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August, 1973

IM41-1108-00
SOFTWARE INSTRUCTION MANUAL
ND4410 PEAK FIND AND GAUSSIAN FIT
W/DOUBLET RESOLUTION OVERLAY PROGRAM

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INSTRUCTION MANUAL CHANGES
IM41-1108-00
ND4410 PEAK FIND AND GAUSSIAN FIT W/DOUBLET
RESOLUTION OVERLAY PROGRAM

Original Issue: August, 1973

Make the change listed below as ERRATA in your Instruction Manual. This change is effective for all programs with part number 41-1108-01.

ERRATA Page 3-3, paragraph 3-4, lines 3, 6, and 9 - change location references from $\emptyset, 4521g$ to $\emptyset, 4552g$.

March 12, 1975

This Instruction Manual Change Sheet supercedes all prior change sheets to this manual.

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SECTION I INTRODUCTION

1-1. PROGRAM SUMMARY

1-2. The ND4410 Peak Find and Gaussian Fit w/Doublet Resolution Overlay Program (41-1108) is written in assembly language for use with the ND4410 Data Acquisition and Display System. The program is an overlay for the ND4410 Basic Physics Analyzer Program (41-1060) containing routines for peak find/fit, energy calibration and data smoothing. The peak find/fit routine uses a peak extraction process to automatically examine the portion of the spectrum contained between the left and right markers of the currently displayed group for peak centroid, full-width-half-maximum (FWHM), background and peak area information. The peak extraction process uses an additive correlation method for peak determination based upon entry of the half width from which it determines the maximum peak width and the convoluted width. Upon extraction of each peak, the peak find routine displays markers at peak limits and prints the following information at the Teletype: the peak number (from left to right), an error code number (if applicable), the channel location of the peak centroid, the number of channels at the FWHM point, the background counts, the net total counts (the total number of counts in the area defined by the peak minus the background counts), and the channel locations of the left and right minimum points (limits) of the peak. The error code list number indicates characteristics of the peak extraction process which can be altered by varying the half width parameter. Upon completion of printout of the information determined for each peak during the peak extraction process, the peak fit process is initiated. The fit process first determines if the peak found during the peak extraction process was a single peak or a doublet. If the peak is a single peak, a least squares Gaussian fit process is performed which uses the centroid, FWHM and height values found by the peak extraction process as initial guesses. Upon completion of the fit process, markers are again displayed at the peak limits, and values for the centroid, FWHM, height and area of the Gaussian are printed at the Teletype. If the peak is a doublet, pairs of input guesses are generated for the double peak which are based upon the skewness of the peak and the centroid, FWHM, height, left and right channel values found by the peak extraction process. The pairs of guesses are then used as input to the Gaussian fit process which separates and fits the doublet, improving the initial guesses by an iterative scheme. Upon completion of the fit, markers are again displayed at the peak limits and new values for the centroid, FWHM, height and

area for each peak are printed at the Teletype. The number of iterations is also printed. The peak fit can also be manually initiated on any single peak or doublet using the Manual Override Command. This command permits selecting any single peak or doublet using the display markers, and entering the channel value(s) of the peak centroid(s). It then initiates the peak fit process, and prints the centroid, FWHM, height and area values of the peak(s) at the Teletype. The energy calibration routine permits energy calibration based upon entry of the known energy in eV for any two peaks determined during the peak find/fit routine. The routine then calculates the energy intercept and the energy per channel (slope). The data smooth routine performs a five-point coefficient smoothing operation on the data spectrum contained in the currently displayed group to reduce the deviation of counts in the spectrum or to compensate for poor statistics. The smooth operation can be performed from 1 to 4095 times.

1-3. PROGRAM AREA

1-4. The program occupies memory locations $0,4000_8 - 0,7777_8$ and $1,0000_8 - 1,2710_8$.

1-5. STARTING ADDRESS

1-6. All routines of this program are called through the command mode of the ND4410 Basic Physics Analyzer Program (41-1060) via Teletype entered single-letter mnemonics.

1-7. EQUIPMENT CONFIGURATION

1-8. The minimum equipment required for proper operation of this program is:

- a. An ADC.
- b. The ND4410 Function Control Module.
- c. A 33ASR Teletype.
- d. A display oscilloscope.
- e. The 8K, ND812 Computer.

1-9. The program will operate with either an 8K, 12K, or 16K ND812 Memory configuration providing maximum data storage configuration of 1K, 3K or 5K (24 bits), respectively.

SECTION II PROGRAM DESCRIPTION

2-1. INTRODUCTION

2-2. The ND4410 Peak Find and Gaussian Fit w/Doublet Resolution Overlay Program (41-1108) consists of three routines for parameter definition and implementation of a peak extraction/fit process, an energy calibration routine and a data smoothing routine. The peak extraction process is described in an article: "Automatic Peak Analysis on Mini-computers" by E. von Meerwall and M.D. Gawlik in Computer Physics Communications 5 (1973) 309.

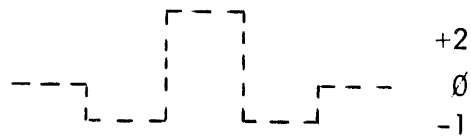
2-3. PEAK EXTRACTION PROCESS

2-4. Peak extraction when dealing with line shapes is usually performed using a mathematical model such as a gaussian for a correlator. This process yields excellent results but also requires use of floating-point arithmetic which significantly increases processing time. In addition, this technique is not easily adaptable for use in a small computer. Therefore, a peak extraction process using an additive correlation procedure similar to the one described in the above article has been used in this program for automatic examination of spectra for peak centroid, FWHM, background and intensity information.

2-5. The process used in this program is designed to be fast (by avoiding floating-point arithmetic, the execution time is significantly reduced), efficient and use a minimum of core.

2-6. The program permits specification of one parameter which is used in the peak extraction process. This is the half width from which the program determines the maximum width of spectral peak and the correlator width. The specification of different half widths allows the analyst considerable flexibility in dealing with individual spectra or in developing a general procedure peculiar to his needs.

2-7. The correlator used in this program is a zero-area rectangular fold-in function as depicted below.



2-8. Implementation of this type of correlation involves only addition and subtraction of data points. The resulting convoluted spectrum is examined for points which alternately exceed and recede through a discrimination level based on the standard deviation. When a pair of points L, R is determined, and refined by testing of the average slopes near these points, four point averages are used to locate the background on either side of the peak for linear interpolation. At this point the background subtracted area (intensity) of the peak can be easily calculated. The centroid is then determined by finding the center of gravity for the respective points in the background subtracted spectrum. If the value of any background subtracted channel content is not significantly greater than the local background statistics, the value is set equal to zero for the channel under consideration. Thus, the center of gravity and area results exclude points which are not significantly above the local background statistics.

2-9. The FWHM is calculated by determining the background subtracted highest channel in the peak. The contents of this channel is then halved and this value is used as a test for determining the channel on either side of the peak which just exceeds this value. Once these channels are determined, the intercepted difference of the two channels (the one just above and the one just below the value) is calculated using similar triangle relations. These positions plus the integer channel difference is then equal to the FWHM.

2-10. PEAK FIT PROCESS

2-11. The peak fit process first determines if the peak found during the peak extraction process is a single peak or doublet. If the peak is a single peak, a least squares Gaussian fit is performed using the centroid, FWHM and height values found by the peak extraction process as initial values.

2-12. The equation of a single Gaussian on zero background is:

$$Y(X) = H * \text{EXP}(-2.7724 * ((X - X_C) / \text{GAMMA}) ** 2).$$

If the spectrum $Y(X)$ is transformed logarithmically, this equation has the form:

$$\text{LN } Y(X) = A + B * X + C * X ** 2,$$

where A, B, and C involve the descriptive parameters H, X_C , and GAMMA.

The details of the method of fitting are described in a paper: "Automatic Spectra Analysis on Minicomputers: Doublet Resolution by Gaussian Fit", by E.D. von Meerwall and M.D. Gawlik, submitted to Computer Physics Communications.

- a. Do a channel-by-channel subtraction of background (and, where appropriate the other Gaussian), to get:

$$Y'(I) = Y(I) - \text{BKG}(I), \text{ where } I = \text{channel number.}$$

- b. Now set the weighting factor for each channel:

$$Q = (Y'(I))^{* * 2}. \text{ Then let } Y'(I) \leftarrow \text{LN}(Y'(I)), \text{ and } X(I) = 1.$$

- c. With the above three substitutions, minimize the following expression:

$$F = \text{Sum of } (Q * Y'(I) - A - B * X(I) - C * X(I) * * 2) * * 2):$$

where $I = L, L + 1, \dots, R$ channels.

This is done by requiring the derivatives of F with respect to A, B, and C to be zero. The resulting three simultaneous linear equations are solved for A, B, and C using the method of determinants.

- d. Using the values of A, B, and C, obtained, solve for GAMMA, XC, H in the equation describing a Gaussian line shape:

$$\begin{aligned} \text{GAMMA} &= \text{SQRT}(-2.7724/C) \\ \text{XC} &= ((\text{GAMMA})^{* * 2}) * B / (2 * 2.7724) \\ \text{H} &= \text{EXP}(A + 2.7724 * \text{XC})^{* * 2} / \text{GAMMA}^{* * 2}). \end{aligned}$$

2-12. If the peak is a doublet, pairs of input guesses are generated for the double peak which are based upon the skewness of the peak, the centroid, FWHM, height, left and right channel values found by the peak extraction process. The pairs of guesses are then used as input to the peak fit process which separates and fits the doublet, improving the initial guesses by an iterative scheme, involving fits (as described above) alternated to each component of the doublet.

2-13. ENERGY CALIBRATION

2-14. Energy calibration is based upon entry of the known energies for any two peaks determined by the peak fit process. The routine then calculates the energy per channel (slope) and the energy intercept. The formula for calculation of the energy per channel is as follows:

$$A1 = \frac{E_2 - E_1}{X_2 - X_1}$$

where
 $A1$ = Energy per channel (slope)
 E_1 = Energy in eV of first known peak channel
 E_2 = Energy in eV of second known peak channel
 X_1 = First known peak channel
 X_2 = Second known peak channel

2-15. The formula for calculation of the energy intercept is as follows.

$$A\emptyset = E_1 - A1X_1$$

where
 $A\emptyset$ = Energy intercept
 E_1 = Energy in eV of first known peak
 $A1$ = Energy per channel (slope) calculated above
 X_1 = First known peak channel

2-16. DATA SMOOTHING

2-17. The purpose of data smoothing is normally to reduce the deviation of counts in the spectrum or to partially compensate for poor statistics. This program incorporates a five-point coefficient smooth routine which can be performed on the spectrum contained in the currently displayed group. Data smoothing is accomplished by successively addressing each channel in the currently displayed group, solving the following equation using the contents of five channels (the currently addressed channel and two channels before and after it), and then re-storing and displaying the results. The contents of the first two channels and the last two channels of the currently displayed group are replaced unaltered. Since the data smoothing routine is time-shared in the background display program other functions can be performed during the time the smooth operation is in progress.

$$S_{(\emptyset)} = 1/35 [17Y_{(\emptyset)} + 12(Y_{(-1)} + Y_{(+1)}) - 3(Y_{(-2)} + Y_{(+2)})]$$

where
 $S_{(\emptyset)}$ = Contents re-stored after smoothing
 $Y_{(\emptyset)}$ = Contents of the currently addressed channel
 $Y_{(-1)}$ = Contents of the currently addressed channel -1
 $Y_{(+1)}$ = Contents of the currently addressed channel +1
 $Y_{(-2)}$ = Contents of the currently addressed channel -2
 $Y_{(+2)}$ = Contents of the currently addressed channel +2

SECTION III OPERATIONAL PROCEDURE

3-1. INITIALIZATION PROCEDURE

3-2. The following is a step-by-step procedure for loading and initializing the ND4410 Peak Find and Gaussian Fit w/Doublet Resolution Overlay Program (41-1108).

NOTE

Prior to performing the following procedure, load and initialize the ND4410 Basic Physics Analyzer Program and, if desired, any one of the following ND4410 overlay programs.

1. Data Manipulation Overlay Program (41-1061)
2. Low/High Speed Paper Tape I/O Overlay Program (41-1062)
3. Magnetic Tape Cassette I/O Overlay Program (41-1063)
4. Magnetic Tape Overlay Program (41-1064)
5. Real Time Clock Overlay Program (41-1065)
6. Franklin Printer Overlay Program (41-1066)
7. Hewlett Packard Overlay Program (41-1067)
8. Block Format Magnetic Tape Cassette I/O Overlay Program (41-1105)

Refer to the respective Software Instruction Manual (IM41-1XXX) for the loading and initialization procedures pertaining to the above listed programs.

- a. Depress the STOP key at the ND812 Computer.
- b. Place the START/STOP/FREE switch at the Teletype in the FREE position.
- c. Load the paper tape of the ND4410 Peak Find and Gaussian Fit w/Doublet Resolution Overlay Program (41-1108) into the Teletype reader with the leader (8-level punches) over the read head.

- d. Set the START/STOP/FREE switch to START.
- e. Simultaneously depress the LOAD AR and NEXT WORD keys at the ND812 Computer. The Teletype will step through the leader and read the program into the ND812 memory. Upon completion of read-in, the reader will stop automatically. When the reader stops, check the J Register for zero. If non-zero, reload.

NOTE

Refer to the ND812 Binary Paper Tape and Cassette Loader Program (41-0005) for loading procedures using a high speed paper tape reader or magnetic tape cassette.

- f. Set the SWITCH REGISTER switches at starting address (0,0200₈) and depress the LOAD AR key.
- g. Depress the START key. The program will cause the Teletype to perform a carriage return/line feed, print ND4410, perform another carriage return/line feed and print PLOTTER?, and then waits for entry of a Y or N to indicate whether or not an X-Y plotter is to be used.
- h. If an X-Y plotter is not used, type N. When N is typed, the program causes the Teletype to print NO, perform a carriage return/line feed and type an asterisk (*).
- i. If an X-Y plotter is used, type Y. When Y is typed, the program causes the Teletype to print YES and supplies a (0,0) calibration voltage to the X-Y plotter.
- j. Adjust the plotter Zero controls to place the pen at the desired (0,0) point.
- k. Depress the SPACE bar at the Teletype. This supplies a full scale X-Y calibration voltage to the X-Y plotter.
- l. Adjust the plotter Vernier controls to place the pen at the desired full scale X-Y point.
- m. Depress the SPACE bar at the Teletype again. This returns the calibration voltage to the (0,0) point. Readjust the plotter Zero controls to place the pen at the desired (0,0) point.

- n. Depress the SPACE bar at the Teletype again. This returns the calibration voltage to the full scale X-Y point. Readjust the plotter Vernier controls to place the pen at the desired full scale X-Y point.
- o. Repeat steps m and n as often as necessary to attain satisfactory calibration. When satisfactory calibration is attained, depress the RETURN key at the Teletype. When the RETURN key is depressed, the program causes the Teletype to perform a carriage return/line feed and type an asterisk (*).
- p. When an asterisk (*) is typed either after step h or after step o, call up the desired routine from the monitor mode by depressing the appropriate pushbutton at the ND4410 Function Control Module or by typing the appropriate single-letter mnemonic at the Teletype keyboard.

3-3. PEAK SENSITIVITY ADJUSTMENT

3-4. The sensitivity level of the program is set at a nominal value for peak extraction using spectra with average background content. The nominal value is defined by the content of location $0,4521_8^*$ and is initially set to 0020_8 . By altering the contents of this location, the sensitivity of the peak extraction process can be increased or decreased, accordingly. To increase sensitivity, i.e., to extract peaks that slightly exceed the average background content; the content of location $0,4521_8^*$ can be changed to any octal value less than 0020_8 , but not 0000_8 since zero is an unacceptable value. Maximum sensitivity would be obtained using a value of 0001_8 . To decrease sensitivity, i.e., to extract only large peaks; the content of location $0,4521_8^*$ could be changed to a value of 0021_8 or greater.

*use $0,4552_8$ in 41-1108-01

SECTION IV OPERATOR OR USER CONTROL

4-1. GENERAL INFORMATION

4-2. The commands of the ND4410 Peak Find and Gaussian Fit w/Doublet Resolution Overlay Program (41-1108) are executed by entering the appropriate single-letter mnemonic at the Teletype after the program causes an asterisk (*) to be typed, signifying the command mode. In the following descriptions, the portion of the command to be typed at the Teletype is underlined. All other information is provided by the program.

4-3. HALF WIDTH COMMAND

4-4. The Half Width Command permits entry of a number equal to the average number of channels at the full-width-half-maximum points of the peaks to be determined during the peak extraction/fit process. The Half Width can be any number of channels from 2 to 85. The following is an example of the entry required for the Half Width command. In this example, 2 is entered as the half width. An estimation of the half width can be made by observing several of the peaks in an expanded display, actually counting the number of channels at the FWHM points of the peaks and then using the average number for the half width.

```
*L  
HW:2 (SPACE)
```

*

4-5. The Half Width command is specified by typing an L after an asterisk (*) is typed. When L is typed, the routine causes the Teletype to perform a carriage return/line feed and print HW:, and then waits for entry of the half width. The half width can be any number of channels from 2 to 85. Entry of the half width must be terminated by depressing the SPACE bar at the Teletype. When the SPACE bar is depressed, the routine causes the Teletype to perform a carriage return/line feed and type an asterisk (*), signifying return to the command mode.

4-6. PEAK FIND/FIT COMMAND

NOTE

Prior to performing the Peak Find/Fit Command, the Half Width command should be performed to enter the half width. The half width is initially set to 4 by the program.

4-7. The Peak Find/Fit command determines the centroid, FWHM and intensity information for each peak contained within the marker defined portion of the spectrum stored in the currently displayed group. Each peak is determined using a peak extraction process which is based upon the entry for the half width parameter. During the peak extraction process, the display is disabled. Upon extraction of each peak, the display is re-enabled with markers at the left and right limits of the peak and the following information is printed at the Teletype: the number of the extracted peak (from left to right), an Error Code List (ECL) number (if applicable), the channel location of the peak centroid, the number of channels at the Full-Width-Half-Maximum (FWHM) point, the background counts, the net total counts (the total number of counts in the area defined by the peak minus the background counts), and the channel locations of the left and right minimum points of the peak. The Error Code List number indicates three characteristics of peak extraction process. ECL #1 indicates that the slopes on either side of the peak do not meet the test criteria either because the half width entered is smaller than the half width of the extracted peak, the extracted peak represents a Compton edge or the extracted peak represents one or more peaks. ECL #2 indicates the left portion of the extracted peak falls beyond the first channel of the group. ECL #3 indicates the right portion of the extracted peak falls beyond the last channel of the group. Upon completing printout of the information determined for each peak during the peak extraction process, the peak fit process is initiated. During the peak fit process, the display is disabled. The peak fit process first determines if the peak found during the peak extraction process is a single peak or doublet. If the peak is a single peak, a least squares Gaussian fit process is performed which uses the centroid, FWHM and height values found by the peak extraction process as initial guesses. Upon completing the fit process, the display is re-enabled with marker at the left and right limits of the peak and values for the centroid, FWHM, height and area of the Gaussian are printed at the Teletype. If the peak is a doublet, pairs of input guesses are generated for the double peak which are based upon the skewness of the peak, the centroid, FWHM, height, left and right channel values found by the peak extraction process. The pairs of guesses are then used as input to the peak fit process which separate and fit the doublet, improving the initial guesses by an iterative least squares Gaussian fit process. Upon completing the iterative fit process, the display is re-enabled with markers at the left and right limits of the peak and fit values for the centroid, FWHM, height and area for each of the two peaks are printed at the Teletype. The number of iterations is also printed. The following is an example of the entry required and the resulting printout at the Teletype. In this example, the peak find/fit routine is performed on

the spectrum shown in Figure 4-1 which was acquired using a solid state (GeLi) detector. The peak extraction/fit process is based upon a half width of 2.

NOTE

The maximum group width (selected using the Group Set Command, 41-1060) in which the peak extraction/fit process can be performed is 4095 channels.

* P

NO.	ECL	CENTROID	FWHM	BKG(HGT)	AREA	LEFT	RIGHT
1		519.99	2.09	7357.50	3104.50	516	524
		519.89	2.15	1392.89	3173.69		
2		538.96	2.13	8166.13	5262.88	534	544
		538.95	2.14	2120.76	4805.80		
3		585.39	4.28	7795.13	8388.87	579	591
		584.27	2.01	2283.66	4865.32		
10		586.85	2.01	1631.12	3475.10		
4		666.16	2.08	2050.13	3109.87	661	671
		666.13	2.12	1312.29	2954.74		
5		682.38	2.32	1897.50	7105.50	677	688
		682.36	2.25	2925.06	6988.68		
6		700.19	2.15	686.00	483.00	697	703
		699.99	1.79	153.86	291.96		
7		729.85	2.32	1301.63	5057.37	724	736
		729.84	2.29	1993.57	4841.52		
8	1	793.38	2.50	1875.52	187.48	789	811
		795.33	3.81	115.08	464.88		

*

888/283
488-808

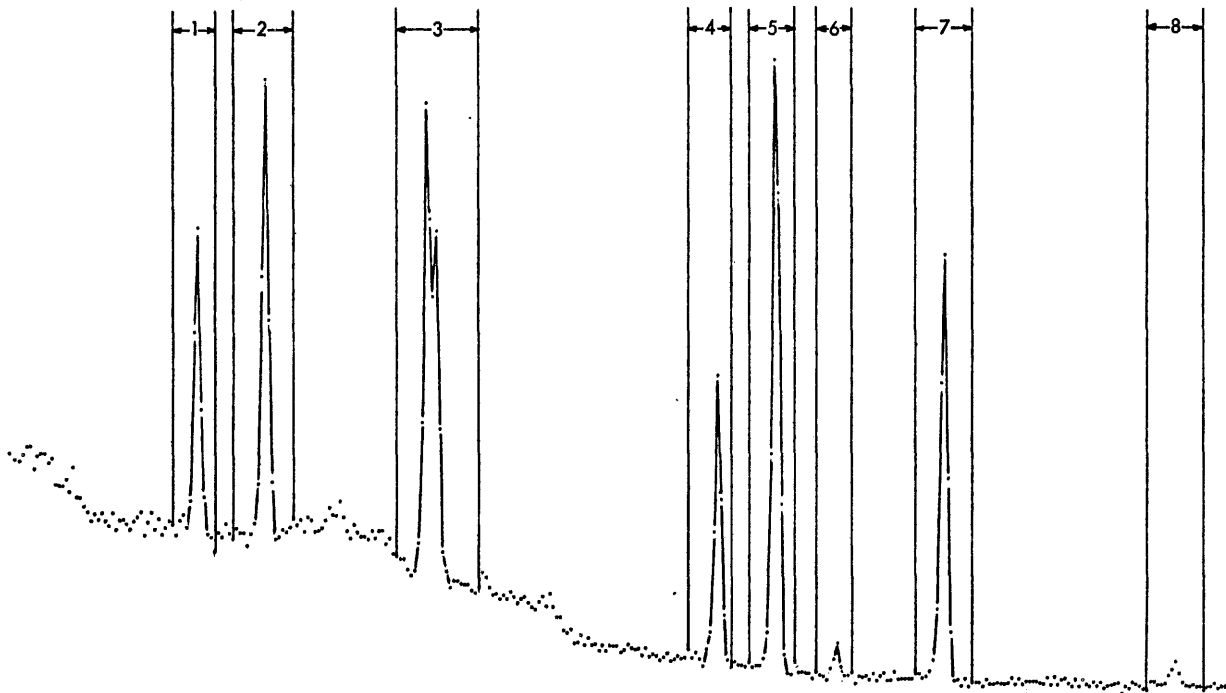


Figure 4-1. Marker Defined Portion of 1024 Channel Spectrum with Markers at the Limits of Eight Extracted Peaks (GeLi Detector)

4-8. The Peak Find/Fit Command is specified by typing P after an asterisk (*) is typed. When P is typed, the routine causes the Teletype to perform a carriage return/line feed, print the column heading NO., ECL, CENTROID, FWHM, BKG(HGT), AREA, LEFT and RIGHT, and perform another carriage return/line feed, and then performs the peak extraction process for the first peak. During the peak extraction process the display is disabled. Upon extraction of the first peak, the routine re-enables the display with markers at the left and right limits of the peak and prints the values under each column heading at the Teletype. Upon completion of printout of the values determined during the peak extraction process for the first peak, the routine initiates the peak fit process. During the peak fit process the display is disabled. Upon completion of the peak fit process the routine re-enables the display with markers at the left and right limits of the peak and prints either one or two lines of values under the column heading: CENTROID, FWHM, BKG(HGT) and AREA. If the peak is a single peak only one line is printed. If the peak is a doublet, two lines are printed with the number of iterations (10, maximum) printed in the second line under the column heading: ECL. Upon completion of printout of the values determined for the first peak, the routine causes the Teletype to perform a carriage return/line feed, performs the peak extraction process for the next peak, displays markers at the peak limits, prints the values determined by the peak extraction process, performs the peak fit process, again displays markers at the peak limits, prints the values determined by the peak fit process and then causes the Teletype to perform another carriage return/line feed. When the peak extraction/fit process, display and printout for the last peak is complete, the routine causes

the Teletype to perform a carriage return/line feed and type an asterisk (*), signifying return to the command mode.

4-9. MANUAL OVERRIDE COMMAND

4-10. The Manual Override Command permits manually performing the peak fit process as any single peak (or doublet) selected using the display markers. After the peak is selected, the channel value(s) of the peak centroid(s) is entered and the peak fit process is initiated using the channel value(s) and the marker channels as initial guesses. Upon completion of the peak fit process, the centroid, FWHM, height and area values of the peak(s) are printed at the Teletype. The following is an example of entries required and the resulting printout at the Teletype. In this example, a single peak (peak 2, Figure 4-1) was selected by setting the left marker at channel 529 and the right marker at channel 549 (approximately 5 channels on either side of the peak limits) using the MARK POS and SPAN pushbuttons. The channel value (539) of the peak centroid (read from the Status display of the center marker by moving the expanded display using the MOTION and WIDTH pushbuttons) was entered. The peak fit process is based upon the channel value entered, the marker channels and a half width of 2 (previously entered using Half Width command).

```
* M: 1 (SPACE) X1: 539 (SPACE)
           538.96    2.07    2097.98    4602.72
*
```

4-11. The following is another example of the Manual Override command but this time it is performed on a doublet (peak 3, Figure 4-1) which was selected by setting the left marker at channel 574 and the right marker at channel 596 (again approximately 5 channels on either side of the peak limits) using the MARK POS and SPAN pushbuttons. In this example, the channel values (584 and 587) of the peak centroids (again read from the Status display of the center marker by moving the expanded display using the MOTION and WIDTH pushbuttons) were entered. The peak fit process (in this case iterative) is based upon the channel values entered, the marker channels and a half width of 2 (previously entered using the half width command). The number of iterations (10) is also printed.

```
* M: 2 (SPACE) X1: 584 (SPACE) X2: 587 (SPACE)
           584.27    2.00    2262.87    4806.40
10      586.85    2.00    1613.79    3427.73
*
```

4-12. The Manual Override Command is specified by typing M after an asterisk (*) is typed. Prior to typing M, select a single peak or doublet using the MARK POS and SPAN pushbuttons, positioning the left and right markers approximately 5 channels on either side of the peak limits (i.e., on representative background data). After a single peak or doublet has been selected, type M. When M is typed, the routine causes the Teletype to print a colon (:), and then waits for entry of a 1 or 2 to specify a single peak or a doublet, respectively. Entry of 1 or 2 must be terminated by depressing the SPACE bar at the Teletype. When the SPACE bar is depressed, the routine causes the Teletype to print X1:, and then waits for entry of the channel value of the centroid of the single peak or the first peak of a doublet. The channel value of the centroid can be read directly from the Status display of the center marker by moving the expanded display using the MOTION and WIDTH pushbuttons. Entry of the channel value must be terminated by depressing the SPACE bar at the Teletype. When the SPACE bar is depressed, the routine either initiates the peak fit process or causes the Teletype to print X2:. If a single peak was specified, the routine initiates the peak fit process on the single peak. If a doublet was specified, the routine causes the Teletype to print X2:, and then waits for entry of the channel value of the centroid of the other peak in the doublet. The channel value of the centroid of the second peak can also be read directly from the Status display of the center marker by moving the expanded display using the MOTION and WIDTH pushbuttons. Entry of the second channel value must also be terminated by depressing the SPACE bar at the Teletype. When the SPACE bar is depressed the routine initiates the peak fit process on the doublet. Upon completion of the peak fit process, the routine prints either one or two lines of values (centroid, FWHM, height and area). If the peak is a single peak, one line is printed. If the peak is a doublet, two lines are printed with the number of iterations printed in the first column of the second line. Upon completion of printout of the values, the routine causes the Teletype to perform a carriage return and line feed and type an asterisk (*), signifying return to the command mode.

4-13. ENERGY CALIBRATE COMMAND

4-14. The Energy Calibrate Command permits entry of the half width and then performs the peak extraction/fit process, marker display and printout in the same manner as the Peak Find/Fit Command. In addition, it permits entry of the known energy in eV for any two peaks and then calculates the energy intercept (A0) and the energy per channel (A1) in eV/channel. Once the energy calibrate command has been executed, the Centroid and FWHM values printed during any ensuing peak extraction/fit process, will be in KeV and will be based on the last two known energy values entered. The following is an example of the entries required and the resulting printout for the Energy Calibrate Command. In this example, the peak extraction process is performed on the spectrum shown in Figure 4-1 using a half width of 2. The energy calibration is based on the energy values entered for the second and fifth peaks which have known energies of 1,938,000 eV and 1,188,000 eV, respectively.

NOTE

To return to the uncalibrated mode once the Energy Calibrate Command has been performed, change the contents of location 0,5722g to 0000g.

* ENERGY CALIBRATE

HW: 2 (SPACE)

NO.	ECL	CENTROID	FWHM	BRK(HGT)	AREA	LEFT	RIGHT
1		519.99	2.09	7357.50	3104.50	516	524
		519.89	2.15	1392.89	3173.69	E(EV):	<u>Ø (SPACE)</u>
2		538.96	2.13	8166.13	5262.88	534	544
		538.95	2.14	2120.76	4805.80	E(EV):	<u>938000 (SPACE)</u>
3		585.39	4.28	7795.13	8388.87	579	591
		584.27	2.01	2283.66	4865.32	E(EV):	<u>Ø (SPACE)</u>
10		586.85	2.01	1631.12	3475.10	E(EV):	<u>Ø (SPACE)</u>
4		666.16	2.08	2050.13	3109.87	661	671
		666.13	2.12	1312.29	2954.74	E(EV):	<u>Ø (SPACE)</u>
5		682.38	2.32	1897.50	7105.50	677	688
		682.36	2.25	2925.06	6988.68	E(EV):	<u>1188000 (SPACE)</u>

A0 = -1514.72

A1 = 1743.24

4-15. The Energy Calibrate Command is specified by typing E after an asterisk (*) is typed. When E is typed, the routine causes the Teletype to print ENERGY CALIBRATE, perform a carriage return/line feed and print HW:. When HW: is printed, the routine waits for entry of the half width. The half width can be any number from 2 to 85. Entry of the half width must be terminated by depressing the SPACE bar at the Teletype. When the SPACE bar is depressed, the routine causes the Teletype to perform a carriage return/line feed, print the column headings NO., ECL, CENTROID, FWHM, BKG(HGT), AREA, LEFT and RIGHT, perform another carriage return/line feed, and then performs the peak extraction/fit process for the first peak. Upon completion of the extraction/fit process for the first peak, the routine displays markers at the left and right limits of the peak and prints the respective information at the Teletype. After the fit process value under the AREA column is printed, the routine causes the Teletype to print E(EV):, and then waits for entry of a known energy value in eV. If the first peak is one of the known peaks for which an energy value is to be entered, enter the energy value after the E(EV): is printed. If not, enter Ø. Entry of an energy value or zero (Ø) must be terminated by depressing the SPACE bar at the Teletype. When the SPACE bar is depressed the routine causes the Teletype to perform a carriage return/line feed, and then performs the peak extraction/fit process for the next peak. Upon completion of the extraction/fit process for the next and each succeeding peak, the routine displays markers at the peak limits, prints values for each column heading and E(EV):, and then waits for entry of a known energy value. An energy value can be entered for any two peaks determined during the peak extraction/fit process with zeroes entered for all other

peaks. The energy value can be any number from 1 to 8,388,607 eV. When the SPACE bar is depressed to terminate entry of an energy value for the second known peak, the routine causes the Teletype to perform a carriage return/line feed, print A0 = and the value of the energy intercept in eV, perform another carriage return/line feed, print A1 = and the value of the slope (energy per channel) in eV/channel, performs another carriage return/line feed, and type an asterisk (*), signifying return to the command mode.

4-16. The following is an example of the performance of the Peak Find/Fit Command after the Energy Calibration Command has been executed. In this example, the peak extraction process is again performed on the spectrum shown in Figure 4-1, but this time the Centroid and FWHM values are printed in KeV, using the values determined for the energy intercept (-1514.72 eV) and the energy per channel (1743.24 eV/channel) in the example described in paragraph 4-7.

* P

NO.	ECL	CENTROID	FWHM	BKG(HGT)	AREA	LEFT	RIGHT
1		904.96 904.78	3.64 3.75	7357.50 1392.89	3104.50 3173.69	516	524
2		938.02 938.00	3.72 3.73	8166.13 2120.76	5262.88 4805.80	534	544
3		1018.97 1017.00	7.46 3.50	7795.13 2283.66	8388.87 4865.32	579	591
10		1021.50	3.50	1631.12	3475.10		
4		1159.75 1159.71	3.62 3.70	2050.13 1312.29	3109.87 2954.74	661	671
5		1188.04 1188.00	4.04 3.93	1897.50 2925.06	7105.50 6988.68	677	688
6		1219.09 1218.74	3.74 3.12	686.00 153.86	483.00 291.96	697	703
7		1270.78 1270.78	4.05 3.99	1301.63 1993.57	5057.37 4841.52	724	736
8	1	1381.54 1384.94	4.35 6.64	1875.52 115.08	187.48 464.88	789	811

*

4-17. SMOOTH COMMAND

4-18. The Smooth command permits performing a five-point coefficient smooth on the data spectrum contained in the currently displayed group to reduce the deviation of counts in the spectrum peaks or to compensate for poor statistics. The smooth operation can be performed from 1 to 4095 times. The following is an example of the entry required to perform a single smooth operation on the spectrum contained in the currently displayed group.

```
*$ : 1 (SPACE)
```

*

NOTE

The Peak Find/Fit and Smooth commands cannot be performed simultaneously. Once the smooth operation is initiated, it must continue until completed before entering the Peak Find/Fit Command, or vice versa.

4-19. The Smooth command is specified by entering a dollar sign (depressing the SHIFT key and then the \$ key) after an asterisk (*) is typed. When \$ is entered, the routine causes the Teletype to print a colon (:), and then waits for entry of the number of times the smooth operation is to be performed. This number can be any number from 1 to 4095. Entry of the number of times must be terminated by depressing the SPACE bar at the Teletype. When the SPACE bar is depressed, the routine initiates the smooth operation and causes the Teletype to perform a carriage return/line feed and type an asterisk (*).

NOTE

When the smooth operation is initiated, lamp B at the ND4410 Function Control Module is turned on. Upon completion of the last specified smooth operation, lamp B is turned off. Thus, to avoid extraneous results, do not initiate acquire or the peak extraction/fit process during the time lamp B is on.

SECTION V ERROR DIAGNOSTICS

5-1. ERROR INDICATION

5-2. Execution of an illegal operation will result in an error message being typed at the Teletype. Table 5-1 lists the error messages and their causes.

Table 5-1. Error Indications

Error Message	Cause
ERROR: 99XXXX	Depressing an unassigned pushbutton.
ERROR: 79XXXXX	Depressing an unassigned Teletype key.
ERROR: 75XXXXX	Current group width is either greater than 4095 channels or it is too small relative to the peak width determined by the program using the half width specified.

NOTE

The least significant digits indicated by X's in Table 5-1 for the ERROR message may change depending upon what illegal command was performed. However, the two most significant digits will be the same for the same type of error.

SECTION VI COMMAND SUMMARY

- 6-1. The following summarizes the commands described in Section IV.
1. L HALF WIDTH COMMAND - Permits entry of a number equal to the average number of channels at the FWHM points of the peaks to be determined during the peak extraction/fit process. The peak width can be any number of channels from 2 to 85.
 2. PEAK FIND/FIT COMMAND - Determines the centroid, FWHM, background and intensity information for each peak contained within the marker-defined portion of the spectrum stored in the currently displayed group using a peak extraction process which is based upon the entry for the half width parameter. Upon extraction of each peak, markers are displayed at the peak limits and the following information is printed at the Teletype: the number of the extracted peak, an error code list number (if applicable), the channel location of the peak centroid, the number of channels at the full-width-half-maximum (FWHM) point, the background counts, the net total (the total number of counts within the peak limits minus the background counts), and the channel locations of the left and right limits of the peak. Upon completion of printout of the information determined for each peak during the peak extraction process, the peak fit process is initiated. The fit process first determines if the peak found is a single peak or doublet. If the peak is found to be a single peak, a least squares Gaussian fit process is performed using the centroid, FWHM and height values found by using the peak extraction process as initial guesses. Upon completion of the fit process, markers are again displayed at the peak limits and values for the centroid, FWHM, height and area of the Gaussian are printed at the Teletype. If the peak is found to be a doublet, pairs of input guesses are generated for the double peak which are based upon the skewness of the peak, the centroid, FWHM, height, left and right channel values found by the peak extraction process. The pairs of guesses are then used as input to the peak fit process which separates and fits the doublet, improving the initial guesses by an iterative

least squares Gaussian fit process. Upon completion of the iterative fit process, markers are again displayed at the peak limits and new values for the centroid, FWHM, height and area for each peak are printed at the Teletype. The number of iterations is also printed.

3. **MANUAL OVERRIDE COMMAND** - Permits manually performing the peak fit process on any single peak (or doublet) selected using the display markers. After the peak is selected, the channel value(s) for the peak centroid(s) is entered and the peak fit process is initiated using the centroid value(s) and the marker channel values as initial guesses. Upon completion of the fit process, the centroid, FWHM, height and area values of the peak(s) are printed at the Teletype.
4. **ENERGY CALIBRATE COMMAND** - Permits entry of the half width and then performs the peak extraction/fit process, marker display and print-out in the same manner as the Peak Find/Fit command. In addition, it permits entry of the known energy in eV for any two peaks and then calculates the values for the energy intercept in eV and the energy per channel (slope) in eV/channel.
5. **\$ SMOOTH COMMAND** - Performs a five-point coefficient smooth on the data spectrum contained in the currently displayed group a specified number (1 to 4095) of times.