARSPC)
0031              CALL PARRD
0032              GOTO 1000
0033          ENDIF
C*
0034          1000 CALL PARLUN
0035          CALL PARFIL
C*
C* Return to calling program
C*
0036          9000 RETURN
0037          *****
          END

```



```

0001 SUBROUTINE FITPEA (X,IBACK)
      *****
      C*
      C* This subroutine calculates at a given -X- the contribution
      C* of the peaks
      C*
      C* < 0 : Only one peak (-IBACK) for display and output
      C* = 0 : All peaks for fit processing
      C* > 0 : All peaks for display and output
      C*
      C*
      C* Ver. 1.0/02-DEC-83 (DR) Original version
      C* Ver. 1.1/25-JAN-84 (TK) Implementation of peak selection
      C* Ver. 1.2/06-FEB-84 (DR) Implementation of folding with complex
      C* error function
    
```

```

0002 INCLUDE 'FIT.COM'
0003 IMPLICIT REAL*8 (A-H,O-Z)
      C*
      C* Logical unit numbers used:
      C*
      C* LUNSPC: Lun to read spectrum
      C* LUNPAR: Lun for PARFIT
      C* LUNPRT: Lun for print output
      C* LUNCAL: Lun for calibration input, and energy table
      C* LUNTRM: Lun for terminal i/o (incl. DLPACK, MNPACK)
    
```

```

0004 PARAMETER LUNSPC=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
0005 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
      NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
    
```

```

0006 BYTE SPESPC(30),PARSPC(30),CALSPC(30),FILPRT(30),ENESPC(30)
    
```

```

0007 CHARACTER*20 HDGLIN
    
```

```

0008 INTEGER*4 JCOUNT
    
```

```

0009 REAL*4 T0,SECNDS
    
```

```

0010 COMMON /SPECTR/ JCOUNT(MAXCHN)
0011 COMMON /SPDESC/ NXCHAN,NYCHAN,IDATIM(9),NRUN,ISPILL,ITARG,
      ITEXT(18),LABEL
0012 COMMON /OPPARS/ MDEV,SPESPC,PARSPC,MXITER,LBPIX,INREG,LIXLO,LIXHI,
      LTYLO,LTYHI,IYPWR,LIFLO,LIFHI,IPEAK,LBACK,LPEAK,
      LPEBA,NCOEFF,COEFF(MAXCO),ITERA,NFREE,
      PEAK(NPPARM,MAXPK),IFLAG(NPPARM,MAXPK),
      INDIR(NPPARM,MAXPK),IDLLEC,IGNOR(MAXPK),NREG,
      KHLGL0(MAXREG),KHLGL1(MAXREG),IMODI,INTCOR,NCALF,
      CALFAC(MXCALF),SIGMA(MAXPK),GAMMA(MAXPK),CALSPC,
      FILPRT,ENESPC
    
```

```

0013 COMMON /OPPART/ IOPARS
0014 COMMON /RESULT/ CHINEW,CHIOLD,FVBACK,FVPEAK
0015 COMMON /ERRCOM/ IERROR
0016 COMMON /PARAM/ ILINK(NPPARM, MXLINK),NPAR,NDIMM,KUSE,KSKIP,
    
```

```

0017 COMMON /ARRAYS/ T0LO(G),T0HI(G)
      VVRT(MAXPAR*(MAXPAR+1)/2),DERIV(MAXPAR),
      RVLC(MAXPAR),HDERIV(MAXPAR)
0018 COMMON /CONST/ PICON,EPSILN,SORTPI,SRLN2
    
```

```

0019 LOGICAL FILOPN
0020 COMMON /GLOBAL/ IOP,T0,IFIT,FILOPN
    
```

```

0021 DATA IOPARS /D/
    
```

```

0022 COMPLEX CWERF,C
    
```

```

      Prepare values
    
```

```

0023 FVPEAK = 0.000
    
```

```

      Determine 'peak range'
    
```

```

0024 IF (IBACK .GE. 0) THEN
0025   IL = 1
0026   IH = MAXPK
0027 ELSE
0028   IL = -IBACK
0029   IH = -IBACK
0030 ENDIF
    
```

```

0031 C*
0032 C* Calculate contribution of peaks
0033 C*
      DO 1015 IP=IL,IH,1
0034   IF (IGNOR(IP) .EQ. 1) GOTO 1015
0035   IF (IBACK .EQ. 0) THEN
0036     I1 = INDEX(1,IP)
0037     I2 = INDEX(2,IP)
0038     I3 = INDEX(3,IP)
0039     I6 = INDEX(6,IP)
0040   ENDIF
0041   XT = X - PEAK(I,IP)
0042   HEIGHT = PEAK(I,IP)
0043   IF (IFLAG(I,IP) .NE. -2) THEN
0044     C*
0045     C* A. Lorentzian peak
0046     ZREAL = XT / SIGMA(IP)
0047     ZIMAG = GAMMA(IP) / SIGMA(IP)
0048     C = CWERF(CMPLX(ZREAL,ZIMAG))
0049     DHEIG = DBLE(REAL(C)) * SORTPI * ZIMAG
0050     IF (IBACK .EQ. 0) THEN
0051       CDERIV = 2.00 * HEIGHT * ZIMAG * SORTPI / SIGMA(IP)
0052       DGAML = CDERIV * (ZREAL * DBLE(AIMAG(C)) +
0053         (ZIMAG + 0.500 / ZIMAG) * DBLE(REAL(C))
0054         - 1.00 / SORTPI)
0055       DPOSI = - CDERIV * (ZIMAG * DBLE(AIMAG(C)) -
0056         ZREAL * DBLE(REAL(C)))
0057     ENDIF
0058   ELSE
0059     C*
0060     C* B. Exponential tail to the left
0061     IF (IFLAG(4,IP) .NE. -2) THEN
0062       F = PEAK(4,IP)
0063       IF (U .LT. F) GOTO 1000
0064     ENDIF
0065     C*
0066     C* C. Exponential tail to the right
0067     IF (IFLAG(5,IP) .NE. -2) THEN
0068       F = PEAK(5,IP)
0069       IF (U .GT. F) GOTO 1000
0070     ENDIF
0071     DHEIG = (F - 2.00 * U) * F
0072     GOTO 1010
0073     C*
0074     C* D. Pure Gaussian peak
0075     IF (ABS(U) .GT. 2.600) GOTO 1015
0076     DHEIG = - U * U
0077     C*
0078     C* Determine derivatives
0079     DHEIG = EXP(DHEIG)
0080     IF (IBACK .EQ. 0) THEN
0081       DPOSI = 2.00 * U / SIGMA(IP) * HEIGHT * DHEIG
0082       DSIGM = U * DPOSI
0083     ENDIF
0084     C*
0085     C* Determine results and update derivatives (if needed)
0086     C*
0087     FUNCT = HEIGHT * DHEIG
0088     FVPEAK = FVPEAK + FUNCT
0089     IF (IBACK .EQ. 0) THEN
0090       IF (IFLAG(3,IP) .GT. 0) DHEIG = FUNCT
0091       IF (I1 .GT. 0) DERIV(I1) = DERIV(I1) + DPOSI
0092       IF (I2 .GT. 0) DERIV(I2) = DERIV(I2) + DSIGM
0093       IF (I3 .GT. 0) DERIV(I3) = DERIV(I3) + DHEIG
0094       IF (I6 .GT. 0) DERIV(I6) = DERIV(I6) + DGAML
0095     ENDIF
0096   1015 CONTINUE
0097     C*
0098     C* Return to calling program
0099     C*
0100   RETURN
0101 *****
0102 END
    
```

```

0001 SUBROUTINE FITPRT
      C=
      C= *****
      C= This subroutine handles the printout of the fit results
      C= to a print file
      C=
      C= Ver. 0.0/12-Oct-83(TK) Preliminary version
0002 INCLUDE 'FIT.COM'
0003 IMPLICIT REAL*8 (A-H,O-Z)
      C=
      C= Logical unit numbers used:
      C=
      C= LUNSPC: Lun to read spectrum
      C= LUNPAR: Lun for PARFIL
      C= LUNPRT: Lun for print output
      C= LUNCAL: Lun for calibration input, and energy table
      C= LUNTRM: Lun for terminal I/O (incl. DLPACK, MNPACK)
0004 PARAMETER LUNSPC=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
0005 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
      C= NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
0006 BYTE SPESPC(30),PARSPC(30),CALSPC(30),FILPRT(30),ENESPC(30)
0007 CHARACTER*20 HDGLIN
0008 INTEGER*4 JCOUNT
0009 REAL*4 T0,SECNDS
      C=
0010 COMMON /SPECTR/ JCOUNT(MAXCHN)
0011 COMMON /SPDESC/ NXCHAN,NYCHAN,IDATIM(9),NRUN,ISPILL,ITARG,
      C= ITEXT(18),LABEL
0012 COMMON /OPPARS/ MDEV,SPESPC,PARSPC,MXITER,LBFI,INREG,LIXLO,LIXHI,
      C= LIYLO,LIYHI,IYPWR,LIFLO,LIFHI,IPEAK,LBACK,LPEAK,
      C= LPEBA,NCOEFF,COEFF(MAXCO),ITERA,NFREE,
      C= PEAK(NPPARM,MAXPK),IFLAG(NPPARM,MAXPK),
      C= INDEX(NPPARM,MAXPK),ISELEC,IGNOR(MAXPK),NREG,
      C= KREGLO(MAXREG),KRECHI(MAXREG),IMODL,INTCOR,NCALF,
      C= CALFAC(MXCALF),SIGMA(MAXPK),GAMMA(MAXPK),CALSPC,
      C= FILPRT,ENESPC
0013 COMMON /OPPART/ IOPARS
0014 COMMON /RESULT/ CHINEM,CHIOLD,FVBACK,FVPEAK
0015 COMMON /ERRCOM/ IERROR
0016 COMMON /PARAM/ ILINK(NPPARM,MXLINK),NPAR,NDIMM,KUSE,KSKIP,
      C= TOLO(6),TOHI(6)
0017 COMMON /ARRAYS/ VMAT(MAXPAR*(MAXPAR+1)/2),DERIV(MAXPAR),
      C= RVEC(MAXPAR),HDERIV(MAXPAR)
0018 COMMON /CONST/ PICON,EPSILN,SQRTPI,SRLN2
      C=
0019 LOGICAL FILOPN
0020 COMMON /GLOBAL/ IOP,T0,IFIT,FILOPN
    
```

```

0021 DATA IOPARS /0/
      C=
      C= Ask for file-name
      C=
0022 CALL MNERAS
0023 CALL DLVIND (' Do you want a new print output-file? ',0,IAN)
0024 IF (.NOT. FILOPN .OR. IAN.EQ.1) THEN
0025   IF (FILOPN) CLOSE (UNIT=LUNPRT)
0026   FILOPN = .FALSE.
0027   CALL DLTXI (' Print output-file name',FILPRT,FILPRT,30,LEN)
0028 ENDIF
      C=
      C= Open print file (if not already open)
      C=
0029 IF (.NOT. FILOPN) THEN
0030   CALL ASSIGN (LUNPRT,FILPRT)
0031   FILOPN = .TRUE.
0032 ENDIF
      C=
      C= Print results (using FITOUT)
      C=
0033 CALL FITOUT (LUNPRT)
      C=
      C= Return to calling program
      C=
0034 RETURN
0035 *****
      C=
      C= END
    
```

```

0001 SUBROUTINE FITROU
      C=
      C= *****
      C= This subroutine routes a print file to the printer
      C=
      C= Ver. 0.0/12-Oct-83(TK) Preliminary version
0002 INCLUDE 'FIT.COM'
0003 IMPLICIT REAL*8 (A-H,O-Z)
      C=
      C= Logical unit numbers used:
      C=
      C= LUNSPC: Lun to read spectrum
      C= LUNPAR: Lun for PARFIL
      C= LUNPRT: Lun for print output
      C= LUNCAL: Lun for calibration input, and energy table
      C= LUNTRM: Lun for terminal I/O (incl. DLPACK, MNPACK)
0004 PARAMETER LUNSPC=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
0005 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
      C= NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
0006 BYTE SPESPC(30),PARSPC(30),CALSPC(30),FILPRT(30),ENESPC(30)
0007 CHARACTER*20 HDGLIN
0008 INTEGER*4 JCOUNT
0009 REAL*4 T0,SECNDS
      C=
0010 COMMON /SPECTR/ JCOUNT(MAXCHN)
0011 COMMON /SPDESC/ NXCHAN,NYCHAN,IDATIM(9),NRUN,ISPILL,ITARG,
      C= ITEXT(18),LABEL
0012 COMMON /OPPARS/ MDEV,SPESPC,PARSPC,MXITER,LBFI,INREG,LIXLO,LIXHI,
      C= LIYLO,LIYHI,IYPWR,LIFLO,LIFHI,IPEAK,LBACK,LPEAK,
      C= LPEBA,NCOEFF,COEFF(MAXCO),ITERA,NFREE,
      C= PEAK(NPPARM,MAXPK),IFLAG(NPPARM,MAXPK),
      C= INDEX(NPPARM,MAXPK),ISELEC,IGNOR(MAXPK),NREG,
      C= KREGLO(MAXREG),KRECHI(MAXREG),IMODL,INTCOR,NCALF,
      C= CALFAC(MXCALF),SIGMA(MAXPK),GAMMA(MAXPK),CALSPC,
      C= FILPRT,ENESPC
0013 COMMON /OPPART/ IOPARS
0014 COMMON /RESULT/ CHINEM,CHIOLD,FVBACK,FVPEAK
0015 COMMON /ERRCOM/ IERROR
0016 COMMON /PARAM/ ILINK(NPPARM,MXLINK),NPAR,NDIMM,KUSE,KSKIP,
      C= TOLO(6),TOHI(6)
0017 COMMON /ARRAYS/ VMAT(MAXPAR*(MAXPAR+1)/2),DERIV(MAXPAR),
      C= RVEC(MAXPAR),HDERIV(MAXPAR)
0018 COMMON /CONST/ PICON,EPSILN,SQRTPI,SRLN2
      C=
0019 LOGICAL FILOPN
0020 COMMON /GLOBAL/ IOP,T0,IFIT,FILOPN
    
```

```

0021 DATA IOPARS /0/
      C=
      C= Check whether a printfile is open or not
      C=
0022 CALL MNERAS
0023 IF (.NOT. FILOPN) THEN
0024   CALL DLOUT ('No print file open.')
0025   CALL DLKEY
0026 ELSE
0027   CLOSE (UNIT=LUNPRT)
0028   CALL ASSIGN (LUNPRT,'FITRES.OMP')
0029 ENDIF
      C=
      C= Return to calling program
      C=
0029 RETURN
0030 *****
0030 END
    
```

```

0001 SUBROUTINE FITSCT
      *****
      C*
      C* This subroutine sets the fit parameters in a dialog mode
      C*
0002 INCLUDE 'FIT.COM'
0003 IMPLICIT REAL*8 (A-H,O-Z)
      C*
      C* Logical unit numbers used:
      C*
      C* LUNSPE: Lun to read spectrum
      C* LUNPAR: Lun for PARFIL
      C* LUNPRT: Lun for print output
      C* LUNCAL: Lun for calibration input, and energy table
      C* LUNTRM: Lun for terminal i/o (incl. DLPACK, MNPACK)
0004 PARAMETER LUNSPE=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
0005 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
      C* MPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
0006 BYTE SPESPC(30),PARSPC(30),CALSPC(30),FILPRT(30),ENESPC(30)
0007 CHARACTER*20 HDGLIN
0008 INTEGER*4 JCOUNT
0009 REAL*4 TO,SECNDS
      C*
0010 COMMON /SPECTR/ JCOUNT(MAXCHN)
0011 COMMON /SPDESC/ NXCHAN,NYCHAN,IDATIM(9),NRUN,ISPILL,ITARG,
      C* ITXT(18),LABEL
0012 COMMON /OPPARS/ MDEV,SPESPC,PARSPC,MXITER,LBFIX,INREG,LIXLO,LIXHI,
      C* LIYLO,LIYHI,IYPWR,LIFLO,LIFHI,IPEAK,LBACK,LPEAK,
      C* LPEBA,NCOEFF,COEFF(MAXCO),ITERA,NFREE,
      C* PEAK(NPPARM,MAXPK),IFLAG(NPPARM,MAXPK),
      C* INDEX(NPPARM,MAXPK),ISELEC,IGNOR(MAXPK),NREG,
      C* KREGLO(MAXREG),KREGHI(MAXREG),IMODE,INTCOR,NCALF,
      C* CALFAC(MXCALF),SIGMA(MAXPK),GAMMA(MAXPK),CALSPC,
      C* FILPRT,ENESPC
0013 COMMON /OPPART/ IOPARS
0014 COMMON /RESULT/ CHINNEW,CHIOLD,FVBACK,FVPEAK
0015 COMMON /ERRCOM/ IERROR
0016 COMMON /PARAM/ ILINK(NPPARM,MXLINK),NPAR,NDIMM,KUSE,KSKIP,
      C* TOL(6),TOHI(6)
0017 COMMON /ARRAYS/ VMAT((MAXPAR*(MAXPAR+1))/2),DERIV(MAXPAR),
      C* RVEC(MAXPAR),HDERIV(MAXPAR)
0018 COMMON /CONST/ PICON,EPSILN,SQRTPI,SRLN2
      C*
0019 LOGICAL FILOPN
0020 COMMON /GLOBAL/ IOP,TO,IFIT,FILOPN
      C*
0021 DATA IOPARS /0/
      C*
0022 COMMON /BUFMEN/ MBUFF(600)
  
```

```

      C*
      C* If no spectrum present: Go home
      C*
0023 IF (NXCHAN .LE. 0) THEN
0024 CALL MNERAG
0025 CALL DLQUT ('0No spectrum to fit')
0026 CALL DLKLY
0027 IERROR = -1
0028 GOTO 9000
0029 ENDDIF
  
```

```

      C*
      C* Display sub menu
      C*
0030 IFIT = 0
0031 CALL MNCLR
0032 CALL MNBUFF (MBUFF,600)
0033 CALL MHEAD ('Set parameters for fit')
0034 CALL MNDEC ( 1, 'Maximum iteration count',MXITER,MXITER,0.32)
0035 CALL MNOPT ( 2, 'Set convergence radius for fit')
0036 CALL MNDEC ( 3, 'No of background coeffs',NCOEFF,NCOEFF,1,MAXCO)
0037 CALL MNYENO ( 4, 'Fixed background',LBFIX,LBFIX)
0038 IF (LBFIX.EQ.1) CALL MNDEC (5, 'Set background coeff.',
      C* ICoeff,ICoeff,1,NCoeff)
0039 CALL MNDEC ( 6, 'No of fit regions',NREG,NREG,1,MAXREG)
0040 CALL MNDEC ( 7, 'Define fit region',INREG,INREG,1,NREG)
0041 CALL MNDEC ( 8, 'Lower end of fit region',
      C* KREGLO(INREG),KREGLO(INREG),1,MAXCHN)
0042 CALL MNDEC ( 9, 'Upper end of fit region',
      C* KREGHI(INREG),KREGHI(INREG),1,MAXCHN)
0043 CALL MNOPT (11, 'Reset peak parameters and disable peaks')
0044 CALL MNYENO (12, 'Do internal start-value corrections',
      C* INTCOR,INTCOR)
0045 CALL MNOPT (14, 'Define peaks by crosshair cursor')
0046 CALL MNOPT (15, 'Define peaks by setting parameters')
0047 CALL MNOPT (17, 'Define flags globally')
0048 CALL MNOPT (19, 'Start the fit')
0049 CALL MNDISP
0050 CALL MNIN (IOP)
0051 IF (IOP) 1065,1000,1005
      C*
      C* The big option switch
      C*
0052 1005 GOTO (1000, 1006, 1000, 1000, 1010, 1000, 1000, 1000,
      C* 1000, 1000, 1020, 1000, 1000, 1020, 1035, 1000,
      C* 1040, 1000, 1045), IOP
      C*
      C* Option B(2): Set convergence radius for fit
      C*
0053 1006 CALL DIPAGE
0054 WRITE (5,1007) EPSILN
0055 1007 FORMAT ('..Old convergence radius = .E15.7./,
      C* ..Enter new value')
0056 READ (5,*) EPSILN
0057 GOTO 1000
  
```

```

      C*
      C* Option E(5): Set background coefficient
      C*
0058 1010 WRITE (5,1015) ICoeff,COEFF(ICoeff)
0059 1015 FORMAT ('..Background coefficient',I3,' = .E15.7./,
      C* ..Enter new value')
0060 READ (5,*) COEFF(ICoeff)
0061 GOTO 1000
      C*
      C* Option K(11): Reset peak parameters and disable peaks
      C*
0062 1020 DO 1025 J=1,MAXPK,1
0063 ICHOR(J) = 1
0064 CONTINUE
0065 CALL VDZERO (PEAK,MAXPK*NPPARM)
0066 CALL VIZERO (IFLAG,MAXPK*NPPARM)
0067 IF (IOP.EQ.14) GOTO 1030
0068 GOTO 1000
      C*
      C* Option N(14): Define peaks by crosshair cursor
      C*
0069 1030 CALL DIPAGE
0070 CALL FITCUR
0071 INTCOR = 1
0072 GOTO 1000
      C*
      C* Option O(15): Define peaks by setting parameters
      C*
0073 1035 CALL DIPAGE
0074 CALL FITST1
0075 GOTO 1000
      C*
      C* Option C(17): Define flags globally
      C*
0076 1040 CALL DIPAGE
0077 CALL FITST2
0078 GOTO 1000
      C*
      C* Option S(19): Start the fit
      C* Set parameters for fit
      C*
0079 1045 IANW = 1
0080 CALL FITPAR (IANW)
0081 IF (IERROR.LT.0) GOTO 9000
0082 IF (IANW.NE.1) GOTO 1000
  
```

```

C*
C* Display peak parameters and ask for confirmation
C*
0083 CALL DIPAGE
0084 WRITE (5,1050)
0085 1050 FORMAT (' ', 'The following peaks will be fitted: ', //,
+ ' ', 'No', 4X, 'Position', 4X, 'Gauss-FWHM', 7X, 'Height', 5X,
+ ' ', 'Lorentz-FWHM')
0086 DO 1060 J=1, MAXPK, 1
0087 IF (IGNOR(J) .EQ. 0) THEN

```

PDP-11 FORTRAN-77 VS. 0-0 09:38:27 26-Sep-86 Page 4
 FITSET.FTN,1 /F77/OP/TR:BLOCKS/WR

```

0088 WRITE (5,1055) J, PEAK(1,J), IFLAG(1,J), PEAK(2,J), IFLAG(2,J),
+ PEAK(3,J), IFLAG(3,J), PEAK(6,J), IFLAG(6,J)
0089 1055 FORMAT (' ', I2, ' ', F8.3, '(', I2, ')', F8.3, '(', I2, ')',
+ F13.2, '(', I2, ')', F8.3, '(', I2, ')')
0090 ENDIF
0091 1060 CONTINUE
0092 CALL DLYENO ('Correct', 1, J)
0093 IF (J .LE. 0) GOTO 1000
0094 CALL DIPAGE
0095 IFIT = 1
0096 GOTO 9000
0097
C*
C* Error return : no fit
C*
0098 1065 IF (IOP .LT. 0) IERROR = -1
C*
C* Return to calling program
C*
0099 9000 RETURN
0100 *****
0100 END

```

PDP-11 FORTRAN-77 VS. 0-0 09:36:47 26-Sep-86 Page 1
 FITSPR.FTN,1 /F77/OP/TR:BLOCKS/WR

```

0001 SUBROUTINE FITSPR
+-----+
C*
C*
C* INCLUDE 'FIT.COM'
0002 INCLUDE 'FIT.COM'
0003 IMPLICIT REAL*8 (A-H,O-Z)
C*
C* Logical unit numbers used:
C*
C* LUNSPE: Lun to read spectrum
C* LUNPAR: Lun for PARFIL
C* LUNPRT: Lun for print output
C* LUNCAL: Lun for calibration input, and energy table
C* LUNTRM: Lun for terminal I/O (incl. DLPACK, MNPACK)
0004 PARAMETER LUNSPE=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
0005 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
+ NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
0006 BYTE SPESPC(30), PARSPC(30), CALSPC(30), FILPRT(30), ENESPC(30)
0007 CHARACTER*20 HDGLIN
0008 INTEGER*4 JCOUNT
0009 REAL*4 TD, SECND9
0010 COMMON /SPECTR/ JCOUNT(MAXCHN)
0011 COMMON /SPDESC/ NXCHAN, NYCHAN, IDATIM(9), NRUN, ISPILL, ITARG,
+ ITEXT(3), LABEL
0012 COMMON /OPPARS/ MDEV, SPESPC, PARSPC, MXITER, LBFIX, INREG, LIXLO, LIXHI,
+ LIYLO, LIYHI, IYPR, LIFLO, LIFHI, IPEAK, LBACK, LPEAK,
+ LPEBA, NCOEFF, COEFF(MAXCO), ITERA, NFREE,
+ PEAK(NPPARM, MAXPK), IFLAG(NPPARM, MAXPK),
+ INDEX(NPPARM, MAXPK), ISELEC, IGNOR(MAXPK), NREG,
+ KREGLO(MAXREG), KREGHI(MAXREG), IMODE, INTCOR, NCALF,
+ CALFAC(MXCALF), SIGMA(MAXPK), GAMMA(MAXPK), CALSPC,
+ FILPRT, ENESPC
0013 COMMON /OPPART/ IOPARS
0014 COMMON /RESULT/ CHINEW, CHIOLD, FVBACK, FVPEAK
0015 COMMON /ERRCOM/ IERROR
0016 COMMON /PARAM/ ILINK(NPPARM, MXLINK), NPAR, NDIMM, KUSE, KSKIP,
+ TOL(6), TOH(6)
0017 COMMON /ARRAYS/ VMAT(MAXPAR*(MAXPAR+1)/2), DERIV(MAXPAR),
+ RVEC(MAXPAR), HDERIV(MAXPAR)
0018 COMMON /CONST/ PICON, EPSILN, SQRTPI, SRLN2
C*
0019 LOGICAL FILOPN
0020 COMMON /GLOBAL/ IOP, TD, IFIT, FILOPN
0021 DATA IOPARS /0/

```

PDP-11 FORTRAN-77 VS. 0-0 09:36:47 26-Sep-86 Page 2
 FITSPR.FTN,1 /F77/OP/TR:BLOCKS/WR

```

0022 1070 CALL MNFRAS
0023 CALL VJZERO (JCOUNT, MAXCHN)
0024 CALL ASSIGN (LUNSPE, SPESPC)
0025 1025 READ (LUNSPE, ERR=2000, END=2000) NXCHAN, NYCHAN, IDATIM,
+ NRUN, ISPILL, ITARG, ITEXT, LABEL
0026 IF (LABEL .NE. ISELEC) THEN
0027 DO 1030 J=1, NYCHAN, 1
0028 READ (LUNSPE, ERR=2000, END=2000) (JCOUNT(I), I=1, NXCHAN)
0029 1030 CONTINUE
0030 GOTO 1025
0031 ENDIF
C*
C* Correct spectrum found
C*
0032 IF (NYCHAN .NE. 1) THEN
0033 CALL DLOUT ('Can work only with one dimensional spectra')
0034 NXCHAN = 0
0035 ELSE
0036 READ (LUNSPE, ERR=2000, END=2000) (JCOUNT(J), J=1, NXCHAN)
C*
0037 WRITE (5,1035) LABEL, IDATIM, NRUN, ISPILL, ITARG, ITEXT, NXCHAN
0038 1035 FORMAT ('0', 'Spectrum with label: ', I6, /,
+ ' ', 'No', 4X, 'Position', 4X, 'Gauss-FWHM', 7X, 'Height', 5X, /,
+ ' ', 'Lorentz-FWHM', 7X, 'No. of channels: ', I5)
0039 ENDIF
0040 CLOSE (UNIT=LUNSPE)
0041 CALL DLKEY
0042 GOTO 9000
C*
C* Disk I/O error
C*
0043 2000 CALL DLOUT ('No such spectrum')
0044 NXCHAN = 0
0045 CLOSE (UNIT=LUNSPE)
0046 CALL DLKEY
C*
C* Return to calling program
C*
0047 9000 RETURN
0048 *****
0048 END

```

FIT-listing

page 61

```

0001 SUBROUTINE FITSFP
      *****
      CE
      CE This subroutine saves and parameters for plotting
      CE on a big machine.
      CE
      CE Ver. 1.0/08-Feb-84(TK) Original version
      CE
0002 INCLUDE 'FIT.COM'
0003 IMPLICIT REAL*8 (A-H,O-Z)
      CE
      CE Logical unit numbers used:
      CE
      CE LUNSPE: Lun to read spectrum
      CE LUNPAR: Lun for PARFIL
      CE LUNPRT: Lun for print output
      CE LUNCAL: Lun for calibration input, and energy table
      CE LUNTRM: Lun for terminal I/O (Incl. DLPACK, MNPACK)
      CE
0004 PARAMETER LUNSPE=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
0005 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
      CE * NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
      CE
0006 BYTE SPESPC(30), PARSPC(30), CALSPC(30), FILPRT(30), ENESPC(30)
      CE
0007 CHARACTER*20 HDGLIN
      CE
0008 INTEGER*4 JCOUNT
      CE
0009 REAL*4 T0, SECNDS
      CE
0010 COMMON /SPECTR/ JCOUNT(MAXCHN)
0011 COMMON /SPDESC/ NXCHAN, NYCHAN, IDATIM(9), NRUN, ISPILL, ITARG,
      CE * ITEXT(18), LABEL
0012 COMMON /OPPARS/ MOEV, SPESPC, PARSPC, MXITER, LBFIX, INREG, LIXLO, LIXHI,
      CE * LIYLO, LIYHI, IYPWR, LIFLO, LIFHI, IPEAK, LBACK, LPEAK,
      CE * LPEDA, NCOEFF, COEFF(MAXCO), ITERA, NFREE,
      CE * PEAK(NPPARM, MAXPK), IFLAG(NPPARM, MAXPK),
      CE * INDEX(NPPARM, MAXPK), ISELEC, IGNOR(MAXPK), NREG,
      CE * KREGLO(MAXREG), KREGHI(MAXREG), IMODE, INTCOR, NCALF,
      CE * CALFAC(MXCALF), SIGMA(MAXPK), GAMMA(MAXPK), CALSPC,
      CE * FILPRT, ENESPC
0013 COMMON /OPPART/ IOPARS
0014 COMMON /RESULT/ CHINEW, CHIOLD, FVBACK, FVPEAK
0015 COMMON /ERRCOM/ IERROR
0016 COMMON /PARAM/ ILINK(NPPARM, MXLINK), NPAR, NOIMM, KUSE, KSKIP,
      CE * TOL0(6), TOH1(6)
0017 COMMON /ARRAYS/ VMAT(MAXPAR*(MAXPAR+1)/2), DERIV(MAXPAR),
      CE * RVCC(MAXPAR), HDERIV(MAXPAR)
0018 COMMON /CONST/ PICON, EPSILN, SQRTPI, SRLN2
      CE
0019 LOGICAL FILOPN
0020 COMMON /GLOBAL/ IOP, T0, IFIT, FILOPN
    
```

```

0021 DATA IOPARS /0/
      CE
0022 BYTE SAVFIL(30)
      CE
      CE Ask for file
      CE
0023 CALL MNERAS
0024 CALL DLTXT ('Specify file:', SAVFIL, 30, LEN)
0025 CALL ASSIGN (LUNSPE, SAVFIL)
      CE
      CE Save some general information
      CE
0026 WRITE (LUNSPC, 1000) LIXLO, LIXHI, LIYLO, LIYHI, IYPWR, LIFLO, LIFHI,
      CE * IMODE, MAXREG, IREG, MAXCO, NCOEFF
0027 1000 FORMAT (8I7, 4IG)
0028 WRITE (LUNSPC, 1005) KREGLO, KREGHI
0029 1005 FORMAT (14IS)
      CE
      CE Save background
      CE
0030 WRITE (LUNSPC, 1010) COEFF
0031 1010 FORMAT (4(1PE20, 13))
    
```

```

0032 CE
0033 CE Save peak parameters
0034 CE
0035 DO 1020 J=1, MAXPK, 1
0036 IF (IGNOR(J) NE. 1) THEN
0037 WRITE (LUNSPC, 1015) J, (PEAK(K, J), K=1, NPPARM)
0038 FORMAT (1Z, 6(1X, 1PE12, 6))
0039 ENDF
0040 1020 CONTINUE
      CE
      CE Write a 'termination record' and close output file
      CE
0041 WRITE (LUNSPC, 1025)
0042 FORMAT ('-1', 78X)
0043 CLOSE (UNIT=LUNSPC)
      CE
      CE Return to calling program
      CE
0044 RETURN
0045 *****
0046 END
    
```

```

0001 SUBROUTINE FITST1
      *****
      C=
      C=
      C=
      C= This subroutine changes the fit parameters if neccessary
      C=
      C=
      C= Ver. 1.0 25-Feb-84 (DR) New menu structure
      C=
0002 INCLUDE 'FIT.COM'
0003 IMPLICIT REAL*8 (A-H,O-Z)
      C=
      C= Logical unit numbers used:
      C=
      C= LUNSPE: Lun to read spectrum
      C= LUNPAR: Lun for PARFIL
      C= LUNPRT: Lun for print output
      C= LUNCAL: Lun for calibration input, and energy table
      C= LUNTRM: Lun for terminal i/o (incl. DLPACK, MNPACK)
      C=
0004 PARAMETER LUNSPE=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
      C=
0005 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
      NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
      C=
0006 BYTE SPESPC(30),PARSPC(30),CALSPC(30),FILPRT(30),ENESPC(30)
      C=
0007 CHARACTER*20 HDGLIN
      C=
0008 INTEGER*4 JCOUNT
      C=
0009 REAL*4 T0,SECNDS
      C=
0010 COMMON /SPECTR/ JCOUNT(MAXCHN)
0011 COMMON /SPDESC/ NXCHAN,NYCHAN,IDATIM(9),NRUN,ISPILL,ITARG,
      ITEXT(18),LABEL
0012 COMMON /OPPARS/ MDEV,SPESPC,PARSPC,MXITER,LBFX,INREG,LIXLO,LIXHI,
      LIYLO,LIYHI,IYPWR,LIFLO,LIFHI,IPEAK,LBACK,LPEAK,
      LPEBA,NCOEFF,COEFF(MAXCO),ITERA,NFREE,
      PEAK(NPPARM,MAXPK),IFLAG(NPPARM,MAXPK),
      INDEX(NPPARM,MAXPK),ISELEC,IGNOR(MAXPK),NREG,
      KREGLO(MAXREG),KREGHI(MAXREG),IMODE,INTCOR,NCALF,
      CALFAC(MXCALF),SIGMA(MAXPK),GAMMA(MAXPK),CALSPC,
      FILPRT,ENESPC
      C=
0013 COMMON /OPPART/ IOPARS
0014 COMMON /RESULT/ CHINW,CHIOLD,FVBACK,FVPEAK
0015 COMMON /ERRCOM/ IERROR
0016 COMMON /PARAM/ ILINK(NPPARM,MXLINK),NPAR,NDIMM,KUSE,KSKIP,
      TOLD(6),TOMI(6)
      C=
0017 COMMON /ARRAYS/ VMAT(MAXPAR*(MAXPAR+1)/2),DERIV(MAXPAR),
      RVEC(MAXPAR),HDERIV(MAXPAR)
0018 COMMON /CONST/ PICON,EPSILN,SQRTPI,SRLN2
      C=
0019 LOGICAL FILOPN

```

```

0020 COMMON /GLOBAL/ IOP,T0,IFIT,FILOPN
      C=
0021 DATA IOPARS /D/
      C=
0022 COMMON /BUFMEN/ MBUFF(600)
      C=
0023 CHARACTER*16 KTEXT(6)
      C=
0024 DATA KTEXT /'Position is      ','Gauss-FWHM is      ','
      ','Height is      ','Low-tail is      ','
      ','High tail is      ','Lorentz-FWHM is      '/
      C=
0025 INTCOR = 0

```

```

      C=
      C= Display menu to ease changings
      C=
0026 1000 CALL MNCLR
0027 CALL MNDUFF (MBUFF,600)
0028 CALL MNHEAD ('Set parameters of peaks')
0029 CALL MNDEC ( 1,'Peak Nr ',IPEAK,IPEAK,1,MAXPK)
0030 CALL MNOPT ( 3,'Set position')
0031 CALL MNOPT ( 4,'Set Gauss-FWHM')
0032 CALL MNOPT ( 5,'Set height')
0033 CALL MNOPT ( 6,'Set low tail')
0034 CALL MNOPT ( 7,'Set high tail')
0035 CALL MNOPT ( 8,'Set Lorentz-FWHM')
0036 CALL MNDEC (10,'Position:      -1*fix, 0*fit, >0*group-ld
      IFLAG(1,IPEAK),IFLAG(1,IPEAK),-1,MXLINK)
0037 * CALL MNDEC (11,'FWHM-Gauss:  -1*fix, 0*fit, >0*group-ld
      IFLAG(2,IPEAK),IFLAG(2,IPEAK),-1,MXLINK)
0038 * CALL MNDEC (12,'Height:      -1*fix, 0*fit, >0*group-ld
      IFLAG(3,IPEAK),IFLAG(3,IPEAK),-1,MXLINK)
0039 * CALL MNDEC (13,'Low tail:    -2*no tail, -1*exp tail, 0*no tail',
      IFLAG(4,IPEAK),IFLAG(4,IPEAK),-2,MXLINK)
0040 * CALL MNDEC (14,'High tail:   -2*no tail, -1*exp tail, 0*no tail',
      IFLAG(5,IPEAK),IFLAG(5,IPEAK),-2,MXLINK)
0041 * CALL MNDEC (15,'FWHM-Lorentz: -1*fix, 0*fit, >0*group-ld
      IFLAG(6,IPEAK),IFLAG(6,IPEAK),-2,MXLINK)
0042 * CALL MNYEND (18,'Ignore this peak (Do not fit)',
      IGNOR(IPEAK),IGNOR(IPEAK),-2,MXLINK)
      C=
0043 CALL MNDISP
0044 CALL MNIN (IOP)
      C=
0045 IF (IOP.LT. 0) GOTO 9000
      C=
      C= The big option switch
      C=
0046 GOTO (1000, 1000, 1005, 1005, 1005, 1005, 1005, 1005,
      1000, 1000, 1000, 1000, 1000, 1000, 1000, 1000,
      1000, 1000), IOP
0047 GOTO 1000
      C=
      C= Option C(3) - M(8): Set peak parameters
      C=

```

```

0048 1005 IOP = IOP - 2
0049 CALL MNERAS
0050 WRITE (5,1010) KTEXT(IOP),PEAK(IOP,IPEAK)
0051 1010 FORMAT ('D',A16,F10.3,' ','Enter new value')
0052 READ (5,*) PEAK(IOP,IPEAK)
0053 IF (IOP.EQ. 2) SIGMA(IPEAK) = PEAK(2,IPEAK) / SRLN2
0054 IF (IOP.EQ. 6) GAMMA(IPEAK) = PEAK(6,IPEAK) / 2.D0
0055 IF (PEAK(4,IPEAK).GT. 0.D0) PEAK(4,IPEAK) = -PEAK(4,IPEAK)
0056 IF (PEAK(5,IPEAK).LT. 0.D0) PEAK(5,IPEAK) = -PEAK(5,IPEAK)
0057 GOTO 1000
      C=
      C= Return to calling program
      C=
0058 9000 RETURN
      C=
0059 END

```

FIT-listing

```

0001 SUBROUTINE FITST2
      *****
      C*
      C*
      C* This subroutine changes the flags globally
      C*
      C*
      C* Ver. 1.0 03-May-84 (DR) Original version
      C*
0002 INCLUDE 'FIT.COM'
0003 IMPLICIT REAL*8 (A-H,O-Z)
      C*
      C* Logical unit numbers used:
      C*
      C* LUNSPC: Lun to read spectrum
      C* LUNPAR: Lun for PARFIL
      C* LUNPRT: Lun for print output
      C* LUNCAL: Lun for calibration input, and energy table
      C* LUNTRM: Lun for terminal I/O (incl. DLPACK, MNPACK)
0004 PARAMETER LUNSPC=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
0005 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
      C*
      C* NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
0006 BYTE SPESPC(30),PARSPC(30),CALSPC(30),FILPRT(30),ENESPC(30)
0007 CHARACTER*20 HDGLIN
0008 INTEGER*4 JCOUNT
0009 REAL*4 TO,SECNDS
0010 COMMON /SPECTR/ JCOUNT(MAXCHN)
0011 COMMON /SPDESC/ NXCHAN,NYCHAN, IDATIM(9),NRUN,ISPILL,ITARG,
      C*
      C* ITEXT(18),LABEL
0012 COMMON /OPPARS/ MDEV,SPESPC,PARSPC,MXITER,LBFIX,INREG,LIXLO,LIXHI,
      C*
      C* LIVLO,LIVHI,IVPWR,LIFLO,LIFHI,IPEAK,LBACK,LPEAK,
      C*
      C* LPEBA,NCOEFF,COEFF(MAXCO),ITERA,NFREE,
      C*
      C* PEAK(NPPARM,MAXPK),IFLAG(NPPARM,MAXPK),
      C*
      C* INDEX(NPPARM,MAXPK),ISELEC,IGNOR(MAXPK),NREG,
      C*
      C* KREGLOC(MAXREG),KREGHI(MAXREG),IMODE,INTCOR,NCALF,
      C*
      C* CALFACC(MXCALF),SIGMA(MAXPK),GAMMA(MAXPK),CALSPC,
      C*
      C* FILPRT,ENESPC
0013 COMMON /OPPART/ IOPARS
0014 COMMON /RESULT/ CHINEW,CHIDL0,FVBACK,FVPEAK
0015 COMMON /ERRCOM/ IERROR
0016 COMMON /PARAM/ ILINK(NPPARM,MXLINK),NPAR,NDIMM,KUSE,KSKIP,
      C*
      C* TOLG(6),TOLH(6)
0017 COMMON /ARRAYS/ VMAT(MAXPAR*(MAXPAR+1)/2),DERIV(MAXPAR),
      C*
      C* RVEC(MAXPAR),HDERIV(MAXPAR)
0018 COMMON /CONST/ PICON,EPSILN,SQRTPI,SRLN2
0019 C*
      LOGICAL FILOPN
    
```

```

0020 COMMON /GLOBAL/ IOP,TO,IFIT,FILOPN
0021 DATA IOPARS /0/
0022 LOGICAL LLINE
0023 CHARACTER*12 KTEXT(8)
0024 DATA KTEXT /'Position', 'Gauss-FWHM',
      C*
      C* 'Height', 'Low tail',
      C*
      C* 'High tail', 'Lorentz-FWHM',
      C*
      C* 'Ignor - flag'/
      C**
      C* Display possible flags
      C*
0025 1000 CALL DIPAGE
0026 CALL DLOUT (' 1: Position: -1=fix, 0=fit, >0=group-id')
0027 CALL DLOUT (' 2: FWHM-Gauss: -1=fix, 0=fit, >0=group-id')
0028 CALL DLOUT (' 3: Height: -1=fix, 0=fit, >0=group-id')
0029 CALL DLOUT (' 4: Low tail: -2.0=no tail, -1=exp tail')
0030 CALL DLOUT (' 5: High tail: -2.0=no tail, -1=exp tail')
0031 CALL DLOUT (' 6: FWHM-Lorentz: -1=fix, 0=fit, >0=group-id')
0032 CALL DLOUT (' ')
0033 CALL DLOUT (' 8: Ignor - flag : YES / NO')
0034 CALL DLOUT (' ')
0035 CALL DLOUT (' Which flag do you want to set')
0036 CALL DLOUT (' 0 = No setting wanted',KFLAG,KFLAG,0.0)
0037 IF (KFLAG.EQ.0) GOTO 9000
0038 IF (KFLAG.GT.6) GOTO 1025
      C*
    
```

```

0039 LLINE = .TRUE.
0040 DO 1020 I=1,MAXPK,1
0041 IF (LLINE) THEN
0042 ILINE = 0
0043 CALL DIPAGE
0044 WRITE (5,1015) KTEXT(KFLAG)
0045 1015 FORMAT (' Set ',A12,' flag :')
0046 ILINE = 1
0047 LLINE = .FALSE.
0048 ENDIF
0049 IF (IGNOR(I).EQ.1) GOTO 1020
0050 ILINE = ILINE + 2
0051 CALL DLOUT (' Peak Nr. ',I)
0052 CALL DLDEC (' to ',IFLAG(KFLAG,I),IFLAG(KFLAG,I),-2,MXLINK)
0053 IF (ILINE.GT.28) THEN
0054 LLINE = .TRUE.
0055 ENDIF
0056 1020 CONTINUE
0057 GOTO 1000
      C*
      C* Set Ignor-flag
      C*
0058 1025 IF (KFLAG.GT.8) GOTO 1000
0059 LLINE = .TRUE.
0060 DO 1040 I=1,MAXPK,1
    
```

```

0061 IF (LLINE) THEN
0062 ILINE = 0
0063 CALL DIPAGE
0064 WRITE (5,1035) KTEXT(KFLAG)
0065 1035 FORMAT (' Set ',A12)
0066 ILINE = 1
0067 LLINE = .FALSE.
0068 ENDIF
0069 ILINE = ILINE + 2
0070 CALL DLOUT (' Peak Nr. ',I)
0071 CALL DLZERO (' to ',IGNOR(I),IGNOR(I),-2,MXLINK)
0072 IF (ILINE.GT.28) THEN
0073 LLINE = .TRUE.
0074 ENDIF
0075 1040 CONTINUE
0076 GOTO 1000
      C*
      C* Return to calling program
      C*
0077 9000 RETURN
0078 *****
      END
    
```

POP-11 FORTRAN-77 VS. 0-0 09:40:17 26-Sep-86 Page 1
 PEKDEF.FTN,1 /F77/OP/TR:BLOCKS/WR

```

0001 SUBROUTINE PEKDEF (IPK)
      *****
      C*
      C* This subroutine sets default values for a selected peak
      C*
      C* Ver. 1.0/22-Nov-83(TK) Original version
      C* Ver. 1.1/17-Jan-84(TK) Better handling of background under peak
  
```

```

0002 INCLUDE 'FIT.COM'
0003 IMPLICIT REAL*8 (A-H,O-Z)
      C*
      C* Logical unit numbers used:
      C*
      C* LUNSPE: Lun to read spectrum
      C* LUNPAR: Lun for PARFIL
      C* LUNPRT: Lun for print output
      C* LUNCAL: Lun for calibration input, and energy table
      C* LUNTRM: Lun for terminal I/O (incl. DLPACK, MNPACK)
      C*
0004 PARAMETER LUNSPE=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
0005 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
      NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
      C*
0006 BYTE SPESPC(30), PARSPC(30), CALSPC(30), FILPRT(30), ENESPC(30)
      C*
0007 CHARACTER=20 HDGLIN
      C*
0008 INTEGER=4 JCOUNT
      C*
0009 REAL=4 TO, SECNDS
      C*
0010 COMMON /SPECTR/ JCOUNT(MAXCHN)
0011 COMMON /SPDESC/ NXCHAN, NYCHAN, IDATIM(9), NRUN, ISPILL, ITARG,
      ITEXT(10), LABEL
0012 COMMON /OPPARS/ MDEV, SPESPC, PARSPC, MXITER, LBFX, INREG, LIXLO, LIXHI,
      LIYLO, LIYHI, IYPWR, LIFLO, LIFHI, IPEAK, LBACK, LPEAK,
      LPEA, MCOEFF, COEFF(MAXCO), ITERA, NFREE,
      PEAK(NPPARM, MAXPK), IFLAG(NPPARM, MAXPK),
      INDEX(NPPARM, MAXPK), ISELEC, IGNOR(MAXPK), NREG,
      KREGLO(MAXREG), KREGHI(MAXREG), IMODE, INTCOR, NCALF,
      CALFAC(MXCALF), SIGMA(MAXPK), GAMMA(MAXPK), CALSPC,
      FILPRT, ENESPC
0013 COMMON /OPPART/ IOPARS
0014 COMMON /RESULT/ CHNEW, CHIOLD, FVBACK, FVPEAK
0015 COMMON /ERRCOM/ IERROR
0016 COMMON /PARAM/ ILINK(NPPARM, MXLINK), NPAR, NDIMM, KUSE, KSKIP,
      TOLO(6), TOHI(6)
0017 COMMON /ARRAYS/ VMAT(MAXPAR=(MAXPAR+1)/2), DERIV(MAXPAR),
      RVEC(MAXPAR), HDERIV(MAXPAR)
0018 COMMON /CONST/ PICON, EPSILN, SORTPI, SRLN2
      C*
0019 LOGICAL FILOPN
0020 COMMON /GLOBAL/ IOP, TO, IFIT, FILOPN
  
```

POP-11 FORTRAN-77 VS. 0-0 09:40:17 26-Sep-86 Page 2
 PEKDEF.FTN,1 /F77/OP/TR:BLOCKS/WR

```

0021 DATA IOPARS /0/
      C*
0022 INTEGER=4 J4
      C*
      C* First do some adjustment of the position (parameter 1)
      C*
0023 IF (IFLAG(1,IPK) .EQ. 0) THEN
0024   I = INT(PEAK(1,IPK)+0.500)
0025   J4 = JCOUNT(I)
0026   IF (JCOUNT(I-1) .GT. J4) THEN
0027     J4 = JCOUNT(I-1)
0028     PEAK(1,IPK) = DBLE(I-1)
0029   ENDIF
0030   IF (JCOUNT(I+1) .GT. J4) PEAK(1,IPK) = I+1
0031 ENDIF
      C*
      C* Find in which fit region the peak is situated
      C*
0032 I = INT(PEAK(1,IPK)+0.500)
0033 DO 1000 J=1, NREG, 1
0034   IF (KREGLO(J) .GT. I .OR. KREGHI(J) .LT. I) GOTO 1000
0035   ICL = KREGLO(J)
0036   ICH = KREGHI(J)
0037   GOTO 1005
0038 1000 CONTINUE
      C*
      C* Then set height (parameter 3)
      C*
0039 1005 IF (IFLAG(3,IPK) .EQ. 0 .OR. PEAK(3,IPK) .LE. 0.000) THEN
0040   PEAK(3,IPK) = JCOUNT(INT(PEAK(1,IPK)+0.500))
0041   CALL FITBAC (PEAK(1,IPK), 1)
0042   PEAK(3,IPK) = PEAK(3,IPK) - (0.900=FVBACK)
0043 ENDIF
  
```

```

      C*
      C* Now try to estimate a Gauss FWHM (parameter 2)
      C* 1. Find nearest peak
      C*
0044 IF (IFLAG(2,IPK) .EQ. 0 .OR. PEAK(2,IPK) .LE. 0.000) THEN
0045   I = 0
0046   DIFF = 1.007
0047   DO 1010 J=1, MAXPK, 1
0048     IF (IGNOR(J) .EQ. 1) GOTO 1010
0049     IF (J .NE. IPK) THEN
0050       IF (ABS(PEAK(1,IPK)-PEAK(1,J)) .LT. DIFF) THEN
0051         DIFF = ABS(PEAK(1,IPK)-PEAK(1,J))
0052       ENDIF
0053     ENDIF
0054 1010 CONTINUE
      C*
      C* If distance to nearest peak is less than 1.5 channels
      C* do some corrections
      C*
0055 IF (I .NE. 0 .AND. DIFF .LT. 1.500) THEN
0056   PEAK(1,IPK) = PEAK(1,IPK)+SIGN(0.7500,DBLE(IPK-I))
  
```

POP-11 FORTRAN-77 VS. 0-0 09:40:17 26-Sep-86 Page 3
 PEKDEF.FTN,1 /F77/OP/TR:BLOCKS/WR

```

0057 PEAK(3,IPK) = JCOUNT(INT(PEAK(1,IPK)+0.500))
0058 DIFF = 1.500
0059 ENDIF
      C*
      C* 2. Set Gauss-FWHM to a reasonable value (straight forward)
      C*
0060 I = INT(PEAK(1,IPK)+0.500)
0061 CALL FITBAC (DFLOAT(I), 1)
0062 R8 = 0.500 * (PEAK(3,IPK)-FVBACK)
0063 IL = I
0064 IH = I
0065 1015 IL = IL-1
0066 IF (IL .GT. ICL) THEN
0067   CALL FITBAC (DFLOAT(IL), 1)
0068   IF ((DBLE(JCOUNT(IL))-FVBACK) .GT. R8) GOTO 1015
0069 ENDIF
0070 1020 IH = IH+1
0071 IF (IH .LT. ICH) THEN
0072   CALL FITBAC (DFLOAT(IH), 1)
0073   IF ((DBLE(JCOUNT(IH))-FVBACK) .GT. R8) GOTO 1020
0074 ENDIF
0075 PEAK(2,IPK) = MIN(DBLE(IH-IL), 15.000)
      C*
      C* 3. Correct first estimate in cases of near peaks
      C*
0076 IF (DIFF .LT. 1.005 .AND. PEAK(2,IPK) .GT. DIFF)
      + PEAK(2,IPK) = DIFF/2.
0077 ENDIF
0078 IF (PEAK(2,IPK) .LE. 0.000) THEN
0079   CALL DLOUT ('Merde', IPK)
0080   CALL DLKEY
0081   PEAK(2,IPK) = 1.500
0082 ENDIF
      C*
      C* Return to calling program
      C*
0083 RETURN
0084 *****
      C* END
  
```



```

0001 SUBROUTINE SETUP
      *****
      C=
      C= This subroutine sets up the fit program
      C=
      C= Ver. 1.0/22-Nov-83(TK) Original version
      C=
0002 INCLUDE 'FIT.CUM'
0003 IMPLICIT REAL*8 (A-H,O-Z)
      C=
      C= Logical unit numbers used:
      C=
      C= LUNSPE: Lun to read spectrum
      C= LUNPAR: Lun for PARFIL
      C= LUNPRT: Lun for print output
      C= LUNCAL: Lun for calibration input, and energy table
      C= LUNTRM: Lun for terminal I/O (incl. DLPACK, MNPACK)
      C=
0004 PARAMETER LUNSPE=1, LUNCAL=2, LUNPRT=3, LUNPAR=4, LUNTRM = 5
      C=
0005 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
      C= NPPARM=6, MXCALF=3, MPOINT=500, MXLINK=20
      C=
0006 BYTE SPESPC(30),PARSPC(30),CALSPC(30),FILPRT(30),ENESPC(30)
0007 CHARACTER*20 HDGLIN
      C=
0008 INTEGER*4 JCOUNT
      C=
0009 REAL*4 TD,SECNDS
      C=
0010 COMMON /SPECTR/ JCOUNT(MAXCHN)
0011 COMMON /SPDESC/ NXCHAN,NYCHAN,IDATIM(9),NRUN,ISPILL,ITARG,
      C= ITEXT(18),LABEL
0012 COMMON /OPPARS/ MDEV,SPESPC,PARSPC,MXITER,LBFIK,INREG,LIXLO,LIXHI,
      C= LIYLO,LIYHI,IYPWR,LIFLO,LIFHI,IPEAK,LBACK,LPEAK,
      C= LPEBA,NCOEFF,COEFF(MAXCO),ITERA,NFREE,
      C= PEAK(NPPARM,MAXPK),IFLAG(NPPARM,MAXPK),
      C= INDEX(NPPARM,MAXPK),ISELEC,IGNOR(MAXPK),NREG,
      C= KREGLO(MAXREG),KREGHI(MAXREG),IMODE,INTCOR,NCALF,
      C= CALFAC(MXCALF),SIGMA(MAXPK),GAMMA(MAXPK),CALSPC,
      C= FILPRT,ENESPC
0013 COMMON /OPPART/ IOPARS
0014 COMMON /RESULT/ CHINEM,CHIOLO,FVBACK,FVPEAK
0015 COMMON /ERRCDM/ IERROR
0016 COMMON /PARAM/ ILINK(NPPARM,MXLINK),NPAR,NDIMM,KUSE,KSKIP,
      C= TOL(6),TOHI(6)
0017 COMMON /ARRAYS/ VMAT(MAXPAR*(MAXPAR+1)/2),DERIV(MAXPAR),
      C= RVEC(MAXPAR),HDERIV(MAXPAR)
0018 COMMON /CONST/ PICON,EPSILN,SQRTPI,SRLN2
      C=
0019 LOGICAL FILOPN
0020 COMMON /GLOBAL/ IOP,TD,IFIT,FILOPN
      C=
  
```

```

0021 DATA IOPARS /0/
      C=
0022 NCALF = 0
0023 CALL PARRD
0024 CALL VJZERO (JCOUNT,MAXCHN)
0025 CALL DIWDM (105,1023,30,700)
0026 CALL ERRSET (29, .TRUE., .FALSE., .TRUE., .FALSE.)
0027 CALL MNLUN (LUNTRM)
      C=
      C= Return to calling program
      C=
0028 RETURN
      C=
0029 END
  
```

```

0001 C* COMPLEX FUNCTION CWERF(Z)
C* .....
C* This function is used for calculating the complex error function
C* where  $w(z) = \exp(-z^2) * \operatorname{erfc}(-iz)$ 
C*  $\operatorname{erfc}(z) = 1 - \operatorname{erf}(z)$ 
C* Literature : Abramowitz, Stegun, chp.7
C* W.Gautschi, comm. dcm 12 (1969) 635
C* K.S.Koelbig, comm. dcm 15 (1972) 465
C* D.H.Wilkinson, NIM 95 (1971) 259
C* C.J.Batty et al. NIM 137 (1976) 179
C*
C* Ver. 1.0 05-Feb-84 (DR) Original version
C* Ver. 1.1 10-Mar-84 (DR) Bug removed
C*
0002 C* IMPLICIT REAL*8 (A-H,O-Z)
0003 C* COMPLEX Z
0004 C* LOGICAL B
0005 C* REAL*8 LAMBDA
0006 C* DATA XLIMIT /5.33D0/, YLIMIT /4.29D0/,
C* DCONST /1.12837916709551D0/
C*
0007 C* XX = DBLE(REAL(Z))
0008 C* YY = DBLE(AIMAG(Z))
0009 C* X = ABS(XX)
0010 C* Y = ABS(YY)
0011 C* IF (Y .LT. YLIMIT .AND. X .LT. XLIMIT) THEN
0012 C* S = (1.0D0 - Y / YLIMIT) * SQRT(1.0D0 - X / XLIMIT)
0013 C* H = 1.6D0 * S
0014 C* H2 = 2.0D0 * H
0015 C* NC = 6 + INT(23.DD * S)
0016 C* NU = 9 + INT(21.DD * S)
0017 C* LAMBDA = H2**NC
0018 C* B = LAMBDA .EG. D.DD
0019 C* ELSE
0020 C* H = 0.DD
0021 C* NC = 0
0022 C* NU = 8
0023 C* LAMBDA = D.DD
0024 C* B = .TRUE.
0025 C* ENDIF
0026 C* R1 = 0.DD
0027 C* R2 = 0.DD
0028 C* S1 = 0.DD
0029 C* S2 = 0.DD
0030 C* N = NU + 1

```

```

0031 C* 1000 N = N - 1
0032 C* FN = DFLOAT(N + 1)
0033 C* T1 = Y * W * FN * R1
0034 C* T2 = X - FN * R2
0035 C* C = 0.5D0 / (T1 * T1 + T2 * T2)
0036 C* R1 = C * T1
0037 C* R2 = C * T2
0038 C* IF (H .GT. 0.DD .AND. N .LE. NC) THEN
0039 C* T1 = LAMBDA * S1
0040 C* S1 = R1 * T1 - R2 * S2
0041 C* S2 = R2 * T1 + R1 * S2
0042 C* LAMBDA = LAMBDA / H2
0043 C* ENDIF
0044 C* IF (N .GT. 0) GOTO 1000
0045 C* IF (B) THEN
0046 C* RS1 = R1
0047 C* RS2 = R2
0048 C* ELSE
0049 C* RS1 = S1
0050 C* RS2 = S2
0051 C* ENDIF
0052 C* RS1 = DCONST * RS1
0053 C* IF (Y .EQ. 0.DD) RS1 = EXP(-X * X)
0054 C* CWERF = CMPLX(RS1, DCONST * RS2)
0055 C* IF (YV .LT. 0.DD) THEN
0056 C* CWERF = 2.DD * CEXP(-CMPLX(X,Y) * CMPLX(X,Y)) - CWERF
0057 C* IF (XX .GT. 0.DD) CWERF = CONJG(CWERF)
0058 C* ELSE
0059 C* IF (XX .LT. 0.DD) CWERF = CONJG(CWERF)
0060 C* ENDIF
C*
C* Return to calling program
C*
0061 C* RETURN
C* *****
0062 C* END

```

```

0001 C* SUBROUTINE DATE (KDATE)
C* .....
C* This program gets the actual date
C* Ver 1.0 10-Jan-85 DR Original Version
C*
0002 C* INTEGER*2 KDATE(5), DATIM(8), CAL1(12), CAL2(12)
0003 C* BYTE STRING,BLANK
0004 C* CHARACTER*10 FORM
0005 C* BYTE FORM1(10)
0006 C* DATA CAL1 /'Ja','Fe','Ma','Ap','Ma','Ju',
C* 'Ju','Au','Se','Oc','No','De'/
0007 C* DATA CAL2 /'n','b','r','r','y','n',
C* 'l','g','p','t','v','c'/
0008 C* DATA STRING /'.'/, BLANK /'.'/
0009 C* EQUIVALENCE (FORM,FORM1(1))
C*
0010 C* CALL GETTIM (DATIM)
0011 C* WRITE (FORM,1000) DATIM(3),STRING,CAL1(DATIM(2)),
C* CAL2(DATIM(2)),DATIM(1),BLANK
0012 C* 1000 FORMAT (I2,A1,A2,A2,I2,A1)
0013 C* IF (FORM1(1) .EQ. BLANK) FORM1(1) = '0'
0014 C* IF (FORM1(2) .EQ. BLANK) FORM1(2) = '0'
0015 C* READ (FORM,1005) (KDATE(I),I=1,5)
0016 C* 1005 FORMAT (5A2)
C*
C* Return to calling program
C*
0017 C* RETURN
C* *****
0018 C* END

```

```

0001 C* SUBROUTINE TIME (KTIME)
C* .....
C* This program gets the actual time
C* Ver 1.0 10-Jan-85 DR Original Version
C*
0002 C* INTEGER*2 KTIME(4), DATIM(8)
0003 C* BYTE STRING,BLANK
0004 C* CHARACTER*8 FORM
0005 C* BYTE FORM1(8)
0006 C* DATA STRING /'.'/, BLANK /'.'/
0007 C* EQUIVALENCE (FORM,FORM1(1))
C*
0008 C* CALL GETTIM (DATIM)
0009 C* WRITE (FORM,1000) DATIM(4),STRING,DATIM(5),STRING,DATIM(6)
0010 C* 1000 FORMAT (I2,A1,I2,A1,I2)
0011 C* IF (FORM1(1) .EQ. BLANK) FORM1(1) = '0'
0012 C* IF (FORM1(4) .EQ. BLANK) FORM1(4) = '0'
0013 C* IF (FORM1(7) .EQ. BLANK) FORM1(7) = '0'
0014 C* READ (FORM,1005) (KTIME(I),I=1,4)
0015 C* 1005 FORMAT (4A2)
C*
C* Return to calling program
C*
0016 C* RETURN
C* *****
0017 C* END

```

```

0001 SUBROUTINE SPXINV (A,NDIM)
      *****
      Inversion of a packed symmetric matrix CERN Lib. F106
      *****
      +1: Everything was ok.
      IERR: -1: Bad matrix
           -2: Invalid dimension parameter (NDIM)
      *****
      Ver. 1.0/16-DEC-79(RG) Implemented under RSX-11-M
      Ver. 1.1/11-SEP-83(TK) Minor modifications
      Ver. 1.2/01-OCT-83(DR) Minor modifications
      Ver. 1.3/08-MAR-84(TK) Some corrections
      *****
0002 IMPLICIT REAL*8 (A-H,D-Z)
0003 PARAMETER MAXDIM = 40
0004 COMMON /ERRCOM/ IERR
0005 DIMENSION INDEX(MAXDIM),RK(MAXDIM),A(MAXDIM*(MAXDIM+1)/2)
0006 DATA TOL/ 1.D-12/
      Set up subroutine
      *****
0007 IERR = 1
0008 IF (NDIM .GT. MAXDIM) .THEN
0009     IERR = -2
0010     GOTO 9000
0011 ENDIF
0012 NMAX = NDIM * (NDIM+1) / 2
0013 NDM1 = NDIM - 1
      *****
0014 DO 1000 I=1,NDIM
0015     INDEX(I) = 1
0016     CONTINUE
0017 DO 1020 I=1,NDIM
      Find pivot
      *****
0018     JJ = 1
0019     MDIM = NDIM
0020     PIVOT = D.D0
0021     DO 1005 J=1,NDIM
0022     IF (INDEX(J) .NE. 0) THEN
0023     AJJ = ABS(A(JJ))
0024     IF (AJJ .GT. PIVOT) THEN
0025     PIVOT = AJJ
0026     K = J
0027     IF KK = JJ
0028     ENDIF
0029     ENDIF
    
```

```

0030     JJ = JJ + MDIM
0031     MDIM = MDIM - 1
0032     CONTINUE
0033     IF (PIVOT/ABS(A(1))) .LT. TOL) THEN
0034     IERR = -1
0035     GOTO 9000
0036     ENDIF
0037     INDEX(K) = 0
0038     PIVOT = - A(KK)
    
```

```

      Elimination
      *****
0039     NP = NDM1
0040     JK = K
0041     NM = 1
0042     DO 1015 J=1,NDIM
0043     IF (J .EQ. K) THEN
0044     A(JK) = 1.D0 / PIVOT
0045     RK(J) = D.D0
0046     NM = 0
0047     NP = 1
0048     ELSE
0049     AJK = SIGN (MAX (TOL,ABS(A(JK))),-A(JK))
0050     RK(J) = AJK / PIVOT
0051     RK(J) = SIGN (MAX (TOL,ABS(RK(J))),RK(J))
0052     IF (AJK .NE. D.D0) THEN
0053     NPC = NDM1
0054     JL = J
0055     DO 1010 L=1,J
0056     A(JL) = A(JL) + AJK * RK(L)
0057     JL = JL + NPC
0058     NPC = NPC - 1
0059     CONTINUE
0060     ENDIF
0061     A(JK) = RK(J)
0062     ENDIF
0063     JK = JK + NP
0064     NP = NP - NM
0065     CONTINUE
0066     CONTINUE
      *****
0067     DO 1025 I=1,NMAX
0068     A(I) = - A(I)
0069     CONTINUE
      *****
0070     RETURN
0071     *****
      END
    
```

```

0001 SUBROUTINE PRTHDR (JMAX,JSUM)
      *****
      This subroutine prints the spectrum header on top of a picture
      *****
0002     Ver. 1.0/08-DEC-83(TK) Original Version
0003     Ver. 1.1/14-DEC-83(TK) LABEL Implemented
      *****
0004     COMMON /SPDESC/ NXCHAN,NYCHAN,IDATIM(9),
0005     IRUN,ISPILL,ITARG,ITEXT(18),LABEL
      *****
0006     INTEGER*4 JMAX,JSUM
0007     Set cursor to homeposition and switch to alpha mode
      *****
0008     CALL DIHOME
0009     CALL DIANU
      *****
0010     Print header
      *****
0011     WRITE (5,1000) IDATIM,IRUN,ISPILL,ITARG,LABEL,JSUM,JMAX,ITEXT
0012     1000 FORMAT ('* * * * * Run: I4, Spill: I3, Target: I3,
0013     * * * * * Label: I4,
0014     * * * * * Sum: I11, * * * * * Maximum: 2X, I10A2)
      *****
0015     Return to calling program
      *****
0016     RETURN
0017     *****
      END
    
```

BEEP MACRO M1200 25-FEB-85 13:23 PAGE 1

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16 000000      007
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18 000002
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22 000006      010046
23 000010
24 000062      012600
25 000064      000207
26 000001      000001

```

```

      TITLE BEEP
      .....
      THIS ROUTINE SENDS A CNTL-G (BEL) TO LUN 5
      CALLING SEQUENCE:  CALL BEEP
      .....
      VER 1.0/03-OCT-83(TK) ORIGINAL VERSION
      .....
      MCALL GIOW%S
BEEP:  BYTE 007          ,CNTL-G (THE BEEP)
      EVEN
      IOSTAT: BLKW 2      ,THE STATUS OF I/O
      .....
      ISSUE GIO TO SEND BEEP
BEEP:  MOV R0, -(SP)      ,SAVE REGISTER
      GIOW%S #IO, WAL, #5, #5, , #IOSTAT, , #BEEP, #1, #0
      MOVS (SP)+, R0      ,RESTORE REGISTER
      RTS PC              ,AND RETURN TO CALLING PROGRAM
      END

```

```

0001 PDP-11 FORTRAN-77 VS. 0-0 /F77/OP/TR:BLOCKS/WR 25-Feb-85 Page 1
      SUBROUTINE VJZERO (IARRAY,N)
      .....
      This subroutine zeroes the integer2 array IARRAY of length N
      On entry:
      IARRAY (I2): Array to be zeroed
      N (I2): Index up to which IARRAY will be zeroed
      On exit:
      IARRAY (I2): Array filled with zeroes up to index N
      Ver. 1.0/29-FEB-83(TK) Original version
      INTEGER2 IARRAY(I2)
      Zero out array
      DO 1000 J=1,N,1
      IARRAY(J) = 0
      1000 CONTINUE
      Return to calling program
      RETURN
      *****
      END
0002
0003
0004
0005
0006
0007

```

```

0001 PDP-11 FORTRAN-77 VS. 0-0 /F77/Op/TR:BLOCKS/WR 25-Feb-85 Page 1
      SUBROUTINE VJZERO (JARRAY,N)
      .....
      This subroutine zeroes the integer2 array JARRAY of length N
      On entry:
      JARRAY (I24): Array to be zeroed
      N (I2): Index up to which JARRAY will be zeroed
      On exit:
      JARRAY (I24): Array filled with zeroes up to index N
      Ver. 1.0/08-Dec-83(TK) Original version
      INTEGER24 JARRAY(I2)
      Zero out array
      DO 1000 J=1,N,1
      JARRAY(J) = 0
      1000 CONTINUE
      Return to calling program
      RETURN
      *****
      END
0002
0003
0004
0005
0006
0007

```

```

0001 PDP-11 FORTRAN-77 VS. 0-0 /F77/OP/TR:BLOCKS/WR 25-Feb-85 Page 1
      SUBROUTINE VDZERO (DARRAY,LENGTH)
      REAL8 DARRAY(LENGTH)
      DO 1000 J=1,LENGTH,1
      DARRAY(J) = 0.000
      1000 CONTINUE
      RETURN
      *****
      END
0002
0003
0004
0005
0006
0007

```

```

0001 SUBROUTINE DJCURI (ICHA,IX,JY)
      *-----*
      C#
      C# This routine displays a crosshair cursor on the screen,
      C# gets the input from the keyboard, converts the (absolute)
      C# screen coordinates to user coordinates and returns them to
      C# the calling program
      C#
      C# Calling sequence: CALL DJCURI (ICHA,IX,JY)
      C#
      C# On exit: ICHAR (I#2): character typed (left justified)
      C#           IX (I#2):  X coordinate of cursor (user system)
      C#           JY (I#4):  Y coordinate of cursor (user system)
      C#
      C# Ver. 1.0/22-Sep-83(TK) Original version
0002 INTEGER*4 JYMIN,JYMAX,JYRAN,JUSERX
0003 COMMON /DICOM / IXMIN,IXMAX,IXRAN,JYMIN,JYMAX,JYRAN,
      C# IMODE,IUSERX,JUSERX,KXLO,KXHI,KXRAN,
      C# KYLO,KVHI,KYRAN
0004 C#
      C# INTEGER*4 JY,JXX
      C#
      C# Call DICURI to get the absolute screen coordinates
0005 CALL DICURI (ICHA,IXX,IYY)
      C#
      C# Convert X coordinate
0006 JXX = IXX-KXLO
0007 JXX = JXX+IXRAN
0008 JXX = JXX/KXRAN
0009 IX = JXX+IXMIN
      C#
      C# Convert Y coordinate
0010 JY = IYY-KYLO
0011 JY = JY+JYRAN
0012 JY = JY/KYRAN
0013 JY = JY+JYMIN
      C#
      C# Return to calling program
0014 RETURN
0015 END
    
```

```

0001 SUBROUTINE PREPDI (JCOUNT,IXL,IXH,IYL,IYH,IYPWR,JMIN,JMAX,JSUM)
      *-----*
      C#
      C# This subroutine prepares the data needed to produce a plot
      C#
      C# Ver. 0.0/07-SEP-83(TK) Original version
0002 INTEGER*4 JMIN,JMAX,JSUM,JCOUNT(=)
      C#
      C# Check Y-limits and prepare them
0003 IF (IYL.GE.IYH) THEN
0004   JMAX = 0
0005   JMIN = 999999
0006   DO 1000 J=IXL,IXH,1
0007     JMIN = MIN(JMIN,JCOUNT(J))
0008     JMAX = MAX(JMAX,JCOUNT(J))
0009   1000 CONTINUE
0010 ELSE
0011   JMIN = IYL
0012   JMAX = IYH
0013   JMIN = JMIN+10**IYPWR
0014   JMAX = JMAX+10**IYPWR
0015 ENDIF
      C#
      C# Calculate integrated contents
0016 JSUM = 0
0017 DO 1005 J=IXL,IXH,1
0018   JSUM = JSUM+JCOUNT(J)
0019 1005 CONTINUE
      C#
      C# Return to calling program
0020 RETURN
0021 END
    
```

```

0001 SUBROUTINE SDISPL (JCOUNT,IXLO,IXHI,JMIN,JMAX,ITYPE)
      *-----*
      C#
      C# This subroutine displays a spectrum -JCOUNT- from
      C# channel IXLO to channel IXHI and sets the Y limits
      C# to JMIN and JMAX. The display type is taken from ITYPE.
      C#
      C# Ver. 0.0/08-SEP-83(TK) Original Version
0002 INTEGER*4 JCOUNT(=),JMIN,JMAX
      C#
      C# Define display window, erase screen, draw frame and axis
0003 CALL DJWNDW (IXLO,IXHI,JMIN,JMAX)
0004 CALL DJPADE
0005 CALL DJFRAM
0006 CALL DJAXIS
      C#
      C# Display spectrum of type ITYPE and "leave the picture open"
0007 CALL DJSPEC (JCOUNT,IXLO,IXHI,ITYPE)
      C#
      C# Return to calling program
0008 RETURN
0009 END
    
```

```

0001 SUBROUTINE DJSPEC (NN,KA,KB,IPLOT)
      C#
      C# *****
      C# DISPLAY INTEGER*4 SPECTRUM BETWEEN CHANNELS KA AND KB ACCORDING TO IPLOT
      C#
      C# IPLOT = 0 HISTOGRAM PLOT
      C#         = 1 ERROR BARS
      C#         = 2 SPECTRUM PLOT
      C#         = 3 POINT PLOT
      C# *****
0002 INTEGER*4 NN(1),JY,JJY
      C#
      C#
0003 JY=NN(KA)
0004 CALL DJMOVA (KA,JY)
0005 DO 200 I=KA,KB
0006   JY=NN(I)
0007   IF (IPLOT.NE.3) GOTO 100
0008   CALL DJPNTA (I,JY)
0009   GOTO 200
0010 100 IF (IPLOT.NE.1) GOTO 150
0011   IF (JY.LE.0) GOTO 150
0012   E=JY
0013   E=SQRT (E)
0014   JJY=JY-E
0015   CALL DJMOVA (I,JJY)
0016   JY=JY+E
0017 150 CALL DJDRWA (I,JY)
0018   IF (IPLOT.NE.0) GOTO 200
0019   I=I-1
0020   CALL DJDRWA (I,JY)
0021 200 CONTINUE
0022 RETURN
0023 END
    
```


DIPACK MACRO M1200 25-FEB-85 13:11 PAGE 2

```

130
131
132 ;-----
133 ; FILL STRING TERMINATED BY A NULL INTO OUTPUT BUFFER WHICH IS
134 ; OUTPUT TO TERMINAL IN A SINGLE BIO IF :
135 ; - FULL - OR <CR> OR <US> OR 377 ENCOUNTERED
136 ;
137 ; CALLING SEQUENCE: JSR PC,DIOUT
138 ; ON ENTRY: RO POINTS TO STRING TO BE OUTPUT
139 ;-----
140 000342 010146 DIOUT: MOV R1, -(SP) ; GAVE R1
141 000344 016701 177450 MOV BUFCNT, R1 ; GET ACTUAL BUFFER COUNT
142 000350 111061 000022 GETCHA: MOVB (RD), BUFFER(R1) ; GET CHARACTER
143 000354 001447 BEQ EXOUT ; NO MORE CHARS IF ZERO
144 000356 005201 INC R1 ; VALID CHAR => INCREMENT COUNT
145 000360 005200 INC R0 ; ... AND POINTER
146
147 ; LOOK WETHER AN OUTPUT IS TO BE DONE OR NOT
148
149 000362 122761 000015 000021 CMPB #15, BUFFER-1(R1) ; IF CARRIAGE RETURN
150 000370 001413 BEQ OUT ; ... THEN FORCE OUTPUT OF BUFFER
151 000372 122761 000037 000021 CMPB #17, BUFFER-1(R1) ; IF US
152 000400 001407 BEQ OUT ; ... THEN FORCE OUTPUT OF BUFFER
153 000402 122761 000377 000021 CMPB #377, BUFFER-1(R1) ; IF 377
154 000410 001403 BEQ OUT ; ... THEN FORCE OUTPUT OF BUFFER
155 000412 020127 000110 CMP R1, #MAXCNT ; IF STILL PLACE IN BUFFER
156 000416 002754 BLT GETCHA ; ... THEN GET NEXT CHAR
157 000420 OUT: QIOVSS #10, RAL, #5, #5, , #IOSTAT, #BUFFER, R1, #0 ; RESET BUFFER COUNT
158 000470 005001 CLR R1 ; RESET BUFFER COUNT
159 000472 000726 BR GETCHA
160 000474 010167 177320 EXOUT: MOV R1, BUFCNT ; SAVE BUFFER POINTER
161 000500 012601 MOV (SP)+, R1 ; RESTORE R1
162 000502 000207 RTS PC

```

DIPACK MACRO M1200 25-FEB-85 13:11 PAGE 3

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164
165 ;
166 ; DIGCUR - SHOW GRAPHICS (CROSSHAIR) CURSOR AND WAIT FOR INPUT
167 ;
168 ; CALLING SEQUENCE: JSR PC,DIGCUR
169 ; ON ENTRY: RO POINTS TO A STRING OF 5 BYTES WHERE
170 ; THE GRAPHIC INPUT WILL BE STORED
171
172 000504 010046 DIGCUR: MOV RO, -(SP) ; GAVE RO FOR A WHILE
173 000512 004767 177624 MOV #GINPUT, RD ; GINPUT PROD. CROSSHAIR CURSOR
174 000516 012600 JSR PC,DIOUT ; OUTPUT (FORCED BY 377 AT END)
175 000520 000207 MOV (SP)+, RD ; RESTORE RD
176 000570 000207 QIOVSS #10, RAL, #5, #5, , #IOSTAT, #RD, #6, #0 ; READ INPUT
; AND RETURN TO CALLING PROGRAM
RTS PC

```

DIPACK MACRO M1200 25-FEB-85 13:11 PAGE 4

```

178 ;-----
179 ;
180 ; FORTRAN COMMON /DICOM/ FOR DISPLAY ROUTINES
181 ;-----
182
183 000000 .PSECT DICOM, RW, D, GBL, OVR, REL
184 000000 IXMIN: .BLKW 1 ; USER LEFT MARGIN
185 000002 IXMAX: .BLKW 1 ; USER RIGHT MARGIN
186 000004 IXRAN: .BLKW 1 ; USER X-RANGE
187 000006 IYMIN: .BLKW 2 ; USER BOTTOM MARGIN (INTEGER*4)
188 000012 IYMAX: .BLKW 2 ; USER TOP MARGIN (INTEGER*4)
189 000016 IYRAN: .BLKW 2 ; USER Y-RANGE (INTEGER*4)
190 000022 IMODE: .BLKW 1 ; CURRENT SOFTWARE DISPLAY MODE
191 000024 IUSERX: .BLKW 1 ; CURRENT USER X-POSITION
192 000026 IUSERY: .BLKW 2 ; CURRENT USER Y-POSITION (INTEGER*4)
193
194 000032 KXLO: .BLKW 1 ; SCREEN LEFT MARGIN
195 000034 KXHI: .BLKW 1 ; SCREEN RIGHT MARGIN
196 000036 KXRAN: .BLKW 1 ; SCREEN X-RANGE
197 000040 KYLO: .BLKW 1 ; SCREEN BOTTOM MARGIN
198 000042 KYHI: .BLKW 1 ; SCREEN TOP MARGIN
199 000044 KYRAN: .BLKW 1 ; SCREEN Y-RANGE
200 000046 KKMDE: .BLKW 1 ; CURRENT HARDWARE DISPLAY MODE
201 000050 KBEAMX: .BLKW 1 ; CURRENT BEAM X-POSITION
202 000052 KBEAMY: .BLKW 1 ; CURRENT BEAM Y-POSITION
203 000054 KSPED: .BLKW 1 ; TERINAL SPEED IN CHARACTERS PER SECOND
204 000056 KPCHAR: .BLKW 4 ; CURRENT BEAM POSITION IN CHARACTER FORMAT
205 000066 ABEAM: .BYTE 2, 0 ; ARGUMENT BLOCK FOR CURRENT SCREEN COORDINATES
206 000070 .WORD KBEAMX
207 000072 .WORD KBEAMY
208 000074 AUSER: .BYTE 2, 0 ; ARGUMENT BLOCK FOR CURRENT USER COORDINATES
209 000076 .WORD IUSERX
210 000100 .WORD IUSERY
211 000102 AKXKY: .BYTE 2, 0 ; ARGUMENT BLOCK TEMPORARY SCREEN COORDINATES
212 000104 .WORD KX
213 000106 .WORD KY
214 000110 KX: .BLKW 1 ; TEMPORARY SCREEN X-COORDINATE
215 000112 KY: .BLKW 1 ; TEMPORARY SCREEN Y-COORDINATE
216 000114 AIXIV: .BYTE 2, 0 ; ARGUMENT BLOCK TEMPORARY USER COORDINATES
217 000116 .WORD IX
218 000120 .WORD IY
219 000122 IX: .BLKW 1 ; TEMPORARY USER X-COORDINATE (INTEGER*2)
220 000124 IY: .BLKW 2 ; TEMPORARY USER Y-COORDINATE (INTEGER*4)
221 000001 .END

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DIABS MACRO M1200 25-FEB-85 13:10 PAGE 1

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21 000000 017567 000006 000022* DIABS:  MOV @6(R5),IMODE           ;GET DESIRED MODE
22 000006 026727 000022* 000002 DIA:  CMP IMODE,@2           ;TAKE ACTION ACCORDING TO MODE
23 000014 003021                                     BGT DIPNTA           ;MODE = 3
24 000016 001403                                     BEQ DIDRWA           ;MODE = 2
25
26 000020 004767 000000G  DIHOVA: JSR PC,DIVEC           ;MODE = 1
27 000024 000423                                     BR GOTOXY
28
29 000026 022767 000001 000046* DIDRWA: CMP @1,KKMODE           ;IF ALREADY IN VECTOR MODE
30 000034 001417                                     BEQ GOTOXY           ;... THEN DRAW VECTOR
31 000036 004767 000000G  JSR PC,DIVEC           ;... ELSE SWITCH TO VECTOR MODE
32 000042 010546                                     MOV R5,-(SP)         ;SAVE ARGUMENT POINTER
33 000044 012705 000066*  JSR @BEAM,R5           ;POINTER TO CURRENT BEAM COORD.
34 000050 004767 000000G  JSR PC,DICNVY         ;DRAW DARK VECTOR TO LAST POSITION
35 000054 012605                                     MOV (SP)+,R5         ;RESTORE POINTER TO (X,Y)
36 000056 000406                                     BR GOTOXY
37
38 000060 022767 000002 000046* DIPNTA: CMP @2,KKMODE           ;IF ALREADY IN POINT MODE
39 000066 001402                                     BEQ GOTOXY           ;... THEN DRAW POINT
40 000070 004767 000000G  JSR PC,DIPNT         ;... ELSE SWITCH TO POINT MODE
41 000074 004767 000000G  GOTOXY: JSR PC,DICNVY         ;DRAW VECTOR TO (X,Y)
42 000100 000207                                     RTS PC
43
44
45
46
47
48 000000
49 000002
50 000002
51 000004
52 000006
53 000012

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DIABS MACRO M1200 25-FEB-85 13:10 PAGE 1-1

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54 000016 IVRAN:  .BLKW 2           ;USER V-RANGE (INTEGER*4)
55 000022 IMODE:  .BLKW 1           ;CURRENT SOFTWARE DISPLAY MODE
56 000024 IUSERX:  .BLKW 1           ;CURRENT USER X-POSITION
57 000026 IUSERY:  .BLKW 2           ;CURRENT USER Y-POSITION (INTEGER*4)
58
59 000032 KXLO:   .BLKW 1           ;SCREEN LEFT MARGIN
60 000034 KXHI:   .BLKW 1           ;SCREEN RIGHT MARGIN
61 000036 KXRAN:  .BLKW 1           ;SCREEN X-RANGE
62 000040 KYLO:   .BLKW 1           ;SCREEN BOTTOM MARGIN
63 000042 KYHI:   .BLKW 1           ;SCREEN TOP MARGIN
64 000044 KYRAN:  .BLKW 1           ;SCREEN Y-RANGE
65 000046 KKMODE: .BLKW 1           ;CURRENT HARDWARE DISPLAY MODE
66 000050 KBEAMX: .BLKW 1           ;CURRENT BEAM X-POSITION
67 000052 KBEAMY: .BLKW 1           ;CURRENT BEAM Y-POSITION
68 000054 KPSPEED: .BLKW 1           ;TERMINAL SPEED IN CHARACTERS PER SECOND
69 000056 KPCHAR:  .BLKW 4           ;CURRENT BEAM POSITION IN CHARACTER FORMAT
70 000066 ABEAM:  .BYTE 2,0           ;ARGUMENT BLOCK FOR CURRENT SCREEN COORDINATES
71 000070 000058* .WORD KBEAMX
72 000072 000052* .WORD KBEAMY
73 000074 002 .BLKW 2           ;ARGUMENT BLOCK FOR CURRENT USER COORDINATES
74 000076 000024* .WORD IUSERX
75 000100 000026* .WORD IUSERY
76 000102 002 .BLKW 2           ;ARGUMENT BLOCK TEMPORARY SCREEN COORDINATES
77 000104 000110* .WORD KX
78 000106 000112* .WORD KY
79 000110 000112* .WORD KX
80 000112 000112* .WORD KY
81 000114 002 .BLKW 2           ;TEMPORARY SCREEN X-COORDINATE
82 000116 000122* .WORD KX
83 000120 000124* .WORD KY
84 000122 .BLKW 1           ;TEMPORARY SCREEN Y-COORDINATE
85 000124 .BLKW 2           ;ARGUMENT BLOCK TEMPORARY USER COORDINATES
86 000001 .WORD IX
87 .BLKW 1           ;TEMPORARY USER X-COORDINATE (INTEGER*2)
88 .BLKW 2           ;TEMPORARY USER Y-COORDINATE (INTEGER*4)
89 END

```


DIREL MACRO M1200 25-FEB-85 13:12 PAGE 1

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22
23 000000 017567 000006 000022' DIREL:: MOV @6(R5),IMODE ;GET DESIRED MODE
24 000006 067567 000002 000050' RELOC: ADD @2(R5),KBEAMX ;ADD X-INCREMENT TO CURRENT POS
25 000014 067567 000004 000052' ADD @4(R5),KBEAMY ;ADD Y-INCREMENT TO CURRENT POS
26 000022 010546 ;MOV R5,-(SP) ;SAVE R5
27 000024 012705 ;MOVI #ABEAM,R5 ;POINTER TO ARGUMENT BLOCK
28 000030 004767 000000 ;JSR PC,DIA ;DRAW ACCORDING TO MODE
29 000034 012605 ;MOV (SP)+,R5 ;RESTORE R5
30 000036 000207 ;RTS PC
31
32 000040 012767 000001 000022' DIMOVR:: MOV #1,IMODE ;MODE=1 => DARK VECTOR
33 000046 000757 ;BR RELOC
34 000050 012767 000002 000022' DIDRWR: MOV #2,IMODE ;MODE=2 => BRIGHT VECTOR
35 000056 000753 ;BR RELOC
36 000060 012767 000003 000022' DIPNTR: MOV #3,IMODE ;MODE=3 => POINT
37 000066 000747 ;BR RELOC
38
39
40
41
42
43 000000 ;PSECT DICOM,RW,D,GBL,OVR,REL
44 000000 IXMIN: .BLKW 1 ;USER LEFT MARGIN
45 000002 IXMAX: .BLKW 1 ;USER RIGHT MARGIN
46 000004 IXRAN: .BLKW 1 ;USER X-RANGE
47 000006 IYMIN: .BLKW 2 ;USER BOTTOM MARGIN (INTEGER**4)
48 000012 IYMAX: .BLKW 2 ;USER TOP MARGIN (INTEGER**4)
49 000016 IYRAN: .BLKW 2 ;USER Y-RANGE (INTEGER**4)
50 000022 IMODE: .BLKW 1 ;CURRENT SOFTWARE DISPLAY MODE
51 000024 IUSERX: .BLKW 1 ;CURRENT USER X-POSITION
52 000026 IUSERY: .BLKW 2 ;CURRENT USER Y-POSITION (INTEGER**4)
53

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DIREL MACRO M1200 25-FEB-85 13:12 PAGE 1-1

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54 000032 KXLD: .BLKW 1 ;SCREEN LEFT MARGIN
55 000034 KXHI: .BLKW 1 ;SCREEN RIGHT MARGIN
56 000036 KXRAN: .BLKW 1 ;SCREEN X-RANGE
57 000040 KYLD: .BLKW 1 ;SCREEN BOTTOM MARGIN
58 000042 KYHI: .BLKW 1 ;SCREEN TOP MARGIN
59 000044 KYRAN: .BLKW 1 ;SCREEN Y-RANGE
60 000046 KKMODE: .BLKW 1 ;CURRENT HARDWARE DISPLAY MODE
61 000050 KBEAMX: .BLKW 1 ;CURRENT BEAM X-POSITION
62 000052 KBEAMY: .BLKW 1 ;CURRENT BEAM Y-POSITION
63 000054 KSPED: .BLKW 1 ;TERINAL SPEED IN CHARACTERS PER SECOND
64 000056 KPCHAR: .BLKW 4 ;CURRENT BEAM POSITION IN CHARACTER FORMAT
65 000066 ABEAM: .BYTE 2,0 ;ARGUMENT BLOCK FOR CURRENT SCREEN COORDINATES
66 000070 .WORD KBEAMX
67 000072 .WORD KBEAMY
68 000074 .WORD 2,0 ;ARGUMENT BLOCK FOR CURRENT USER COORDINATES
69 000076 .WORD IUSERX
70 000100 .WORD IUSERY
71 000102 .WORD 2,0 ;ARGUMENT BLOCK TEMPORARY SCREEN COORDINATES
72 000104 .WORD KX
73 000106 .WORD KY
74 000110 KX: .BLKW 1 ;TEMPORARY SCREEN X-COORDINATE
75 000112 KY: .BLKW 1 ;TEMPORARY SCREEN Y-COORDINATE
76 000114 .WORD 2,0 ;ARGUMENT BLOCK TEMPORARY USER COORDINATES
77 000116 .WORD IX
78 000120 .WORD IY
79 000122 IX: .BLKW 1 ;TEMPORARY USER X-COORDINATE (INTEGER**2)
80 000124 IY: .BLKW 2 ;TEMPORARY USER Y-COORDINATE (INTEGER**4)
81 000001 .END

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DJABS MACRO M1200 25-FEB-85 13:12 PAGE 1

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          .TITLE DJABS
          -----
          DRAW VECTOR OR POINT TO ABSOLUTE USER COORDINATES (IX,JY)
          ROLF GUIGAS      FEB-1982
          CALLING SEQUENCE: CALL DJABS (IX,JY,IMODE) ;POINT OR VECTOR
          CALL DJMOVA (IX,JY) ;DARK VECTOR
          CALL DJDRWA (IX,JY) ;BRIGHT VECTOR
          CALL DJPNTA (IX,JY) ;POINT
          ON ENTRY:      IX      = USER X-COORDINATE (INTEGER*2)
          JY             = USER Y-COORDINATE (INTEGER*4)
          IMODE = 1 => DARK VECTOR
                   2 => BRIGHT VECTOR
                   3 => POINT
          -----
          .GLOBL DJCNVT
          DJABS:  MOV  #6(R5),IMODE ;GET DESIRED MODE
          CNVT:  JSR  PC,DJCNVT ;CONVERT TO SCREEN COORD.
                   RTS  PC
          DJMOVA: MOV  #1,IMODE ;MODE=1 => DARK VECTOR
                   BR  CNVT
          DJDRWA: MOV  #2,IMODE ;MODE=2 => BRIGHT VECTOR
                   BR  CNVT
          DJPNTA: MOV  #3,IMODE ;MODE=3 => POINT
                   BR  CNVT
          -----
          FORTRAN COMMON /DICOM/ FOR DISPLAY ROUTINES
          .PSECT DICOM, RW, D, GBL, DVR, REL
          IXMIN: .BLKW 1 ;USER LEFT MARGIN
          IXMAX: .BLKW 1 ;USER RIGHT MARGIN
          IXRAN: .BLKW 1 ;USER X-RANGE
          IYMIN: .BLKW 2 ;USER BOTTOM MARGIN (INTEGER*4)
          IYMAX: .BLKW 2 ;USER TOP MARGIN (INTEGER*4)
          IYRAN: .BLKW 2 ;USER Y-RANGE (INTEGER*4)
          IMODE: .BLKW 1 ;CURRENT SOFTWARE DISPLAY MODE
          IUSERX: .BLKW 1 ;CURRENT USER X-POSITION
          IUSERY: .BLKW 2 ;CURRENT USER Y-POSITION (INTEGER*4)
          KXLO: .BLKW 1 ;SCREEN LEFT MARGIN
          KXHI: .BLKW 1 ;SCREEN RIGHT MARGIN
          KYRAN: .BLKW 1 ;SCREEN X-RANGE
          KYLO: .BLKW 1 ;SCREEN BOTTOM MARGIN
          KYHI: .BLKW 1 ;SCREEN TOP MARGIN
          KYRAN: .BLKW 1 ;SCREEN Y-RANGE
          KMODE: .BLKW 1 ;CURRENT HARDWARE DISPLAY MODE
          KBEAMX: .BLKW 1 ;CURRENT BEAM X-POSITION
          KBEAMY: .BLKW 1 ;CURRENT BEAM Y-POSITION
          KSPEED: .BLKW 1 ;TERMINAL SPEED IN CHARACTERS PER SECOND
          KPCHAR: .BLKW 4 ;CURRENT BEAM POSITION IN CHARACTER FORMAT
          ABEAM: .BYTE 2,0 ;ARGUMENT BLOCK FOR CURRENT SCREEN COORDINATES
                   .WORD KBEAMX
                   .WORD KBEAMY
          AUSER: .BYTE 2,0 ;ARGUMENT BLOCK FOR CURRENT USER COORDINATES
                   .WORD IUSERX
                   .WORD IUSERY
          AKXKY: .BYTE 2,0 ;ARGUMENT BLOCK TEMPORARY SCREEN COORDINATES
                   .WORD KX
                   .WORD KY
          KX: .BLKW 1 ;TEMPORARY SCREEN X-COORDINATE
          KY: .BLKW 1 ;TEMPORARY SCREEN Y-COORDINATE
          AIXIV: .BYTE 2,0 ;ARGUMENT BLOCK TEMPORARY USER COORDINATES
                   .WORD IX
                   .WORD IY
          IX: .BLKW 1 ;TEMPORARY USER X-COORDINATE (INTEGER*2)
          IY: .BLKW 2 ;TEMPORARY USER Y-COORDINATE (INTEGER*4)
          .END

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DJABS MACRO M1200 25-FEB-85 13:12 PAGE 1-1

DJREL MACRO M1200 25-FEB-85 13:12 PAGE 1

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          .TITLE DJREL
          -----
          DRAW VECTOR OR POINT TO RELATIVE USER COORDINATES (INCX,INCY)
          ROLF GUIGAS      FEB-1982
          CALLING SEQUENCE: CALL DJREL (INCX,INCY,IMODE) ; POINT OR VECTOR
                           CALL DJMOVR (INCX,INCY)      ; DARK VECTOR
                           CALL DJDRWR (INCX,INCY)      ; BRIGHT VECTOR
                           CALL DJPNTR (INCX,INCY)      ; POINT
          ON ENTRY:      INCX = USER X-INCREMENT (INTEGER*2)
                           INCY = USER Y-INCREMENT (INTEGER*4)
                           IMODE = 1 => DARK VECTOR
                               2 => BRIGHT VECTOR
                               3 => POINT
          -----
          .GLOBL DJCNVT
          DJREL:  MOV  #6(R5),IMODE ; GET DESIRED MODE
                  ADD  #2(R5),IUSERX ; ADD X-INCREMENT TO CURRENT POS.
                  MOV  R5,-(SP) ; SAVE R5
                  MOV  4(R5),R5 ; POINTER TO LOW Y
                  ADD  (R5)+,IUSERY ; ADD Y-INCREMENT TO CURRENT POS.
                  ADC  IUSERY+2 ; IN
                  ADD  (R5),IUSERY+2 ; DOUBLE PRECISION
                  MOV  #AUSER,R5 ; POINTER TO ARGUMENT BLOCK
                  JSR  PC,DJCNVT ; DISPLAY ACCORDING TO MODE
                  MOV  (SP)+,R5 ; RESTORE R5
                  RTS  PC
          DJMOVR: MOV  #1,IMODE ; MODE=1 => DARK VECTOR
                  BR   RELOC
          DJDRWR: MOV  #2,IMODE ; MODE=2 => BRIGHT VECTOR
                  BR   RELOC
          DJPNTR: MOV  #3,IMODE ; MODE=3 => POINT
                  BR   RELOC
          -----
          FORTRAN COMMON /DICOM/ FOR DISPLAY ROUTINES
          .PSECT DICOM,RW,D,GBL,DVR,REL
          IXMIN: .BLKW 1 ; USER LEFT MARGIN
          IXMAX: .BLKW 1 ; USER RIGHT MARGIN
          IXRAN: .BLKW 1 ; USER X-RANGE
          IYMIN: .BLKW 2 ; USER BOTTOM MARGIN (INTEGER**4)
          IYMAX: .BLKW 2 ; USER TOP MARGIN (INTEGER**4)
          IYRAN: .BLKW 2 ; USER Y-RANGE (INTEGER**4)
          IMODE: .BLKW 1 ; CURRENT SOFTWARE DISPLAY MODE

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DJREL MACRO M1200 25-FEB-85 13:12 PAGE 1-1

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          IUSERX: .BLKW 1 ; CURRENT USER X-POSITION
          IUSERY: .BLKW 2 ; CURRENT USER Y-POSITION (INTEGER**4)
          KXLO: .BLKW 1 ; SCREEN LEFT MARGIN
          KXHI: .BLKW 1 ; SCREEN RIGHT MARGIN
          KXRAN: .BLKW 1 ; SCREEN X-RANGE
          KYLO: .BLKW 1 ; SCREEN BOTTOM MARGIN
          KYHI: .BLKW 1 ; SCREEN TOP MARGIN
          KYRAN: .BLKW 1 ; SCREEN Y-RANGE
          KKMODE: .BLKW 1 ; CURRENT HARDWARE DISPLAY MODE
          KBEAMX: .BLKW 1 ; CURRENT BEAM X-POSITION
          KBEAMY: .BLKW 1 ; CURRENT BEAM Y-POSITION
          KSPD: .BLKW 1 ; TERMINAL SPEED IN CHARACTERS PER SECOND
          KPCHAR: .BLKW 4 ; CURRENT BEAM POSITION IN CHARACTER FORMAT
          ABEAM: .BYTE 2,D ; ARGUMENT BLOCK FOR CURRENT SCREEN COORDINATES
                  .WORD KBEAMX
                  .WORD KBEAMY
          AUSER: .BYTE 2,D ; ARGUMENT BLOCK FOR CURRENT USER COORDINATES
                  .WORD IUSERX
                  .WORD IUSERY
          AKXKY: .BYTE 2,D ; ARGUMENT BLOCK TEMPORARY SCREEN COORDINATES
                  .WORD KX
                  .WORD KY
          KX: .BLKW 1 ; TEMPORARY SCREEN X-COORDINATE
          KY: .BLKW 1 ; TEMPORARY SCREEN Y-COORDINATE
          AIXIV: .BYTE 2,D ; ARGUMENT BLOCK TEMPORARY USER COORDINATES
                  .WORD IX
                  .WORD IY
          IX: .BLKW 1 ; TEMPORARY USER X-COORDINATE (INTEGER*2)
          IY: .BLKW 2 ; TEMPORARY USER Y-COORDINATE (INTEGER**4)
          .END

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DIAXIS MACRO M1200 25-FEB-85 13:10 PAGE 1-2

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107 000410 070227 036411      M:      MUL  #15625.,R2      ; JINC = INC * 5**6
108 000414 073227 000006      ASHC  #6,R2              ; ... * 2**6
109 000420 073027 177772      ASHC  #6,R0              ; ILAB = IYMIN / 2**6
110 000424 071027 036411      DIV   #15625.,R0        ; FIRST LABEL VALUE / 5**6
111 000430 010067 177370      MOV   R0,ILAB           ; LONG WORD
112 000434 010367 177370      MOV   R3,JINC           ; INCREMENT
113 000440 010267 177366      MOV   R2,JINC+2
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117 000444 012705 000000      ; DRAW Y-AXIS WITH TIC MARKS AND LABELS
118 000450 004767 000000      NEXTY: MOV  #AXY,R5       ; POINTER TO ARGUMENTS
119 000454 012767 177772 000110' JSR   PC,DJHOVA         ; GO TO TIC POSITION
120 000462 005067 000112' MOV   #LTIC,KX         ; LOAD OFFSETS
121 000466 012705 000102' CLR   KY               ; ... FOR TIC MARK
122 000472 004767 000000      JSR   PC,DIDRWR        ; DRAW TIC MARK
123 000476 012767 177635 000110' MOV   #LABYX,KX        ; LOAD OFFSETS
124 000504 012767 177770 000112' MOV   #LABVY,KY        ; ... FOR LABEL POSITION
125 000532 004767 000000      JSR   PC,DIHOVR        ; MOVE BEAM TO LABEL START
126 000516 012705 000020' MOV   #LABY,R5         ; ARGUMENT POINTER FOR LABEL
127 000522 004767 000000      JSR   PC,DIDEC        ; PRINT LABEL
128 000526 012705 000034' MOV   #AUNIT,R5       ; PRINT UNIT OF LABEL VALUE
129 000532 004767 000000      JSR   PC,DITXT        ; INCREMENT LABEL VALUE
130 000536 0666767 177264 177260 ADD   INC,ILAB         ; ADVANCE
131 000544 0666767 177260 177236 ADD   JINC,VY          ; ... TO
132 000552 004767 177234      DC   VY+2              ; ... NEXT TIC MARK
133 000556 0666767 177250 177226 ADD   JINC+2,VY+2      ; IF STILL IN RANGE
134 000564 026767 177222 000014' CMP   VY+2,IYMAX+2    ; ... THEN DRAW NEXT Y-TIC
135 000572 000274      BLT   NEXTY
136 000574 003004      BGT   EXAX
137 000576 026767 177206 000012' CMP   VY,IYMAX
138 000604 161717      BLOS  NEXTY
139 000606 000207      RTS   PC
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151 000610 012703 000001      ; CALCULATE SUITABLE INCREMENT BETWEEN TIC MARKS
152 000614 020127 000012      ON ENTRY: R1 = NUMBER TO SCALE
153 000620 003425      ON EXIT:  R3 = INCREMENT
154 000622 070327 000012      METHOD:  NUMBER = A * 10**I + B
155 000626 005000      A < 2      => INC = 2 * 10**(I-1)
156 000630 071027 000012      1 < A < 5  => INC = 5 * 10**(I-1)
157 000634 010001      A > 4      => INC = 10**I
158 000636 020127 000012      DELTA:  MOV  #1,R3      ; START WITH 10**0
159 000642 002367      CMP   R1,#10         ; IF < 10
BLE   EXDEL           ; ... THEN INCREMENT = 1
POWER:  MOV  #10,R3     ; NEXT POWER OF TEN
CLR   R0              ; ZERO HIGH ORDER PART FOR DIVISION
DIV   #10.,R0         ; DIVIDE BY TEN
MOV   R0,R1           ; LOAD RESULT FOR NEXT DIVISION
CMP   R1,#10         ; IF STILL > TEN
BGE   POWER          ; ... THEN TRY NEXT POWER

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DIAXIS MACRO M1200 25-FEB-85 13:10 PAGE 1-3

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160 000644 020127 000004      CMP   R1,#4          ; IF > 4
161 000650 003011      BGT   EXDEL         ; ... THEN INC = 10**I
162 000652 020127 000002      CMP   R1,#2          ; IF > 1
163 000656 002402      BLT   1             ; ... THEN INC = 5 * 10**(I-1)
164 000660 006203      ASR   R3
165 000662 000404      BR   EXDEL
166 000664 005002      13:  CLR   R2
167 000666 071227 000005      DIV   #5,R2          ; INC = 2 * 10**(I-1)
168 000672 010203      MOV   R2,R3
169 000674 000207      EXDEL: RTS   PC
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175 000000      ; FORTRAN COMMON /DICOM/ FOR DISPLAY ROUTINES
176 000000      ; PSECT DICOM,RW,D,GBL,OVR,REL
177 000002      IYMIN: .BLKW 1       ; USER LEFT MARGIN
178 000004      IXMAX: .BLKW 1       ; USER RIGHT MARGIN
179 000006      IXRAN: .BLKW 1       ; USER X-RANGE
180 000012      IYMIN: .BLKW 2       ; USER BOTTOM MARGIN (INTEGER**4)
181 000016      IYMAX: .BLKW 2       ; USER TOP MARGIN (INTEGER**4)
182 000022      IVRAN: .BLKW 2       ; USER Y-RANGE (INTEGER**4)
183 000024      IHODE: .BLKW 1       ; CURRENT SOFTWARE DISPLAY MODE
184 000026      IUSERX: .BLKW 1     ; CURRENT USER X-POSITION
185
186 000032      IXLO: .BLKW 1       ; SCREEN LEFT MARGIN
187 000034      KXHI: .BLKW 1       ; SCREEN RIGHT MARGIN
188 000036      KXRAN: .BLKW 1       ; SCREEN X-RANGE
189 000040      KYLO: .BLKW 1       ; SCREEN BOTTOM MARGIN
190 000042      KYHI: .BLKW 1       ; SCREEN TOP MARGIN
191 000044      KYRAN: .BLKW 1       ; SCREEN Y-RANGE
192 000046      KKMODE: .BLKW 1     ; CURRENT HARDWARE DISPLAY MODE
193 000050      KBEAMX: .BLKW 1     ; CURRENT BEAM X-POSITION
194 000052      KBEAMY: .BLKW 1     ; CURRENT BEAM Y-POSITION
195 000054      KSPEED: .BLKW 1     ; TERMINAL SPEED IN CHARACTERS PER SECOND
196 000056      KPCHAR: .BLKW 4     ; CURRENT BEAM POSITION IN CHARACTER FORMAT
197 000066      ABEAM: .BYTE 2,0   ; ARGUMENT BLOCK FOR CURRENT SCREEN COORDINATES
198 000070      ;
199 000072      ;
200 000074      ;
201 000076      ;
202 000100      ;
203 000102      ;
204 000104      ;
205 000106      ;
206 000110      ;
207 000112      ;
208 000114      ;
209 000116      ;
210 000120      ;
211 000122      ;
212 000124      ;
AUSER:  .WORD 2,0       ; ARGUMENT BLOCK FOR CURRENT USER COORDINATES
IUSERX: .WORD IUSERX
IUSERY: .WORD IUSERY
AKKXY:  .BYTE 2,0       ; ARGUMENT BLOCK TEMPORARY SCREEN COORDINATES
        .WORD IY
        .WORD KY
KX:     .BLKW 1         ; TEMPORARY SCREEN X-COORDINATE
KY:     .BLKW 1         ; TEMPORARY SCREEN Y-COORDINATE
AIXIV:  .BYTE 2,0       ; ARGUMENT BLOCK TEMPORARY USER COORDINATES
        .WORD IX
        .WORD IY
IX:     .BLKW 1         ; TEMPORARY USER X-COORDINATE (INTEGER**2)
IY:     .BLKW 2         ; TEMPORARY USER Y-COORDINATE (INTEGER**4)

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DIAXIS MACRO M1200 25-FEB-85 13:10 PAGE 1-4

213 000001 .END

DICNVY MACRO M1200 25-FEB-85 13:10 PAGE 1

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16 000000
17 000000 000
18 000001 000
19 000002
20 000002 000
21 000003 000
22 000004 000 000 000
23 000007 000 000
24 000011 035 000
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26 000014 010046
27 000016 010146
28 000020 010246
29 000022 017501 000022
30 000026 020127 002000
31 000032 010462
32 000034 012701 001777
33 000040 072127 000023
34 000044 106001
35 000046 106001
36 000050 106001
37 000052 052701 020000
38 000056 010167 177672
39 000062 017501 000022
40 000066 072127 000023
41 000072 106001
42 000074 106001
43 000076 106001
44 000100 052701 020000
45 000104 010167 177672
46 000110 012702 000022
47 000114 116742 177655
48 000120 126767 177655 000060
49 000126 001403
50 000130 116742 177655
51 000134 000404
52 000136 126767 177655 000062

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          . TITLE DICNVY
          ;
          ;-----
          ; CONVERT SCREEN COORDINATES (IX,IY) TO CHARACTERS AND OUTPUT THEM
          ;
          ; CALLING SEQUENCE:          CALL DICNVY (IX,IY)
          ;-----
          ;
          . GLOBL DIOUT
          ;
          ; OLD LO X = KPCHAR
          ; OLD HI X = KPCHAR+2
          ; OLD LO Y = KPCHAR+4
          ; OLD HI Y = KPCHAR+6
          ;
          NEWX:
          NLX: .BYTE 0
          NHX: .BYTE 0
          NEWY:
          NLY: .BYTE 0
          NHY: .BYTE 0
          BYTSTK: .BYTE 0,0,0,0,0
          GSBUF: .BYTE 29,0
          .EVEN
          DICNVY: MOV R0,-(SP)          ;SAVE REGISTERS
                  MOV R1,-(SP)
                  MOV R2,-(SP)
                  MOV @2(R5),R1      ;GET SCREEN X-COORDINATE
                  CMP R1,#1024
                  BL 1$
                  MOV #1023,R1
          1$:     ASH #3,R1
                  RORB R1
                  RORB R1
                  RORB R1
                  BIS #20100,R1      ;FLAG X
                  MOV R1,NEWX       ;STORE NEW X
                  MOV @4(R5),R1     ;GET SCREEN Y-COORDINATE
                  ASH #3,R1
                  RORB R1
                  RORB R1
                  RORB R1
                  BIS #20140,R1      ;FLAG Y
                  MOV R1,NEWY       ;STORE NEW Y
                  MOV #BYTSTK+4,R2   ;POINTER TO BYTE STACK
                  MOVB NLX,-(R2)
                  CMPB NHX,KPCHAR+2
                  BEQ LYCK
                  MOVB NHY,-(R2)
                  BR PUSHLV
          LYCK:  CMPB NLY,KPCHAR+4

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DICNVY MACRO M1200 25-FEB-85 13:10 PAGE 1-1

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53 000144 001402
54 000146 116742 177630
55 000152 126767 177625 000064
56 000160 001402
57 000162 116742 177615
58 000166 000166 000022
59 000174 001004 000046
60 000176 012700 000022
61 000202 004767 000022
62 000206 010200
63 000210 004767 000022
64 000214 022767 000022 000046
65 000222 010004
66 000224 012700 000022
67 000230 004767 000022
68 000234 116767 177655 000056
69 000242 116767 177633 000060
70 000250 116767 177626 000062
71 000256 116767 177621 000064
72 000264 017567 000022 000050
73 000272 017567 000022 000052
74 000300 012602
75 000302 012601
76 000304 012600
77 000306 000207
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83 000000
84 000000
85 000002
86 000004
87 000006
88 000012
89 000016
90 000022
91 000024
92 000026
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94 000032
95 000034
96 000036
97 000040
98 000042
99 000044
100 000046
101 000050
102 000052
103 000054
104 000056
105 000066 002 000

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          BEQ HYCK
          MOV NLY,-(R2)
          CMPB NHY,KPCHAR+6
          BEQ DMPBS
          MOV NLY,-(R2)
          CMP #2,KKMODE
          BNE PASSA
          MOV #GSBUF,R0
          JSR PC,DIOUT
          MOV R2,R0
          JSR PC,DIOUT
          CMP #2,KKMODE
          BNE PASSA
          MOV #BYTSTK+3,R0
          JSR PC,DIOUT
          MOVB NLX,KPCHAR
          MOVB NHX,KPCHAR+2
          MOVB NLY,KPCHAR+4
          MOVB NHY,KPCHAR+6
          MOV @2(R5),KBEAMX
          MOV @4(R5),KBEAMY
          MOV (SP)+,R2
          MOV (SP)+,R1
          MOV (SP)+,R0
          RTS PC
          ;-----
          ; FORTRAN COMMON /DICOM/ FOR DISPLAY ROUTINES
          ;
          . PSECT DICOM,RW,D,GBL,OVR,REL
          IXMIN: .BLKW 1 ;USER LEFT MARGIN
          IXMAX: .BLKW 1 ;USER RIGHT MARGIN
          IXRAN: .BLKW 1 ;USER X-RANGE
          IYMIN: .BLKW 2 ;USER BOTTOM MARGIN (INTEGER#4)
          IYMAX: .BLKW 2 ;USER TOP MARGIN (INTEGER#4)
          IYRAN: .BLKW 2 ;USER Y-RANGE (INTEGER#4)
          IMODE: .BLKW 1 ;CURRENT SOFTWARE DISPLAY MODE
          IUSERX: .BLKW 1 ;CURRENT USER X-POSITION
          IUSERY: .BLKW 2 ;CURRENT USER Y-POSITION (INTEGER#4)
          KXLO: .BLKW 1 ;SCREEN LEFT MARGIN
          KXHI: .BLKW 1 ;SCREEN RIGHT MARGIN
          KXRAN: .BLKW 1 ;SCREEN X-RANGE
          KYLO: .BLKW 1 ;SCREEN BOTTOM MARGIN
          KYHI: .BLKW 1 ;SCREEN TOP MARGIN
          KYRAN: .BLKW 1 ;SCREEN Y-RANGE
          KMODE: .BLKW 1 ;CURRENT HARDWARE DISPLAY MODE
          KBEAMX: .BLKW 1 ;CURRENT BEAM X-POSITION
          KBEAMY: .BLKW 1 ;CURRENT BEAM Y-POSITION
          KSPED: .BLKW 1 ;TERMINAL SPEED IN CHARACTERS PER SECOND
          KPCHAR: .BLKW 4 ;CURRENT BEAM POSITION IN CHARACTER FORMAT
          ABEAM: .BYTE 2,0 ;ARGUMENT BLOCK FOR CURRENT SCREEN COORDINATES

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DICNVY MACRO M1200 25-FEB-85 13:10 PAGE 1-2

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106 000070 000050
107 000072 000052
108 000074 002 000
109 000076 000024
110 000100 000026
111 000102 002 000
112 000104 000110
113 000106 000112
114 000110
115 000112
116 000114 002 000
117 000116 000122
118 000120 000124
119 000122
120 000124
121 000001

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          .WORD KBEAMX
          .WORD KBEAMY
          AUSER: .BYTE 2,0 ;ARGUMENT BLOCK FOR CURRENT USER COORDINATES
                  .WORD IUSERX
                  .WORD IUSERY
          AKXKY: .BYTE 2,0 ;ARGUMENT BLOCK TEMPORARY SCREEN COORDINATES
                  .WORD KX
                  .WORD KY
          KX: .BLKW 1 ;TEMPORARY SCREEN X-COORDINATE
          KY: .BLKW 1 ;TEMPORARY SCREEN Y-COORDINATE
          AIXIV: .BYTE 2,0 ;ARGUMENT BLOCK TEMPORARY USER COORDINATES
                  .WORD IX
                  .WORD IY
          IX: .BLKW 1 ;TEMPORARY USER X-COORDINATE (INTEGER#2)
          IY: .BLKW 2 ;TEMPORARY USER Y-COORDINATE (INTEGER#4)
          .END

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DJCNVT MACRO M1200 25-FEB-85 13:12 PAGE 1

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17 000000 004767 000000G DJCNVT: JSR PC,RCSAVE ;SAVE REGISTERS
18 000004 017500 000002 MOV @2(R5),R0 ;GET X-COORDINATE
19 000010 010067 000024* MOV R0,IUSERX ;UPDATE USER X
20 000014 166700 000000* SUB IXMIN,R0 ;SUBTRACT LEFT MARGIN
21 000020 070067 000036* MUL KXRAN,R0 ;SCALE
22 000024 071067 000004* DIV IXRAN,R0 ;... USER DISTANCE
23 000030 066700 000032* ADD KXLO,R0 ;... TO SCREEN DISTANCE
24 000034 010067 000110* MOV R0,KX ;SAVE CONVERTED X
25
26
27
28 000040 016500 000004 ; CONVERT Y COORDINATE
29 000044 012001 000000 MOV 4(R5),R0 ;POINTER TO Y COORDINATE
30 000046 011000 000000 MOV (R0),R0 ;GET LOW PART
31 000050 010167 000026* MOV R1,IUSERY ;GET HIGH PART
32 000054 010067 000030* MOV R0,IUSERY+2 ;UPDATE
33 000060 166701 000006* SUB IYMIN,R1 ;... USER Y
34 000064 005600 000000* SBC R0 ;DOUBLE PRECISION
35 000066 016700 000010* SBC IYMIN+2,R0 ;... SUBTRACTION
36 000072 016703 000016* MOV IYRAN,R0 ;... OF BOTTOM MARGIN
37 000076 016702 000020* MOV IYRAN+2,R2 ;GET LOW DIVISOR
38 ; GET HIGH DIVISOR
39
40 ; NORMALIZE DOUBLE INTEGERS SO THAT MSB = BIT 31
41 000102 073227 000001 SHIFT: ASHC #1,R2 ;SHIFT DIVISOR
42 000106 102403 000000 BVS NORM ;... UNTIL BIT 31 SET
43 000110 073027 000001 ASHC #1,R0 ;SHIFT DIVIDENT
44 000114 000772 000000 BR SHIFT
45 000116 006002 000000 NORM: R0 R2 ;RESTORE SIGN BIT
46 000120 070067 000044* MUL KYRAN,R0 ;SCALE
47 000124 071002 000040* DIV R2,R0 ;... USER Y DISTANCE
48 000126 066700 000040* ADD KYLO,R0 ;... TO SCREEN Y DISTANCE
49 000132 010067 000112* MOV R0,KV ;SAVE CONVERTED Y
50 000136 012705 000102* MOV #AKKXY,R5 ;POINTER TO SCREEN ARGUMENTS
51 000142 004767 000000G JSR PC,DIA ;DISPLAY ACCORDING TO MODE
52 000146 004767 000000G JSR PC,RGREST ;RESTORE REGISTERS
53 000152 000207 RTS PC

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DJCNVT MACRO M1200 25-FEB-85 13:12 PAGE 1-1

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59 000000 ;
60 000000 ;
61 000002 ;
62 000004 ;
63 000006 ;
64 000012 ;
65 000016 ;
66 000022 ;
67 000024 ;
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70 000032 ;
71 000034 ;
72 000036 ;
73 000040 ;
74 000042 ;
75 000044 ;
76 000046 ;
77 000050 ;
78 000052 ;
79 000054 ;
80 000056 ;
81 000066 002 000 ;
82 000070 000050* ;
83 000072 000052* ;
84 000074 002 000 ;
85 000076 000024* ;
86 000100 000026* ;
87 000102 002 000 ;
88 000104 000110* ;
89 000106 000112* ;
90 000110 ;
91 000112 ;
92 000114 002 000 ;
93 000116 000122* ;
94 000120 000124* ;
95 000122 ;
96 000124 ;
97 000001 ;

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;
;-----
;
; FORTRAN COMMON /DICOM/ FOR DISPLAY ROUTINES
;
; PSECT DICOM,RW,D,GBL,OVR,REL
IXMIN: .BLKW 1 ;USER LEFT MARGIN
IXMAX: .BLKW 1 ;USER RIGHT MARGIN
IXRAN: .BLKW 1 ;USER X-RANGE
IYMIN: .BLKW 2 ;USER BOTTOM MARGIN (INTEGER*4)
IYMAX: .BLKW 2 ;USER TOP MARGIN (INTEGER*4)
IYRAN: .BLKW 2 ;USER Y-RANGE
IMODE: .BLKW 1 ;CURRENT SOFTWARE DISPLAY MODE
IUSERX: .BLKW 1 ;CURRENT USER X-POSITION
IUSERY: .BLKW 2 ;CURRENT USER Y-POSITION (INTEGER*4)
;
KXLO: .BLKW 1 ;SCREEN LEFT MARGIN
KXHI: .BLKW 1 ;SCREEN RIGHT MARGIN
KXRAN: .BLKW 1 ;SCREEN X-RANGE
KYLO: .BLKW 1 ;SCREEN BOTTOM MARGIN
KYHI: .BLKW 1 ;SCREEN TOP MARGIN
KYRAN: .BLKW 1 ;SCREEN Y-RANGE
KKMODE: .BLKW 1 ;CURRENT HARDWARE DISPLAY MODE
KBEAMX: .BLKW 1 ;CURRENT BEAM X-POSITION
KBEAMY: .BLKW 1 ;CURRENT BEAM Y-POSITION
KSPPEED: .BLKW 1 ;TERMINAL SPEED IN CHARACTERS PER SECOND
KPCCHAR: .BLKW 4 ;CURRENT BEAM POSITION IN CHARACTER FORMAT
ABEAM: .BYTE 2,0 ;ARGUMENT BLOCK FOR CURRENT SCREEN COORDINATES
;
WORD KBEAMX
WORD KBEAMY
;
AUSER: .BYTE 2,0 ;ARGUMENT BLOCK FOR CURRENT USER COORDINATES
WORD IUSERX
WORD IUSERY
;
AKKXY: .BYTE 2,0 ;ARGUMENT BLOCK TEMPORARY SCREEN COORDINATES
WORD KX
WORD KY
;
KX: .BLKW 1 ;TEMPORARY SCREEN X-COORDINATE
KY: .BLKW 1 ;TEMPORARY SCREEN Y-COORDINATE
AIXIV: .BYTE 2,0 ;ARGUMENT BLOCK TEMPORARY USER COORDINATES
WORD IX
WORD IY
;
IX: .BLKW 1 ;TEMPORARY USER X-COORDINATE (INTEGER*2)
IY: .BLKW 2 ;TEMPORARY USER Y-COORDINATE (INTEGER*4)
END

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DICURI MACRO M1200 25-FEB-85 13:10 PAGE 1

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```

; TITLE DICURI
;
; THIS SUBROUTINE DISPLAYS A CROSSHAIR CURSOR ON THE SCREEN, WAITS
; UNTIL A CHARACTER IS TYPED AT THE KEYBOARD AND RETURNS THE CURSOR
; COORDINATES (IN ABSOLUTE SCREEN COORDINATES) TO THE CALLER.
; CALLING SEQUENCE: CALL DICURI (ICHR,IX,IV)
; ON EXIT: ICHAR (I#2): CHARACTER TYPED ('RIGHT JUSTIFIED')
; IX: X SCREEN COORDINATE
; IV: Y SCREEN COORDINATE
;
; VER. 1.0/21-SEP-83(1K) ORIGINAL VERSION
;
; GLOBL DIGCUR, RGSAVE, RGREST
;
; GIBUFF: .BLKB 6. ; TEMPORARY STORAGE FOR GINPUT
DICURI:: JSR PC,RGSAVE ; SAVE REGISTERS
; WHERE TO STORE GRAPH. INPUT
MOV @GIBUFF,R0 ; GET GRAPHICS INPUT
JSR PC,DIGCUR ; MASK OFF 8TH BIT
BIC @200,GIBUFF ; STORE SENT CHARACTER
MOV GIBUFF,@2(R5)
; PROCESS X COORDINATE
;
; MOVB GIBUFF+1,R0 ; PICK UP FIRST CHARACTER
; MOVB GIBUFF+2,R1 ; PICK UP SECOND CHARACTER
JSR PC,EXTRA ; PRODUCE 16 BIT COORDINATE (R0)
MOV R0,@4(R5) ; STORE X COORDINATE
; PROCESS Y COORDINATE
;
; MOVB GIBUFF+3,R0 ; PICK UP FIRST CHARACTER
; MOVB GIBUFF+4,R1 ; PICK UP SECOND CHARACTER
JSR PC,EXTRA ; PRODUCE 16 BIT COORDINATE (R0)
MOV R0,@6(R5) ; STORE Y COORDINATE
; RESTORE REGISTERS
JSR PC,RGREST ; AND RETURN TO CALLING PROGRAM
RTS PC

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DICURI MACRO M1200 25-FEB-85 13:10 PAGE 2

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; INTERNAL SUBROUTINE TO PRODUCE 16 BIT COORDINATE FROM 2 CHARACTERS
; ON ENTRY: R0: FIRST CHARACTER, R1: SECOND CHARACTER
; ON EXIT: R0: 16 BIT COORDINATE, R1: DESTROYED
;
EXTRA: BIC @177740,R0 ; MASK OFF ALL UNUSED STUFF
SWAB R0 ; MOVE IT TO UPPER BYTE
ROR R0 ; AND MOVE
ROR R0 ; IT BACK TO
ROR R0 ; POSITION TO 16 BIT
BIC @177740,R1 ; CLEAN LOWER PART
BIS R1,R0 ; MOVE IT INTO OUTPUT VALUE
RTS PC ; AND RETURN TO MAINLINE CODE
.END

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DIFRAM MACRO M1200 25-FEB-85 13:11 PAGE 1

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; TITLE DIFRAM
;-----
; DRAW A RECTANGULAR BOX ACCORDING TO SCREEN WINDOW
;
; ROLF GUIGAS 17-FEB-1982
;
; CALLING SEQUENCE: CALL DIFRAM
;-----
; GLOBL DIDRWA, DIMOVA
DIFRAM: MOV @AKXKY, R5 ; POINTER TO ARGUMENTS
MOV KXLO, KX ; START WITH LOWER LEFT CORNER
MOV KYLO, KY
JSR PC, DIMOVA ; DARK VECTOR TO LOWER LEFT CORNER
MOV KXHI, KX
JSR PC, DIDRWA ; VECTOR TO LOWER RIGHT CORNER
MOV KYHI, KY
JSR PC, DIDRWA ; VECTOR TO UPPER RIGHT CORNER
MOV KXLO, KX ; VECTOR TO UPPER LEFT CORNER
JSR PC, DIDRWA ; VECTOR TO LOWER LEFT CORNER
RTS PC
;-----
; FORTRAN COMMON /DICOM/ FOR DISPLAY ROUTINES
;
; PSECT DICOM, RW, D, GBL, OVR, REL
IXMIN: .BLKW 1 ; USER LEFT MARGIN
IXMAX: .BLKW 1 ; USER RIGHT MARGIN
IXRAN: .BLKW 1 ; USER X-RANGE
IYMIN: .BLKW 2 ; USER BOTTOM MARGIN (INTEGER*4)
IYMAX: .BLKW 2 ; USER TOP MARGIN (INTEGER*4)
IYRAN: .BLKW 2 ; USER Y-RANGE (INTEGER*4)
IMODE: .BLKW 1 ; CURRENT SOFTWARE DISPLAY MODE
IUSERX: .BLKW 1 ; CURRENT USER X-POSITION
IUSERY: .BLKW 2 ; CURRENT USER Y-POSITION (INTEGER*4)
;
KXLO: .BLKW 1 ; SCREEN LEFT MARGIN
KXHI: .BLKW 1 ; SCREEN RIGHT MARGIN
KXRAN: .BLKW 1 ; SCREEN X-RANGE
KYLO: .BLKW 1 ; SCREEN BOTTOM MARGIN
KYHI: .BLKW 1 ; SCREEN TOP MARGIN
KYRAN: .BLKW 1 ; SCREEN Y-RANGE
KKMODE: .BLKW 1 ; CURRENT HARDWARE DISPLAY MODE
KBEAMX: .BLKW 1 ; CURRENT BEAM X-POSITION
KBEAMY: .BLKW 1 ; CURRENT BEAM Y-POSITION
KSPEED: .BLKW 1 ; TERMINAL SPEED IN CHARACTERS PER SECOND
KPCHAR: .BLKW 4 ; CURRENT BEAM POSITION IN CHARACTER FORMAT

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DIFRAM MACRO M1200 25-FEB-85 13 11 PAGE 1-1

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ABEAM: .BYTE 2,0 ; ARGUMENT BLOCK FOR CURRENT SCREEN COORDINATES
; WORD KBEAMX
; WORD KBEAMY
AUSER: .BYTE 2,0 ; ARGUMENT BLOCK FOR CURRENT USER COORDINATES
; WORD IUSERX
; WORD IUSERY
AKXKY: .BYTE 2,0 ; ARGUMENT BLOCK TEMPORARY SCREEN COORDINATES
; WORD KX
; WORD KY
KX: .BLKW 1 ; TEMPORARY SCREEN X-COORDINATE
KY: .BLKW 1 ; TEMPORARY SCREEN Y-COORDINATE
AIXIY: .BYTE 2,0 ; ARGUMENT BLOCK TEMPORARY USER COORDINATES
; WORD IX
; WORD IY
IX: .BLKW 1 ; TEMPORARY USER X-COORDINATE (INTEGER*2)
IY: .BLKW 2 ; TEMPORARY USER Y-COORDINATE (INTEGER*4)
END

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DIWNDD MACRO H1200 25-FEB-85 13:12 PAGE 1

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000000 005725
000002 012704 000032
000006 013524
000010 017524 000000
000014 013514
000016 166714 000032
000022 005224
000024 013524
000026 017524 000000
000032 013514
000034 166714 000040
000040 005214
000042 000207
    
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      .TITLE DIWNDD
      -----
      ; DEFINE SCREEN WINDOW (SCREEN UNITS)
      ; ROLF GUIGAS      17-FEB-1982
      ;
      ; CALLING SEQUENCE:  CALL DIWNDD (KXLO,KXHI,KXLO,KYHI)
      ;
      ; ON ENTRY:  ABSOLUTE COORDINATES OF SCREEN WINDOW
      -----
DIWNDD: TST  (R5)+          ; SKIP NUMBER OF ARGUMENTS
        MOV  @KXLO,R4      ; POINTER TO ENTRY IN COMMON
        MOV  @R5+,(R4)+    ; GET KXLO
        MOV  @R5+,(R4)+    ; GET KXHI
        MOV  @R5+,(R4)+    ; GET KXHI AGAIN
        SUB  KXLO,(R4)     ; CALCULATE X-RANGE
        INC  (R4)+         ; KXRAN := KXHI-KXLO+1
        MOV  @R5+,(R4)+    ; GET KYLO
        MOV  @R5+,(R4)+    ; GET KYHI
        MOV  @R5+,(R4)+    ; GET KYHI AGAIN
        SUB  KYLO,(R4)     ; CALCULATE Y-RANGE
        INC  (R4)         ; KYRAN := KYHI-KYLO+1
        RTS  PC
    
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      ;
      ; FORTRAN COMMON /DICOM/ FOR DISPLAY ROUTINES
      ;
      ; PSECT DICOM,RV,D.GBL,OVR,REL
      ;
      ; IXXIN:  .BLKW 1      ; USER LEFT MARGIN
      ; IXMAX:  .BLKW 1      ; USER RIGHT MARGIN
      ; IXRAN:  .BLKW 1      ; USER X-RANGE
      ; IYMIN:  .BLKW 2      ; USER BOTTOM MARGIN (INTEGER**4)
      ; IYMAX:  .BLKW 2      ; USER TOP MARGIN (INTEGER**4)
      ; IYRAN:  .BLKW 2      ; USER Y-RANGE (INTEGER**4)
      ; IMODE:  .BLKW 1      ; CURRENT SOFTWARE DISPLAY MODE
      ; IUSERX: .BLKW 1      ; CURRENT USER X-POSITION
      ; IUSERY: .BLKW 2      ; CURRENT USER Y-POSITION (INTEGER**4)
      ;
      ; KXLO:   .BLKW 1      ; SCREEN LEFT MARGIN
      ; KXHI:   .BLKW 1      ; SCREEN RIGHT MARGIN
      ; KXRAN:  .BLKW 1      ; SCREEN X-RANGE
      ; KYLO:   .BLKW 1      ; SCREEN BOTTOM MARGIN
      ; KYHI:   .BLKW 1      ; SCREEN TOP MARGIN
      ; KYRAN:  .BLKW 1      ; SCREEN Y-RANGE
      ; KMODE:  .BLKW 1      ; CURRENT HARDWARE DISPLAY MODE
      ; KBEAMX: .BLKW 1      ; CURRENT BEAM X-POSITION
      ; KBEAMY: .BLKW 1      ; CURRENT BEAM Y-POSITION
      ; KSPEED: .BLKW 1      ; TERINAL SPEED IN CHARACTERS PER SECOND
      ; KPCHAR: .BLKW 4      ; CURRENT BEAM POSITION IN CHARACTER FORMAT
      ; ABEAM:  .BYTE 2,0    ; ARGUMENT BLOCK FOR CURRENT SCREEN COORDINATES
      ; WORD KBEAMX
    
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DIWNDD MACRO H1200 25-FEB-85 13:12 PAGE 1-1

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000072 000052
000074 002 000
000076 000024
000100 000026
000102 002 000
000104 000110
000106 000112
000110
000112
000114 002 000
000116 000122
000120 000124
000122
000124 000001
    
```

```

      ;
      ; WORD KBEAMY
      ; .BYTE 2,0          ; ARGUMENT BLOCK FOR CURRENT USER COORDINATES
      ; WORD IUSERX
      ; WORD IUSERY
      ;
      ; AKXKV:  .BYTE 2,0    ; ARGUMENT BLOCK TEMPORARY SCREEN COORDINATES
      ; WORD KX
      ; WORD KY
      ;
      ; KX:     .BLKW 1      ; TEMPORARY SCREEN X-COORDINATE
      ; KY:     .BLKW 1      ; TEMPORARY SCREEN Y-COORDINATE
      ;
      ; AIXIV:  .BYTE 2,0    ; ARGUMENT BLOCK TEMPORARY USER COORDINATES
      ; WORD IX
      ; WORD IY
      ;
      ; IX:     .BLKW 2      ; TEMPORARY USER X-COORDINATE (INTEGER**2)
      ; IY:     .BLKW 2      ; TEMPORARY USER Y-COORDINATE (INTEGER**2)
      ; END
    
```

DJWNDV MACRO H1200 25-FEB-85 13:12 PAGE 1

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15 000000 005725
16 000002 012704 000000
17 000006 013524
18 000010 017524 000000
19 000014 013514
20 000016 011467 000024
21 000022 166714 000000
22
23 000026 005724
24
25 000030 012503
26 000032 011324
27 000034 012367 000026
28 000040 011367 000030
29 000044 011324
30 000046 011503
31 000050 011324
32 000052 012367 000016
33 000056 011324
34 000060 011367 000020
35 000064 166724 000006
36 000070 005614
37 000072 166714 000010
38 000076 005744
39 000100 062724 000001
40 000104 005514
41 000106 000207
42
43
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47 000000
48 000000
49 000002
50 000004
51 000006
52 000012
53 000016

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          .TITLE DJWNDV
          -----
          DEFINE USER WINDOW
          ROLF GUIGAS      FEB-1982
          BUG TAKEN OUT (IXRAN=IXMAX-IXMIN, NOT IXRAN=IXMAX-IXMIN+1)
          THOMAS KOEHLER  MAY-1983
          CALLING SEQUENCE: CALL DJWNDV (IXMIN,IXMAX,JVMIN,JVMAX)
          ON ENTRY:        USER COORDINATES OF WINDOW (Y IN INTEGER**4)
          -----
          DJWNDV: TST (R5)+          ; SKIP NUMBER OF ARGUMENTS
                  MOV 8IXMIN,R4    ; POINTER TO ENTRY IN COMMON
                  MOV 8(R5)+,(R4)+  ; GET IXMIN
                  MOV 8(R5)+,(R4)+  ; GET IXMAX
                  MOV 8(R5)+,(R4)+  ; GET IXMAX AGAIN
                  MOV (R4),IUSERX   ; IUSERX := IXMIN
                  SUB IXMIN,(R4)    ; CALCULATE USER X-RANGE
                  INC (R4)         ; IXRAN := IXMAX-IXMIN+1
                  TST (R4)+        ; POINT CORRECT
          ;
          MOV (R5)+,R3             ; POINTER TO IVMIN
          MOV (R3),(R4)+          ; GET IVMIN LOW
          MOV (R3)+,IUSERY        ; IUSERY := IVMIN
          MOV (R3),IUSERY+2       ; ... DOUBLE PRECISION
          MOV (R3),(R4)+          ; GET IVMIN HIGH
          MOV (R5),R3             ; POINTER TO IWMAX
          MOV (R3),(R4)+          ; GET IWMAX LOW
          MOV (R3)+,IYRAN         ; ... AGAIN
          MOV (R3),(R4)+          ; GET IWMAX HIGH
          MOV (R3),IYRAN+2        ; ... AGAIN
          SUB IYMIN,(R4)+         ; DOUBLE PRECISION
          MOV (R4)                ; ... CALCULATION
          SUB IYMIN+2,(R4)        ; ... OF USER Y-RANGE
          TST -(R4)
          ADD 8I,(R4)+            ; IYRAN := IYMAX-IYMIN+1
          ADC (R4)
          RTS PC
          -----
          ;
          ; FORTRAN COMMON /DICOM/ FOR DISPLAY ROUTINES
          ;
          ; PSECT DICOM,RW,D,GBL,OVR,REL
          IXMIN: .BLKW 1          ; USER LEFT MARGIN
          IXMAX: .BLKW 1          ; USER RIGHT MARGIN
          IXRAN: .BLKW 1          ; USER X-RANGE
          IVMIN: .BLKW 2          ; USER BOTTOM MARGIN (INTEGER**4)
          IWMAX: .BLKW 2          ; USER TOP MARGIN (INTEGER**4)
          IYRAN: .BLKW 2          ; USER Y-RANGE (INTEGER**4)

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DJWNDV MACRO H1200 25-FEB-85 13:12 PAGE 1-1

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55 000024
56 000026
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58 000032
59 000034
60 000036
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62 000042
63 000044
64 000046
65 000050
66 000052
67 000054
68 000056
69 000066
70 000070 000050 000
71 000072 000052
72 000074 002 000
73 000076 000024
74 000100 000026
75 000102 002 000
76 000104 000110
77 000106 000112
78 000110
79 000112
80 000114 002 000
81 000116 000122
82 000120 000124
83 000122
84 000124
85 000001

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IMODE: .BLKW 1          ; CURRENT SOFTWARE DISPLAY MODE
IUSERX: .BLKW 1          ; CURRENT USER X-POSITION
IUSERY: .BLKW 2          ; CURRENT USER Y-POSITION (INTEGER**4)
;
KXLD: .BLKW 1           ; SCREEN LEFT MARGIN
KXHI: .BLKW 1           ; SCREEN RIGHT MARGIN
KXRRAN: .BLKW 1         ; SCREEN X-RANGE
KYLD: .BLKW 1           ; SCREEN BOTTOM MARGIN
KYHI: .BLKW 1           ; SCREEN TOP MARGIN
KYRAN: .BLKW 1          ; SCREEN Y-RANGE
KKMODE: .BLKW 1         ; CURRENT HARDWARE DISPLAY MODE
KBEAMX: .BLKW 1         ; CURRENT BEAM X-POSITION
KBEAMY: .BLKW 1         ; CURRENT BEAM Y-POSITION
KSPEED: .BLKW 1         ; TERINAL SPEED IN CHARACTERS PER SECOND
KPCHAR: .BLKW 4         ; CURRENT BEAM POSITION IN CHARACTER FORMAT
ABEAM: .BYTE 2,0        ; ARGUMENT BLOCK FOR CURRENT SCREEN COORDINATES
;
AUSER: .WORD KBEAMX     ; WORD KBEAMX
        .BYTE 2,0        ; ARGUMENT BLOCK FOR CURRENT USER COORDINATES
        .WORD IUSERX
        .WORD IUSERY
;
AKXKY: .BYTE 2,0        ; ARGUMENT BLOCK TEMPORARY SCREEN COORDINATES
        .WORD KX
        .WORD KY
;
KX: .BLKW 1             ; TEMPORARY SCREEN X-COORDINATE
KY: .BLKW 1             ; TEMPORARY SCREEN Y-COORDINATE
AIXIV: .BYTE 2,0        ; ARGUMENT BLOCK TEMPORARY USER COORDINATES
        .WORD IX
        .WORD IY
;
IX: .BLKW 2             ; TEMPORARY USER X-COORDINATE (INTEGER**2)
IY: .BLKW 2             ; TEMPORARY USER Y-COORDINATE (INTEGER**4)
END

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```

0001 PROGRAM FITSPY
      *****
      CE
      CE This routine prints the results on the line-printer
      CE
      CE Ver. 1.0 29-Feb-84 (OR) Original version
      CE
0002 IMPLICIT REAL*8 (A-H,O-Z)
0003 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
      * LUNSP=1, LUNPAR=2, LUNPRT=3, NPPARM=6, MXCALF=3,
      * MPOINT=500, MXLINK=20, MAXLIN=10, LUN=6
      CE
0004 BYTE SPESPC(30), PARSPC(30)
0005 COMMON /OPPARS/ MDEV, SPESPC, PARSPC, MXITER, LBFIX, IREG, IXLO, IXHI,
      * IYLO, IYHI, IYPWR, IFLO, IFHI, IPEAK, LBACK, LPEAK, LALL,
      * NCOEFF, COEFF(MAXCO), ITER, NDF, PEAK(NPPARM, MAXPK),
      * IFLAG(NPPARM, MAXPK), INDEX(NPPARM, MAXPK), ISEL,
      * IGNOR(MAXPK), NREG, KREGLO(MAXREG), KREGHI(MAXREG),
      * IMODE, INTCOR, NCALF, CALFAC(MXCALF), SIGMA(MAXPK),
      * GAMMA(MAXPK)
0006 COMMON /OPPART/ IOPARS
0007 COMMON /ERRCOM/ IERR
      CE
0008 DATA IOPARS /0/, DT /1000.D0/, PI /3.141592654D0/,
      * SRPI /1.772453851D0/
      CE
      CE Read FIT parameter file
      CE
0009 CALL PARNAM ('FIT')
0010 CALL PARRD
      CE
      CE Start printout with header lines
      CE
0011 WRITE (LUN,1000)
0012 1000 FORMAT ('1')
      CE
      CE Printout of FIT regions
      CE
0013 WRITE (LUN,1005) ITER, ((KREGLO(J), KREGHI(J)), J=1, NREG)
0014 1005 FORMAT ('0', I2, ' Iteration /
      * '0', 'FIT regions used: ', /, ' ', 6(I5, '- ', I4))
      CE
      CE Printout of background
      CE
0015 WRITE (LUN,1010) NCOEFF
0016 1010 FORMAT ('0', 'Background with', I3, ' coefficients:')
0017 WRITE (LUN,1015) (COEFF(J), J=1, NCOEFF)
0018 1015 FORMAT (' ', 3(IPE16.8) /
      * ' ', 3(IPE16.8))
      CE
      CE Printout of calibration polynomial
      CE
PDP-11 FORTRAN-77 VS. 0-0 13:05:59 3-May-84 Page 2
FITSPY.FTN;1 /F77/OP/TR:BLOCKS/WR
0019 IF (NCALF GT 0) THEN
0020 WRITE (LUN,1020)
0021 1020 FORMAT ('0', 'Calibration polynomial:')
0022 WRITE (LUN,1015) (CALFAC(J), J=1, NCALF)
0023 ENDDI
      CE
      CE Printout of peaks
      CE
0024 NPLINE = 0
0025 DO 1050 IPEAK=1, MAXPK, 1
0026 IF (IGNOR(IPEAK) .EQ. 1) GOTO 1050
      CE
      CE Convert width to FWHM
      CE
0027 IHTIG = INDEX(3, IPEAK)
      CE
      CE Gaussian
      CE
0028 IPARM = 0
0029 XPI = SRPI
0030 WIDTH = SIGMA(IPEAK)
      CE
      CE Lorentzian
      CE
0031 IF (IFLAG(G, IPEAK) .NE. -2) THEN
0032 IPARM = 4
0033 XPI = PI
0034 WIDTH = GAMMA(IPEAK)
0035 ENDDI
      CE
      CE Area
      CE
0037 AREA = XPI * PEAK(3, IPEAK) * WIDTH
    
```

```

      CE
      CE Start output
      CE
0038 IF (NPLINE.EQ.0) THEN
0039 WRITE (LUN,1025)
0040 1025 FORMAT (' ')
0041 WRITE (LUN,1030)
0042 1030 FORMAT (' ', 'Position', 2X, 'Gauss-FWHM', 3X, 'Height', 1X,
      * 'Low-tail', 1X, 'High-tail', 1X, 'Lorentz-FWHM',
      * 'Intensity')
      CE
0043 ENDDI
0044 WRITE (LUN,1035) IPEAK, (IFLAG(I, IPEAK), I=1, NPPARM)
0045 1035 FORMAT ('0', 'Peak', 3, I2, ' (Flags: ', 5(I2, ' ', I2, '))')
0046 WRITE (LUN,1040) (PEAK(I, IPEAK), I=1, NPPARM), AREA
0047 1040 FORMAT (' ', F3.1X, F7.3, 1X, F13.2, 2X, OPFF.3, 2X, F7.3, 2X, F7.3,
      * 1X, F13.2)
      CE
      CE Print calibration (if any)
      CE
0048 IF (NCALF GT 0) THEN
0049 XPI = PEAK(1, IPEAK)
PDP-11 FORTRAN-77 VS. 0-0 13:05:59 3-May-84 Page 3
FITSPY.FTN;1 /F77/OP/TR:BLOCKS/WR
0050 WIDTH = 0.500*PEAK(2, IPEAK)
0051 DWIDTH = 0.500*PEAK(6, IPEAK)
0052 WRITE (LUN,1045) CALVAL(XPI),
      * DT*(CALVAL(XPI+WIDTH)-CALVAL(XPI-WIDTH)),
      * DT*(CALVAL(XPI+DWIDTH)-CALVAL(XPI-DWIDTH))
0053 1045 FORMAT (' ', 'E', F9.4, ' ', 'G', F8.1, ' ', 'L', F8.1)
0054 ENDDI
      CE
      CE Make a nice paging
      CE
0055 NPLINE = NPLINE + 1
0056 IF (NPLINE GE MAXLIN) THEN
0057 WRITE (LUN,1047)
0058 1047 FORMAT ('1')
0059 NPLINE = 0
0060 ENDDI
0061 1050 CONTINUE
      CE
      CE Terminate silently
      CE
0062 9000 END
    
```

```

PDP-11 FORTRAN-77 VS. 0-0 13:06:16 3-May-84 Page 6
FITSPY.FTN;1 /F77/OP/TR:BLOCKS/WR
0001 DOUBLE PRECISION FUNCTION CALVAL (DCHAN)
      *****
      CE
      CE This function returns the ...
      CE
0002 IMPLICIT REAL*8 (A-H,O-Z)
0003 PARAMETER MAXCHN=4096, MAXPK=30, MAXCO=6, MAXREG=7, MAXPAR=40,
      * LUNSP=1, LUNPAR=2, LUNPRT=3, NPPARM=6, MXCALF=3,
      * MPOINT=500, MXLINK=20, MAXLIN=6, LUN=6
      CE
0004 BYTE SPESPC(30), PARSPC(30)
0005 COMMON /OPPARS/ MDEV, SPESPC, PARSPC, MXITER, LBFIX, IREG, IXLO, IXHI,
      * IYLO, IYHI, IYPWR, IFLO, IFHI, IPEAK, LBACK, LPEAK, LALL,
      * NCOEFF, COEFF(MAXCO), ITER, NDF, PEAK(NPPARM, MAXPK),
      * IFLAG(NPPARM, MAXPK), INDEX(NPPARM, MAXPK), ISEL,
      * IGNOR(MAXPK), NREG, KREGLO(MAXREG), KREGHI(MAXREG),
      * IMODE, INTCOR, NCALF, CALFAC(MXCALF), SIGMA(MAXPK),
      * GAMMA(MAXPK)
0006 COMMON /OPPART/ IOPARS
0007 COMMON /ERRCOM/ IERR
      CE
      CE Apply calibration (if any)
      CE
0008 IF (NCALF GT 0) THEN
0009 DTEMP = DCHAN
0010 CALVAL = CALFAC(1)
0011 DO 1000 J=2, NCALF+1
0012 CALVAL = CALVAL + (DTEMP*CALFAC(J))
0013 DTEMP = DTEMP*DTEMP
0014 1000 CONTINUE
0015 ELSE
0016 CALVAL = 0.000
0017 ENDDI
      CE
      CE Return to calling program
      CE
0018 RETURN
      CE
0019 *****
      CE
      CE END
    
```