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PLOTSPEC

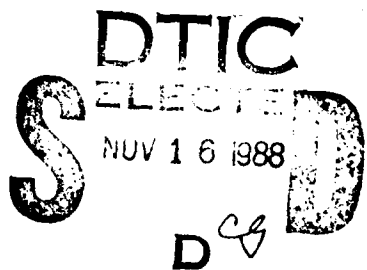
A FORTRAN 77 Program for Plotting Spectral Data from The Varian CARY 2390 UV-VIS-NIR Spectrophotometer

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PLOTSPEC is a FORTRAN 77 program designed to plot UV-VIS-NIR spectra using data obtained from the CARY 2300 - 2400 series spectrophotometers. The program is written to operate on a Hewlett-Packard 1000 computer system but with very few system dependent features to enable easy conversion for operation on other host systems. PLOTSPEC supports a wide range of Hewlett-Packard digital plotters using the HP-GL command language. The program uses a menu driven environment with automatic scaling and axes setup in the					
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19. ABSTRACTS (Continued)

ordinate and abscissa modes of choice. PLOTSPEC offers abscissa choices of Wavelength (nm) or Wavenumbers $\times 10^{-3}$ and ordinate choices of Absorbance, Extinction Coefficient, % Reflectance or % Transmission. Annotation and digitizing facilities are also included for easy labelling and peak determinations.

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CONTENTS

Section	Description	Page
INTRODUCTION		1
IMPLEMENTATION		
1.0	Hardware Interface	2
1.1	System Handshaking	2
1.2	HP-GL Software Control Of HP Plotters	3
1.3	HP-GL Commands Summary	4
1.4	Default Plotting Parameters	6
SOFTWARE DESCRIPTION		
2.0	Purpose Of PLOTSPEC	7
2.1	Program Structure	8
2.2	Plotting Menu Commands	13
2.3	COMMON DATA	16
2.4	SUBROUTINES	18
2.5	FUNCTIONS	23

... cont'd

Section	Description	Page
PROGRAM CODE		
3.0	Source Code Availability	23
3.1	Variable Names And Usage	23
3.2	Program Listing	29
APPENDIX	Sample Plots	68

LIST OF TABLES

TABLE	Description	Page
I	Data File Format	10
II	Glossary Of Integer Variables	24
III	Glossary Of Real Variables	25
IV	Glossary Of Real Array Variables	26
V	Glossary Of Character Variables	27

PLOTSPEC

A FORTRAN 77 Program For Plotting Spectral Data From The Varian CARY 2390 UV-VIS-NIR Spectrophotometer

INTRODUCTION

Spectral data acquisition from the CARY 2300 and 2400 series spectrophotometers has been implemented successfully using a Hewlett-Packard 1000 minicomputer system using the FORTRAN 77 program CARYSPEC, which is described in a separate report. The ability to acquire high quality UV-VIS-NIR spectra must be complemented with flexible data analysis and plotting software to make full use of the spectroscopic data. This report describes a fully tested FORTRAN 77 program PLOTSPEC which fulfills the plotting requirements of most users in a simple to use menu driven environment. The program supports Absorbance, Extinction Coefficient, % Transmission and % Reflectance ordinates vs linear Wavelength (nm) or Energy (cm^{-1}) abscissa. Automatic *data rescaling* is provided between Absorbance units and % Transmission so that either type of data file from CARYSPEC may be plotted in the ordinate of choice. PLOTSPEC supports two concurrent spectra, of up to 10001 data points each, allowing difference spectra to be obtained with automatic scaling for differences in concentration and pathlength. This mode is only valid for Absorbance or Extinction Coefficient ordinate choices and % Transmission data files will be automatically rescaled before plotting. Data treatment in the % Reflectance mode is identical to % Transmission with only the plotting label altered to match the use of this measurement technique. The abscissa axis scaling is bidirectional to suit individual preferences for the direction of increasing wavelength or energy units.

PLOTSPEC has been developed for use with an HP 1000 minicomputer system running the RTE-6/VM operating system and CI shell. In this environment the program communicates with Hewlett-Packard model 9872A and 7550A digital plotters via the IEEE-488 and RS-232C I/O subsystems, respectively. These communication functions are transparent to high level languages on the HP 1000 enabling simple READ/WRITE statements from FORTRAN to control the external plotting operations. The program resides in a single 32K word memory segment and utilizes 79 pages of Extended Memory Addressing (EMA) memory for the large data arrays. Since PLOTSPEC makes use of very few special features of the HP 1000 computer system the program could be modified easily to run on other host systems supporting the FORTRAN 77 language and either the IEEE-488 or RS-232C interface standards.

Manuscript approved August 9, 1988.

IMPLEMENTATION

1.0 Hardware Interface:

The IEEE-488 interface for the HP 1000 system is implemented with an HP 59310B interface card which utilizes 4 Logical Unit (LU) addresses in the system. The LU addresses used within the program are system dependent and are defined during the system generation. The interface card accessed by PLOTSPEC occupies LU addresses 31-34, corresponding to card addresses 0-3. Address 0 enables a special addressing mode for sending low level bus command sequences. Addresses 1-3 are predefined automatic READ/WRITE channels which select device numbers 1-3 on the bus. PLOTSPEC uses LU 33 to automatically address device #2 on the bus (HP 9872A plotter). To simplify alterations to the plotter address the program uses the INTEGER variable PU for the unit number in all READ/WRITE operations with the plotter.

The RS-232C interface to the HP 7550A plotter is implemented via a standard HP 1000 8 channel multiplexer card (MUX) operating at 9600 baud with 8 data bits and XON/XOFF software handshaking protocol. PLOTSPEC does not send device control commands to set these communications parameters within the HP 7550A since these are easy to select from the front panel control of the plotter. In this application the HP 7550A plotter is operated in the STANDALONE mode with DIRECT connection to the MUX output of the HP 1000.

1.1 System Handshaking:

The IEEE-488 subsystem of the HP 1000 is operated by the RTE driver DVA37 configured for ASCII Data Record mode, enabling automatic ASCII $\longleftrightarrow$ NUMERIC conversion on I/O. This mode sends and expects to receive an End Of Record (EOR) with data transmission in the form of a Carriage Return/Line Feed (CR/LF) sequence which matches the requirements of Hewlett-Packard digital plotters.

The RS-232C subsystem is operated by the RTE driver DDV00 which also performs automatic ASCII $\longleftrightarrow$ NUMERIC conversions for FORTRAN I/O statements. This allows PLOTSPEC to control either plotter without regard for differences in the handshaking protocols. Character labelling mode on these plotters requires a special terminator character and PLOTSPEC issues the default Etx character, ASCII 3.

1.2 HP-GL Software Control Of HP Plotters:

PLOTSPEC uses a subset of the Hewlett-Packard Graphics Language (HP-GL) to control the operations of the HP 9872A and HP 7550A digital plotters. The early generation of HP plotters often only allow scaling and plotting commands to use integer units which restricts the utility of the automatic scaling command 'SC' in these plotters. This lack of utility is so severe that the operating manual for the HP 9872A plotter does not even document the existence of the 'SC' command in the HP-GL syntax. However, PLOTSPEC utilizes a general scaling procedure with the 'SC' command which functions on *all models* of HP plotters, maintaining a 0-10000 unit scale on each axis at all times. The 'SC' command has the advantage of automatically mapping these user units onto the scaling points P1 (lower left) and P2 (upper right). In order to map the real user units onto this 10000 x 10000 unit grid the program only needs to use a multiplier (XMULT,YMULT) for the data on each axis. For example, a % Transmission range of 0-100% would require YMULT = 100 for correct scaling of the user's data. This technique maintains software resolution at 1 in 10000 units regardless of the range of the user's MIN,MAX values.

PLOTSPEC also supports *bidirectional* plotting on the X-axis even though the 'SC' scaling command of early HP plotters does not permit setting $X_{min} > X_{max}$, i.e. numbers increasing towards the left. In order to accomplish this task in a general manner the program uses two X_{min}, X_{max} ranges, 0 - +10000 (increasing to the right) and -10000 - 0 (increasing to the left). The change in sign has the effect of reversing the direction of plotting. This scheme is known to work on HP 9872A, 7225A, 7470A, 7475A and 7550A model plotters.

The HP-GL commands used within PLOTSPEC are summarized below together with their syntax and parameter types. The type labels INTEGER and DECIMAL should be interpreted as their ASCII representations. All data sent to or received from the plotters is in ASCII code. Therefore, where the command syntax below indicates a program variable, a parameter value enclosed within literal string delimiters is equally applicable. The HP 1000 computer system performs the conversion between numeric and ASCII representations automatically on I/O operations allowing liberal mixtures of literal string and numeric variables to appear in HP-GL instructions, with a few exceptions. For example, the character plot instruction 'CP' fails on receipt of the value 0.0 from a program variable but happily accepts the literal '0.0'. Where HP-GL commands are known fail to function correctly for valid ranges of parameters PLOTSPEC first converts the values to their string representation before sending them to the plotters.

1.3 HP-GL Commands Summary:

- 'AP' Automatic Pen Pickup
Syntax = 'AP;'
- 'CP' Character Plot...moves the pen in units of character width, height
Syntax = 'CP',X,',',Y',';
DECIMAL X,Y
- 'DF' Default Settings...sets the plotter to default parameters
Syntax = 'DF;'
- 'DI' Direction...sets the labeling direction
Syntax = 'DI',X,',',Y',';
DECIMAL X,Y
where $X,Y = \cos(\theta), \sin(\theta)$
DEFAULT = 1,0
- 'IP' Input P1,P2 Scaling Points...sets the size of the plot
Syntax = 'IP',X1,',',Y1,',',X2,',',Y2',';
where (X1,Y1) = lower left scaling coordinate (plotter units)
where (X2,Y2) = upper right scaling coordinate (plotter units)
INTEGER X1,Y1,X2,Y2
- 'IW' Input Window...sets the size of the plotting window
Syntax = 'IW',X1,',',Y1,',',X2,',',Y2',';
where (X1,Y1) = lower left soft clip coordinate (plotter units)
where (X2,Y2) = upper right soft clip coordinate (plotter units)
INTEGER X1,Y1,X2,Y2
- 'LB' Label...draws the following literal characters
Syntax = 'LB',string,Etx
ASCII string
where Etx = CHAR(3) terminates LB
- 'LT' Line Type...solid or broken lines styles
Syntax = 'LT',PN,',',PL',';
INTEGER PN, DECIMAL PL
where PN = Pattern number (1-6)
where PL = Pattern length (0-100%)

- 'OA' Output Actual Pen Position...sends the current coordinate position
 Syntax = 'OA;' followed by READ (...) X,Y,Z
 where (X,Y) = current position (plotter units)
 where Z = 0 or 1 for pen status (up/down)
 INTEGER X,Y,Z
- 'OP' Output Scaling Points P1,P2...sends the coordinates of plot limits
 Syntax = 'OP;' followed by READ (...) X1,Y1,X2,Y2
 where (X1,Y1) = lower left scaling point
 where (X2,Y2) = upper right scaling point
 INTEGER X1,Y1,X2,Y2
- 'PA' Plot Absolute...moves the pen to an absolute coordinate
 Syntax = 'PA',X,',',Y,',' where X,Y = coordinates (plotter units)
 HP 9872A: INTEGER X,Y
 HP 7550A: INTEGER X,Y or DECIMAL X,Y if user scaling is on
- 'PD' Pen Down...sets the pen on the plotting surface
 Syntax = 'PD;'
- 'PU' Pen Up...picks up the pen from the plotting surface
 Syntax = 'PU;'
- 'SC' Scale Plot...maps user units for X,Y axes onto P1,P2 scaling points
 Syntax = 'SC',X1,',',X2,',',Y1,',',Y2,','
 where (X1,Y1) = coordinate of scaling point P1 (user units)
 where (X2,Y2) = coordinate of scaling point P2 (user units)
 HP 9872A: INTEGER X1,Y1,X2,Y2
 HP 7550A: DECIMAL X1,Y1,X2,Y2
- 'SR' Size Relative...sets the character size in proportion to axes scaling
 Syntax = 'SR',WIDTH,',',HEIGHT,','
 DECIMAL WIDTH,HEIGHT

- 'SP' Select Pen...picks up the pen from selected stall or carousel position
 Syntax = 'SP',X,',' where X = pen number (0-8)
 INTEGER X
- 'TL' Tick Length...sets the length of positive tick marks for axes
 Syntax = 'TL',X,',' where X = % of full scale (0-100)
 DECIMAL X
- 'VS' Velocity Select....sets the pen down speed
 Syntax = 'VS',X,',' where X = velocity (cm/sec)
 INTEGER X
- 'XT' X-tick...draws a vertical tick mark at the current pen position
 Syntax = 'XT;'
- 'YT' Y-tick...draws a horizontal tick mark at the current pen position
 Syntax = 'YT;'

1.4 Default Plotting Parameters:

PLOTSPEC initializes the HP plotters using the 'DF' default parameters command and then sets up the following plotting style:

- LABELS** The initial label direction is set to horizontal with nominal character fields of 1 x 2 cm and the size relative option is selected.
- PEN** Pen #1 is selected with automatic pen pickup and set to the UP state. The pen down velocity is set to 5 cm/sec for best line quality with felt tip pens on graphics paper.
- SCALE** Initial scaling coordinates for the HP 9872A plotter are (1350,1000) and (8500,7000) corresponding to the NOTEBOOK size plot on A-size paper while the plotting window is set to the hard clip limits.
- TICKS** Tick marks are set to +1% of full scale.

2.0 Purpose Of PLOTSPEC:

This program is intended to provide a flexible plotting facility for spectral data acquired from the Cary 2390 spectrophotometer using the program CARYSPEC, which is described in a separate report. The HP 1000 computer system provides a large EMA area to hold data arrays and PLOTSPEC makes use of this feature to access two concurrent spectra of up to 10001 points each. This allow for difference spectra to be plotted with relative ease compared with the experimental difficulties incurred with real time subtraction. While the raw data from the spectrophotometer consists of Absorbance or % Transmission measurements vs Wavelength (nm), PLOTSPEC allows for presentation of the data in more meaningful units as well. The abscissa may be scaled in Wavelength (nm) or Wavenumbers $\times 10^{-3}$ with increasing values towards the left or right. The ordinate may be presented in Absorbance, Extinction Coefficient (Molar Absorptivity), % Transmission or % Reflectance. PLOTSPEC automatically rescales the original ordinate data to match the choice of plotting ordinate. Furthermore, automatic range, tick and label position selection is provided for fast and efficient setup of a neat and tidy plot. However, the user can easily alter the default selections in the menu driven plotting environment.

PLOTSPEC also provides some useful annotation facilities for documenting the plot and for producing presentation material. A digitizing routine is interwoven with the annotation commands to enable semi-automatic labelling of peak maxima with the ease of a *point and shoot* technique. More accurate determinations of peak maxima can also be made using a page scrolling data listing routine, though the digitizing facility seems to be perfectly adequate in most cases. The default plotting mode produces a small NOTEBOOK size plot on A-size paper, together with a list of spectral parameters for documentation purposes. A FULL size plotting mode can also be selected to produce a larger plot on A-size paper without a parameter list. Both modes include sufficient space for a centered title over the plot. Additionally, the program provides a USER SET plotting size with default boundaries suited for a full size plot on B-size paper. This mode is ideal for producing poster presentation material. PLOTSPEC supports output to two generic types of Hewlett-Packard digital plotters, the older HP 9872A and the more recent HP 7550A model. However, PLOTSPEC is designed to function with all generations of HP plotters with only minor differences in the position of the plotting origin.

2.1 Program Structure:

PLOTSPEC comprises a large main program unit containing the console menu displays, string data for the instrument settings variables and a number of subroutines that perform string processing, input validation and communication with the HP 9872A and HP 7550A digital plotters. The main program unit is responsible for all the logic flow and the subroutines execute specific support tasks, which are summarized below:

The main program unit of PLOTSPEC comprises 6 distinct segments of code to carry out the the functions of disk file data retrieval, instrument settings display, plotting mode setup and actual plotting operations. The code fragments appear under the following assigned labels: MENU, READ, SETTINGS, DIFF, PLOT and EXIT.

MAIN PROGRAM

MENU:

This is the first and main control menu of the program, selecting entry to the data retrieval, instrument settings, plotting mode and exit routines. The choices are as follows:

'R1'Read Spectrum #1

This command branches to label READ and the program performs logical tests for the presence of a valid spectrum in memory before allowing previous data to be overwritten by a new file. The data file format is listed below in Table I. Files are read into the first dimension of the data arrays and may be plotted using the 'P1' command.

'R2'Read Spectrum #2

This command performs the same operation as 'R1' but the file is read into the second dimension of the data arrays. The second spectrum can be plotted independently of the first or used for difference spectroscopy.

'IS'Instrument Settings

This option branches to label SETTINGS and prompts for the number of the spectrum. This routine allows for display of the most important operating conditions of the Cary 2390 spectrophotometer during acquisition of the selected spectrum. This provides an on-line reference when comparing a number of spectra.

'PS'Plotter Selection

This option allows the user to select either the HP 9872A (default) or HP 7550A plotter as the output device. Digitizing is more convenient with the older HP 9872A plotter but output quality and plotting speed are much improved with the HP 7550A.

'P1'Plot Spectrum #1

Selection of this command branches to label PLOT which performs a check for the presence of a valid file in memory. The routine then starts the plotting mode setup for the first spectrum with selection of the abscissa and ordinate scaling modes. The user has a choice of *Nanometres* and *Wavenumbers* for the abscissa and a choice of *ABSORBANCE*, *Extinction Coefficient*, *% Transmission* and *% Reflectance* for the ordinate. The program then proceeds to scale the data and set default plotter operating modes before presenting a menu of plotting options. The original data file may have been recorded in either Absorbance or % Transmission units so the data will be rescaled if the choice of plotting ordinate differs from the file ordinate.

'P2'Plot Spectrum #2

This command performs the same operations as 'P1' but uses data residing in the second dimension of the data arrays.

'DS'Difference Spectrum (1-2)

Selection of this option causes a branch to label DIFF which first checks for the presence of two valid spectra in memory and then tests for matching of their wavelength range and step size (nm). If the spectra are matched the program continues to label PLOT in the normal fashion. In this case, however, all plotting operations will use the scaled difference between the two data sets. The data from the second spectrum are scaled for differences in concentration or pathlength before subtraction during plotting.

'EX'Exit

The final option causes an unconditional branch to the label EXIT which terminates the program.

TABLE I

Data File Format

Line	File Variables ^a	Format Type ^b
1	TITLE(2)	CHARACTER (A72)
2	DATE(2)	CHARACTER (A8)
3	FMIN(2),FMAX(2),FSTEP(2),CONC(2), PATH(2)	REAL (*)
4	ORD(2),ABSC(2),CELL(2),CYCLE(2), SAMPLE(2),WAVE(2),TIMER(2), TEMP(2),DIST(2)	REAL (*)
5	J,K,NDATA(2,I)	INTEGER (I3,I3,I6)
6-54	PARAM(2,I)	INTEGER (I2)
55	VARIABLE(2,I)	REAL (*)
56-/	A(2,I)	REAL (*)
/-eof	W(2,I)	REAL (*)

^a: Disk data files are read into either half of the data arrays

^b: (*) indicates free field format

READ:

This section of PLOTSPEC opens a disk file previously stored by the data acquisition program CARYSPEC. The data are stored in ASCII code and contain a complete description of the instrument parameter settings as well as the spectral data. The format of the data file is listed above in Table I. The program prompts the user for both the filename and subdirectory. The latter defaults to the user's directory if only a RETURN character is entered. If a directory name is given the program builds a complete CI pathname for use in the OPEN statement. If the file cannot be found or the file is already open the program displays an error message and then returns to the main MENU. Otherwise, the file is read and the file descriptors are displayed on the console while the remainder of the data are being transferred. After completion of the data transfer the program prompts for changes to the concentration or pathlength variables. This feature allows for on-line corrections to the file variables before plotting, though permanent corrections should be made using the file editing program EDITSPEC. The program then returns to the main MENU.

SETTINGS:

This section of code displays a list of the most important instrument settings of the Cary 2390 spectrophotometer during acquisition of the specified spectrum. The program includes a large amount of string data for the various settings in the CHARACTER array Pstr. The INTEGER array PARAM is used as an index to this string data while numeric data for the table are obtained from the REAL array VARIABLES.

DIFF:

Entry into this section of code is made prior to plotting in order to verify that the data in memory are suitable for difference spectral plots. The program first checks that there are two spectra present and proceeds to test for exact matching of the wavelength limits and step size. The editing program EDITSPEC includes routines for preparing subset data files to support the difference plotting mode of PLOTSPEC.

PLOT:

This section of PLOTSPEC allows the user to set up the axes scaling to suit the type of data to be plotted. If the selected spectrum is not present in memory an error message is displayed and the program returns to the main MENU. Otherwise, a prompt is displayed for the choice of abscissa. PLOTSPEC supports two abscissa modes, Wavelength (nm) and Wavenumbers $\times 10^{-3}$. After this selection the program sets a number of X-axis plotting variables and calls Subroutine Xaxis to setup the default tick and label positioning. The abscissa is *bidirectional* allowing the user to select the direction of increasing values. However, the default direction is for values to increase towards the right.

The following prompt is for the choice of ordinate mode. Data may be plotted in a choice of ABSORBANCE, Extinction Coefficient, % Transmission and % Reflectance. The latter pair are identical except for the label on the Y-axis. Data files from the CARYSPEC program may contain either Absorbance or % Transmission values so that rescaling is provided automatically to suit the user's choice of plotting ordinate. If the Difference Spectrum mode has been invoked only the Absorbance and Extinction Coefficient ordinates are valid. If the plotting ordinate uses Absorbance data the program will search the data array for the maximum value to provide automatic ranging on the Y-axis. If Extinction Coefficient mode is specified the program also calculates a suitable Y-axis exponent. Otherwise, the Y-axis defaults to 0-100% limits. The default tick and label positions are then set by calling Subroutine Yaxis.

The user is then prompted to check that the selected plotter is connected and turned on before proceeding to send plotter commands. Finally, the user is presented with the plotting menu with default settings for axis and label sizes, line type, pen velocity, the location of tick marks and axis labels and the command interface for plotting, annotating and digitizing.

EXIT:

The final portion of PLOTSPEC issue an erase command line instruction and then terminates the program unconditionally.

2.2 Plotting Menu Commands:

The interactive plotting control menu is designed both for flexibility and ease of use in setting quite a large number of plotting parameters. On most occasions, the default limits and spacing between tick marks and labels will be perfectly satisfactory. However, the user has complete control over these parameters to suit individual preferences. The various command selections are listed below:

'PL'Plot Limits

This command sets the actual range of the data file to be plotted. The default value is the full scan range. If the plotting scale is made smaller than the scan range the plot limits are reduced to match in order to prevent attempts to plot off scale data. If the plotting scale is made larger than the scan range the plot limits are set to the actual scan limits.

'XS'X-scale

The range of the X-axis plotting scale defaults to the scan range of the spectrum but may be made larger or smaller than the scan limits. The XMIN,XMAX values may be entered in reverse order to produce a plot with values increasing towards the left. These limits are passed to Subroutine Xaxis to reset the plot limits, tick marks and label positions automatically.

'XT'X-tick Spacing

This option allows for customizing the X-axis tick mark spacing with prompts for First, Last and Space. The limits are validated to lie within the current X-scale range and the label positions are automatically reset to match the tick positions.

'XL'X-label Spacing

This option allows the user to reset the automatic label positioning. The entries for First, Last and Space are treated in a similar manner to the tick marks.

'YS'Y-scale

The range of the Y-axis plotting scale defaults to the MIN,MAX scale appropriate for the selected ordinate. For %R and %T scales the default scale is 0-100%. For Absorbance and Extinction Coefficient ordinates autoranging is used to fit the entire spectrum on scale. The scale range is passed to Subroutine Yaxis to reset the plot limits, tick marks and label positions automatically.

'YT'Y-tick Spacing

This option allows for customizing the Y-axis tick mark spacing with prompts for First, Last and Space. The label positions are automatically reset to match the tick marks. No input validation is provided for the limits as it is assumed the user can read the updated console display before plotting.

'YL'Y-label Spacing

This option allows the user to reset the automatic label positioning. The entries for First, Last and Space are treated in a similar manner to the tick marks.

'CS'Char.Size

The size of character labels can be altered to suit individual preferences. However, the size should not be made much larger than the default fields (1x2 cm) when using the NOTEBOOK or FULL size axes definitions since the labels may not fit within the hard clip limits of the plotters.

'PV'Pen Velocity

Plotting quality is very dependent on the pen speed, the type of pen and plotting medium chosen. The program uses a default pen speed of 5 cm/sec for both the axes and spectrum plots. The user can alter these within the range 1-36 cm/sec. While the manual for the HP 7550A plotter *recommends* a speed of 50 cm/sec for the combination of felt tip pen and graphics paper there is no doubt that this is determined more by the quest for throughput than quality. Roller ball pens also work well at the 5 cm/sec pen speed. Thus, there is little need to alter the default values in most cases though transparency plots can benefit from a higher speed (10 cm/sec).

'LT'Line Type

The plotters have 6 inbuilt line type functions. The default value specifies a SOLID line. Since PLOTSPEC can plot multiple spectra on the same graph the BROKEN line type function is quite useful. The various patterns can be found by reference to the plotter manuals. The length of the patterns is entered as a % of full scale and a useful guide is to select the same length as the pattern number.

'AX'Axes Size

The program includes three, predefined plot types NOTEBOOK, FULL and USER SET. The plotting boundaries vary to suit different functions and paper sizes. The default NOTEBOOK size is a small, A-size plot which allows room for labelling a list of spectral file parameters on the right hand margin. The FULL size plot nicely fills the plotting area of A-size paper with sufficient space for a centered Title over the plot. The USER SET size allows for custom size plots up to the limits of B-size paper. This mode has predefined limits which produce a FULL size plot on B-size paper but the scaling coordinates can be easily altered by the user to suit individual needs.

'AN'Annotate Plot

This command allows the use to enter, move and plot Labels, a list of spectral Parameters or a centered Title. The Title defaults to the data file descriptor but the user can enter a new Title if required. The Parameters option is only valid for the NOTEBOOK size plot which allocates room for these descriptors in the right hand margin. The Labelling options allows for entry of descriptive text (up to 40 chars.) which may be positioned and drawn anywhere on the plotting surface. The character size and labelling direction are selectable while the plotting mode supports centered, left and right justification. The character size for labels defaults to 0.6*Normal plot size.

'PA'Plot Axes

This command draws the axes grid according to the selected tick and label positions listed in the plotting menu.

'PS'Plot Spectrum

Before proceeding with the plot this command pauses for the possible entry of a step multiplier. This allows the user to speed plotting for very large data files.

'DD'Digitize/Display Data

The program supports manual use of the plotters for digitizing peak positions from the plot. This routine will allow the user to annotate the plot at these positions with either the X coordinate, the Y coordinate or Both. Labels are drawn with small characters in the vertical direction and may be plotted in centered, left or right justified format. In this case, the annotation routine provides offsets to avoid writing over the spectrum.

2.3 COMMON DATA:

All COMMON variables used by PLOTSPEC are held in named COMMON blocks. The variables contained within the COMMON blocks are listed below:

/DATA/ Contains EMA REAL Arrays of spectroscopic data

A Array containing the Absorbance or %T data
 Values read from disk data file
 Values used in main program unit

W Array containing the wavelength data (nm)
 Values read from disk data file
 Values used in main program unit

/DIGIT/ Contains REAL and INTEGER variables for scaling digitized data

FACTOR REAL variable for scaling absorbance to extinction coefficient units
 Values set in main program unit (from data file variables)
 Values used in main program unit and Subroutine Digitize

XMIN, REAL variables containing the current X-axis limits

XMAX Values set in main program unit
 Values used in main program unit, Subroutine Digitize, Subroutine Order and
 Subroutine Xaxis

YOFF, REAL variables containing the current Y-axis offset & scale length

YSCALE Values set in main program unit
 Values used in main program unit, Subroutine Digitize, Subroutine Order and
 Subroutine Yaxis

IX,IY INTEGER variables containing the coordinates of the digitized point

X1,Y1 INTEGER variables containing the coordinates of the scaling points P1,P2

X2,Y2 Values set in main program unit and Subroutine Digitize
 Values used in main program unit and Subroutine Digitize

/XPARAM/ Contains REAL variables for plotting control

LMIN, Current X-axis plotting limits for validation of Tick or Label entries

LMAX

WN,WX Current plotting limits for Wavelength or Wavenumber scale

Xtick, X-axis tick mark spacing

FXT,LXT First and Last X-axis tick marks

Xlabel, X-axis label spacing

FXL,LXL First and Last X-axis labels

Values set in Subroutine Xaxis

Values used in main program unit

/YPARAM/ Contains REAL variables for plotting control

Ytick, Y-axis tick mark spacing

FYT,LYT First and Last Y-axis tick marks

Ylabel Y-axis label spacing

FYL,LYL First and Last Y-axis labels

Values set in Subroutine Yaxis

Values used in main program unit

2.4 SUBROUTINES:

PLOTSPEC uses subroutines to perform specific tasks which are required more than once, including string manipulations, input validation, digitizing and data rescaling. The purpose and calling sequences are listed below:

Center(TITLE)

Prints a string on the user console centred within a 72 column line.

TITLE CHARACTER*72 string, contents set by calling unit

CALLED BY: Main program unit

CALLS: None

Coeff(E,String,K)

Converts a numeric extinction coefficient into a rounded string with exponent, if required. Special handling is executed for 0.0000 and 1.0000 values.

E REAL variable input from calling unit

String CHARACTER*(*) output containing floating point string
DIMENSION is set by the calling unit

K INTEGER variable input from calling unit specifying the number of digits of precision required in string. Output value returns the number of characters in string to the calling unit.

CALLED BY: SUBROUTINE Digitize

CALLS: SUBROUTINE Str

Digitize(X,Xcode,Y,Ext,K)

Reads the current pen position from the plotter and converts the coordinates to the user's units. The routine also converts the Y-coordinate to extinction coefficient format. The main program determines whether the latter value is valid for the ordinate mode in use.

X REAL variable output containing the abscissa value in user units

Xcode CHARACTER variable input used to select scaling of the abscissa units

Y REAL variable output containing the ordinate value in user units

Ext CHARACTER*(*) output string containing the extinction coefficient
DIMENSION is set by the calling unit

K INTEGER variable input to specify the number of digits precision in Ext
Output value contains the number of characters in the returned string

CALLED BY: Main program unit

CALLS: SUBROUTINE Coeff

Exponent(N,Mult)

Converts the scale factor (power of 10) for extinction coefficient mode into string exponents for labelling the Y-axis in the screen menu and on the plotted graph (e.g. '1E-3' or '1 ...').

N REAL variable input, power of 10

Mult CHARACTER*(*) output string containing multiplier
DIMENSION is set by the calling unit

CALLED BY: Main program unit

CALLS: SUBROUTINE Str

Line(N)

Prints a line of '-' characters to the user console N columns wide and centred within a 72 column line.

N INTEGER variable input from calling unit

CALLED BY: Main program unit

CALLS: None

Order(MIN,MAX)

Validates the input arguments so that MIN < MAX

MIN,MAX REAL variables input and output with order swapped if required

CALLED BY: Main program unit

CALLS: None

Rescale(J,K,ND)

Converts ordinate data array between Absorbance units and % Transmission. The data array A(J,I) is accessed from EMA COMMON.

J INTEGER variable input (1 or 2) to specify the spectrum

K INTEGER variable input (0 or 1) to specify the scaling procedure. The original value for K is obtained from PARAM(J,1) in the data file. On return to the main program unit the latter parameter is altered to reflect the current data format.

ND INTEGER variable input containing the number of data points in A(J,I)

CALLED BY: Main program unit

CALLS: None

Str(VALUE,String,PREC)

Performs a conversion from numeric value to a string number for floating point numbers only with up to 12 digits precision.

VALUE REAL variable input to be processed by the routine

String CHARACTER*14 string output corresponding to VALUE

PREC INTEGER variable input to set the rounding precision for string

CALLED BY: Main program unit, SUBROUTINE Coeff, SUBROUTINE Exponent

CALLS: None

Upper(Code)

Performs a check for lower case characters in a string of arbitrary length and converts to upper case if necessary.

Code CHARACTER*(*) variable passed into routine and UPPER case on exit
DIMENSION is set by the calling unit

CALLED BY: Main program unit

CALLS: None

EXTENSION: LEN(string) function, an HP extension to FORTRAN 77

Val(String,VALUE)

Performs a conversion from string to numeric value for a string number containing up to 10 digits. This is more than required by PLOTSPEC.

String CHARACTER*(*) string input to be processed by routine
DIMENSION is set by calling unit

VALUE REAL variable output

CALLED BY: Main program unit

CALLS: None

Wait(DELAY)

Performs a loop which tests the system clock until DELAY seconds have elapsed. The routine does not make provision for the special case at the transition to 2400 hours.

DELAY REAL variable holding the value of the delay period in seconds

CALLED BY: Main program unit

CALLS: FUNCTION Time(I)

Xaxis(XL,XH)

Performs both limits settings for the X-axis range variables and selection of the default Tick and Label positions. The routine starts with Xtick set to 1/10 of the full scale range and then compares this with a table of preferred values. If the range is anomalously small or large the Tick and Label positions are based on the 1/10 scale spacing. Otherwise, a neat and tidy spacing is selected from the table values with a label at every other tick position.

Yaxis(YSCALE)

Performs Tick and Label position selection using preferred table values, if possible. The routine start with Ytick equal to 1/10 of YSCALE. If the ordinate uses Extinction Coefficient scaling or the range is anomalously small or large the Tick and Label positions are based on the 1/10 scale spacing. Otherwise, a neat and tidy spacing is selected from the table values with a label at every other tick position.

2.5 FUNCTIONS:

PLOTSPEC uses only one function subprogram that makes an EXEC call to read the system time.

Time(I)

Performs an EXEC call to read the system clock and converts the reading to seconds and centiseconds.

I Dummy argument

CALLED BY: SUBROUTINE Wait only

CALLS: EXEC(ICODE,ITIME) system level command

PROGRAM CODE

3.0 Source Code Availability:

The source code for program PLOTSPEC is a 73K ASCII text file available on either a Hewlett-Packard cartridge, 9 track tape or an IBM 360K format floppy disk. All requests should be accompanied by the blank medium desired. A printed copy of the source code is listed below.

3.1 Variable Names And Usage:

A complete listing of the INTEGER, REAL, REAL Array and CHARACTER variables for the MAIN segment of PLOTSPEC is given below in Tables II, III, IV & V, respectively. The subroutines use the same names as the main program for the same variables. Additional variables in the subroutines and simple integers, I-N, are not documented since their usage is rather obvious. The logical variable MATCH is used within the program when comparing two spectra for the difference spectrum mode.

Table II

Glossary of INTEGER Variables

Name	Description	Value
DIFF	Assigned Label - Difference Spectrum	370
EXIT	Assigned Label - Terminate Program	9000
MENU	Assigned Label - Main Control Menu	10
PLOT	Assigned Label - Plot Spectrum, 1 or 2	400
READ	Assigned Label - Read Spectrum, 1 or 2	570
SETTINGS	Assigned Label - Scan Conditions, 1 or 2	300
ASCII	ASCII equivalent of digits in Str	48-57
FINISH	Index of final abscissa value to plot	1-10001
IX,IY,IZ	Plotter position variables READ/WRITE	0-16000
NCOL	Number of screen columns in menu display	50-70
ND	Number of data points in plotted spectrum	1-10001
NP	Number of parameters to read from file	49
NV	Number of variables to read from file	14
PREC	Precision for rounding function in Str	3,4
PN	Plotter model selection number	1,2
PU	Plotter Logical Unit #, READ/WRITE	17,33
PXOFF	Plotter X-zero position offset	0,200
PYOFF	Plotter Y-zero position offset	0,100
START	Index of first abscissa value to plot	1-10001
UX1,UX2	Absolute Plotter scaling coordinates,	0-16000
UY1,UY2	USER size plot dimensions	0-10100
X1,X2	Plotter X & Y coordinates for reading	0-16000
Y1,Y2	soft clip windowing points	0-10100
XP1,XP2	Absolute Plotter scaling coordinates,	0-16000
YP1,YP2	for WRITE to plotter	0-10100
NDATA(2)	Number of data points in spectrum	1-10001
PARAM(2,49)	Instrument operating modes table	1-16

Table III

Glossary of REAL Variables

Name	Description
BAND	Spectral Bandwidth (nm) - AUTO GAIN mode
BHEIGHT	Large label character height
BWIDTH	Large label character width
COFF	Character offset variable, labelling mode
ESCALE	Y-axis scale length, Ext. Coeff. mode
EMULT	Power of 10 for scaling, Ext. Coeff. mode
EOFF	Y-axis offset, Ext. Coeff. mode
FXL,LXL	First & last X-axis labels
FXT,LXT	First & last X-axis tick marks
FYL,LYL	First & last Y-axis labels
FYT,LYT	First & last Y-axis tick marks
GAIN	Instrument gain - AUTO SLIT mode
HEIGHT	Normal label character height
LHEIGHT	Small label character height
LWIDTH	Small label character width
LMIN	Current X-axis lower limit, data entry check
LMAX	Current X-axis upper limit, data entry check
NUMBER	General purpose data entry variable
PMIN	Pen scale minimum limit
PMAX	Pen scale maximum limit
RATIO	General purpose scaling variable
STEP	Step size (nm) interval, plotting mode
T1,...,T4	Powers of 10 (10,...,1E4)
WIDTH	Normal label character width
WN,WX	Current plot limits, default = WMIN,WMAX
WMIN,XMAX	Absolute scan limits (nm) or (kK)
X,Y	General purpose plotting variables
Xlabel	X-axis label spacing
XMIN,XMAX	Left & Right edges of X-scale on plot
XMULT	Multiplier to scale user X-scale to 10000 units
XOFF	Offset to user X-scale units to set min'm at 0
Xtick	X-axis tick spacing
XN,XX	Data entry variables for X-scale, ticks & labels
YN,YX	Data entry variables for Y-scale, ticks & labels
Ylabel	Y-axis label spacing
YMULT	Scales Y-axis data & labels for Ext. Coeff. mode
YOFF	Offset variable on current Y-axis scale
YSCALE	Current Y-axis scale length
Ytick	Y-axis tick spacing

Table IV

Glossary of REAL Array Variables

Name	Description
ORD(2)	Final ordinate value in file
ABSC(2)	Final abscissa value in file
CELL(2)	Final cell # value in file
CYCLE(2)	Final cycle # value in file
SAMPLE(2)	Final sample # value in file
WAVE(2)	Final wavelength value in file
TIMER(2)	Final time value in file
DIST(2)	Final distance value in file
A(2,10001)	Absorbance or %T array
CONC(2)	Concentration of sample (M), from data file
FACTOR(2)	Concentration * Pathlength for scaling spectra
FMAX(2)	Starting wavelength of scan (nm)
FMIN(2)	Ending wavelength of scan (nm)
FSTEP(2)	Step size (nm), from data file
PATH(2)	Pathlength of sample cell (cm), from data file
VARIABLE(2,14)	Instrument operating conditions table
W(2,10001)	Wavelength array

Table V

Glossary Of CHARACTER Variables

Name	Description
Screen Control:	
BELL	CHAR(7) bell character
CLR*2	Clear screen
DOWN*2	Move cursor down 1 line
ESC	CHAR(27) escape character
HOME*2	Move cursor to upper left corner
UP*2	Move cursor up 1 line
File Status:	
DATE(2)*8	Date (mm/dd/yy)
Fname(2)*20	Filename, CI convention
LABEL(2)*72	Descriptor of spectrum
Pstr(23,16)*14	Table of parameter setting names
Smin(2)*4	Spectrum ending wavelength (nm)
Smax(2)*4	Spectrum starting wavelength (nm)
Sinc(2)*4	Step size interval (nm)
Sstat(2)*10	Spectrum status (VALID, INVALID)
Program Control:	
C	Literal comma ','
Code*2	Main menu selection, valid until reset
Directory*40	User directory name, CI convention
Ext*14	Extinction Coefficient, digitize & label modes
Filespec*63	Full pathname, CI convention
Icode	General purpose selection key entry
Mult*5	Y-axis multiplier label, Ext. Coeff. mode
Pcode*2	Plotting menu option, valid until reset
Psize*8	Screen label for axes type selected
Size	Select type of plotted axes, 'N', 'F' or 'U'
String*14	String to pass data to or from subroutines
Text*40	General purpose string for labelling plot
TITLE*72	String to be printed to screen
Xcode	Selects X-axis scale, (nm) or (kK)
Xord*7	X-axis label (nm) or (cm ⁻¹), digitize mode
Ycode	Selects Y-axis scale, 'A', 'E', 'R' or 'T'

...cont'd

Plotter Control:

CR	CHAR(13), carriage return
Etx	CHAR(3), Terminator for label mode on plotter
LF	CHAR(10), line feed
Length*6	Broken line style pattern length (%)
Lmode*8	Line type mode (SOLID or BROKEN)
Pattern*6	Broken line type number
Plotter*10	Literal 'HP 9872A' or 'HP 7550A' identifier
Vaxes*2	Pen velocity (cm/sec), axes vectors
Vspec*2	Pen velocity (cm/sec), spectrum
Xleft*6	Literal '0' or '-10000', for scale command SC
Xright*6	Literal '10000' or '0', for scale command SC
Xstring*15	X-axis label, plotter output
Ylow*6	Literal '0'
Ystring*15	Y-axis label, screen and plotter output
Ytop*6	Literal '10000'

```

1 FTN7X,L
2 $FILES 0,1
3 $EMA/DATA/
4 PROGRAM PLOTSPEC
5 C -----
6 C
7 C This Program Is Designed To Plot Spectral Data Acquired From
8 C The CARY 2390 UV-VIS-NIR Spectrophotometer With CARYSPEC.RUN
9 C
10 C The Program Supports Output To HP 9872A And HP 7550A Plotters
11 C The HP 9872A Is Plotter #1 At Address LU 33 (IEEE-488 Device #2)
12 C The HP 7550A Is Plotter #2 At Address LU 17 (RS-232C Device)
13 C
14 C -----
15 C
16 C AUTHOR: Dr. Robert A. Binstead,
17 C Chemistry Division, Code 6125,
18 C Naval Research Laboratory,
19 C Washington. D.C. 20375-5000
20 C
21 C WRITTEN: February, 1987
22 C
23 C VERSION: 1.72
24 C
25 C REVISED: March, 1987:
26 C - Debugged plotting DO loops
27 C - Added Ordinate/Abscissa mode checks
28 C - Added ending wavelength check
29 C
30 C April, 1987:
31 C - Altered to use expt'l X-values
32 C - Added screen display routine
33 C - Removed rounding from SUB Xlimits
34 C - Altered rounding to use NINT function
35 C
36 C May, 1987:
37 C - Altered annotation mode to support
38 C Title, Parameters & Labels on plot
39 C - Altered AXES selection to provide
40 C default USER values & easy updates
41 C - Changed FFRCL to 79 characters to
42 C prevent unwanted line wrapping
43 C
44 C June, 1987:
45 C - Altered Filename convention to match
46 C the directory structure of the new CI
47 C operating system
48 C - The program had to be stripped down
49 C to run under the CI operating system
50 C by eliminating most I/O error checks
51 C
52 C July, 1987:
53 C - SEGMENTED versions of the full size

```

54 C	program failed with Memory Protect
55 C	errors at the INQUIRE statement if
56 C	the file existed already
57 C	
58 C	August, 1987:
59 C	- Eliminated INQUIRE statement for file
60 C	exists or open check to avoid system
61 C	crash in the segmented version of the
62 C	program. The error checks are now made
63 C	using error numbers returned in the
64 C	OPEN statement.
65 C	
66 C	April, 1988:
67 C	- Removed needless DATA for Pstr, unused
68 C	arrays and most I/O error checks on
69 C	WRITE to allow room for the complete
70 C	program in a single 32K word segment.
71 C	- Added Uppercase string conversion
72 C	routine for all string entries.
73 C	- Subroutines Xlimits & Ylimits were
74 C	replaced by Subroutine Order(MIN,MAX)
75 C	- Subroutine Xaxis was added to avoid
76 C	duplication in setting X-axis Limits,
77 C	Xtick and Xlabel spacing.
78 C	- Subroutine Yaxis was added to avoid
79 C	duplication in setting Y-axis Limits,
80 C	Ytick and Ylabel spacing.
81 C	- Altered Annotation Mode For Labels Up
82 C	To 40 Characters In Centered, Left &
83 C	Right Justified Formats. Positioning
84 C	& Character Size Commands Were Added.
85 C	- The Pen Position Digitizing Routine
86 C	Was Rewritten In Subroutine Form And
87 C	A Labelling Command Added To The Menu.
88 C	- The Annotation Routine Was Augmented
89 C	To Support Peak Position Labels In
90 C	Centered, Left & Right Justified Modes
91 C	With Special Offset Features To Avoid
92 C	Writing Over The Spectrum.
93 C	- % Transmission & % Reflectance Modes
94 C	Were Added To The Y-scale Selections.
95 C	- Re-scaling Between %T & Absorbance
96 C	Was Added To Support Both Plotting
97 C	Modes From Either Type Of Data File.
98 C	- Rounding Functions Were Altered To
99 C	Use ANINT (Whole Number) Command To
100 C	Avoid Integer Overflow With %T & %R
101 C	Labelling.
102 C	- Added Automatic Tick & Label Routines
103 C	To Select Preferred Values Based On
104 C	X & Y Scale Ranges. Defaults To 1/10
105 C	Of Scale For Entry Of An Anomously
106 C	Small Or Large Range.

```

107 C                                     - Added Code For Selection Of Plotter
108 C                                     Type (HP 9872A / HP 7550A) And Made
109 C                                     Adjustments To The P1,P2 Scaling
110 C                                     Points To Fit Output Within The Hard
111 C                                     Clip Limits Of Both Plotters.
112 C
113 C      Y-AXIS: Absorbance or Extinction Coefficient
114 C
115 C      X-AXIS: Wavelength or Wavenumbers x 1E-3
116 C
117 C      MEMORY: 30,000 Words (PROGRAM) + 80,000 Words EMA (DATA)
118 C
119 C      -----
120 C
121      INTEGER DIFF,EXIT,MENU,PLOT,READ,SETTINGS,PARAM(2,49)
122      INTEGER FINISH,IX,IY,IZ,NCOL,ND,NDATA(2),NP,NV,PN,PU,PXOFF,PYOFF
123      INTEGER START,UX1,UX2,UY1,UY2,X1,X2,Y1,Y2,XP1,XP2,YP1,YP2
124      REAL BAND,COFF,ESCALE,EMULT,EOFF,GAIN,LMIN,LMAX,NUMBER
125      REAL PMIN,PMAX,RATIO,SCALE,STEP,V,WN,WX,WMIN,WMAX
126      REAL XMIN,XMAX,XMULT,XOFF,X,XN,XX,Y,YN,YX,YMULT,YOFF,YSCALE
127      REAL Xtick,FXT,LXT,Ytick,FYT,LYT,Xlabel,FXL,LXL,Ylabel,FYL,LYL
128      REAL T1,T2,T3,T4,LWIDTH,WIDTH,BWIDTH,LHEIGHT,HEIGHT,BHEIGHT
129      REAL ABSC(2),CELL(2),CONC(2),CYCLE(2),DIST(2),ORD(2),PATH(2)
130      REAL SAMPLE(2),TIMER(2),TEMP(2),WAVE(2),FMIN(2),FMAX(2),FSTEP(2)
131      REAL FACTOR(2),VARIABLE(2,14),A(2,10001),W(2,10001)
132      LOGICAL MATCH
133 C
134 C      Dimension Screen Control String Variables
135 C
136      CHARACTER BELL,CLR*2,DOWN*2,ERASE*2,ESC,HOME*2,UP*2
137 C
138 C      Dimension Program Parameter Variables
139 C
140      CHARACTER DATE(2)*8,Fname(2)*20,LABEL(2)*72,Plotter(2)*10
141      CHARACTER Smin(2)*4,Smax(2)*4,Sinc(2)* ,Sstat(2)*10
142      CHARACTER C,CR,Code*2,Directory*40,Ex,Ext*14,Filespec*63
143      CHARACTER Icode,Length*6,LF,Lmode*8,Mult*5,Pcode*2,Pattern*6
144      CHARACTER Psize*8,Size,String*14,Text*40,TITLE*72,Vaxes*2
145      CHARACTER Vspec*2,Xcode,Xleft*6,Xord*7,Xright*6,Xstring*15
146      CHARACTER Ycode,Ylow*6,Ystring*15,Ytop*6,Pstr(23,16)*14
147 C
148 C      -----
149 C
150      COMMON /DATA/A,W
151      COMMON /XPARAM/LMIN,LMAX,WN,WX,Xtick,FXT,LXT,Xlabel,FXL,LXL
152      COMMON /YPARAM/Ytick,FYT,LYT,Ylabel,FYL,LYL
153      COMMON /DIGIT/FACTOR,XMIN,XMAX,YOFF,YSCALE,IX,IY,J,PU,X1,X2,Y1,Y2
154 C
155 C      -----
156 C
157 C      Define Rounding Functions Using Nearest Integer Commands
158 C
159      R0(X)=NINT(X)                                ! Type = INTEGER

```

```

160      R1(X)=ANINT(X*10.0)/10.0          ! Type = REAL
161      R2(X)=ANINT(X*100.0)/100.0        ! Type = REAL
162      R3(X)=ANINT(X*1.0E3)/1.0E3        ! Type = REAL
163 C
164 C      -----
165 C
166 C      Initialize String Variables
167 C
168      DATA (Plotter(1),I=1,2)/'HP 9872A ','HP 7550A '/
169      DATA (Pstr(1,I),I=1,6)/'ABSORBANCE','% TRANSMISSION',
170      &'TEMPERATURE','% REFLECTANCE','CONCENTRATION','EMISSION'/
171      DATA (Pstr(2,I),I=1,4)/'WAVELENGTH','TIME','TEMPERATURE',
172      &'DISTANCE'/
173      DATA (Pstr(3,I),I=1,11)/'OFF','0.01','0.02','0.05','0.1','0.2',
174      &'0.5','1.0','2.0','5.0','10.0'/
175      DATA Pstr(4,1)/'OFF'/
176      DATA (Pstr(4,I),I=6,15)/'0.2','0.5','1.0','2.0','5.0',
177      &'10','20','50','100','200'/
178      DATA (Pstr(5,I),I=1,4)/'AUTO SELECT','AUTO GAIN','AUTO SLIT',
179      &'SINGLE BEAM'/
180      DATA (Pstr(6,I),I=1,5)/'OFF','NORMAL','1ST DERIV','2ND DERIV',
181      &'LOG'/
182      DATA (Pstr(7,I),I=1,9)/'0.01','0.02','0.05','0.1','0.2','0.5',
183      &'1.0','2.0','4.0'/
184      DATA (Pstr(8,I),I=10,16)/'2','5','10','20','50','100','200'/
185      DATA (Pstr(9,I),I=12,15)/'10','20','50','100'/
186      DATA (Pstr(10,I),I=1,5)/'-1.9 TO 0.6','-2.0 TO 0.5',
187      &' -2.1 TO 0.4', '-2.2 TO 0.3', '-2.3 TO 0.2'/
188      DATA (Pstr(11,I),I=1,16)/'+/-0.01','+/-0.02','+/-0.05','+/-0.1',
189      &' +/-0.2', '+/-0.5', '+/-1.0', '+/-2.0', '+/-5.0', '+/-10', '+/-20',
190      &' +/-50', '+/-100', '+/-200', '+/-500', '+/-1000'/
191      DATA (Pstr(12,I),I=1,16)/'+/-0.01','+/-0.02','+/-0.05','+/-0.1',
192      &' +/-0.2', '+/-0.5', '+/-1.0', '+/-2.0', '+/-5.0', '+/-10', '+/-20',
193      &' +/-50', '+/-100', '+/-200', '+/-500', '+/-1000'/
194      DATA (Pstr(14,I),I=1,10)/'0','10','20','30','40','50','60','70',
195      &'80','90'/
196      DATA (Pstr(15,I),I=1,4)/'0.5','1.0','3.0','10'/
197      DATA (Pstr(16,I),I=1,2)/'NORMAL','REVERSE'/
198      DATA (Pstr(17,I),I=1,2)/'OFF','ON'/
199      DATA (Pstr(18,I),I=1,2)/'REPEAT SCAN','SGL/MULTI'/
200      DATA (Pstr(19,I),I=1,2)/'SERIAL','OVERLAY'/
201      DATA (Pstr(20,I),I=1,4)/'BOTH ON','UV ONLY','VIS/NIR ONLY',
202      &' BOTH OFF'/
203      DATA (Pstr(21,I),I=1,3)/'AUTO','UV','VIS/NIR'/
204      DATA (Pstr(22,I),I=1,3)/'AUTO','UV/VIS','NIR'/
205      DATA (Pstr(23,I),I=1,2)/'FULL','1/3'/
206 C
207      BELL=CHAR(7)
208      ESC=CHAR(27)
209      CLR=ESC// 'J'
210      HOME=ESC// 'h'
211      UP=ESC// 'A'
212      DOWN=ESC// 'B'
213      ERASE=ESC// 'K'

```

```

214 C
215         PN=1                                ! Select Plotter #1 (HP 9872A)
216         T1=10.0
217         T2=100.0
218         T3=1000.0
219         T4=10000.0
220 C
221 C -----
222 C
223 C         Assign Statement Labels
224 C
225 C -----
226 C
227         ASSIGN 10 TO MENU
228         ASSIGN 100 TO READ
229         ASSIGN 300 TO SETTINGS
230         ASSIGN 370 TO PLOT
231         ASSIGN 390 TO DIFF
232         ASSIGN 9000 TO EXIT
233 C
234 C -----
235 C
236 C         Data Transfer and Plot Control Menu
237 C
238 C -----
239 C
240         CALL FFRCL(79)                        ! Set Fields to 79 Characters
241 10 WRITE (1,*) HOME,CLR,'_'
242         NCOL=70
243         TITLE='Cary 2390 Spectral Data Plotting'
244         CALL Center(TITLE)
245         WRITE (1, '(T61,A2,A9)') UP, 'Rev: 1.72'
246         CALL Line(NCOL)
247         WRITE (1,20) 'CODE', 'FUNCTION', 'STATUS', 'MIN', 'MAX', 'INC'
248 20 FORMAT (T4,A4,T18,A8,T38,A7,T50,A3,T58,A3,T66,A3)
249         CALL Line(NCOL)
250         WRITE (1,30) 'R1', '.....Read Spectrum #1.....', Sstat(1),
251         &Smin(1), Smax(1), Sinc(1)
252         WRITE (1,30) 'R2', '.....Read Spectrum #2.....', Sstat(2),
253         &Smin(2), Smax(2), Sinc(2)
254         WRITE (1,50) 'IS', '.....Instrument Settings.....'
255         WRITE (1,30) 'PS', '.....Plotter Selection.....', Plotter(PN)
256         WRITE (1,40) 'P1', '.....Plot Spectrum #1.....', Fname(1)
257         WRITE (1,40) 'P2', '.....Plot Spectrum #2.....', Fname(2)
258         WRITE (1,50) 'DS', '.....Difference Spectrum.....'
259         WRITE (1,50) 'EX', '.....EXIT Menu.....'
260 30 FORMAT (/ ,T5,A2,T7,A30,T39,A10,T50,A4,T58,A4,T66,A4)
261 40 FORMAT (/ ,T5,A2,T7,A30,T39,A16)
262 50 FORMAT (/ ,T5,A2,T7,A30)
263         WRITE (1,*)
264         CALL Line(NCOL)
265         WRITE (1,*)
266 70 WRITE (1,*) UP,ERASE,'_'

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```

267      WRITE (1, '(T3,A15,A,A2)') 'Enter the CODE:', BELL, '_'
268      READ (1, 80) Code
269      80 FORMAT (A2)
270      CALL Upper(Code)
271 C      -----
272      IF ((Code.EQ.'R1').OR.(Code.EQ.'R2')) THEN
273          J=ICHAR(Code(2:2))-48
274          GO TO READ
275      END IF
276      IF (Code.EQ.'IS') GO TO SETTINGS
277      IF (Code.EQ.'PS') THEN
278          90 WRITE (1,*) UP,ERASE,' Select: 1...HP 9872A,',
279          & ' 2...HP 7550A ? ', BELL, '_'
280          READ (1,99) Icode
281          IF ((Icode.NE.'1').AND.(Icode.NE.'2')) THEN
282              GO TO 90
283          END IF
284          PN=ICHAR(Icode)-48
285          GO TO MENU
286      END IF
287      IF ((Code.EQ.'P1').OR.(Code.EQ.'P2')) THEN
288          J=ICHAR(Code(2:2))-48
289          GO TO PLOT
290      END IF
291      IF (Code.EQ.'DS') THEN
292          J=1
293          GO TO DIFF
294      END IF
295      IF (Code.EQ.'EX') GO TO EXIT
296      GO TO 70
297 C
298 C      -----
299 C
300 C          Read Spectrum: (J = 1 or 2)
301 C
302 C      -----
303 C
304      99 FORMAT (A1)
305      100 IF (Sstat(J).EQ.'VALID') THEN
306          WRITE (1,*) UP,ERASE,' Spectrum is PRESENT: ',
307          & ' Proceed (Y or N) ? ', BELL, '_'
308          READ (1,99) Icode
309          CALL Upper(Icode)
310          IF (Icode.EQ.'N') GO TO 70
311          IF (Icode.NE.'Y') GO TO 100
312      END IF
313      WRITE (1,*) HOME,CLR,'_'
314      TITLE='Read Spectrum #'//Code(2:2)
315      CALL Center(TITLE)
316      CALL Line(NCOL)
317      WRITE (1,*) DOWN,' Enter Filename: ', BELL, '_'
318      READ (1, '(A20)') Fname(J)
319      CALL Upper(Fname(J))

```

```

320 WRITE (1,*) DOWN,' Directory, (Return = /DEFAULT/) ',BELL,'_'
321 READ (1,'(A40)') Directory
322 IF (Directory.EQ.' ') THEN
323     Filespec=Fname(J)
324     GO TO 110
325 END IF
326 K=40
327 DO WHILE (Directory(K:K).EQ.' ')
328     K=K-1
329 END DO
330 IF (Directory(K:K).EQ.'/') K=K-1
331 Filespec=Directory(1:K)//'/'//Fname(J)
332 110 K=63
333 DO WHILE (Filespec(K:K).EQ.' ')
334     K=K-1
335 END DO
336 WRITE (1,*) UP,ERASE,' Validating: ',Filespec(1:K),'_'
337 CALL Wait(1.0)
338 OPEN (UNIT=66,FILE=Filespec(1:K),IOSTAT=N,STATUS='OLD')
339 WRITE (1,*)
340 IF (N.NE.0) THEN
341     WRITE (1,*) UP,ERASE,'_'
342     N=N-500
343     IF (N.EQ.6) WRITE (1,*) ' File does NOT EXIST: ',BELL,'_'
344     IF (N.EQ.8) WRITE (1,*) ' File is already OPEN: ',BELL,'_'
345     IF ((N.NE.6).AND.(N.NE.8)) WRITE (1,*) ' Disk Error = ',N,
346     & BELL,'_'
347     CLOSE (UNIT=66,STATUS='DELETE')
348     CALL Wait(2.0)
349     WRITE (1,*)
350     Sstat(J)='INVALID'
351     GO TO MENU
352 END IF
353 WRITE (1,*) UP,ERASE,' Reading File: ',Filespec(1:K)
354 READ (66,FMT=120,IOSTAT=N,ERR=210) LABEL(J)
355 120 FORMAT (A72)
356 WRITE (1,*) DOWN,' Title:'
357 WRITE (1,*) ' ',LABEL(J)
358 READ (66,FMT=130) DATE(J)
359 130 FORMAT (A8)
360 WRITE (1,*) DOWN,' Date: ',DATE(J)
361 READ (66,*) FMIN(J),FMAX(J),FSTEP(J),
362 &CONC(J),PATH(J)
363 READ (66,*) ORD(J),ABSC(J),CELL(J),CYCLE(J),
364 &SAMPLE(J),WAVE(J),TIMER(J),TEMP(J),DIST(J)
365 WRITE (1,140) DOWN,' Scan Range: ',FMAX(J),' to ',FMIN(J),
366 & ' nm at ',FSTEP(J),' nm steps'
367 WRITE (1,'(T4,A2,A12,2X,G9.4)') DOWN,' Conc. (M) : ',CONC(J)
368 WRITE (1,150) DOWN,' Path (cm) : ',PATH(J)
369 WRITE (1,150) DOWN,' Temp. (C) : ',TEMP(J)
370 140 FORMAT (T4,A2,A12,F6.2,A4,F6.2,A7,F4.2,A9)
371 150 FORMAT (T4,A2,A12,F6.2)

```



```

372     CALL Str(FMIN(J),String,4)
373     Smin(J)=String(2:5)
374     CALL Str(FMAX(J),String,4)
375     Smax(J)=String(2:5)
376     CALL Str(FSTEP(J),String,4)
377     Sinc(J)=String(2:5)
378     READ (66,FMT=160,IOSTAT=N,ERR=210) NP,NV,NDATA(J)
379 160  FORMAT (13,13,16)
380     IF ((NP.NE.49).OR.(NV.NE.14)) GO TO 200
381     IF (ABS(FMIN(J)-WAVE(J)).GT.0.1) THEN
382         WRITE (1,*) DOWN,' Warning! Scan ended at ',WAVE(J),' nm',BELL
383         CALL Wait(2.0)
384     END IF
385     WRITE (1,*)
386     TITLE='### READING SPECTRUM ###'
387     WRITE (1,*) HOME,'_'
388     CALL Center(TITLE)
389     READ (66,FMT=170) (PARAM(J,K),K=1,NP)
390 170  FORMAT (12)
391     READ (66,*) (VARIABLE(J,K),K=1,NV)
392     READ (66,*) (A(J,K),K=1,NDATA(J))
393     READ (66,*) (W(J,K),K=1,NDATA(J))
394     Sstat(J)='VALID'
395 180  CLOSE (UNIT=66,IOSTAT=N,ERR=210)
396     IF (Sstat(J).NE.'VALID') GO TO MENU
397 190  WRITE (1,*) UP,ERASE,' EDIT Conc./Path: (Y or N) ? ',BELL,'_'
398     READ (1,99) Icode
399     CALL Upper(Icode)
400     IF (Icode.EQ..'Y') GO TO 230
401     IF (Icode.NE..'N') GO TO 190
402     GO TO MENU
403 C -----
404 200  WRITE (1,*) UP,ERASE,' Data Format Error: ',BELL,'_'
405     Sstat(J)='ABORTED'
406     GO TO 220
407 210  WRITE (1,*) UP,ERASE,' Disk Error =',N,BELL,'_'
408     Sstat(J)='INVALID'
409 220  CALL Wait(2.0)
410     WRITE (1,*)
411     GO TO 180
412 C -----
413 230  WRITE (1,*) UP,ERASE,' (C...Conc. , P...Path) ? ',BELL,'_'
414     READ (1,99) Icode
415     CALL Upper(Icode)
416     IF (Icode.EQ..'P') GO TO 250
417     IF (Icode.NE..'C') GO TO 230
418 240  WRITE (1,*) UP,ERASE,' Concentration, (M): ',BELL,'_'
419     READ (1,*,ERR=240) CONC(J)
420     GO TO 190
421 250  WRITE (1,*) UP,ERASE,' Pathlength, (cm): ',BELL,'_'
422     READ (1,*,ERR=250) PATH(J)
423     GO TO 190

```

```

424 C
425 C -----
426 C
427 C      Error Messages & Returns To Menu
428 C
429 C -----
430 C
431 260 TITLE=' Conc. or Path = 0.0 '
432 GO TO 290
433 270 TITLE=' Spectra are MISMATCHED: '
434 GO TO 290
435 280 TITLE=' Spectrum is ABSENT: '
436 290 WRITE (1,*) UP,ERASE,TITLE(1:26),BELL,'_'
437 CALL Wait(2.0)
438 WRITE (1,*)
439 GO TO 70
440 C
441 C -----
442 C
443 C      Display Instrument Settings
444 C
445 C -----
446 C
447 300 IF ((Sstat(1).NE.'VALID').AND.(Sstat(2).NE.'VALID')) GO TO 280
448 310 WRITE (1,*) UP,ERASE,' Spectrum #, (1 or 2): ',BELL,'_'
449 READ (1,'(I2)',ERR=310) J
450 IF ((J.NE.1).AND.(J.NE.2)) GO TO 310
451 IF (Sstat(J).NE.'VALID') GO TO 280
452 BAND=VARIABLE(J,10)
453 GAIN=VARIABLE(J,6)
454 String=Pstr(7,PARAM(J,7)+1)
455 K=1
456 IF (PARAM(J,1).NE.0) THEN
457 String=Pstr(8,PARAM(J,8)+1)
458 K=11
459 END IF
460 CALL Val(String,PMAX)
461 PMIN=VARIABLE(J,K)
462 PMAX=PMIN+PMAX
463 K=11
464 IF (PARAM(J,6).EQ.4) K=10
465 String=Pstr(K,PARAM(J,K)+1)
466 WRITE (1,*) HOME,CLR,'_'
467 TITLE='Instrument Settings'
468 CALL Center(TITLE)
469 CALL Line(50)
470 WRITE (1,'(T20,A8,T40,A7)') 'FUNCTION','SETTING'
471 CALL LINE(50)
472 WRITE (1,*)
473 WRITE (1,320) 'WAVELENGTH LIMITS.....',FMIN(J),', ',FMAX(J)
474 WRITE (1,330) 'ORDINATE.....',Pstr(1,PARAM(J,1)+1)
475 WRITE (1,330) 'ABSCISSA.....',Pstr(2,PARAM(J,2)+1)
476 WRITE (1,330) 'SCAN RATE (nm/sec).....',Pstr(3,PARAM(J,3)+1)

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477 WRITE (1,330) 'CHART DISPLAY (nm/cm)...',Pstr(4,PARAM(J,4)+1)
478 WRITE (1,330) 'REFERENCE MODE.....',Pstr(5,PARAM(J,5)+1)
479 WRITE (1,340) 'SBW (nm), GAIN.....',BAND,',',',C:IN
480 WRITE (1,330) 'PEN FUNCTION.....',Pstr(6,PARAM(J,6)+1)
481 WRITE (1,340) 'PEN LIMITS (Min,Max)...',PMIN,',',',PMAX
482 IF (PARAM(J,6).GT.1) WRITE (1,350) UP,ERASE,String
483 WRITE (1,330) 'RESPONSE TIME (sec)....',Pstr(15,PARAM(J,15)+1)
484 WRITE (1,330) 'BEAM INTERCHANGE.....',Pstr(16,PARAM(J,16)+1)
485 WRITE (1,330) 'SLIT HEIGHT.....',Pstr(23,PARAM(J,23)+1)
486 WRITE (1,330) 'LAMP SELECT.....',Pstr(21,PARAM(J,21)+1)
487 WRITE (1,330) 'DETECTOR SELECT.....',Pstr(22,PARAM(J,22)+1)
488 320 FORMAT (T15,A23,T40,F5.2,A,F5.2)
489 330 FORMAT (T15,A23,T40,A14)
490 340 FORMAT (T15,A23,T40,F4.2,A,F5.2)
491 350 FORMAT (T40,A2,A2,A14)
492 WRITE (1,*)
493 CALL Line(50)
494 WRITE (1,*)
495 360 WRITE (1, '(T14,A2,A2,A23,A,A)') UP,ERASE,
496 &'Press RETURN for MENU: ',BELL, '_'
497 READ (1,99) Icode
498 IF (Icode.NE.' ') GO TO 360
499 GO TO MENU
500 C
501 C -----
502 C
503 C Plot Mode Setup
504 C
505 C -----
506 C
507 370 IF (Sstat(J).NE.'VALID') GO TO 280
508 GO TO 400
509 390 IF ((Sstat(1).NE.'VALID').OR.(Sstat(2).NE.'VALID')) GO TO 280
510 MATCH=.TRUE.
511 IF (FSTEP(1).NE.FSTEP(2)) MATCH=.FALSE.
512 IF (FMIN(1).NE.FMIN(2)) MATCH=.FALSE.
513 IF (FMAX(1).NE.FMAX(2)) MATCH=.FALSE.
514 IF (MATCH) GO TO 400
515 GO TO 270
516 C -----
517 400 TITLE='Plot Spectrum # '//CHAR(J+48)
518 FACTOR(1)=CONC(1)*PATH(1)
519 FACTOR(2)=CONC(2)*PATH(2)
520 IF (Code.EQ.'DS') THEN
521 IF ((FACTOR(1).EQ.0.0).OR.(FACTOR(2).EQ.0.0)) GO TO 260
522 RATIO=FACTOR(1)/FACTOR(2) ! Temporary Scaling Factor
523 TITLE='Difference Spectrum Plot'
524 END IF
525 IF (FACTOR(J).EQ.0.0) FACTOR(J)=1.0 ! Avoid Division By Zero
526 WRITE (1,*) HOME,CLR, '_'
527 CALL Center(TITLE)
528 CALL Line(NCOL)
529 WRITE (1,*) DOWN,DOWN

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530      WRITE (1, '(T10,A32)') 'X-scale units:  N.....Nanometres'
531      WRITE (1,*)
532      WRITE (1, '(T26,A17)') 'W.....Wavenumbers'
533      WRITE (1,*) DOWN
534 410  WRITE (1,420) UP,ERASE,'Code:  ',BELL,'_'
535 420  FORMAT (T19,A2,A2,A7,A,A)
536      READ (1,99) Xcode
537      CALL Upper(Xcode)
538      IF (Xcode.EQ.'W') THEN
539          WRITE (1,*) UP,ERASE,UP,UP,ERASE,UP,UP
540          WRITE (1, '(T26,A2,A2,A11)') UP,ERASE,'Wavenumbers'
541          Xord=' (cm-1)'
542          WMAX=R2(T4/FMIN(J))
543          WMIN=R2(T4/FMAX(J))
544          GO TO 430
545      END IF
546      IF (Xcode.NE.'N') GO TO 410
547      WRITE (1,*) UP,ERASE,UP,UP,ERASE,UP,UP
548      WRITE (1, '(T26,A2,A2,A10)') UP,ERASE,'Nanometres'
549      Xord=' (nm)'
550      WMAX=R1(FMAX(J))
551      WMIN=R1(FMIN(J))
552 430  ND=NDATA(J)                ! Number Of Data Points
553      STEP=STEP(J)              ! Step Size (nm)
554      XMIN=WMIN                 ! X-scale MIN/MAX = Scan Limits
555      XMAX=WMAX
556      CALL Xaxis(XMIN,XMAX)      ! Set Limits, Tick & Label Spacing
557 C  -----
558      WRITE (1,*) DOWN,DOWN
559      WRITE (1, '(T10,A32)') 'Y-scale units:  A.....Absorbance'
560      WRITE (1,*)
561      WRITE (1, '(T26,A28)') 'E.....Extinction Coefficient'
562      WRITE (1,*)
563      WRITE (1, '(T26,A19)') 'R.....% Reflectance'
564      WRITE (1,*)
565      WRITE (1, '(T26,A20)') 'T.....% Transmission'
566      WRITE (1,*) DOWN
567 440  WRITE (1,420) UP,ERASE,'Code:  ',BELL,'_'
568      READ (1,99) Ycode
569      CALL Upper(Ycode)
570      Text=UP//ERASE//UP//UP//ERASE//UP//UP//ERASE//UP//UP//ERASE//UP
571 C  -----
572      IF (Code.EQ.'DS') THEN
573          IF ((Ycode.EQ.'R').OR.(Ycode.EQ.'T')) GO TO 440
574      END IF
575 C  -----
576      IF (Ycode.EQ.'A') THEN
577          Ystring='ABSORBANCE'    ! Select Y-axis Label For Plot
578          K=0                    ! Ordinate Mode = Absorbance
579      ELSE IF (Ycode.EQ.'E') THEN
580          K=0                    ! Ordinate Mode = Absorbance
581      ELSE IF (Ycode.EQ.'R') THEN
582          Ystring='% Reflectance'
583          K=1                    ! Ordinate Mode = % Transmission

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584 ELSE IF (Ycode.EQ.'T') THEN
585     Ystring='% Transmission'
586     K=1 ! Ordinate Mode = % Transmission
587 ELSE
588     GO TO 440
589 END IF
590 C -----
591 IF (PARAM(J,1).NE.K) THEN ! Test Ordinate Mode Of Spectrum =J
592     CALL Rescale(J,K,ND) ! Rescale Between Absorbance & %T
593     PARAM(J,1)=K ! Reset Ordinate Variable To Match
594 END IF
595 IF (Code.EQ.'DS') THEN ! Difference Spectrum Mode
596     K=0 ! Only Absorbance Mode Allowed
597     IF (PARAM(2,1).NE.K) THEN ! Test Ordinate Mode Of Spectrum =2
598         CALL Rescale(2,K,ND) ! Rescale To Absorbance If Required
599         PARAM(2,1)=K ! Reset Ordinate Variable To Match
600     END IF
601 END IF
602 C -----
603 IF (Ycode.NE.'E') THEN
604     WRITE (1,*) Text(1:24),UP ! Erase Unwanted Labels
605     WRITE (1, '(T26,A2,A2,A15)') UP,ERASE,Ystring
606     YMULT=1.0 ! YMULT Scales Ext.Coeff. Mode
607     IF (Ycode.EQ.'A') GO TO 450
608     YOFF=0.0
609     YSCALE=100.0
610     CALL Yaxis(YSCALE,Ycode)
611     GO TO 460
612 END IF
613 C -----
614 IF (FACTOR(J).EQ.0.0) THEN
615     WRITE (1, '(T19,A2,A2,T30,A19,A,A)') UP,ERASE,
616     & 'Conc. or Path = 0.0',BELL,'_'
617     CALL Wait(2.0)
618     WRITE (1,*)
619     GO TO 440
620 END IF
621 WRITE (1,*) Text(1:24),UP ! Erase Unwanted Labels
622 WRITE (1, '(T26,A2,A2,A22)') UP,ERASE,'Extinction Coefficient'
623 C -----
624 450 K=1
625 PMAX=0.0
626 DO WHILE (K.LE.ND) ! Find Maximum Absorbance
627     NUMBER=A(J,K)
628     IF (Code.EQ.'DS') THEN
629         NUMBER=ABS(A(1,K)-A(2,K)*RATIO)
630     END IF
631     IF (PMAX.LT.NUMBER) PMAX=NUMBER
632     K=K+1
633 END DO
634 SCALE=R3(PMAX+0.001) ! Round Up Absorbance Max'm
635 IF (PMAX.GT.0.01) SCALE=R2(PMAX+0.01)
636 IF (PMAX.GT.0.10) SCALE=R1(PMAX+0.10)

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637      YOFF=0.0                ! Initial Y-scale Min'm
638      YSCALE=SCALE            ! Initial Y-scale Max'm
639      ESCALE=SCALE            ! Initial E-scale Max'm
640      IF (Code.EQ.'DS') THEN
641          YSCALE=2.0*SCALE      ! 2 x Y-scale for +/- Max'm Range
642          YOFF=SCALE           ! Set Zero Position At Half Y-scale
643      END IF
644      CALL Yaxis(YSCALE,Ycode)  ! Set Tick & Label Spacing
645      IF (Ycode.EQ.'A') GO TO 460
646 C
647 C -----
648 C
649 C      Scale YMULT for Extinction Coefficient Mode
650 C
651 C -----
652 C
653      DO WHILE (ESCALE/FACTOR(J).LT.1.0)
654          ESCALE=ESCALE*10.0
655      END DO
656      DO WHILE (ESCALE/FACTOR(J).GT.10.0)
657          ESCALE=ESCALE/10.0
658      END DO
659      RATIO=ESCALE/SCALE        ! Power Of 10 For Exponent
660      YMULT=RATIO/FACTOR(J)    ! Scaling Factor For Ext. Coeff.
661      CALL Exponent(RATIO,Mult) ! Convert Exponent To String
662 C
663 C -----
664 C
665 C      Plotting Routine: HP 9872A & HP 7550A
666 C
667 C -----
668 C
669      460 PU=33                 ! Plotter Logical Unit # (HP 9872A)
670          PXOFF=0              ! X-zero Position Offset (HP 9872A)
671          PYOFF=0              ! Y-zero Position Offset (HP 9872A)
672          IF (PN.EQ.2) THEN
673              PU=17            ! Plotter Logical Unit # (HP 7550A)
674              PXOFF=200        ! X-zero Position Offset (HP 7550A)
675              PYOFF=100        ! Y-zero Position Offset (HP 7550A)
676          END IF
677          WIDTH=1.0            ! Character Field Width (cm)
678          HEIGHT=2.0           ! Character Field Height (cm)
679          Lmode='SOLID'        ! Solid Line Type ON
680          Pattern=' '          ! Broken Line Type OFF
681          Length=' '           ! Not Used For Solid Pattern
682          LF=CHAR(10)          ! Linefeed Character
683          CR=CHAR(13)          ! Carriage Return Character
684          C=', '               ! Data Separator In HP-GL Commands
685          Etx=CHAR(3)          ! Label Mode Terminator (HP Default)
686          Size='N'             ! Plot Size Default Is NOTEBOOK
687          Vaxes='5'            ! Pen Speed (cm/sec) For Axes Vectors
688          Vspec='5'            ! Pen Speed (cm/sec) For Spectrum
689 C -----

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```

690      WRITE (1,*) DOWN,DOWN,DOWN
691 470 WRITE (1,480) UP,ERASE,'Press RETURN if plotter is ON: ',BELL,'_'
692 480 FORMAT (T10,A2,A2,A31,A,A)
693      READ (1,99) Icode
694      IF (Icode.NE.' ') GO TO 470
695      WRITE (1, '(T10,A2,A2,A21)') UP,ERASE,'Initializing Plotter:'
696      WRITE (PU,*,IOSTAT=N,ERR=9999) 'DF;'
697      UX1=1800
698      UX2=15500                ! Default User Set Plotting Boundaries
699      UY1=1200                ! P1 = (1800,1200) & P2 = (15500,9500)
700      UY2=9500                ! For B-size Paper On HP 7550A Plotter
701 490 IF (Size.EQ.'F') THEN
702      Psize='FULL'
703      XP1=1350-PXOFF
704      XP2=10000-PXOFF        ! FULL A-size Paper Plotting Boundaries
705      YP1=1000-PYOFF        ! P1 = (1350,1000) & P2 = (10000,7500)
706      YP2=7500-PYOFF        ! Offset P1,P2 For HP 7550A Plotter
707      GO TO 500
708  END IF
709      Psize='NOTEBOOK'
710      XP1=1350-PXOFF
711      XP2=8500-PXOFF        ! NOTEBOOK Size Plotting Boundaries
712      YP1=1000-PYOFF        ! P1 = (1350,1000) & P2 = (8500,7000)
713      YP2=7000-PYOFF        ! Offset P1,P2 For HP 7550A Plotter
714 C      -----
715 C      LU #33 is device #2 on IEEE-488 interface #1
716 C      LU #17 is serial device on HP MUX (9600 Baud, XON/XOFF)
717 C      -----
718 500 WRITE (PU,FMT=510)
719 510 FORMAT ('SP1;PU;AP;TL1;DI1,0;IW;')
720      WRITE (PU,*) 'IP',XP1,C,YP1,C,XP2,C,YP2,',';
721      Xleft='0'
722      Xright='10000'
723      XOFF=XMIN
724      IF (XMIN.GT.XMAX) THEN
725          Xleft='-10000'
726          Xright='0'
727          XOFF=XMAX
728      END IF
729      XMULT=T4/(XMAX-XMIN)    ! Scales User Units To 0-10000 Range
730      Ylow='0'               ! YMULT Is Set In Y-scale Routines
731      Ytop='10000'           ! For A Scaled Range Of 0-10000 Units
732      WRITE (PU,*) 'SC',Xleft,',',Xright,',',Ylow,',',Ytop,',';
733      RATIO=0.6
734      LWIDTH=WIDTH*RATIO    ! LITTLE Size Characters Default To
735      LHEIGHT=HEIGHT*RATIO  ! 0.6 Of The User Set Character Size
736      RATIO=4.0/3.0
737      BWIDTH=WIDTH*RATIO    ! BIG Size Characters Are Kept In
738      BHEIGHT=HEIGHT*RATIO  ! Proportion To The User Set Size
739      WRITE (PU,*) 'SR',WIDTH,',',HEIGHT,',';VS',Vaxes,',';
740 C      -----
741 520 WRITE (1,*) HOME,CLR,'_'
742      CALL Line(NCOL)

```

```

743      WRITE (1,530) 'CODE','FUNCTION','MIN','MAX','INC'
744 530 FORMAT (T4,A4,T18,A8,T40,A3,T50,A3,T60,A3)
745      CALL Line(NCOL)
746      WRITE (1,540) 'PL','.....Plot Limits.....',WN,WX
747      WRITE (1,540) 'XS','.....X-scale.....',XMIN,XMAX
748      IF (Xcode.EQ.'N') WRITE (1,'(T20,A2,A5)') UP,' (nm)'
749      IF (Xcode.EQ.'W') WRITE (1,'(T20,A2,A14)') UP,' (cm-1) x 1E-3'
750      WRITE (1,550) 'XT','.....X-tick Spacing.....',FXT,LXT,Xtick
751      WRITE (1,550) 'XL','.....X-label Spacing.....',FXL,LXL,Xlabel
752      WRITE (1,*)
753      WRITE (1,560) 'YS','.....Y-scale.....',
754      &(-YOFF*YMULT),(YSCALE-YOFF)*YMULT
755      IF (Ycode.EQ.'E') WRITE (1,'(T20,A2,A9,A5)') UP,' (Ext) x ',Mult
756      WRITE (1,570) 'YT','.....Y-tick Spacing.....',
757      &(FYT-YOFF)*YMULT,(LYT-YOFF)*YMULT,Ytick*YMULT
758      WRITE (1,570) 'YL','.....Y-label Spacing.....',
759      &(FYL-YOFF)*YMULT,(LYL-YOFF)*YMULT,Ylabel*YMULT
760      WRITE (1,*)
761      WRITE (1,580) 'CS','.....Char.Size (Width,Height)',WIDTH,HEIGHT
762      WRITE (1,600) 'PV','.....Pen Velocity (Axes,Spec)',Vaxes,Vspec
763      WRITE (1,590) 'LT','.....Line Type.....',Lmode,Pattern,
764      &Length
765      WRITE (1,590) 'AX','.....Axes Size.....',Psize,' ',' '
766      WRITE (1,610) 'AN','.....Annotate Plot.....'
767      WRITE (1,610) 'PA','.....PLOT AXES.....'
768      WRITE (1,610) 'PS','.....PLOT SPECTRUM.....'
769      WRITE (1,610) 'DD','.....DIGITIZE/DISPLAY DATA...'
770      WRITE (1,610) 'EX','.....EXIT PLOTTING MODE.....'
771 540 FORMAT (T5,A2,T7,A30,T40,F4.1,T50,F4.1)
772 550 FORMAT (T5,A2,T7,A30,T40,F4.2,T50,F4.2,T60,F4.2)
773 560 FORMAT (T5,A2,T7,A30,T40,F5.3,T50,F5.3)
774 570 FORMAT (T5,A2,T7,A30,T40,F5.3,T50,F5.3,T60,F4.3)
775 580 FORMAT (T5,A2,T7,A30,T40,F4.2,T50,F4.2)
776 590 FORMAT (T5,A2,T7,A30,T40,A8,T50,A6,T60,A6)
777 600 FOFMAT (T5,A2,T7,A30,T40,A2,T50,A2)
778 610 FORMAT (T5,A2,T7,A30)
779      CALL Line(NCOL)
780      WRITE (1,*)
781 620 WRITE (1,*) UP,ERASE,'_'
782      WRITE (1,'(T3,A15,A,A2)') 'Enter the CODE:',BELL,'_'
783      READ (1,80) Pcode
784      CALL Upper(Pcode)
785 C -----
786      IF (Pcode.EQ.'PL') GO TO 700
787      IF (Pcode.EQ.'XS') GO TO 720
788      IF (Pcode.EQ.'XT') GO TO 730
789      IF (Pcode.EQ.'XL') GO TO 740
790      IF (Pcode.EQ.'YS') GO TO 760
791      IF (Pcode.EQ.'YT') GO TO 810
792      IF (Pcode.EQ.'YL') GO TO 820
793      IF (Pcode.EQ.'CS') GO TO 840
794      IF (Pcode.EQ.'PV') GO TO 850
795      IF (Pcode.EQ.'LT') GO TO 860

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796      IF (Pcode.EQ.'AX') GO TO 890
797      IF (Pcode.EQ.'EX') GO TO 980
798      IF (Pcode.EQ.'PA') GO TO 1000
799      IF (Pcode.EQ.'AN') GO TO 1100
800      IF (Pcode.EQ.'PS') GO TO 2000
801      IF (Pcode.EQ.'DD') GO TO 3000
802      GO TO 500
803 C -----
804 700 WRITE (1,*) UP,ERASE,' Plot Limits: (Min,Max) ',BELL,'_'
805      READ (1,*,ERR=700) WN,WX
806      CALL Order(WN,WX)
807 710 IF ((WN.LT.WMIN).OR.(WN.GT.WMAX)) WN=WMIN
808      IF ((WX.LT.WMIN).OR.(WX.GT.WMAX)) WX=WMAX
809      GO TO 500
810 C -----
811 720 WRITE (1,*) UP,ERASE,' X-scale: (Min,Max) ',BELL,'_'
812      READ (1,*,ERR=720) XMIN,XMAX
813      XN=XMIN ! X-axis Is Bidirectional So Only
814      XX=XMAX ! XN,XX Are Ordered For Tick & Label
815      CALL Order(XN,XX)
816      CALL Xaxis(XN,XX) ! Set Limits, Tick & Label Spacing
817      GO TO 710
818 C -----
819 730 WRITE (1,*) UP,ERASE,' X-tick: (First,Last,Space) ',BELL,'_'
820      READ (1,*,ERR=730) XN,XX,Xtick
821      CALL Order(XN,XX)
822      IF ((XN.LT.LMIN).OR.(XX.GT.LMAX)) GO TO 730
823      Xtick=ABS(Xtick)
824      FXT=XN
825      LXT=XX
826      Xlabel=Xtick
827      GO TO 750
828 C -----
829 740 WRITE (1,*) UP,ERASE,' X-label: (First,Last,Space) ',BELL,'_'
830      READ (1,*,ERR=740) XN,XX,Xlabel
831      CALL Order(XN,XX)
832      IF ((XN.LT.LMIN).OR.(XX.GT.LMAX)) GO TO 740
833      Xlabel=ABS(Xlabel)
834 750 FXL=XN
835      LXL=XX
836      GO TO 500
837 C -----
838 760 WRITE (1,*) UP,ERASE,' Y-scale: (Min,Max) ',BELL,'_'
839      READ (1,*,ERR=760) YN,YX
840      CALL Order(YN,YX) ! Y-scale Is Unidirectional
841      EOFF=-YN
842      IF (Ycode.NE.'E') GO TO 800
843 770 WRITE (1,780) UP,ERASE,' Ext.Coeff.Scale: ',Mult,
844      &': (U...UP / D...Down / A...Accept) ? ',BELL,'_'
845 780 FORMAT (A2,A2,A20,A6,A37,A.A)
846      READ (1,99) Icode
847      CALL Upper(Icode)
848      IF (Icode.EQ.'A') GO TO 800

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849      IF (Icode.EQ.'U') THEN
850          EMULT=10.0
851          GO TO 790
852      END IF
853      IF (Icode.EQ.'D') THEN
854          EMULT=0.1
855          GO TO 790
856      END IF
857      GO TO 770
858 790 ESCALE=ESCALE*EMULT          ! Update Ext. Coeff. Scale
859      RATIO=ESCALE/SCALE          ! Power Of 10 For Exponent
860      YMULT=RATIO/FACTOR(J)       ! Scaling Factor For Ext. Coeff.
861      CALL Exponent(RATIO,Mult)   ! Convert Exponent To String
862      GO TO 770
863 800 YSCALE=(YX-YN)/YMULT         ! YMULT Alters Scaling For The
864      YOFF=EOFF/YMULT            ! Extinction Coefficient Mode
865      CALL Yaxis(YSCALE,Ycode)    ! Set Tick & Label Spacing
866      GO TO 500
867 C -----
868 810 WRITE (1,*) UP,ERASE,' Y-tick: (First,Last,Space) ',BELL,'_'
869      READ (1,*,ERR=810) YN,YX,Ytick
870      CALL Order(YN,YX)
871      Ytick=ABS(Ytick)/YMULT
872      FYT=(YN+EOFF)/YMULT
873      LYT=(YX+EOFF)/YMULT
874      Ylabel=Ytick
875      GO TO 830
876 C -----
877 820 WRITE (1,*) UP,ERASE,' Y-label: (First,Last,Space) ',BELL,'_'
878      READ (1,*,ERR=820) YN,YX,Ylabel
879      CALL Order(YN,YX)
880      Ylabel=ABS(Ylabel)/YMULT
881 830 FYL=(YN+EOFF)/YMULT
882      LYL=(YX+EOFF)/YMULT
883      GO TO 500
884 C -----
885 840 WRITE (1,*) UP,ERASE,' Char.size: (Width,Height) ',BELL,'_'
886      READ (1,*,ERR=840) WIDTH,HEIGHT
887      IF (Pcode.EQ.'AN') GO TO 1140 ! Return To Annotation Mode
888      GO TO 500
889 C -----
890 850 WRITE (1,*) UP,ERASE,' Pen Velocity, (Axes,Spectrum): ',BELL,'_'
891      READ (1,*,ERR=850) X,Y
892      IF ((X.LT.1.0).OR.(X.GT.36.0)) GO TO 850
893      IF ((Y.LT.1.0).OR.(Y.GT.36.0)) GO TO 850
894      CALL Str(X,String,2)
895      Vaxes=String(2:3)
896      CALL Str(Y,String,2)
897      Vspec=String(2:3)
898      GO TO 500
899 C -----

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900 860 WRITE (1,*) UP,ERASE,' Line Type: (S.....Solid, B.....Broken) ',
901 &BELL,'_'
902 READ (1,99) Icode
903 CALL Upper(Icode)
904 IF (Icode.EQ.'S') THEN
905     Lmode='SOLID'
906     Pattern=' '
907     Length=' '
908     WRITE (PU,*) 'LT;'
909     GO TO 500
910 END IF
911 IF (Icode.NE.'B') GO TO 860
912 Lmode='PATTERN'
913 870 WRITE (1,*) UP,ERASE,' Pattern #: (1-6) ',BELL,'_'
914 READ (1,'(12)',ERR=870) N
915 IF ((N.LT.1).OR.(N.GT.6)) GO TO 870
916 NUMBER=FLOAT(N)
917 CALL Str(NUMBER,String,1)
918 Pattern(1:1)='#'
919 Pattern(3:3)=String(2:2)
920 880 WRITE (1,*) UP,ERASE,' Pattern Length: (0-10)% ',BELL,'_'
921 READ (1,*,ERR=880) NUMBER
922 IF ((NUMBER.LT.0.0).OR.(NUMBER.GT.10.0)) GO TO 880
923 CALL Str(NUMBER,String,2)
924 K=2
925 DO WHILE (String(K:K).NE.' ')
926     K=K+1
927 END DO
928 Length=String(2:K)
929 WRITE (PU,*) 'LT',Pattern(3:3),',',',',Length,';'
930 Length(K:K)='% '
931 GO TO 500
932 C -----
933 890 WRITE (1,*) UP,ERASE,' F...FULL, N...NOTEBOOK, U...USER SET ? ',
934 &BELL,'_'
935 READ (1,99) Size
936 CALL Upper(Size)
937 IF (Size.EQ.'F') GO TO 490
938 IF (Size.EQ.'N') GO TO 490
939 IF (Size.NE.'U') GO TO 890
940 Psize='USER SET'
941 900 WRITE (1,*) UP,ERASE,' Lower Left: (X,Y) = '
942 WRITE (1,910) UX1,',',UY1,BELL,'_'
943 910 FORMAT (15,A,15,' : A...Alter or RETURN ? ',A,A)
944 READ (1,99) Icode
945 CALL Upper(Icode)
946 IF (Icode.EQ.' ') GO TO 940
947 IF (Icode.NE.'A') GO TO 900
948 920 WRITE (1,930) UP,ERASE,BELL,'? '
949 930 FORMAT (T23,A2,A2,A,A3)
950 READ (1,*,ERR=920) UX1,UY1
951 UX1=ABS(UX1)
952 UY1=ABS(UY1)

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953 940 XP1=UX1
954      YP1=UY1
955      IF (XP1.GT.16000) GO TO 920
956      IF (YP1.GT.11400) GO TO 920
957 950 WRITE (1,*) UP,ERASE,' Upper Right: (X,Y) = '
958      WRITE (1,910) UX2,',',UY2,BELL,'_'
959      READ (1,99) lcode
960      CALL Upper(lcode)
961      IF (lcode.EQ.' ') GO TO 970
962      IF (lcode.NE.'A') GO TO 950
963 960 WRITE (1,930) UP,ERASE,BELL,'? '
964      READ (1,*,ERR=960) UX2,UY2
965      UX2=ABS(UX2)
966      UY2=ABS(UY2)
967 970 XP2=UX2
968      YP2=UY2
969      IF (XP2.GT.16000) GO TO 960
970      IF (YP2.GT.10100) GO TO 960
971      IF ((XP1.GE.XP2).OR.(YP1.GE.YP2)) GO TO 900
972      IF ((XP2-XP1).LT.1000) GO TO 900
973      IF ((YP2-YP1).LT.1000) GO TO 900
974      GO TO 500
975 C -----
976 980 WRITE (PU,*) 'SP0;'
977      CLOSE (PU,IOSTAT=N,ERR=9999)
978      GO TO MENU
979 C
980 C -----
981 C
982 C          AXES PLOTTING ROUTINE
983 C
984 C          - Scaling is ON -
985 C
986 C          Y-axis: 0-10000 user units
987 C          X-axis: 0-10000 user units (increasing -> right)
988 C                  -10000-0 user units (decreasing -> right)
989 C
990 C          - Only integral position values are sent in PA commands
991 C            for compatibility with early model HP plotters.
992 C
993 C          - XMULT & YMULT variables scale data to 10000 digits
994 C            for full scale, ensuring that no round-off errors
995 C            affect plotting resolution on early model HP plotters
996 C            which do not accept decimal fractions in SC or PA.
997 C
998 C          - Real & Integer values are sent within the HP-GL commands
999 C            as appropriate - some computers send extra nulls in these
1000 C            modes causing errors on early HP plotters. In such
1001 C            cases the values must be converted to string literals
1002 C            first. The present form works correctly on the HP1000.
1003 C
1004 C -----
1005 C

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1006 1000 WRITE (1,*) UP,ERASE,' Plotting Axes: ',BELL,'_'
1007      WRITE (PU,*) 'VS',Vaxes,';LT;PA',Xleft,C,Ylow,';PD;'
1008      WRITE (PU,*) 'PA',Xright,C,Ylow,C,Xright,C,Ytop,C,Xleft,C,Ytop,C,
1009      &Xleft,C,Ylow,';PU;'
1010      DX=1E-5*ABS(XMAX)           ! Delta X & Y ensure completion of
1011      DY=1E-5*ABS(YSCALE)         ! DO loops with fractional steps
1012 C      -----
1013      DO 1010 V=FXT,LXT+DX,Xtick
1014          I=R0((V-XOFF)*XMULT)
1015          WRITE (PU,*) 'PA',I,' ',Ylow,';XT;'
1016 1010 CONTINUE
1017 C      -----
1018      DO 1020 V=FXL,LXL+DX,Xlabel
1019          I=R0((V-XOFF)*XMULT)
1020          WRITE (PU,*) 'PA',I,' ',Ylow,';'
1021          X=R2(V)
1022          CALL Str(X,String,4)
1023 C
1024 C      Find # of digits in string, ignoring sign & trailing blanks
1025 C
1026          K=2
1027          DO WHILE (String(K:K).NE.' ')
1028              K=K+1
1029          END DO
1030          X=(FLOAT(K-2)-0.33)/2.0
1031          WRITE (PU,*) 'CP',-X,' ',-1;LB',String(2:K-1),EtX
1032 1020 CONTINUE
1033 C      -----
1034      IF (Xcode.EQ.'N') THEN
1035          Xstring='Wavelength (nm)'
1036          COFF=7.5-0.33
1037      END IF
1038      IF (Xcode.EQ.'W') THEN
1039          Xstring='Wavenumber x 10'
1040          COFF=7.5+0.75-0.33
1041      END IF
1042      String=' 5000'
1043      IF (XMULT.LT.0.0) String='-5000'
1044      WRITE (PU,*) 'PA',String(1:5),' ',Ylow,';SR',BWIDTH,C,BHEIGHT,';'
1045      WRITE (PU,*) 'CP',-COFF,' ',-2;LB',Xstring,EtX,
1046      &'SR',WIDTH,' ',HEIGHT,';'
1047      IF (Xcode.EQ.'N') GO TO 1030
1048      WRITE (PU,*) 'CP0,.5;LB-3',EtX
1049 C      -----
1050 1030 DO 1040 V=FYT,LYT+DY,Ytick
1051          I=R0(V*T4/YSCALE)
1052          WRITE (PU,*) 'PA',Xleft,' ',I,';YT;'
1053 1040 CONTINUE
1054 C      -----
1055      DO 1050 V=FYL,LYL+DY,Ylabel
1056          Y=R3(V-YOFF)
1057          IF (Ycode.EQ.'E') THEN
1058              Y=R2((V-YOFF)*ESCALE/FACTOR(J)/SCALE)
1059          END IF

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1060      I=R0(V*T4/YSCALE)
1061      WRITE (PU,*) 'PA',Xleft,',',I,','
1062      CALL Str(Y,String,4)
1063      IF (String.EQ.' 0.0') String=' 0'
1064 C
1065 C      Find # of digits in string, ignoring sign & trailing blanks
1066 C
1067      K=2
1068      DO WHILE (String(K:K).NE.' ')
1069          K=K+1
1070      END DO
1071      Y=FLOAT(K-1)+.33
1072      WRITE (PU,*) 'CP',-Y,',',-.25;LB',String(1:K-1),EtX
1073 1050 CONTINUE
1074 C -----
1075      WRITE (PU,*) 'PA',Xleft,',',5000;SR',BWIDTH,',',BHEIGHT,
1076      &';CP-5,0;DI0,1;'
1077      IF (Ycode.EQ.'E') THEN
1078          K=5
1079          IF (Mult(5:5).EQ.' ') K=4
1080          IF (Mult(5:5).EQ.'.') K=1
1081          Ystring=' x '//Mult(1:K)
1082          COFF=(FLOAT(K)+13.5)/2.0-1.5
1083          IF (K.EQ.1) COFF=COFF-0.5
1084          WRITE (PU,*) 'CP',-COFF,',',0;CP-.33,.5;DR0,-1;LB3',EtX
1085          WRITE (PU,*) 'DR0,1;CP.33,-.5;LB',Ystring(1:K+4),'(M',EtX
1086          WRITE (PU,*) 'CP0,.25;SR',WIDTH,',',HEIGHT,',',LB-1',EtX
1087          WRITE (PU,*) 'SR',BWIDTH,',',BHEIGHT,',',CP.5,-.25;LBcm',EtX
1088          WRITE (PU,*) 'CP0,.25;SR',WIDTH,',',HEIGHT,',',LB-1',EtX
1089          WRITE (PU,*) 'SR',BWIDTH,',',BHEIGHT,',',
1090          WRITE (PU,*) 'CP0,-.25;LB)',EtX,',',DI1,0;'
1091          GO TO 1060
1092      END IF
1093      IF (Ycode.EQ.'A') K=10
1094      IF (Ycode.EQ.'R') K=13
1095      IF (Ycode.EQ.'T') K=14
1096      COFF=FLOAT(K)/2.0-0.167
1097      WRITE (PU,*) 'CP',-COFF,',',0;LB',Ystring(1:K),EtX,',',DI1,0;'
1098 1060 WRITE (1,*)
1099      IF (YOFF.EQ.0.0) GO TO 1090
1100 C -----
1101 1070 WRITE (1,*) UP,ERASE,' Plot a dashed baseline, (Y or N) ? ',
1102      &BELL,'_'
1103      READ (1,99) Icode
1104      CALL Upper(Icode)
1105      IF (Icode.EQ.'N') GO TO 1090
1106      IF (Icode.NE.'Y') GO TO 1070
1107 1080 WRITE (1,*) UP,ERASE,' Dash Length: (1-5)% ',BELL,'_'
1108      READ (1,*) X
1109      IF ((X.LT.1.0).OR.(X.GT.5.0)) GO TO 1080
1110      IX=R0(X)
1111      IZ=R0(YOFF*T4/YSCALE)

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1112     WRITE (PU,*) 'LT2,',IX,',';PA',Xright,',',IZ,',';PD;PA',Xleft,
1113     &',',IZ,',';PU;LT;
1114 1090 IF (Psize.EQ.'NOTEBOOK') GO TO 1200
1115     GO TO 2080
1116 C
1117 C -----
1118 C
1119 C     Annotation: - Labels, Parameters, Title
1120 C
1121 C -----
1122 C
1123 1100 WRITE (1,*) UP,ERASE,' L...Labels, P...Parameters, T...Title',
1124     &', X...Exit ? ',BELL,'_'
1125     READ (1,99) Icode
1126     CALL Upper(Icode)
1127     IF (Icode.EQ.'T') GO TO 1110
1128     IF (Icode.EQ.'L') GO TO 1120
1129     IF (Icode.EQ.'P') GO TO 1200
1130     IF (Icode.EQ.'X') GO TO 2080
1131     GO TO 1100
1132 C -----
1133 1110 TITLE=LABEL(J)
1134     WRITE (1, '(A2,A2,A4,A72,T76,A)') UP,ERASE,' ? <',TITLE,'>'
1135     WRITE (1, '(T5,A2,A,A)') UP,BELL,'_'
1136     READ (1,120) TITLE
1137     IF (TITLE.EQ.' ') TITLE=LABEL(J)
1138     WRITE (1,*) UP,ERASE,' Plotting Title:',BELL
1139     K=72
1140     DO WHILE (TITLE(K:K).EQ.' ')
1141         K=K-1
1142     END DO
1143     COFF=FLOAT(K)/2.0
1144     IX=5000
1145     IF (XMULT.LT.0.0) IX=-5000
1146     IY=-1
1147     IF (Psize.EQ.'NOTEBOOK') IY=2
1148     WRITE (PU,*) 'PA',IX,C,Ytop,',';SR1,2;CP',-COFF,',',IY,','
1149     WRITE (PU,*) 'LB',TITLE(1:K),EtX
1150     GO TO 1100
1151 C -----
1152 1120 WRITE (1, '(A2,A2,A13,T58,A)') UP,ERASE,' Label: ? <',>'
1153     WRITE (1, '(T14,A2,A,A)') UP,BELL,'_'
1154     READ (1, '(A40)') Text
1155     IF (Text.EQ.' ') GO TO 1100
1156     K=40
1157     DO WHILE (Text(K:K).EQ.' ')
1158         K=K-1
1159     END DO
1160 1130 WRITE (1,*) UP,ERASE,' Label: ',Text(1:K),': OK (Y or N) ? ',
1161     &BELL,'_'
1162     READ (1,99) Icode
1163     CALL Upper(Icode)
1164     IF (Icode.EQ.'N') GO TO 1120
1165     IF (Icode.NE.'Y') GO TO 1130

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1166 1140 WRITE (1,*) UP,ERASE,' C...Char.size, M...Move, P...Plot, ',
1167      &'V...Vplot, X...Exit ? ',BELL,'_'
1168      READ (1,99) Icode
1169      CALL Upper(Icode)
1170      IF (Icode.EQ.'C') GO TO 1150
1171      IF (Icode.EQ.'M') GO TO 1160
1172      IF (Icode.EQ.'V') GO TO 1170
1173      IF (Icode.EQ.'P') GO TO 1180
1174      IF (Icode.NE.'X') GO TO 1140
1175      GO TO 1100
1176 C -----
1177 1150 WRITE (1,*) UP,ERASE,' Char.Size (Width,Height) ? ',BELL,'_'
1178      READ (1,*,ERR=1150) LWIDTH,LHEIGHT
1179      GO TO 1140
1180 C -----
1181 1160 WRITE (1,*) UP,ERASE,' Coordinate, 0-100%: (X,Y) ? ',BELL,'_'
1182      READ (1,*,ERR=1160) X,Y
1183      IX=R0(X*100.0+(XMIN-XOFF)*XMULT)
1184      IY=R0(Y*100.0)
1185      WRITE (PU,*) 'PA',IX,',',IY,','
1186      GO TO 1140
1187 C -----
1188 C      Special Entry Point From Digitize Routine (Pcode.EQ.'DD')
1189 C      Special Offset Controls Are Used For Digitize Mode Labels
1190 C -----
1191 1170 WRITE (PU,*) 'DIO,1;' ! Rotate Labelling Axis 90 Degrees
1192 1180 WRITE (1,*) UP,ERASE,' C...Centered, L...Left Justified, ',
1193      &'R...Right Justified ? ',BELL,'_'
1194      READ (1,99) Icode
1195      CALL Upper(Icode)
1196      IF (Icode.EQ.'C') THEN
1197          X=-FLOAT(K)/2.0
1198          IF (Pcode.EQ.'DD') THEN
1199              X=X-0.5 ! Alter Centering For Leading Blank
1200              IF (K.GT.8) THEN ! Alter Centering For Labelling Both
1201                  I=2 ! X & Y Coordinates In Digitize Mode
1202                  DO WHILE (Text(I:I).NE.' ')
1203                      I=I+1
1204                  END DO ! Find Space Between X & Y Labels
1205                  X=-FLOAT(I+1)
1206              END IF
1207          END IF
1208          GO TO 1190
1209      END IF
1210      IF (Icode.EQ.'R') THEN
1211          X=-FLOAT(K)
1212          IF (Pcode.EQ.'DD') THEN
1213              X=X-2.0 ! Alter Right Justification To Stop
1214              END IF ! Peak Label Writing Over Spectrum
1215          GO TO 1190
1216      END IF
1217      IF (Icode.NE.'L') GO TO 1180
1218      X=0.0 ! Convert X=0.0 To '0.0' With Str

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1219      IF (Pcode.EQ.'DD') THEN
1220          X=1.0                                ! Alter Left Justification To Stop
1221      END IF                                    ! Peak Label Writing Over Spectrum
1222 C      -----
1223 1190 CALL Str(X,String,4)
1224      WRITE (1,*) UP,ERASE,' Plotting Label:',BELL
1225      WRITE (PU,*) 'SR',LWIDTH,',',LHEIGHT,',';CP',String(1:5),',-.25;'
1226      WRITE (PU,*) 'LB',Text(1:K),Etx,',';CP0,.25;DI1,0;'
1227      IF (Pcode.EQ.'DD') THEN
1228          IX=NINT(T4*FLOAT(IX-X1)/FLOAT(X2-X1)+(XMIN-XOFF)*XMULT)
1229          IY=NINT(T4*FLOAT(IY-Y1)/FLOAT(Y2-Y1))
1230          WRITE (PU,*) 'PA',IX,',',IY,',';PU;'
1231          GO TO 3000                                ! Return To Digitize Routine
1232      END IF
1233      GO TO 1100
1234 C      -----
1235 1200 IF (Psize.EQ.'FULL') GO TO 1100
1236 1210 WRITE (1,*) UP,ERASE,' Plot Parameters, (Y or N) ? ',BELL,'_'
1237      READ (1,99) Icode
1238      CALL Upper(Icode)
1239      IF (Icode.EQ.'N') GO TO 1100
1240      IF (Icode.NE.'Y') GO TO 1210
1241      WRITE (1,*) UP,ERASE,' Plotting Parameters:',BELL
1242      WRITE (PU,*) 'PA',Xright,C,Ytop,',';
1243      WRITE (PU,*) 'SR.75,2;CP0,-.5;LB',LF,LF,' File: ',Fname(J),
1244      &CR,LF,LF,Etx
1245      WRITE (PU,*) 'LB Date: ',DATE(J),CR,LF,LF,Etx
1246      WRITE (PU,*) 'LB Conc.(M): ',CONC(J),CR,LF,LF,Etx
1247      WRITE (PU,*) 'LB Path (cm): ',PATH(J),CR,LF,LF,Etx
1248      WRITE (PU,*) 'LB Rate (nm/sec): ',
1249      &Pstr(3,PARAM(J,3)+1),CR,LF,LF,Etx
1250      WRITE (PU,*) 'LB Period (sec): ',
1251      &Pstr(15,PARAM(J,15)+1),CR,LF,LF,Etx
1252      WRITE (PU,*) 'LB Ref. Mode: ',
1253      &Pstr(5,PARAM(J,5)+1),CR,LF,LF,E x
1254      WRITE (PU,*) 'LB Beam Mode: ',
1255      &Pstr(16,PARAM(J,16)+1),CR,LF,LF,Etx
1256      WRITE (PU,*) 'LB SBW (nm) :',VARIABLE(J,10),CR,LF,LF,Etx
1257      WRITE (PU,*) 'LB Slit Gain:',VARIABLE(J,6),CR,LF,LF,Etx
1258      WRITE (PU,*) 'LB Slit Height: ',
1259      &Pstr(23,PARAM(J,23)+1),Etx
1260      GO TO 1100
1261 C
1262 C      ***** END OF AXES PLOTTING *****
1263 C
1264 C      SPECTRUM PLOTTING ROUTINE
1265 C
1266 C      - Velocity Select = 5 cm/sec (Paper). 10 cm/sec (Acetate)
1267 C      - Real variables are used in 'VS' commands
1268 C      - Scaling in ON with Absorbance x 1E4 to match axes
1269 C      - Both Integer and String Numbers are used in 'PA' commands
1270 C      - HP I/O Subsystem Performs Binary <==> ASCII Conversions
1271 C
1272 C      -----

```

```

1273 C
1274 2000 M=1
1275     WRITE (1,*) UP,ERASE,'  Increase step size, (Y or N) ? ',BELL,'_'
1276     READ (1,99) Icode
1277     CALL Upper(Icode)
1278     IF (Icode.EQ.'N') GO TO 2020
1279     IF (Icode.NE.'Y') GO TO 2000
1280 2010 WRITE (1,*) UP,ERASE,'  Step Multiplier, (>1): ',BELL,'_'
1281     READ (1,'(I3)',ERR=2010) M
1282     IF (M.LT.1) M=1
1283 2020 X=STEP*FLOAT(M)
1284     CALL Str(X,String,4)
1285 C
1286 C       Find # of digits, ignoring sign & trailing blanks
1287 C
1288     K=2
1289     DO WHILE (String(K:K).NE.' ')
1290       K=K+1
1291     END DO
1292     WRITE (1,*) UP,ERASE,'  Plotting Spectrum @ ',String(2:K-1),
1293     &' nm steps: ',BELL,'_'
1294 C
1295 C -----
1296 C
1297 C       WINDOW SETTING ROUTINE
1298 C
1299 C       - Soft clip limits are set to P1 & P2 scaling coordinates
1300 C       so that off scale data do not plot on graph. This should
1301 C       not happen normally since the plot boundaries are made to
1302 C       match the X-scale limits automatically if the latter are
1303 C       smaller than the scan range.
1304 C       - Plotter sends output parameters as A,B,C,D,CR,LF
1305 C       where (A-D) are string integers (ASCII), which are read
1306 C       into integer variables (ASCII translation is automatic).
1307 C       - Some computers handshake on CR leaving Li in buffer.
1308 C       In these cases use READ A,B,C,D,E (N.B. CHARACTER E*1)
1309 C       to clear plotter buffer before the next READ cycle.
1310 C
1311 C -----
1312 C
1313 2030 WRITE (PU,*) 'VS',Vspec,';OP;'
1314     READ (PU,*) X1,Y1,X2,Y2
1315     WRITE (PU,*) 'IW',X1,C,Y1,C,X2,C,Y2,';'
1316     IF (Xcode.EQ.'N') THEN
1317       START=R0((WMAX-WX)/STEP)+1
1318       FINISH=R0(FLOAT(ND)-(WN-WMIN)/STEP)
1319       GO TO 2040
1320     END IF
1321     START=R0((T4/WMIN-T4/WN)/STEP)+1
1322     FINISH=R0(FLOAT(ND)-(T4/WX-T4/WMAX)/STEP)
1323 C -----
1324 2040 I=0
1325     RATIO=FACTOR(1)/FACTOR(2)

```

```

1326      DO 2070 K=START,FINISH,M
1327          X=W(J,K)                      ! Acquired Wavelength
1328          IF (Xcode.EQ.'N') THEN
1329 C          X=WX-FLOAT(I)*STEP            ! Calculated Wavelength
1330              IX=R0((X-XOFF)*XMULT)
1331              GO TO 2050
1332          END IF
1333 C          X=T4/WN-FLOAT(I)*STEP          ! Calculated Wavelength
1334              IX=R0((T4/X-XOFF)*XMULT)
1335      2050  IF (Code.EQ.'DS') THEN
1336              IY=R0(((A(1,K)-A(2,K)*RATIO)+YOFF)*T4/YSCALE)
1337              GO TO 2060
1338          END IF
1339              IY=R0((A(J,K)+YOFF)*T4/YSCALE)
1340      2060  WRITE (PU,*) 'PA',IX,C,IY,',';PD;'
1341              I=I+M
1342      2070  CONTINUE
1343 C      -----
1344      2080  WRITE (PU,*) 'PU;LT;'
1345              Lmode='SOLID'
1346              Pattern=' '
1347              Length=' '
1348              GO TO 500
1349 C
1350 C      -----
1351 C
1352 C          PLOTTER DIGITIZING ROUTINE
1353 C
1354 C          - HP-GL command 'OA' provides pen position without using
1355 C            the clumsy ENTER key on the plotter.
1356 C          - The 'DP' & 'OD' commands are used with ENTER in cases
1357 C            where the plotter is remote from the keyboard.
1358 C
1359 C      -----
1360 C
1361      3000  WRITE (1,*) HOME,CLR,'_'
1362              TITLE='Digitize Pen Position'
1363              CALL Center(TITLE)
1364              CALL Line(NCOL)
1365              CALL Digitize(X,Xcode,Y,Ext,K)
1366              WRITE (1,3010) 'X-position = ',X,Xord
1367              String=' Absorbance = '
1368              IF (Ycode.EQ.'R') String=' % Reflect. = '
1369              IF (Ycode.EQ.'T') String=' % Transmit. = '
1370              WRITE (1,3020) String,Y
1371              IF ((Ycode.EQ.'A').OR.(Ycode.EQ.'E')) THEN
1372                  WRITE (1,3030) 'Ext.Coeff. = '
1373                  WRITE (1,*) Ext(1:K),' /M/cm'
1374              END IF
1375      3010  FORMAT (/ ,T5,A14,T20,F5.3,A7)
1376      3020  FORMAT (/ ,T5,A14,T20,F6.4)
1377      3030  FORMAT (/ ,T5,A14)
1378              WRITE (1,*) DOWN

```

```

1379     WRITE (1,3040) 'D....Digitize Position'
1380     WRITE (1,3040) 'L....Label At Position'
1381     WRITE (1,3040) 'S....Segment Display '
1382     WRITE (1,3040) 'X....EXIT To Plotting '
1383 3040 FORMAT (/,T16,A23)
1384     WRITE (1,*) DOWN,DOWN
1385 3050 WRITE (1,'(T10,A2,A2,A6,A,A)') UP,ERASE,'Code: ',BELL,'_'
1386     READ (1,99) Icode
1387     CALL Upper(Icode)
1388     IF (Icode.EQ.'X') GO TO 500
1389     IF (Icode.EQ.'D') GO TO 3000
1390     IF (Icode.EQ.'S') GO TO 4000
1391     IF (Icode.NE.'L') GO TO 3050
1392 3060 WRITE (1,*) UP,ERASE,'      Place PEN In Stall #1, ',
1393 &'Then Press RETURN ',BELL,'_'
1394     READ (1,99) Icode
1395     IF (Icode.NE.' ') GO TO 3060
1396     WRITE (PU,*) 'PU;SP1;'
1397     CALL Digitize(X,Xcode,Y,Ext,K)
1398 3070 WRITE (1,*) UP,ERASE,'      X...X-label, Y...Y-label, B...Both',
1399 &' Q...Quit ? ',BELL,'_'
1400     READ (1,99) Icode
1401     CALL Upper(Icode)
1402     IF (Icode.EQ.'Q') GO TO 3000
1403     IF (Icode.EQ.'Y') GO TO 3080
1404     IF ((Icode.NE.'X').AND.(Icode.NE.'B')) GO TO 3070
1405     CALL Str(X,String,5)
1406     Text=String                      ! String*14, Text*40 And TITLE*72
1407     K=40                             ! Are Reuseable String Variables
1408     DO WHILE (Text(K:K).EQ.' ')
1409         K=K-1                        ! Find Start Of Trailing Blanks
1410     END DO
1411     IF (Icode.EQ.'X') GO TO 3110
1412 C -----
1413 3080 IF (Ycode.EQ.'E') THEN
1414     String=Ext
1415     GO TO 3090
1416 END IF
1417 CALL Str(Y,String,5)
1418 3090 IF (Icode.EQ.'B') THEN
1419     TITLE=Text(1:K)//' ('//String
1420     Text=TITLE(1:40)
1421     GO TO 3100
1422 END IF
1423 Text=String
1424 3100 K=40
1425 DO WHILE (Text(K:K).EQ.' ')
1426     K=K-1                        ! Find Start Of Trailing Blanks
1427 END DO
1428 IF (Icode.EQ.'B') THEN
1429     Text(K+1:K+2)=' )'
1430     K=K+2
1431 END IF
1432 3110 GO TO 1170                      ! Transfer To Vertical Label Routine

```

```

1433 C
1434 C -----
1435 C
1436 C         Display Segment Of Spectrum
1437 C
1438 C -----
1439 C
1440 4000 String=' (nm)'
1441       IF (Xcode.EQ.'W') String=' (cm-1) x 1E-3'
1442       WRITE (1,*) UP,ERASE,' Scan Range: ',WMIN,' to ',WMAX,'_'
1443       WRITE (1,*) String,DOWN,DOWN
1444 4010 WRITE (1,*) UP,ERASE,' DISPLAY Range: (MIN,MAX) ? ',BELL,'_'
1445       READ (1,*,ERR=4010) W1,W2
1446       CALL Order(W1,W2)
1447       IF ((W1.LT.WMIN).OR.(W1.GT.WMAX)) GO TO 4010
1448       IF ((W2.LT.WMIN).OR.(W2.GT.WMAX)) GO TO 4010
1449       IF (Xcode.EQ.'N') THEN
1450           START=R0((WMAX-W2)/STEP)+1
1451           FINISH=R0(FLOAT(ND)-(W1-WMIN)/STEP)
1452           GO TO 4020
1453       END IF
1454       START=R0((T4/WMIN-T4/W1)/STEP)+1
1455       FINISH=R0(FLOAT(ND)-(T4/W2-T4/WMAX)/STEP)
1456 4020 IF ((Ycode.EQ.'R').OR.(Ycode.EQ.'T')) THEN
1457         Text=Ystring
1458         IF (Ycode.EQ.'R') Text=' '//Ystring
1459         TITLE='Energy      Wavelength      '//Text(1:15)
1460         GO TO 4030
1461     END IF
1462     TITLE='Energy      Wavelength      Absorbance      Ext.Coeff. (/M/cm)'
1463 4030 WRITE (1,*) HOME,CLR,'_'
1464       CALL Center(TITLE)
1465       CALL Line(60)
1466       L=1
1467       DO 4050 I=START,FINISH
1468         X=T4/W(J,I)
1469         Y=A(J,I)
1470         IF (Code.EQ.'DS') Y=A(1,I)-A(2,I)*FACTOR(1)/FACTOR(2)
1471         WRITE (1,*)
1472         IF ((Ycode.EQ.'A').OR.(Ycode.EQ.'E')) THEN
1473             WRITE (1,4060) X,W(J,I),Y,Y/FACTOR(J)
1474         ELSE
1475             WRITE (1,4070) X,W(J,I),Y
1476         END IF
1477         L=L+1
1478         IF (L.EQ.10) THEN
1479             WRITE (1,*) DOWN
1480 4040 WRITE (1,4080) UP,ERASE,'Press RETURN to Continue ',BELL,'_'
1481             READ (1,99) Icode
1482             IF (Icode.NE.' ') GO TO 4040
1483             WRITE (1,*) HOME,CLR,'_'
1484             CALL Center(TITLE)
1485             CALL Line(60)
1486             L=1

```

```

1487         END IF
1488 4050 CONTINUE
1489 4060 FORMAT (T9,F7.3,T21,F7.2,T35,F7.4,T49,G10.4)
1490 4070 FORMAT (T14,F7.3,T30,F7.2,T47,F7.2)
1491 4080 FORMAT (T10,A2,A2,A25,A,A)
1492     WRITE (1,*) DOWN
1493 4090 WRITE (1,4080) UP,ERASE,'Press RETURN for MENU    ',BELL,'_'
1494     READ (1,99) lcode
1495     IF (lcode.NE.' ') GO TO 4090
1496     GO TO 3000
1497 C
1498 C -----
1499 C
1500 C         Exit Program
1501 C
1502 C -----
1503 C
1504 9000 WRITE (1,*) UP,ERASE,UP
1505     STOP
1506 C
1507 C -----
1508 C
1509 C         IEEE-488 Error Exit
1510 C
1511 C -----
1512 C
1513 9999 WRITE (1,*) ' Error #',N
1514     STOP
1515     END
1516 C
1517 C ***** END OF MAIN PROGRAM *****
1518 C
1519 C         Print a TITLE Centered in 72 columns
1520 C
1521 C *****
1522 C
1523     SUBROUTINE Center(TITLE)
1524     INTEGER I,J,N
1525     CHARACTER TITLE*72,BLANK*36
1526     BLANK='
1527     I=72
1528     J=0
1529     DO WHILE (ICHAR(TITLE(I:I)).EQ.32)
1530         J=J+1
1531         I=72-J
1532     END DO
1533     N=J/2
1534     WRITE (1,*) BLANK(1:N),TITLE(1:I)
1535     RETURN
1536     END

```

```

1537 C
1538 C -----
1539 C
1540 C      Extinction Coefficient Rounding
1541 C
1542 C -----
1543 C
1544 SUBROUTINE Coeff(E,String,K)
1545 INTEGER F,K,M
1546 REAL E,S
1547 CHARACTER*(*)String
1548 CHARACTER Mult*3
1549 F=0
1550 S=1.0
1551 IF (E.LT.0.0) S=-1.0
1552 E=ABS(E)
1553 IF ((E.NE.0.0).AND.(E.NE.1.0)) GO TO 10
1554 String=' 0.0000'
1555 IF (E.EQ.1.0) String=' 1.0000'
1556 K=7
1557 GO TO 50
1558 10 IF ((E.GT.1.0).AND.(E.LT.10.0)) THEN
1559     K=K+1
1560     GO TO 30
1561 END IF
1562 IF (E.GE.10.0) GO TO 20
1563 DO WHILE (E.LT.1.0)
1564     E=E*10.0
1565     F=F+1
1566 END DO
1567 GO TO 30
1568 20 DO WHILE (E.GE.10.0)
1569     E=E/10.0
1570     F=F+1
1571 END DO
1572 30 E=E*S
1573 CALL Str(E,String,K)
1574 40 K=2
1575 DO WHILE (String(K:K).NE.' ')
1576     K=K+1
1577 END DO
1578 IF (F.EQ.0) GO TO 50
1579 E=FLOAT(F)
1580 CALL Str(E,Mult,2)
1581 IF (Mult(1:1).EQ.' ') Mult(1:1)='+'
1582 M=3
1583 IF (Mult(3:3).EQ.' ') M=2
1584 String(K:K+M)='E'//Mult(1:M)
1585 K=K+M
1586 50 RETURN
1587 END

```

```

1588 C
1589 C -----
1590 C
1591 C       Digitize Pen Position
1592 C
1593 C -----
1594 C
1595 SUBROUTINE Digitize(X,Xcode,Y,Ext,K)
1596 INTEGER IX,IY,IZ,J,K,PU,X1,X2,Y1,Y2
1597 REAL FACTOR(2),NUMBER,XMIN,XMAX,YOFF,YSCALE,X,Y
1598 CHARACTER*(*) Ext,Xcode
1599 COMMON /DIGIT/FACTOR,XMIN,XMAX,YOFF,YSCALE,IX,IY,J,PU,X1,X2,Y1,Y2
1600 WRITE (PU,*) 'OP;'
1601 READ (PU,*) X1,Y1,X2,Y2
1602 WRITE (PU,*) 'OA;'
1603 READ (PU,*) IX,IY,IZ
1604 X=(XMAX-XMIN)*FLOAT(IX-X1)/FLOAT(X2-X1)+XMIN
1605 IF (Xcode.EQ.'W') THEN
1606     X=ANINT(X*1000.0)
1607     GO TO 10
1608 END IF
1609 X=ANINT(X*10.0)/10.0
1610 10 Y=YSCALE*FLOAT(IY-Y1)/FLOAT(Y2-Y1)-YOFF
1611     K=4                                ! K = # Of Digits Precision
1612     NUMBER=Y/FACTOR(J)
1613     CALL Coeff(NUMBER,Ext,K)          ! K = # Of Characters In String
1614     RETURN
1615     END
1616 C
1617 C -----
1618 C
1619 C       Extinction Coefficient Scale Multiplier
1620 C
1621 C -----
1622 C
1623 SUBROUTINE Exponent(N,Mult)
1624 INTEGER I
1625 REAL M,N
1626 CHARACTER String*14
1627 CHARACTER*(*) Mult
1628 M=0.0
1629 N=ABS(N)
1630 I=INT(N+.5)
1631 IF (I.EQ.1) THEN
1632     Mult='1 ...'
1633     GO TO 20
1634 END IF
1635 IF (I.GT.1) GO TO 10
1636 DO WHILE (I.LT.1)
1637     N=N*10.0
1638     M=M-1.0
1639     I=INT(N+.5)
1640 END DO

```



```

1641      CALL Str(M,String,2)
1642      Mult='1E-'//String(2:3)
1643      GO TO 20
1644 10 DO WHILE (I.GT.1)
1645      N=N/10.0
1646      M=M+1.0
1647      I=INT(N+.5)
1648      END DO
1649      CALL Str(M,String,2)
1650      Mult='1E+'//String(2:3)
1651 20 RETURN
1652      END
1653 C
1654 C -----
1655 C
1656 C      Print a line of N '-' characters (72 columns max)
1657 C
1658 C -----
1659 C
1660      SUBROUTINE Line(N)
1661      INTEGER I,N
1662      CHARACTER BLANK*72,DLINE*72,SPACE*36
1663      SPACE='
1664      BLANK=SPACE//SPACE
1665      SPACE='-----'
1666      DLINE=SPACE//SPACE
1667      IF (N.GT.72) N=72
1668      I=(72-N)/2
1669      WRITE (1,*) BLANK(1:I),DLINE(1:N)
1670      RETURN
1671      END
1672 C
1673 C -----
1674 C
1675 C      Order MIN,MAX Entries If Required
1676 C
1677 C -----
1678 C
1679      SUBROUTINE Order(MIN,MAX)
1680      REAL MIN,MAX,SWAP
1681      IF (MIN.LT.MAX) GO TO 10
1682      SWAP=MIN
1683      MIN=MAX
1684      MAX=SWAP
1685 10 RETURN
1686      END

```

```

1687 C
1688 C -----
1689 C
1690 C           Rescale Data Array Between Absorbance And Transmission
1691 C
1692 C -----
1693 C
1694 $EMA/DATA/
1695     SUBROUTINE Rescale(J,K,ND)
1696     INTEGER J,K,ND
1697     REAL A(2,10001)
1698     COMMON /DATA/A
1699     IF (K.EQ.1) GO TO 20
1700     DO 10 I=1,ND
1701         A(J,I)=ALOG10(100.0/A(J,I))
1702     10 CONTINUE
1703     RETURN
1704     20 DO 30 I=1,ND
1705         A(J,I)=100.0/10.0**(A(J,I))
1706     30 CONTINUE
1707     RETURN
1708     END
1709 C
1710 C -----
1711 C
1712 C           Convert Number To ASCII String
1713 C
1714 C -----
1715 C
1716     SUBROUTINE Str(VALUE,String,PREC)
1717     INTEGER ASCII,DECPT,I,J,LENSTR,NDIGIT,NUMBER,PREC
1718     REAL VALUE
1719     DOUBLE PRECISION DECIMAL,FRACTION,TEN
1720     CHARACTER Concat*14,Digit(12),Sign,String*14
1721     LOGICAL INTEGER
1722 C     LOGICAL TEST
1723     INTEGER=.TRUE.
1724 C     TEST=.FALSE.
1725     DECPT=0
1726     J=0
1727     TEN=10.0
1728     Sign=' '
1729     Concat=' '
1730 C     IF (TEST) WRITE (1,*) ' Value Entered = ',VALUE
1731     IF (VALUE.LT.0.0) Sign='- '
1732     IF (VALUE.EQ.0.0) GO TO 100
1733     DECIMAL=ABS(VALUE)
1734     DO WHILE (DECIMAL.GE.1.0)
1735         DECIMAL=DECIMAL/TEN
1736         J=J+1
1737     END DO
1738     DECPT=J
1739 C     IF (TEST) WRITE (1,*) ' # of Whole Digits: ',DECPT

```

```

1740      IF (DECPT.EQ.0) GO TO 30
1741      DO 20 J=1,DECPT
1742          DECIMAL=DECIMAL*TEN
1743          NUMBER=INT(DECIMAL)
1744          ASCII=NUMBER+48
1745          Digit(J)=CHAR(ASCII)
1746          FRACTION=DECIMAL-NUMBER
1747          DECIMAL=DINT(FRACTION*TEN**(PREC-J)+.5)/TEN**(PREC-J)
1748      20 CONTINUE
1749 C      IF (.NOT.TEST) GO TO 30
1750 C      WRITE (1,*) ' The Whole Digits = ',(Digit(I), I=1,DECPT)
1751      30 J=DECPT
1752 C      IF (TEST) WRITE (1,*) ' Decimal Fraction = ',DECIMAL
1753      IF (DECIMAL.NE.0.0) INTEGER=.FALSE.
1754      IF (DECPT.GE.12) GO TO 40
1755      DO WHILE (DECIMAL.NE.0.0)
1756          J=J+1
1757          DECIMAL=DECIMAL*TEN
1758          NUMBER=INT(DECIMAL)
1759          ASCII=NUMBER+48
1760          Digit(J)=CHAR(ASCII)
1761          FRACTION=DECIMAL-NUMBER
1762          DECIMAL=DINT(FRACTION*TEN**(PREC-J)+.5)/TEN**(PREC-J)
1763          IF (DECIMAL.EQ.1.0) THEN
1764              DIGIT(J)=CHAR(ASCII+1)
1765              DECIMAL=0.0
1766          END IF
1767          IF (J.GE.12) DECIMAL=0.0
1768      END DO
1769      40 NDIGIT=J
1770 C      IF (.NOT.TEST) GO TO 50
1771 C      WRITE (1,*) ' The Characters = ',(Digit(I), I=1,NDIGIT)
1772      50 IF (NDIGIT.GT.12) GO TO 200
1773      DO 60 I=1,NDIGIT
1774          Concat(I:I)=Digit(I)
1775      60 CONTINUE
1776      IF (INTEGER) GO TO 80
1777      IF (DECPT.EQ.0) GO TO 70
1778      String=Sign//Concat(1:DECPT)//'.'//Concat(DECPT+1:14)
1779      RETURN
1780      70 String=Sign//'.'//Concat
1781      RETURN
1782      80 String=Sign//Concat
1783      RETURN
1784      100 String=' 0.0'
1785      RETURN
1786      200 WRITE (1,*) ' Error in data: (too many digits)'
1787      STOP
1788      END

```

```

1789 C
1790 C -----
1791 C
1792 C      Convert String Entry To Uppercase If Required
1793 C
1794 C -----
1795 C
1796 SUBROUTINE Upper(Code)
1797 INTEGER LENSTR,N
1798 CHARACTER*(*) Code
1799 LENSTR=LEN(Code)
1800 DO 10 I=1,LENSTR
1801     N=ICHAR(Code(I:I))
1802     IF (N.GT.96) Code(I:I)=CHAR(N-32)
1803 10 CONTINUE
1804 RETURN
1805 END

```

```

1806 C
1807 C -----
1808 C
1809 C         Convert ASCII String To Numeric Value (10 Digits Max'm)
1810 C
1811 C -----
1812 C
1813 SUBROUTINE Val(String,VALUE)
1814 INTEGER DECPT,EXPON,LENSTR,N,NUM(10)
1815 REAL VALUE
1816 DOUBLE PRECISION MULT,SIGN,TEN,DECIMAL
1817 CHARACTER Ascii
1818 CHARACTER*(*) String
1819 LOGICAL INTEGER
1820 C LOGICAL TEST
1821 INTEGER=.TRUE.
1822 C TEST=.FALSE.
1823 J=1
1824 K=0
1825 DECPT=0
1826 SIGN=1.0
1827 TEN=10.0
1828 DECIMAL=0.0
1829 LENSTR=LEN(String)
1830 C IF (TEST) WRITE (1,*) ' String Number = ',String
1831 C IF (TEST) WRITE (1,*) ' String Length = ',LENSTR
1832 DO 100 I=1,LENSTR
1833     Ascii=String(I:I)
1834     N=ICHAR(Ascii)
1835     IF ((N.GE.48).AND.(N.LE.57)) GO TO 20
1836     IF (N.EQ.46) INTEGER=.FALSE.
1837     IF (N.EQ.46) DECPT=K
1838     IF (N.EQ.45) SIGN=-1.0
1839     GO TO 100
1840 20 NUM(J)=N-48
1841     K=J
1842     J=J+1
1843 100 CONTINUE
1844     IF ((DECPT.EQ.0).AND.(INTEGER), DECPT=K
1845     DO 200 J=1,K
1846         EXPON=DECPT-J
1847         MULT=TEN**EXPON
1848         DECIMAL=DECIMAL+NUM(J)*MULT
1849 200 CONTINUE
1850     VALUE=SIGN*DECIMAL
1851 C IF (TEST) WRITE (1,*) ' Value = ',VALUE
1852     RETURN
1853     END

```

```

1854 C
1855 C -----
1856 C
1857 C       Set X-axis Plotting Parameters
1858 C
1859 C -----
1860 C
1861 SUBROUTINE Xaxis(XL,XH)
1862 REAL LMIN,LMAX,WN,WX,Xtick,FXT,LXT,Xlabel,FXL,LXL,XH,XL,XS(17)
1863 COMMON /XPARAM/LMIN,LMAX,WN,WX,Xtick,FXT,LXT,Xlabel,FXL,LXL
1864 DATA (XS(I),I=1,17)/.05,.1,.2,.25,.5,1.,2.,2.5,5.,10.,20.,25.,
1865 &50.,100.,200.,250.,500./
1866 LMIN=XL                                ! Set Limits To X-scale Range
1867 LMAX=XH                                ! Defined By XL,XH Arguments
1868 WN=XL
1869 WX=XH
1870 C -----
1871 Xtick=0.1*(XH-XL)                      ! Set Xtick To 1/10 X-scale
1872 IF ((Xtick.LT.XS(2)).OR.(Xtick.GT.XS(17))) THEN
1873     FXT=XL+Xtick                        ! Test For Xtick Outside The
1874     LXT=XH-Xtick                        ! Preferred Interval Range
1875     Xlabel=Xtick
1876     FXL=FXT
1877     LXL=LXT
1878     GO TO 10                            ! Use Default 1/10 Interval
1879 END IF
1880 C -----
1881 I=1
1882 DO WHILE (Xtick.GT.XS(I))                ! Compare 1/10 Scale Xtick Value
1883     I=I+1                                ! To Find The Nearest Preferred
1884 END DO                                    ! Interval < 1/10 Of X-scale
1885 Xtick=XS(I-1)
1886 C -----
1887 FXT=Xtick*AIN(T(XL/Xtick))+Xtick        ! Truncate -> FXT <= XL (+Xtick)
1888 LXT=Xtick*AIN(T(XH/Xtick))              ! Truncate -> LXT <= XH
1889 IF (ABS(XH-LXT).LT.0.01) THEN
1890     LXT=LXT-Xtick                        ! Decrement If LXT = XH
1891 END IF
1892 Xlabel=Xtick*2.0                         ! Truncate -> FXL <= XL (+Xlabel)
1893 FXL=Xlabel*AIN(T(XL/Xlabel))+Xlabel
1894 LXL=Xlabel*AIN(T(XH/Xlabel))             ! Truncate -> LXL <= XH
1895 IF (ABS(XH-LXL).LT.0.01) THEN
1896     LXL=LXL-Xlabel                       ! Decrement If LXL = XH
1897 END IF
1898 10 RETURN
1899 END

```

```

1900 C
1901 C -----
1902 C
1903 C       Set Y-axis Plotting Parameters
1904 C
1905 C -----
1906 C
1907 SUBROUTINE Yaxis(YSCALE,Ycode)
1908 REAL Ytick,FYT,LYT,Ylabel,FYL,LYL,YSCALE,YS(17)
1909 CHARACTER Ycode
1910 COMMON /YPARAM/Ytick,FYT,LYT,Ylabel,FYL,LYL
1911 DATA (YS(I),I=1,17)/.0005,.001,.002,.005,.01,.02,.05,.1,.2,.5,
1912 &1.,2.,5.,10.,20.,50.,100./
1913 Ytick=0.1*YSCALE
1914 IF ((Ytick.LT.YS(2)).OR.(Ytick.GT.YS(17)).OR.(Ycode.EQ.'E')) THEN
1915     FYT=Ytick
1916     LYT=YSCALE-Ytick
1917     Ylabel=Ytick
1918     FYL=FYT
1919     LYL=LYT
1920     GO TO 10
1921 END IF
1922 C -----
1923 I=1
1924 DO WHILE (Ytick.GT.YS(I))      ! Compare 1/10 Scale Ytick Value
1925     I=I+1                    ! To Find The Nearest Preferred
1926 END DO                        ! Interval < 1/10 YSCALE
1927 Ytick=YS(I-1)
1928 FYT=Ytick
1929 LYT=Ytick*AINT(YSCALE/Ytick)   ! Truncate -> LYT <= YSCALE
1930 IF (ABS(YSCALE-LYT).LT.1E-4) THEN ! Decrement If LYT = YS
1931     LYT=LYT-Ytick
1932 END IF
1933 Ylabel=Ytick*2.0
1934 FYL=Ylabel
1935 LYL=Ylabel*AINT(YSCALE/Ylabel) ! Truncate -> LYL <= YSCALE
1936 IF (ABS(YSCALE-LYL).LT.1E-4) THEN ! Decrement If LYL = YSCALE
1937     LYL=LYL-Ylabel
1938 END IF
1939 10 RETURN
1940 END

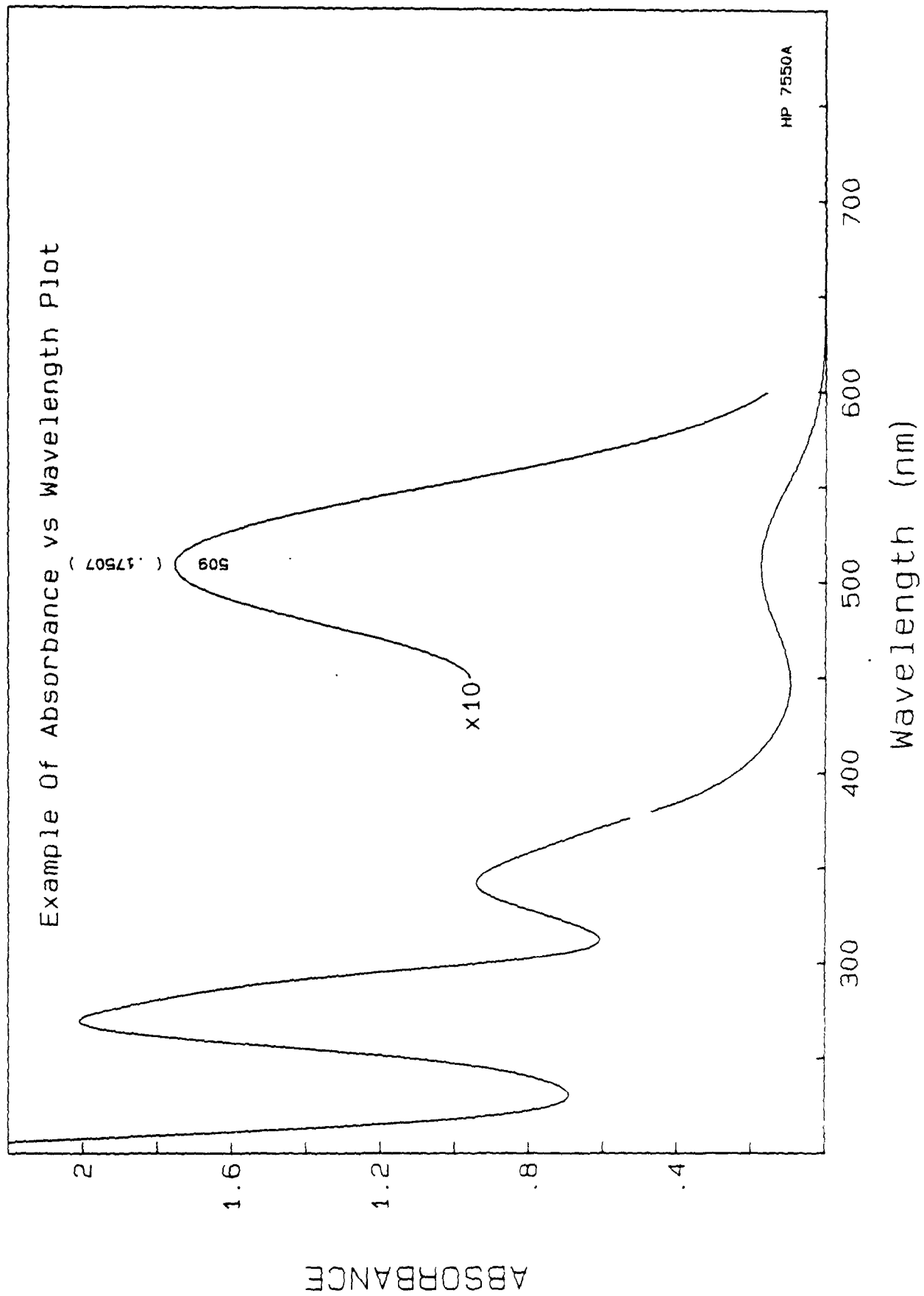
```

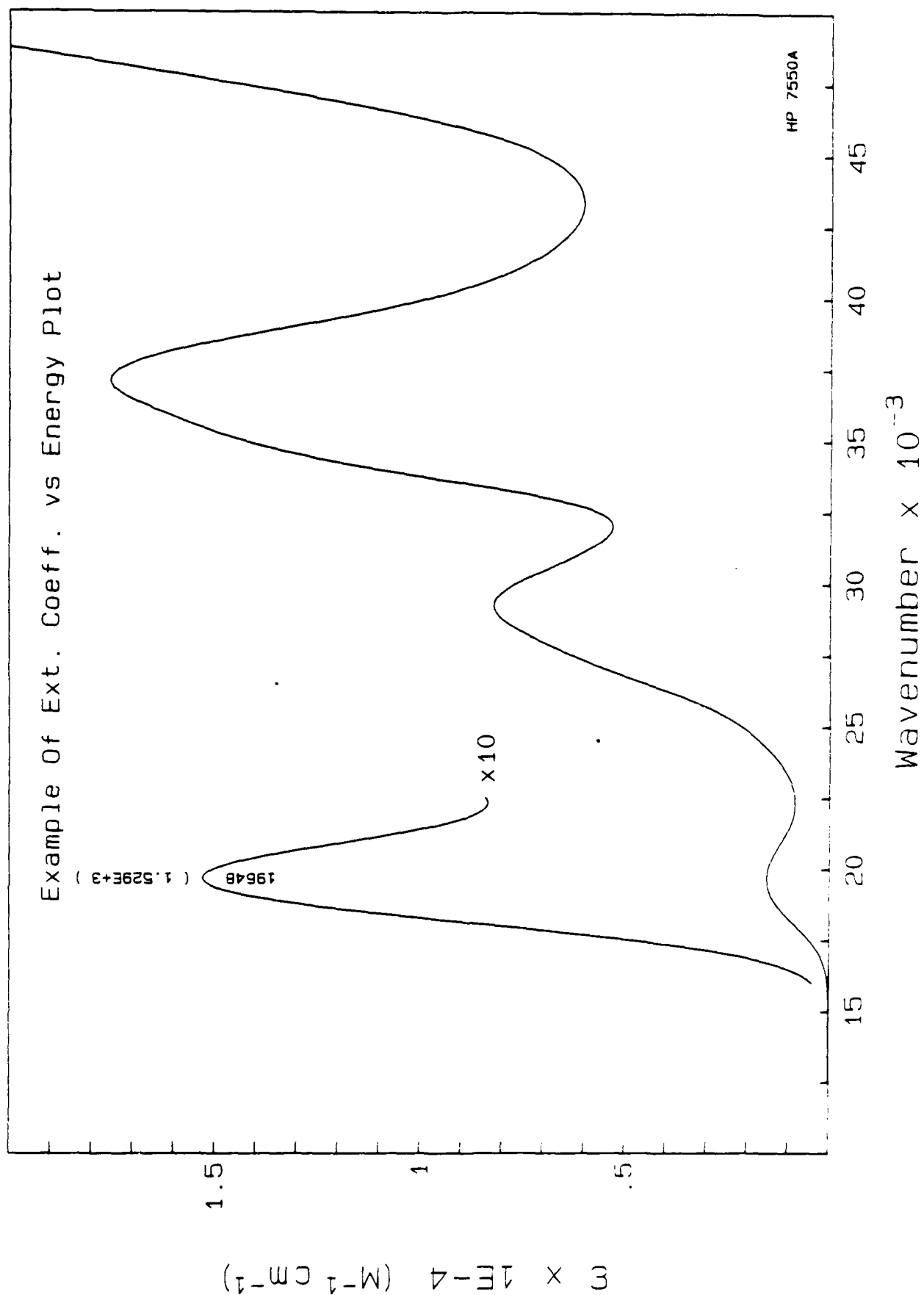
```

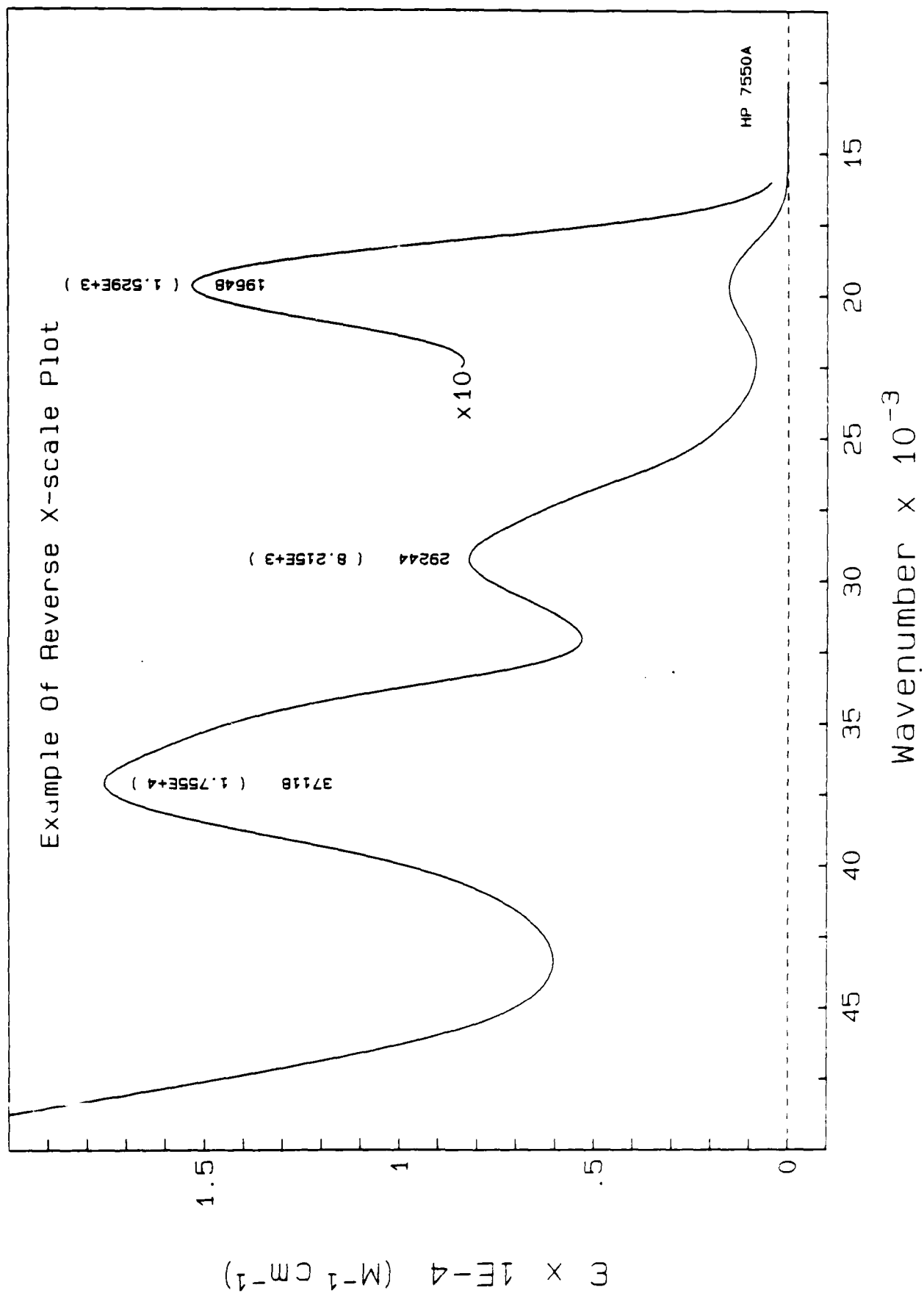
1941 C
1942 C -----
1943 C
1944 C     Wait Specified Delay (sec)
1945 C
1946 C -----
1947 C
1948 SUBROUTINE Wait(DELAY)
1949 REAL DELAY,PERIOD,Tzero,Time
1950 PERIOD=0.0
1951 Tzero=Time(I)
1952 DO WHILE (PERIOD.LT.DELAY)
1953     PERIOD=Time(I)-Tzero
1954 END DO
1955 RETURN
1956 END
1957 C
1958 C -----
1959 C
1960 C     Read Time (sec) from the HP 1000's RTE-6 Operating System
1961 C
1962 C     Note: I is a dummy argument, no values are passed
1963 C
1964 C -----
1965 C
1966 REAL FUNCTION Time(I)
1967 INTEGER ICODE,ITIME(5)
1968 ICODE=11
1969 CALL EXEC(ICODE,ITIME)
1970 Time=FLOAT(ITIME(1))/100.0+FLOAT(ITIME(2))+FLOAT(ITIME(3))*60.0
1971 &+FLOAT(ITIME(4))*3600.0
1972 RETURN
1973 END

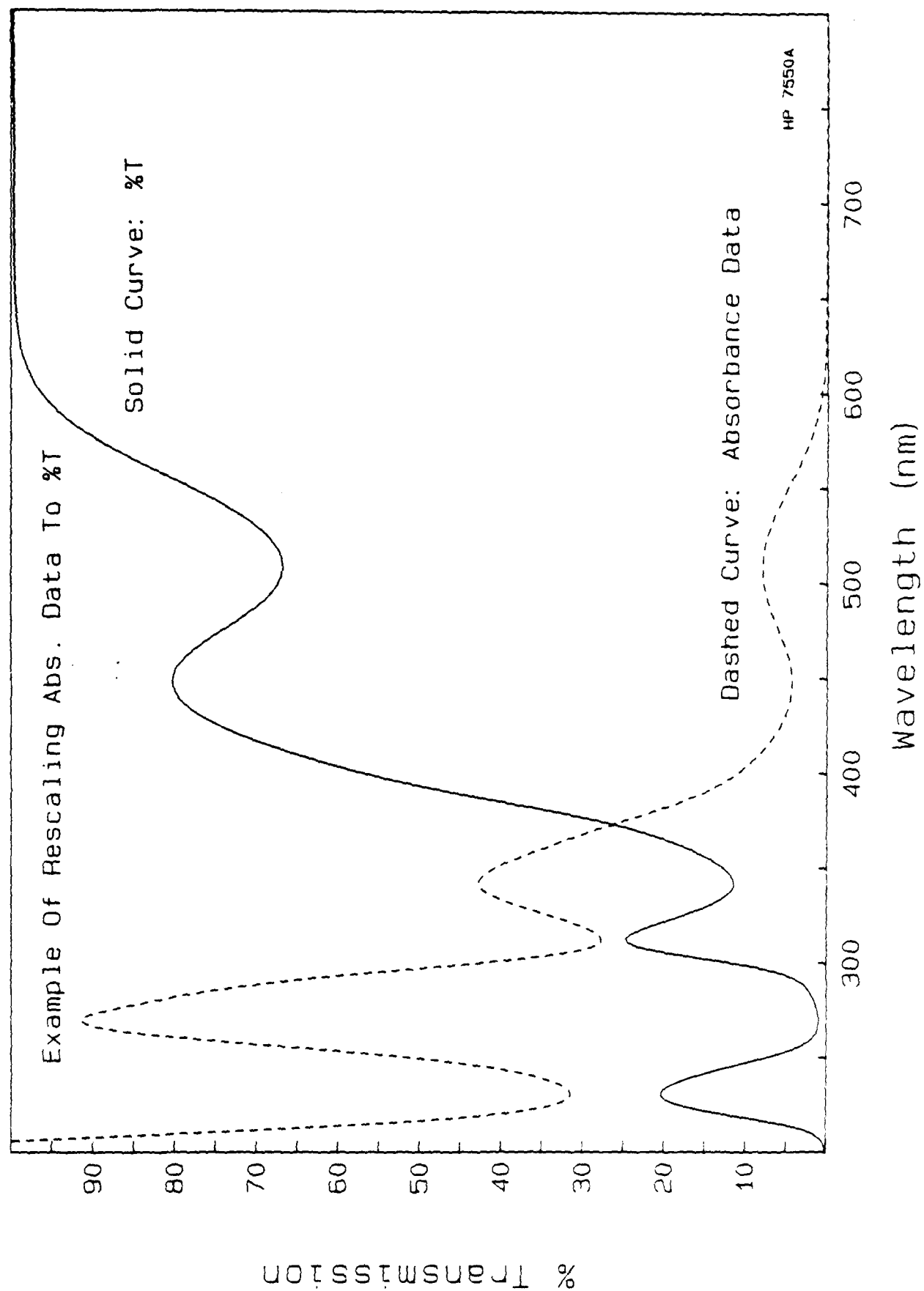
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Appendix
Sample Plots









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