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A Computer Method for the Automatic Reduction of Spectroscopic Data

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ABSTRACT

A computer program, for use with an associated spectral comparator, has been developed at the Naval Research Laboratory for automatically reducing spectroscopic data. A Datex digitizing magnetic-tape recorder, in conjunction with a Jarrel-Ash microphotometer, allows wavelength and intensity information to be read from a photographic plate at 25 data pairs per second. A computer program written in Fortran IV was designed to facilitate processing the information into a usable form.

The computer program permits analysis of spectroscopic data by making simple specifications on a control card. Spectra of local interest are (a) absorption, (b) emission, (c) plasma type, obtained from time-resolved spectroscopic techniques, and (d) solar echellegrams obtained from rocket probings of the upper atmosphere.

Markedly useful features of the program are its capabilities of (a) recognizing spectral peaks from a background of variable density and (b) obtaining absolute values for the radiance or irradiance. The program's essential characteristic is the significant amount of time saved in reducing photographic spectroscopic data. As a rough estimate of the time-saving advantage, one may obtain thirty times the information in 1/100 of the time, as compared to manual reduction of spectroscopic data.

PROBLEM STATUS

This is a final report on one phase of the problem; the results of this phase will be applied to other spectroscopic problems as well.

AUTHORIZATION

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A COMPUTER METHOD FOR THE AUTOMATIC REDUCTION OF SPECTROSCOPIC DATA

INTRODUCTION

A problem associated with investigations in spectroscopy involves the time required to reduce large amounts of data contained in the Photographic spectrograms. It was for this reason that a method for automatic reduction of spectral data was developed at NRL. This technique was the outgrowth of two independent spectroscopic problems undertaken in the Applied Optics and Rocket Spectroscopy Branches. The work in the former branch was under the direction of Dr. Francis Harrington and concerned investigating energy profiles from flash tubes, using time-resolved spectroscopy (work sponsored by ARPA). In the Rocket Spectroscopy Branch an analysis of solar echellegrams obtained from the NRL 1961 and 1964 flights was necessary. In addition, high-resolution spectrograms, related to the work of Dr. Shelby Tilford, required analysis. Computerization of the data reduction was initiated by Dr. Tilford in a calibration program for spectral radiance obtained from the flash-tube spectrograms. Ultimately this work developed into the present large computer program, the combined programs being capable of analyzing much of the spectral work of both branches.

The equipment for the automatic data reduction method was purchased for the time-resolved spectroscopy program and consists of a Datex microphotometer data recording system (system 17,050) and a Jarrel-Ash microphotometer, model 23-500.

FINDING SPECTRAL LINES ON PHOTOGRAPHIC PLATES AUTOMATICALLY

Several automatic comparators have been designed to simplify the task of finding and measuring spectral lines (1-4). These are photoelectric comparators with a rotating prism and an oscilloscopic screen display. More recently, Steinhaus (5-7) has described an automatic comparator which uses a list of transmission values obtained at equal intervals along the spectrum plate by using a precision densitometer. This list is then programmed into a digital computer, along with formulas relating position to wave number and transmission to intensity. Steinhaus, however, describes this program only in a general way, and until now the program has not been written in any widely used computer language (6-8).

A computer program has been designed for processing the output of the NRL comparator-densitometer using magnetic-tape output. The program converts the transmission, position, and neutral-density-filter information from this instrument into various useful forms which will be obvious from the program-description portion of this report.

The outstanding feature of the program is its ability to recognize spectral lines. Using this feature is still somewhat of an art, however; and several factors must be adjusted empirically to the nature of the particular spectrum and to the requirements of the spectroscopist.

Applicability

In certain cases spectra can be interpreted nearly perfectly. The heavy vertical lines at the spectral peaks are the linefind marks generated by the program. Figure 1

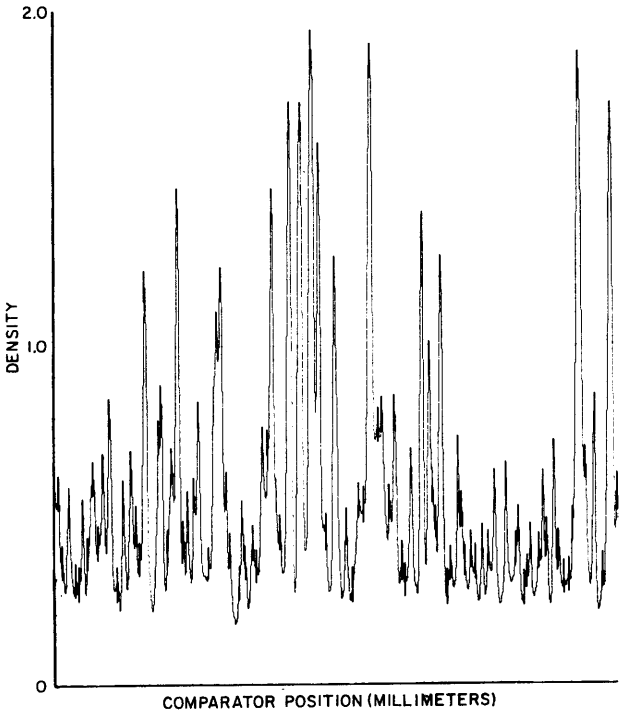


Fig. 1 - An ideal spectrum for linefind analysis

shows such a case. This grazing-incidence spectrum about (245-Å to 250-Å wide) is complex; it does not have extreme contrast; and its weakest recognizable lines have good relief. Such a spectrum can apparently be measured better by the automatic comparator method than by manual setting, assuming equal instrument precision. The comparator and the human eye, however, will vary somewhat in the interpretation of weak features.

The absorption band of CO at 1088 Å, shown in Fig. 2, is another favorable case (the three emission lines are/reference lines). Because of rapid density changes and the scale factor used in the plotting procedure, the darker portions of the spectrum are "stepped." Despite this the lines are well identified. Again the spectrum shows good contrast, and weaker features have reasonable relief.

High-contrast spectra can exceed the effective range of the densitometer. For a very opaque line center, adjacent readings are stepped because of rapid transmission changes. For example, a transmission of 0.5% and 0.4% produces a change of 20% of the 0.5% value. This appears as a distinct step in the density curve. It is impractical to compensate by changing filters because of the narrowness of a line, unless spectra are scanned extremely slowly. Nevertheless, high-contrast spectra are reasonably well analyzed by this automatic process. It is equally difficult for the human eye to find a precise position for many of these lines.

Figure 3 shows the least promising type of spectrum for automatic analysis; the weakest lines have low relief. This spectrum sometimes causes the linefinder to miss certain lines and, in other instances, to falsely identify noise as lines. These defects can be overcome in the computer program, but, presently, only the eye can adequately interpret such spectra.

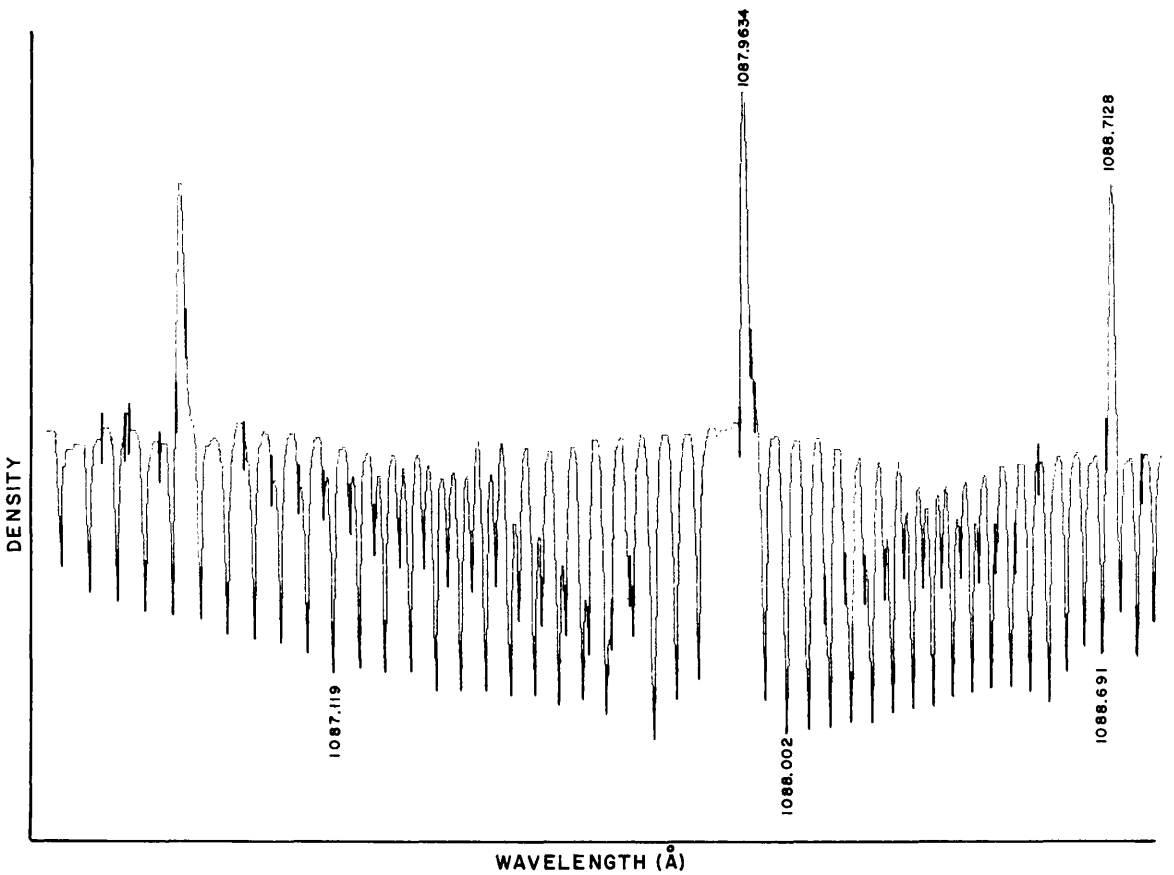


Fig. 2 - CO band at 1880Å

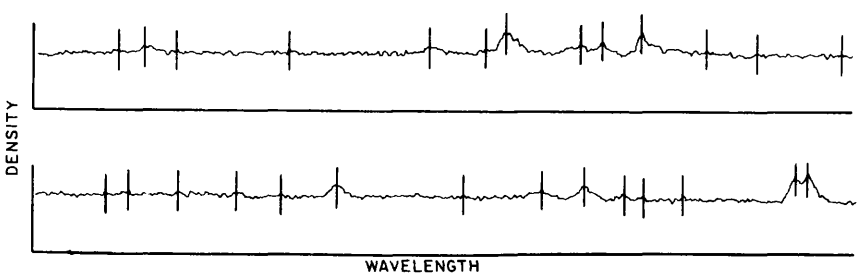


Fig. 3 - An unpromising spectrum
for automatic analysis

In addition, certain broad features which are obvious to the eye are not recognized by this automatic procedure. Figure 4 shows one such feature. The relief is low, and the second-derivative curve becomes insignificant. Here, as before, the eye is the only adequate interpreter.

Parameters for Finding Lines

It is necessary to specify a searching interval (coded N SEARCH on the IBM control card to be described later) before processing a tape to find lines. This interval is a function of the recording speed, the line width, the separation of composite features, and other variables. If the interval is not specified it is automatically set by the program to 12, which implies a searching interval of 25 consecutive data.

Figures 5 and 6 show the effects of varying N SEARCH on a given spectrum. A and B represent two different portions of a spectrum. Note that, with the larger value, certain adjacent features are not distinguished. Also note that sometimes the unrecognized feature is the stronger feature.

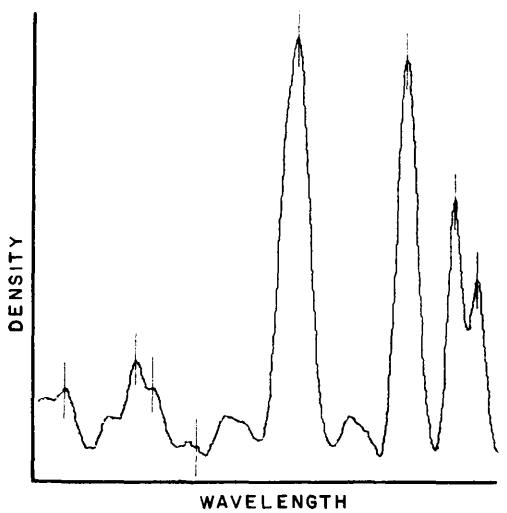


Fig. 4 - Weak lines that are not identified

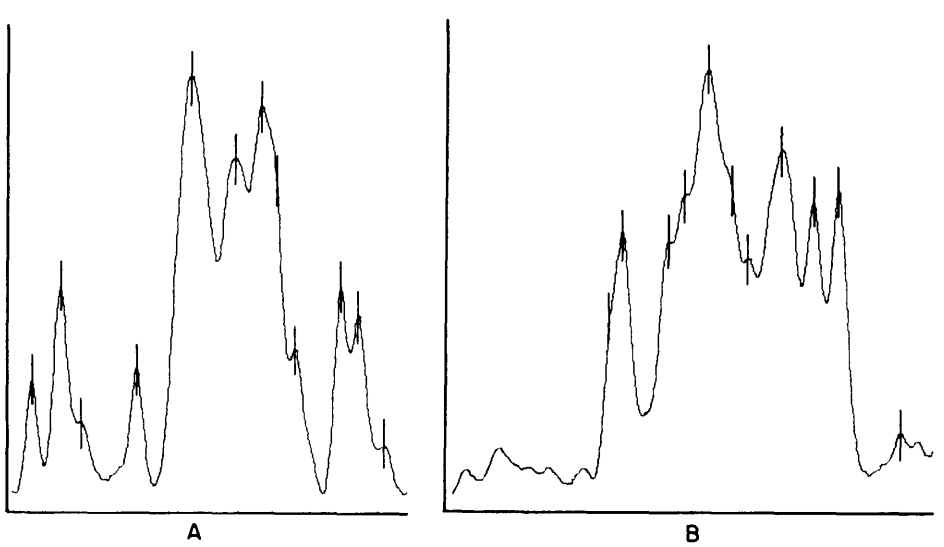


Fig. 5 - Results for the line-searching interval set at N SEARCH = 15

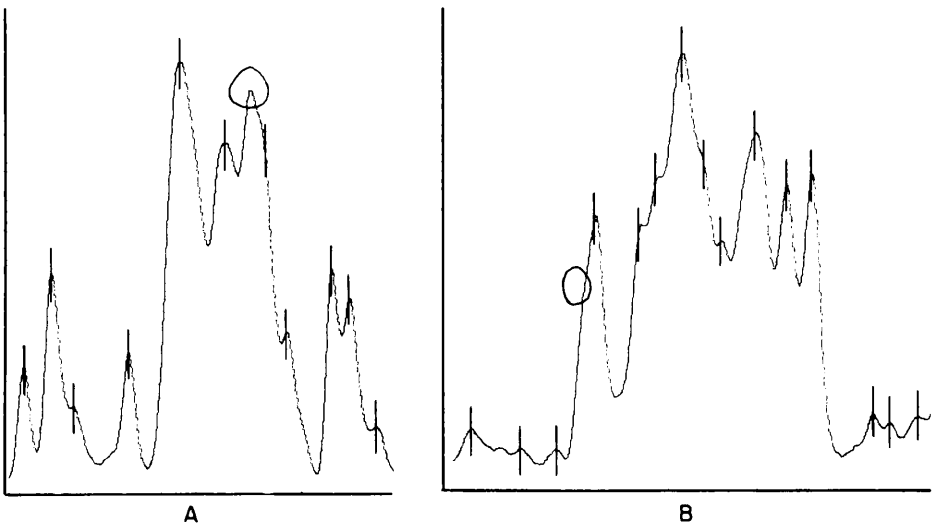


Fig. 6 - Results for the line-searching interval set at N SEARCH = 30

A proper value for N SEARCH can only be determined empirically. The value of this parameter has some relation to the line width and the closeness of the blended features which can be distinguished. Our experience to date indicates that 12 is usually a good value for well-resolved atomic spectra or band spectra which have been scanned at 1 mm/min (recording 25 readings/sec). If similar spectra are scanned faster or slower, N SEARCH must be adjusted to yield the same distance on the plate; for example, if the same spectra were recorded at 0.5 mm/min the equivalent N SEARCH would be 24 (yielding 49 consecutive points as the interval). A trial-and-error determination must be made for different spectra.

Another parameter, the minimum second difference, must also be determined empirically. It is a strong function of N SEARCH, along with many other factors. This parameter must be adjusted, after the data is plotted out, by examining the plot for the minimum density of acceptable lines; the minimum second difference is then set on the basis of this information. A useful lower limit, 0.021, is provided by the program if no value is specified.

A minimum acceptable density for a line (maximum density for absorption spectra) may also be provided. If the background density, in the form of noise above the continuum, is determined, then all such "lines" with a peak value less than this may be rejected; also, minimum acceptable, bonafide lines may be eliminated from the spectrum by the program. Lines are rejected by assigning an appropriate value in the DEN MIN position on the control card. Spectra for which this minimum density rejection is best suited have a constant continuum or a continuum which slowly changes as a function of wavelength. (At present, the same N-SEARCH value is used for constructing both first-differential curves and second-differential curves. Possibly a smaller number would be preferable for the second derivative.)

EQUIPMENT

Components of the System

A high-precision Jarrel-Ash microphotometer has been equipped with a Datex tape recording system 17,050 built according to the special requirements of NRL. The Datex recorder converts the position information of a spectroscopic plate and the plate

transmission, represented by a voltage level, from analog form to digital form. A shaft-position encoder is attached to the precision screw drive of the JACO instrument and produces 1000 counts of digital data for each revolution of the screw. The output signal from the photomultiplier stage is converted to 1000 counts of digital data representing transmission; a light-bank provides a digital readout of the transmission data, for monitoring purposes. The ten-position filter-selector switch on the JACO microphotometer provides one decimal digit for each setting, thereby yielding scale information for recording purposes.

The plate-position data, transmission data, and scale data are automatically recorded on magnetic tape at 1500 readings/min. In addition, 18 characters of parameter data are recorded as heading information at the beginning of each recording cycle. Recording-cycle length is selectable and may be 1500 characters, 3000 characters, 7500 characters, 15,000 characters, 30,000 characters, or 60,000 characters. (In our program the last two are not used.)

Upon receiving a command to record, the system produces and stores, on tape, position data from the encoder and transmission data from the microphotometer. Control circuits and logic circuits in the programmer unit provide sequencing of each data-input character to the magnetic-tape recorder. The format for recording the binary-coded-decimal (BCD) data on the magnetic tape is comprised of (a) Heading: 18 characters of parameter data, (b) Position: six characters of encoded data, (c) Transmission: three characters of data, (d) Fixed zeros: two characters, and (e) Scale: one character from filter scale selector on JACO unit.

This record format, excluding the heading, constitutes one data reading. It is repeated for the selected length of the recording cycle. The heading entry is recorded only once at the beginning of each file, consisting of the specified number of records. Table 1 shows the tape code. Although the position record is made in terms of microns, it is easily converted to wavelength by knowing the spectrograph's dispersion formula and by making the appropriate entry on the control card.

Table 1
Digitizer Character Format

Character	Code						
	1	2	4	8	A	B	C
0		x		x			
1	x						x
2		x					x
3	x	x					
4			x				x
5	x		x				
6		x	x				
7	x	x	x				x
8				x			x
9	x			x			
Space					x		x
End of File	x	x	x	x			

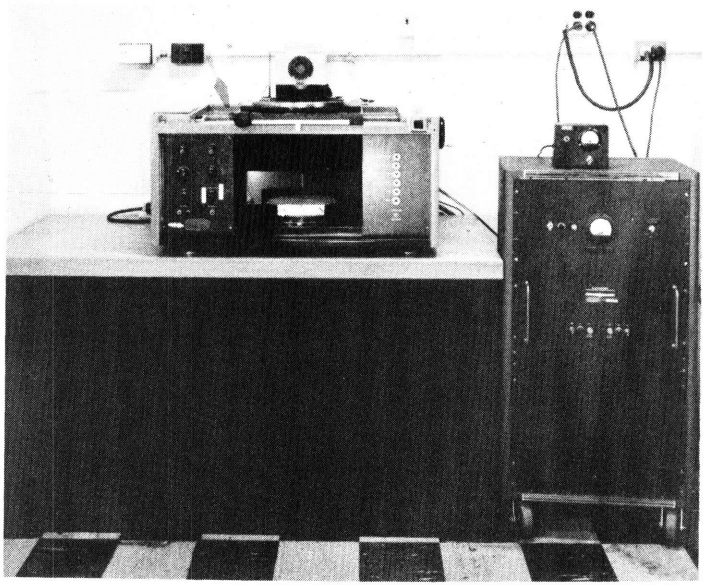


Fig. 7 - Modified Jarrel-Ash microphotometer

Figure 7 shows the JACO Model 23-500 microphotometer with the associated power supplies for the photomultiplier tube, light source, and comparator screw drive mechanism. The modifications to the original equipment, for reducing the noise level in the output signal and for better monitoring and control of the JACO unit, consisted of (a) a switch to permit operating the light source at a reduced dc voltage (76 volts) in a "standby" position or in an "operating" position (120 volts), (b) a shorting switch for zero setting of the Datex input, (c) a meter for monitoring the current output of the PM tube and an outlet for monitoring with a chart recorder, and (d) a regulated power supply substituted for the PM power supply permitting the noise level to be reduced 30 times. This noise-level has a relatively insignificant effect as far as data accumulation is concerned.

Figure 8 shows the Datex digitizing tape recorder. The parameter, record length, end of file, and the data recording switches are on the left panel; controls for the differential dc amplifier are also located here. The power and tape-operating switches for the Potter Model MT-SW magnetic-tape recorder are on the right panel. The tape recorder places digital data on a magnetic tape, one character at a time, with constant spacing.

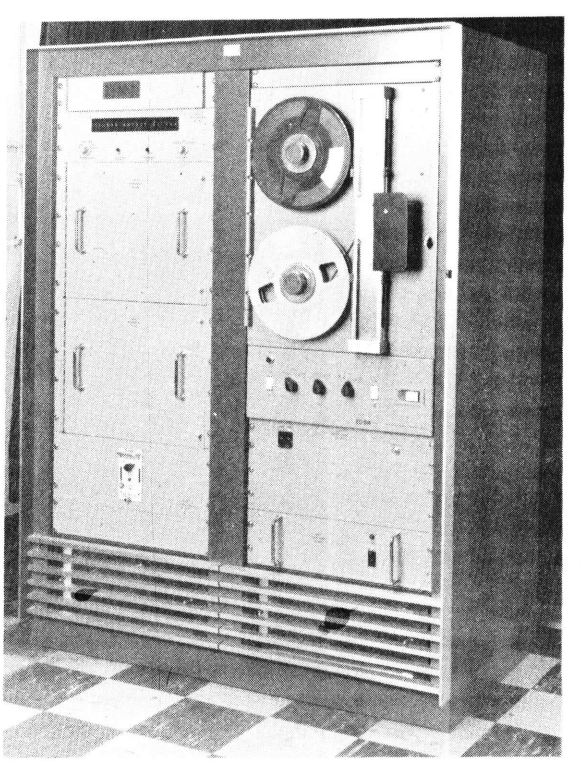


Fig. 8 - Datex digital tape recorder

Basis of Operation

A diagram of the automatic comparator is presented in Fig. 9. The system, upon receiving a record command, simultaneously acquires and stores plate-position data and transmission data from the microphotometer. The transmission data and the plate-position data are stored at the same time. This is required for data acquisition timing to be maintained in 1 msec.

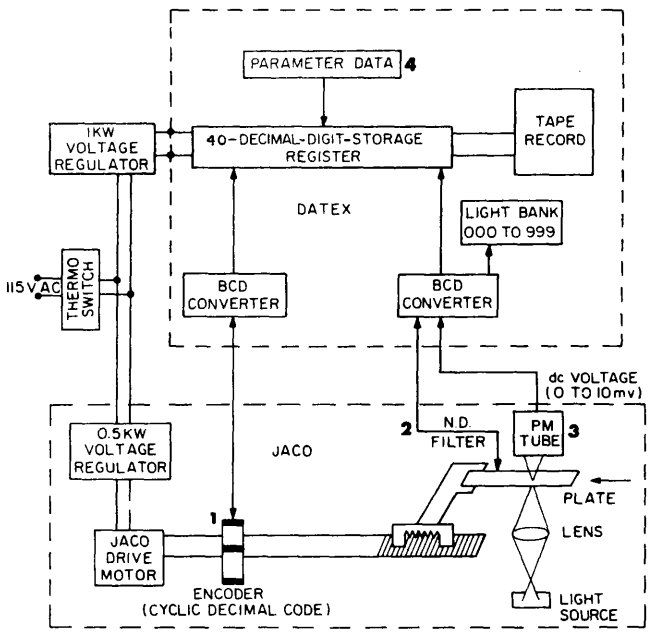


Fig. 9 - The automatic comparator

The plate-position data from the encoder is in Datex cyclic decimal code and consists of six digits. These data bits are first stored and then converted to BCD (binary coded decimal) for storage in part of a 40-decimal-digit storage register.

The transmission-data input is in the form of a dc voltage varying between 0 mv and 10 mv. This analog signal is converted to 1000 counts consisting of three decimal digits in BCD from 000 to 999. The BCD output is stored in a portion of the BCD storage register, to be read out for recording at the proper sequence by program logic in the Datex system. Eighteen digits of parameter data, including one digit of scale data, is read serially from the decimal-selector switches and converted to BCD by code converter circuits. The BCD is again read out for recording, when the program logic is at the proper sequence.

Figure 10 presents some typical program logic circuits and matrix configurations used in the Datex unit. The printed circuit module is a general-purpose, solid-state, plug-in-type board providing for 22 input or output inverters, and a 16 × 20 diode matrix.

COMPUTER PROGRAM DESCRIPTION

Main Program (Spectra From a Tape Densitometer)

The program was written for the CDC 3800 computer and converts the magnetic-tape output of the tape densitometer to several useful forms. The program output can be any

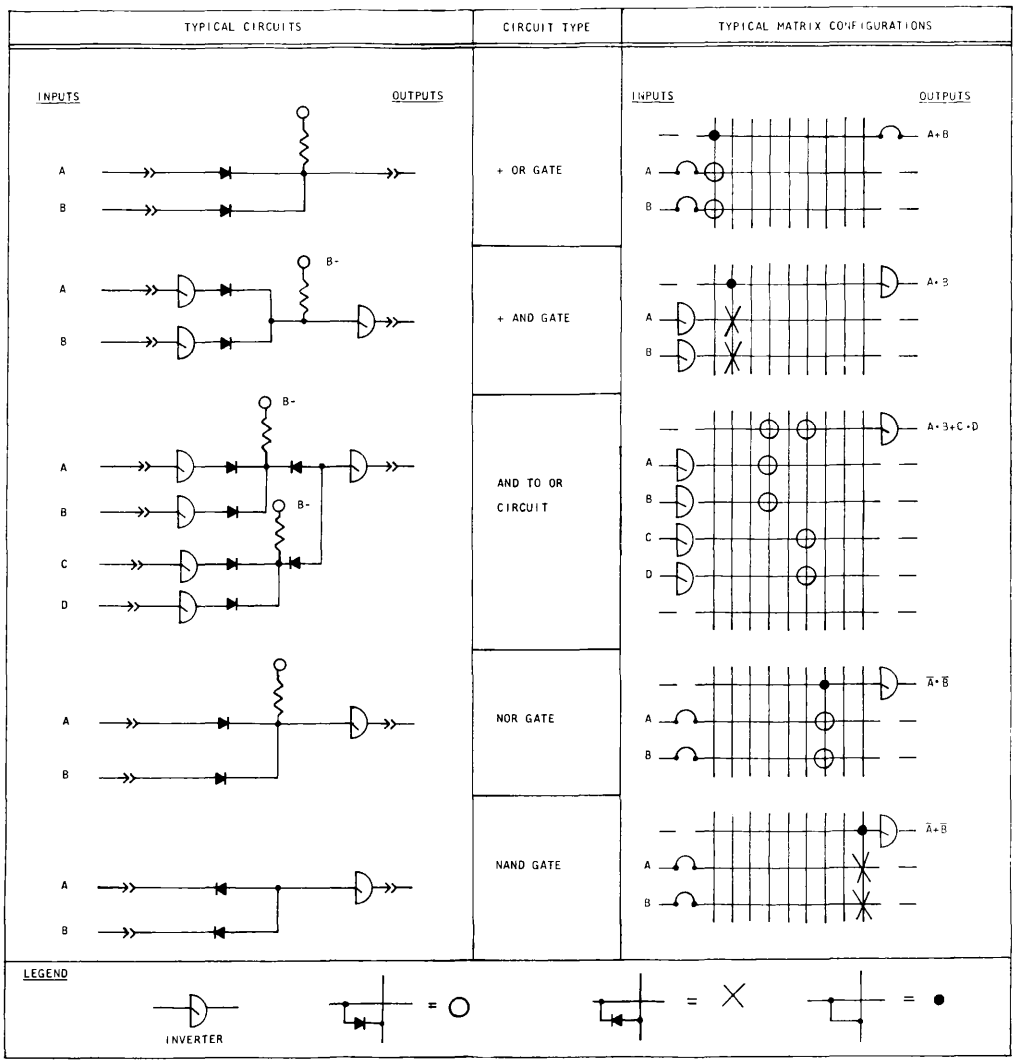


Fig. 10 - Typical program logic circuits in the Datex unit

combination of (a) a paper printout containing the density (or spectral radiance), position, and wavelength of all data points, or of selected data points and the line-finding results, (b) a list of lines, as identified by second derivatives, with a card punched in standard form for each line, and (c) punch cards in "9-card" format from which the spectra can be plotted on the Calcomp plotter of the CDC 3100 computer.

Four different types of spectral modes may be processed with this program by making a specified entry on the control card. The most general of these are for absorption and emission. Calibration of wavelength is achieved by using a quadratic interpolation from three known lines and is provided as an option. (A logical modification could be controlled by a NO WL STD entry, which could signal a cubic interpolation by a value of 3 on the control card.)

The other two modes are very specialized. One is for the solar echellegrams obtained from the NRL 1961 and 1964 rocket flights, using an approximate internal

wavelength calibration. The other is designed according to the specifications of Dr. Francis Harrington and uses his conversion to wavelength and spectral radiance.

The program depends strongly on the large memory and the fast operation of the NRL CDC 3800 computer. The magnetic-tape output, obtained from a Datex microphotometer, is a low-density tape and contains parameter records, data records, end-of-file records, and inter-record gaps. These records consist of strings of digits written at low density in the standard BCD form. Program operation is from a single control card, mentioned in the previous section.

Computer statements are written in the modification of Fortran 63 and are compiled to give a binary program deck. The latter is used routinely for processing tapes. Modifications of the program must be made to the Fortran statements and a new binary deck generated. The Fortran statements can be used as a direct "load and go" operation at the cost of compilation time. Adapting this program to a smaller computer would require shortening the acceptable record length. On a slower computer it might not be feasible – on the fast CDC 3800 the calculations for a complete tape containing a complex spectrum takes up to 25 min. Modification for use with a different tape densitometer could be possible; all decode operations and decode logic would have to be changed. The program includes many features and tests necessary due to the error-proneness of the densitometer; many of these would have to be changed.

Output Data – The printed output is controlled by NO PRINT and related specifications on the control card; the use of NO PRINT will be explained in the description of the control card. Output for the punched data is in the "9-card" format and is controlled by NO CARDS, described later. Either millimeters or wavelengths can be specified as "position" output, assuming that the wavelengths have been defined. Density is the normal "intensity" output, but spectral radiance is provided in the plasma-tube mode.

Plotting Output – To ensure efficient plotting (matching data points with the plotting characteristics applied to the Calcomp 3100 plotter) the plotting frequency can be controlled. If necessary, every point on the original tape can be plotted; normally every tenth or twentieth point will suffice. The Fortran deck must be compiled to give a binary deck for the CDC 3100 computer. A "load and go" program is being developed for Fortran plotting decks. (A logical modification would allow plotting with the Calcomp 3800 plotter directly without the use of cards. This could be specified by the control card.)

Linefind and Linetype – The most useful feature of this program is its ability to find and analyze lines, and it is controlled by a NO LINES specification on the control card. If the linefind portion is not bypassed, the program constructs a first-derivative curve and from it a second-derivative curve using parameters entered on the control card for zeros, minima and maxima. A zero-minimum combination for absorption spectra and a zero-maximum combination for emission spectra are tentatively defined as lines. Certain of these features are rejected by internal criteria, others by control-card criteria. The surviving features are then analyzed by the linetype subroutine, which classifies the lines and refines the peaks of certain lines by a least-squares polynomial fit of the position-intensity coordinates.

For each line a card is punched, using a format compatible with the programs of Dr. Shelby Tilford and personnel of NBS and the University of Maryland. A line of data is also printed, giving many valuable criteria for analyzing the line.

If desired, the linetype command can be bypassed by making an entry in NO REFINE, to leave only unrefined line positions. This feature is included because the linetype subroutine is the greatest time consumer in the entire program; it may occasionally be necessary only to find lines for classification. (A logical next step would be to fit lines

with Gaussian or Laurentian functions to obtain half-widths of more theoretical significance than the present width derived from zero points of the second-derivative curve.)

Control Card Format

Figure 11 is a photograph of an IBM card showing the format used for the program control card. Two examples of control-card application are given below.

1. The control card for an emission spectrum finds lines and punches cards in one scan (one file*) and also punches cards for plotting. The fiducial mark is set internally at 10.000 mm. The space assignment is (a) 1-3 = emission.† (b) 4-5 = 1, (c) 31-32 = 1, and (d) 33-34 = 10. The remainder of the card is blank.

1a. The following control card can find lines and punch cards in three files. The fiducial mark is set at 254.00. This card applies wavelength standards with the space assignment (a) 1-3 = emission, (b) 4-5 = 1, (c) 25 = 3, (d) 31-32 = 1, (e) 38 = 1, and (f) 75-80 = 254.00. The remainder of the card is blank. It is followed by three wavelength-position cards.

1b. This control card generates cards for plotting only and suppresses the fiducial. For this operation the spaces are assigned as (a) 1-3 = emission, (b) 4-5 = 0 or blank, (c) 32 = 0 or blank, (d) 33-34 = 1, and (e) 75-80 = 1. The remainder of the card is blank.

2. The control card for spectra from a tape densitometer has its spaces assigned for 21 separate functions.

Spaces 1-3 hold SPECTRUM (A3), which refers to the type of spectrum encoded on the tape. ABS is written for absorption spectra, EMI is written for emission spectra, ECH is written for echellegrams, and PLA is written for flash-lamp experiments.

Spaces 4-5 hold LINECARD (I2), a positive integer which causes linecards to be punched. A zero or negative integer prevents cards from being punched. For paper printout and cards this must be used with NO LINES.

Spaces 6-10 hold N SEARCH (I5), which is the interval (in data points, not in mm or A) used in finding first differences in the linefind program. If N SEARCH is zero or blank, the program is internally set to 12, a normally acceptable value. For complex spectra,

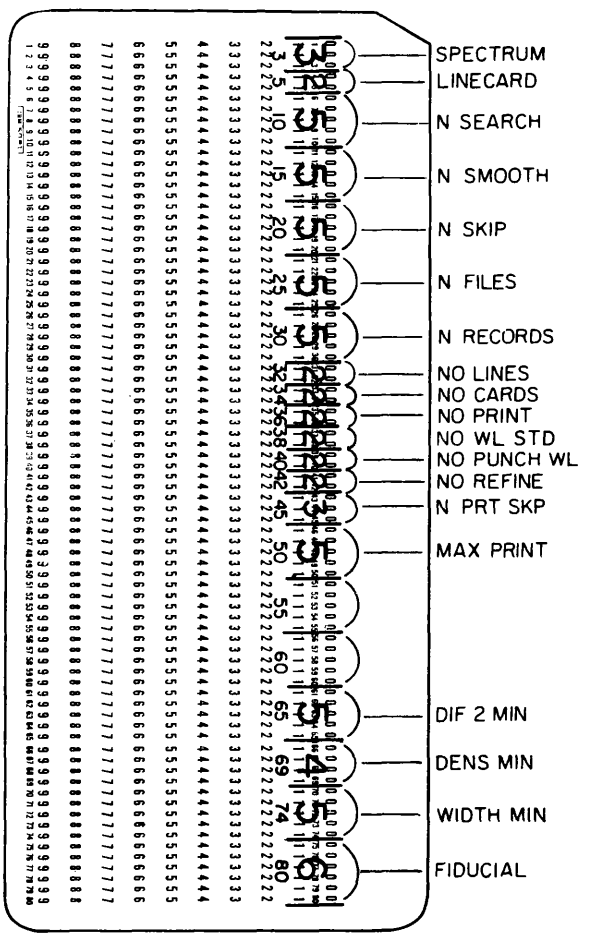


Fig. 11 - Control card for the main program

*A file is a number of records, on magnetic tape, sandwiched by the parameter record heading and the end-of-file (EOF) mark. The number of records in a file is selected at the Datex unit.

†EMI = emission.

and the 1961 echellegrams scanned at 0.5 mm/min, and for complex emission spectra scanned at 0.5 mm/min, a suggested value is 12. For coarse spectra larger values should be used.

The value of N SEARCH has some relation to the line width and the closeness of distinguishable blended features. If its value is larger than, say, twice or three times the suggested values, minor features such as shoulders or components of compound lines will not be identified, and only strong features will be detected. In any case, the numerical value of N SEARCH must be less than (1/5) [3000 - (record length/6)]. This means that for a densitometer record length of 15,000 (digits per record) N SEARCH should not be greater than 100. The maximum record length for this program is 15,000.

Spaces 11-15 hold N SMOOTH (I5), which refers to the degree of smoothing applied to the spectral data. The number of sequential data averaged together is 2* (N SMOOTH) + 1; i.e., if N = 5, each point will be replaced by the average of 11 points (moving successively point by point through the data). If the densitometer was run at 0.5 mm/min and N SMOOTH = 1, there will be no loss of resolution, since each micron is read about three times and, after smoothing, each reading is the average of three readings.

If the densitometer is run at 1 mm/min and N SMOOTH = 0 or blank, data will be processed at maximum resolution, without smoothing. In general, large values of N SMOOTH lead to loss of resolution.

Spaces 16-20 hold N SKIP (I5), which is the number of files skipped before processing begins. A file is a number of records beginning with the parameter heading and ending with the end-of-file mark. For example, if the desired spectrum is in the third file, N SKIP = 2. To process only the first file, this entry is left blank or is set equal to zero.

Spaces 21-25 hold N FILES (I5), which specifies the number of files to be processed. If the desired spectra are in the second and third files, then, for example, N SKIP = 1 and N FILES = 2.

If N FILES is left blank, the program internally sets the value to 1, and only one file will be processed. If a tape contains n files, all of which must be processed, then the minimum value for N FILES is n.

Spaces 26-30 hold N RECORDS (I5), an entry which permits skipping records, such as when the processing is to begin in middle of a file at some particular record.

The first three preliminary records, containing initial values, etc., however, will always be read by the program. If N RECORDS is 60, for example, records 1, 2, and 3 will be processed; then record 64, etc., will be processed to the end. N RECORDS is set internally to zero after processing one file.

Spaces 31-32 hold NO LINES (I2). A zero or blank in NO LINES will cause the line-finding portion of the program to be bypassed. A nonzero number will punch a card for each line obtained, if a positive entry is made in LINECARD. Otherwise, only a paper printout results.

Spaces 33-34 hold NO CARDS (I2). A zero or blank in NO CARDS prevents card punching. If NO CARDS is 1, every datum will be punched; if it is 4, every fourth datum will be punched, etc.

In general, NO CARDS is conveniently set to about 10 (this is slightly redundant, however) for plotting, if every micron is recorded once (a densitometer speed of 1 mm/min, plotting at 1 mm/in.). Output cards are in the specialized "9-card" form. If the

cards from linefind are punched and produced from this section, a zero will be found in column 2 of all "9-cards," while column 2 is blank on the linefind cards. This permits separation in the card sorter.

Spaces 35-36 hold NO PRINT (I2). If a nonzero number is found here, records will be printed. The quantity of printout, however, depends on the values placed in N PRNT SKP and MAX PRINT.

Spaces 37-38 hold NO WL STD (I2). If a nonzero number is given here, three more cards, after the control card, will be read for quadratic wavelength standards, and positions for each file will be processed. This is related to N FILE; e.g., if N FILE is 2, there must be six such cards.

Spaces 39-40 hold N PUNCH WL (I2). If a nonzero number is found here, the "9-cards" are punched with wavelengths instead of millimeter positions.

Spaces 41-42 hold NO REFINE (I2). If a nonzero number is entered here, lines will be identified by the linefind section, but they will not be analyzed by the linetype subroutine.

Spaces 43-45 hold N PRNT SKP (I5). A number here controls the density of printing. If this number is zero, blank, or 1, every datum will be printed. If it is, say, 20, every twentieth datum will be printed, etc.

Spaces 46-50 hold MAX PRINT (I5), which controls the printout, i.e., the maximum number of records to be printed. If MAX PRINT is zero or blank, it is set internally to 50,000, which is not likely to be exceeded in practice. If it is five, the first five records will be printed, etc.

Spaces 51-55 hold MIN WIDTH (I5), and spaces 56-60 hold N DUMMY (I5). These are not presently being used.

Spaces 61-65 hold DIF 2 MIN (F5.3), which is the minimum acceptable second difference. In the linefind portion apparent lines with a second difference less than this entry are bypassed. If DIF 2 MIN is zero or blank, the value is set internally to 0.021, a generally useful value. To allow analyzing all apparent lines, insert any negative number.

Spaces 66-70 hold DENS MIN (F5.2), which is the minimum acceptable density. In the linefind portion apparent lines with a peak density less than this entry are bypassed.

Spaces 71-74 hold WIDTH MIN (F4.3), which is the minimum acceptable width. In the linefind portion apparent lines with a width, in millimeters, less than this are bypassed.

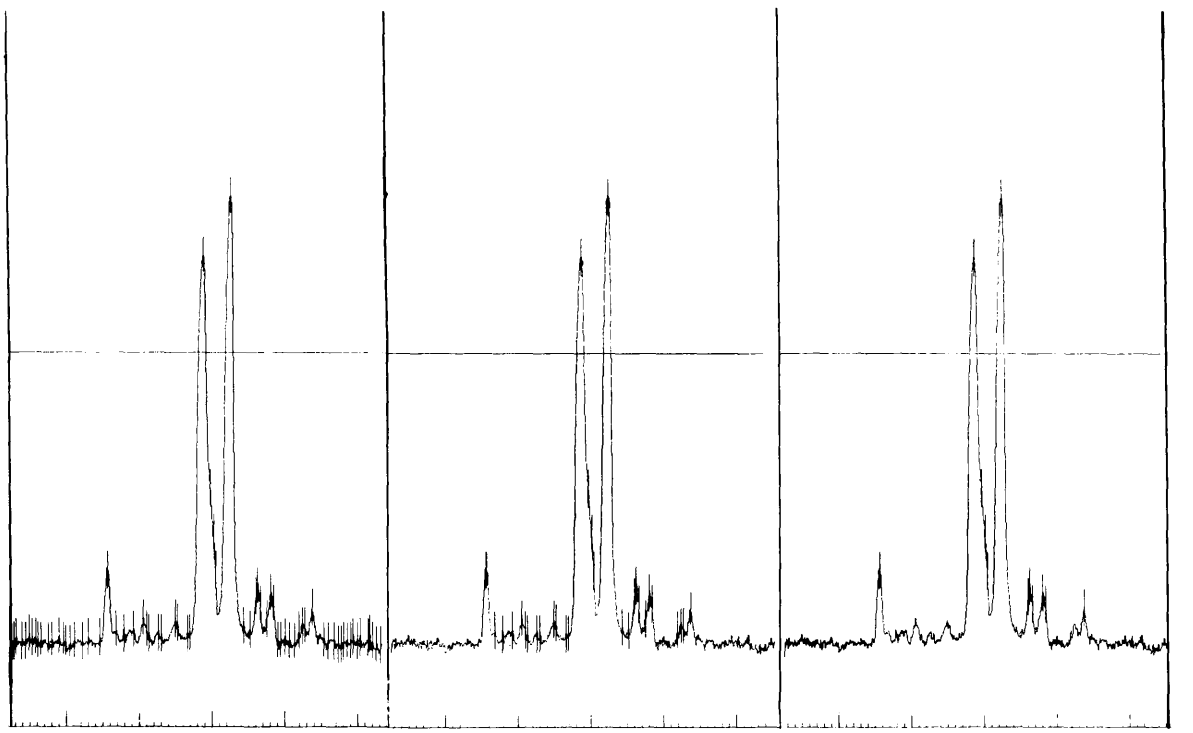
Spaces 75-80 hold FIDUCIAL (F6.3), which converts all millimeter positions so that the first position (coded START POS) on record one is equal to this number. The conversion of all other positions is achieved by using POSN(L) = POSN(L) - START + FIDUCIAL. If the entry is zero or blank, then the FIDUCIAL is set internally to 10.000. A negative number in this field will bypass the conversion expression by setting both START POS and FIDUCIAL to zero.

In this description seven entries influence the linefind analysis. One has already been described – the effect of varying the N SEARCH interval (see Figs. 5 and 6). The following examples will illustrate how some other control card entries also modify the computer trace, when applying the linefind analysis.

Variation of the Minimum Density (DENS MIN) – Figure 12 is a computer trace representing a UV emission spectrum obtained from a plasma (about 2400 Å). In (a),

the left trace, no variation was made. In (b) the trace was given a value of 0.25 mm, while in (c) the trace was produced from a value of 0.30 mm.

This particular entry provides a convenient way of eliminating or minimizing the identification of noise by the linefind analysis as spectral features from the data. Generally, this entry is most effective when the background continuum has a constant value.



a b c

Fig. 12 - Variation of the minimum density

Minimum Width Variation (WIDTH MIN) - The WIDTH MIN entry permits the spectroscopist to select lines, which are greater than a minimum width in millimeters, for the linefind analysis. Figure 13 shows a series of three traces in which the last two have been altered while the first is the original.

Trace (a) represents an unmodified spectrum. In trace (b) a value of 0.025 mm was punched on the control card, and in trace (c) a value of 0.05 mm was assigned. It is noted that, essentially, all the significant lines were analyzed in (b). In the third trace, however, some peaks, and the shoulder between the strong peaks, were missed.

Second Derivative Minimum (DIF 2 MIN) - In Fig. 14 trace (a) is unaltered. In trace (b) the value for the control card entry was 0.03, and in trace (c) the value 0.05 was given. This entry permits all apparent lines with second derivatives less than these values to be bypassed by the linefind analysis. In the trace on the left a value of 0.021 was automatically assigned by the program when no specification was made in the column on the control card. This is a useful value for the echellegrams.

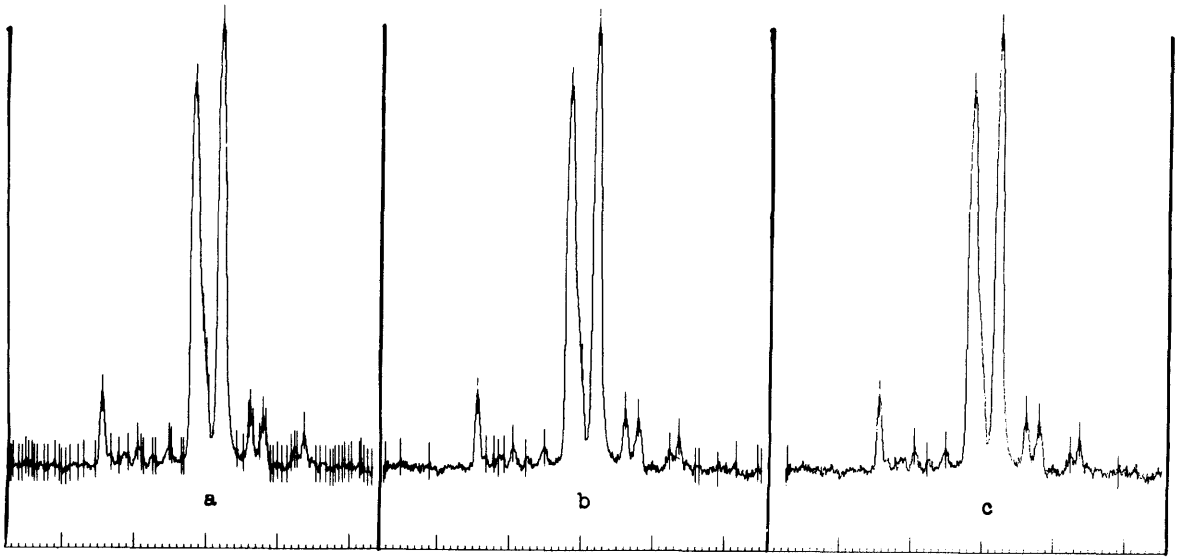


Fig. 13 - Minimum width variation

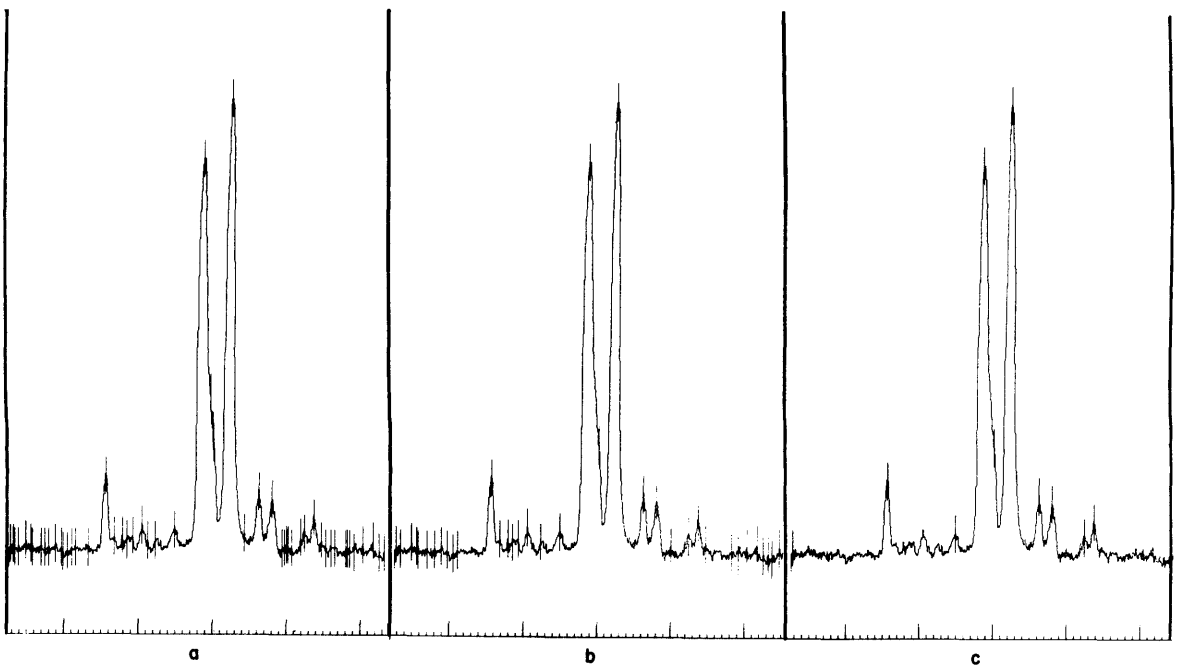


Fig. 14 - Effect of varying the second-derivative minimum

Interpretation of the Program Content

1. The coefficients for a quadratic interpolation of wavelengths used for the echellegrams are generated from three standard lines designated by WLS(I,1), WLS(I,2), and WLS(I,3); these values are obtained from preliminary calculations and based on the assumption that the spectrum is 28.0 mm wide.

Using the quadratic relation

$$WL = A * (POSN)^2 + B * (POSN) + C,$$

the constants are determined as follows:

$$AY1 = \frac{[WLS(N\ ORDER,\ 1) - WLS\ (N\ ORDER,\ 2)]}{(X1 - X2)}$$

and

$$AY2 = \frac{[WLS\ (N\ ORDER,\ 2) - WLS\ (N\ ORDER,\ 3)]}{(X2 - X3)}$$

from which one obtains the relations

$$A = \frac{(AY1 - AY2)}{(X1 - X3)},$$

$$B = AY1 - AAA\ (X1 + X2),$$

and

$$C = WLS\ (N\ ORDER,\ 1) - AAA\ (X1)\ (X1) - BBB\ (X1),$$

where X1, X2, and X3 are the positions of the corresponding wavelength. The meaning of these constants will be found in paragraph 8 of this section.

2. Filter densities from the Jarrel-Ash densitometer are input data to the program in the form of differences from adjacent filter settings, experimentally obtained.

3. Transmission data are corrected by obtaining an average transmission value for the first record, which represents the transmission of the first medium. A second record is made of the transmission values of the second medium, which may be the plate edge at 40% transmission, or the emulsion in the case of the plasma spectrum. From this a correction factor is generated for 100% transmission, which is applied to all following records.

If an improper neutral-density-filter setting has been made in this calibration, the program internally assigns a value of 1, to permit further calculations by the program. Also, a sudden shift of the filter position, electronically or mechanically, will cause the program to assign the value 1.

4. For spectra other than the echellegrams (absorption, emission, and flash tube) the program permits a quadratic interpolation based on externally introducing three known spectral features by specifying a nonzero number in the NO WL STD columns of the control card. Three wavelength-position cards, in standard format, are required, and they must follow the control card. The three positions must be relative to the fiducial mark.

For example, if the edge of the plate is at 2.135 mm, according to the densitometer, and this position is set to 10.00 by the fiducial conversion, a line at 15.145 mm on the densitometer will be at (15.145 - 2.135) + 10.00 = 23.010 mm relative to the fiducial mark.

5. The program prepares a filter-density table on the basis of the filter number assigned by the first record. The parameters

$$K1 = N\ FILTER\ (1)$$

and

$$K2 = K1 - 1$$

are used in the calculations, where the argument of N FILTER is the number of the particular record.

A false switching of the filter by the densitometer or an error in the tape drive will cause a change in the filter value. The erroneous data are eliminated from the filter-density table from which calculations are to be made.

6. Errors in the tape-record data are assumed to appear only as a parity error, i.e., a deviation from the BCD mode. These errors are detected by defining the expressions

$$KAY = LENGTH\ F(1)$$

and

$$LL = 2 * KAY/3\ ,$$

where LL is a running index used for scanning the data stored in the computer memory.

The parity error is identified by the "if" statement:

IF (KAY .LE. 4) GO TO ... ,

since each acceptable record must consist of four eight-digit words. Any record containing more words is assumed to constitute a parity error. The program then recovers as many good records as possible.

7. If any or all of the 21 parameters on the control card are not specified (excluding the two not used), the program assigns a value to them to enable the data processing to continue (this has been oriented in favor of the echellegram spectra). This internal assignment appears in printed form as the "Effective Control Card." The SPECTRUM column entries of EMI, PLA, and ECH internally assigns a +1 to statement 97 plus 2 to indicate emission type spectra, while ABS assigns a -1.

8. The data records from the magnetic tape, which include position, transmission, and filter position, are arranged into three separate tables defined by certain intervals within the program. A running parameter, designated as LL, is used to search through the tables.

These tables are represented in Fig. 15. The middle and lower tables are filled only once with raw data. The upper table is filled repetitively with new data from each record. As new data flow into the upper table, the old data from this table moves down into the middle table, while the old data in the middle table move down into the lower table. This gives three new tables of data for transmission, plate position, and filter setting.

To prevent data gaps or omissions during the linefind analysis, an interval is used which is defined by N OVERLAP = 5 * N SEARCH + 1. This interval overlaps the upper and middle tables, and the middle and lower tables.

The arrangement of the data into tables is necessary so that (a) incoming raw data can be monitored for errors and rejected, if necessary, before calculations are made and (b) a correct time sequence can be achieved among the different calculations.

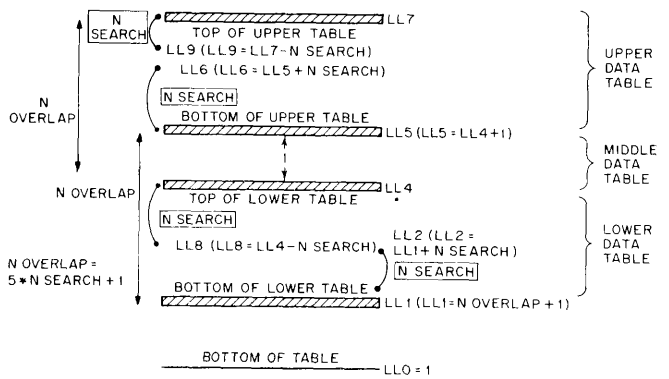


Fig. 15 - Data tables used in the analysis of input data

A zero initial value is assigned to the traveling index LL used for establishing the data tables, to the index used for scanning the records JJ, and to the constants used in the wavelength interpolation AAA, BBB, and CCC. Data are then buffered into the computer memory and decoded for filling in the top data table. A check is then made for parity errors, for the proper length of the records being stored, and for an incorrect setting of the neutral-density filter. The middle data zone is filled and stored in the computer. A check is again made for proper record length and for the number of characters for the shortest possible recording cycle (1500). When these operations are finished, the program determines the plate position with respect to the comparator screw, and the quadratic wavelength interpolation begins.

The next portion of the program is used for smoothing data by taking the average of 2n + 1 points, where n is the assigned value on the control card.

The linefind analysis uses the "N option" for the running index to find the first and second-derivative expressions used for detecting and identifying the spectral peaks. These expressions are defined as follows:

$$\text{DIF (N)} = \text{DENSITY (J2)} - \text{DENSITY (J1)},$$

$$\text{DIF 2 (N)} = \text{SIGN} * (\text{DIF (J1)} - \text{DIF (J2)},$$

where J1 is the first zero point of the curve and is defined by J1 = N - N SEARCH, J2 is the second zero point of the curve and is given by J2 = N + N SEARCH, and N scans across the three data tables by using the interval defined by N = LL8, LL9. The details comprising these data tables are shown in Fig. 15.

New data are fed into the linefind analysis by defining the following parameters in terms of the running index N:

$$\text{N} = \text{L} = \text{LL4},$$

$$\text{LL3} = \text{LL4} = \text{N OVERLAP} + 1,$$

$$\text{LL5} = \text{LL4} + 1,$$

$$\text{LL6} = \text{LL4} + \text{N SEARCH},$$

$$\text{JJ1} = \text{LL4} + \text{N OVERLAP} + 1,$$

and

$$\text{LL8} = \text{LL4} - \text{N SEARCH},$$

where JJ1 is now defined as the first zero point of the curve.

Figure 16 shows how the linefind analysis uses the interval N SEARCH on the lines produced by the quadratic interpolation to obtain the first and second derivatives and, from the latter, the zero points J1 and J2 used for interpreting the peak characteristics. A variable "linefind" is used to analyze the second derivative curve and is given by LINEFIND (N) = -1 * SIGNF (1., DIF 2 (N)), where we have defined DIF 2 above. SIGNF is the function used to extract the sign of the second derivative.

In the second-derivative expression, SIGN is the factor used to indicate that the spectrum is emission if it is +1, or that it is absorption if it is -1. This assignment is done internally by the program when an entry is made for SPECTRUM on the control card.

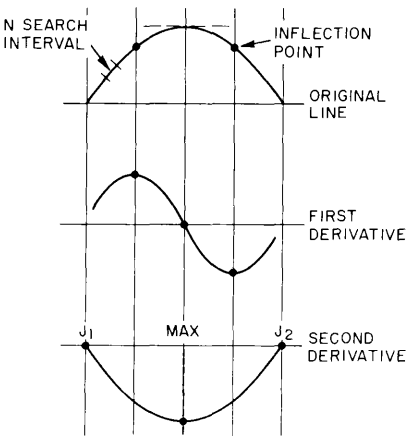


Fig. 16 - Differentiation used in the linefind analysis

9. The criteria for classifying the spectral peaks are those used by Steinhaus, except for the omission of classes 3, 5, and 6. These criteria are (a) 0 - completely acceptable, symmetric, (b) 1 - asymmetric, shaded to red, acceptable, (c) 2 - asymmetric, shaded to blue, acceptable, (d) 4 - wide line, (f) 7 - shoulder, (i) 8 - poor line, fit out of range, and (j) 9 - nothing.

10. Noise-level contributions will be interpreted as false lines by the linefind and linetype routines, but for spectra where the continuum is constant or changes by a constant small factor, this difficulty can be minimized by introducing an appropriate value in the DEN MIN column.

11. A root-mean-square deviation is calculated and printed out as a measure of the noise level in the transmission measurements.

12. Input data for the flash-lamp spectra are calculated from a least-squares fit of a cubic polynomial. This permits absolute values to be obtained for the density in terms of spectral radiance (energy per unit area per solid angle).

Interpretation of the Linefind Printout

The paper printout from the linefind analysis is reproduced in Fig. 17. Information from this analysis is comprised of fourteen groupings and twenty-three separate columns. The groupings are to be interpreted as follows:

Indices – Column 1 contains the lower limit of the line. Column 2 is the maximum of the second derivative. Column 3 gives the refined value of the peak. Column 4 contains the upper limit of the line, and the difference 4-1 is a measure of the line width.

INDICES				POSITION	DENSITY	WL	LINEFIND	WIDTH	PEAK	NCODE	FIRST DIFFERENCES			SECOND DIFFERENCES			JJ1	TYPE	REC	NO
155	171	171	192	54.485	[illegible]	4362.642	1 0 -1	0.011	0.005	8	0.026	0.013	0.000	-0.003	0.026	0.001	1	POOR	6	5
243	288	288	319	54.[illegible]	[illegible]	4363.427	1 0 -1	0.025	0.032	8	0.025	-0.029	-0.077	-0.002	0.098	0.008	192	POOR	6	6
463	494	494	544	54.[illegible]	[illegible]	4364.810	1 0 -1	0.026	0.027	8	0.060	0.010	-0.045	-0.001	0.083	0.002	319	POOR	6	7
588	610	610	628	54.[illegible]	[illegible]	4365.595	1 0 -1	0.018	0.007	8	-0.011	-0.030	-0.046	-0.003	0.036	0.007	544	POOR	6	8
691	752	752	778	54.[illegible]	[illegible]	4366.545	1 0 -1	0.027	0.006	8	0.008	-0.006	-0.019	-0.002	0.025	0.005	698	POOR	6	9

Fig. 17 - Interpretation of the linefind analysis printout

Position – The position in mm is given in column 5.

Density – Density information is calculated to three significant figures and is printed in column 6.

Wavelength – In column 7 the wavelength is given, in angstroms, to three-decimal-place accuracy.

Linefind – Column 8 contains the left limit of the line. Column 9 gives the maximum of the line. Column 10 contains the right limit of the line.

Width – Column 11 gives the apparent width of the line.

Peak – The peak for a complex spectrum is given in column 12.

N Code – Column 13 codes the line using the system developed by Steinhaus. In this instance NCODE = 8 refers to a line peak with poor characteristics.

First Differences (Derivatives) – Column 14 contains the first derivative evaluated at J1. The first derivative evaluated at the maximum is in column 15. Column 16 contains the first derivative evaluated at J2.

Second Differences (Derivatives) – Column 17 contains the second derivative evaluated at J1. The second derivative evaluated at the maximum is in column 18. Column 19 contains the second derivative evaluated at J2.

JJ1 – JJ1 is the value of J2, the second zero point of the second derivative curve, and it is printed in column 20.

Type – The type of the spectral peak is obtained from the linetype portion of the program, and it is given in column 21. The nomenclature is after Steinhaus.

Record – Column 22 gives the record number from which the linefind analysis was made.

Number – The last column numbers the total number of peaks analyzed.

OUTPUT CARDS

The "9-Card" Format (Card Data)

Since data are handled on the CDC 3100 and the CDC 3800 computers, a communication medium is necessary between the two computers. For convenience in reading and flexibility, IBM cards in regular format were chosen; their chief disadvantage is low capacity (by contrast, binary cards can handle ten floating-point data pairs or twenty fixed data pairs). With the special 9-card format used in this program, nine data pairs are placed on a single card.

The intensity part of a data pair usually contains three significant figures, since there is a maximum number of digits readable from the digital voltmeter of the tape densitometer. (Intensity here refers to photographic density, spectral radiance, microwatts, or other such data.) By suppressing the decimal point and coding the range elsewhere, four columns on a card are more than sufficient for one intensity datum.

A scaling number on the data card specifies the position of the decimal point in the intensity; it is zero if the point is between the first and second columns of all intensity data

on a card, and it is 1 if the point is between the second and third columns, etc. Negative scaling numbers are illegal. All intensities on a given card are identically scaled according to the largest value.

Similarly, the position data never vary in more than four significant figures in the nine consecutive data points used for plotting. (Position refers to millimeters, angstroms, etc.) Therefore, positions can be separated into constant and variable parts; the constant parts are recorded only once on a card. The constant part is a whole number without a decimal, while the variable part occupies four card columns with a decimal point assumed between the first and second columns. If the position varies by more than 9.999 units in the nine consecutive points on a card, difficulties will arise, since then there is no scaling in the position data. (If it becomes necessary, a scaling number for position may be placed in column 3, but all programs would have to be modified to reflect this change.)

To separate 9-cards from the line cards, the latter generated in the linefind subroutine of the main program, a zero is always punched in column 2 of the 9-cards. The corresponding position of the line cards is always blank.

The format of 9-cards is then: Column 1, scaling number (JKL); column 2, a zero; columns 3 through 8, constant part of position (FNY); columns 9 through 12, position 1 (to be added to FNY)(POSN); columns 13 through 16, intensity 1 (scaled according to JKL) (DENSITY); columns 17 through 20, position 2 (to be added to FNY)(POSN); columns 21 through 24, intensity 2 (scaled according to JKL)(DENSITY); ...; and in columns 76 through 80, intensity 9 (scaled according to JKL)(DENSITY). The 9-cards formats are used for all position-intensity data in programs related to the use of the tape densitometer. (The programmer should note that in some earlier programs it may be necessary to alter the format statements to allow the zero in column 2; this was added after most programs were prepared, and it seldom caused problems.)

Most programs using 9-cards automatically skip positions in which both intensity and position are blank or zero. Defective cards may be edited by running such cards through the interpreter of an IBM card-punch machine. Programs using 9-cards presuppose that position data will always be positive. Care must be taken to avoid negative numbers in columns 3 through 8, since these are used as operational signals in certain programs.

Types of Cards in the Output

If cards for plotting are generated and the linefind subroutine is not suppressed, the 9-cards and line cards will be intermixed. They can be separated by discarding the extraneous cards found at the start and at the end of the punched deck (these consist of sequence cards, end-of-file cards, etc.) and by placing the rest in a card sorter and sorting on column 2; plotting cards (9-cards) have a zero punched in column 2, while line cards are blank in column 2. For plotting, the two decks are recombined: 9-cards first, then a blank card, and finally the line cards.

Suppressing the Card Output

If plotting cards (9-cards) are suppressed, the only output is print, and the spectroscopic data is now complete. The printed output will consist of lists with all indices available for interpreting the lines: position, density, wavelength (if specified), a width value, a peak function, type code (see program comments in the linetype subroutine of the "Spectra From a Tape Densitometer" program), first differences of the line and its extreme points, second differences, the type of line written in words, and other data useful to the programmer.

Each line will yield a line card, if specified on the control card, punched in standard format, with the linetype code in column 1, density in columns 3 through 5, position in columns 30 through 36, and the identification at the end of the card. These line cards may be used in the standard wavelength extrapolation programs, without modification. The option is given to have either paper, cards, or both for the linefind output. All output can be suppressed.

There are several sources of defects in the 9-cards and the line cards. Most of these are caused by defective tape records which, in turn, are usually produced by electrical transients that cause spurious characters to be written on the tape. Some irregularities in tape motion are caused by defective capstan operation. Both the internal and external capstan should be cleaned regularly with Freon solvent.

In general, defective cards may be fairly easily identified by scanning the paper output for repeated lines or by checking the list of lines for first and second differences that are very large compared to the average value. These incorrect line cards should be eliminated, and then the corresponding 9-cards should be examined for defects.

Defective 9-cards are usually apparent: position values will be unreasonably large or small, or asterisks may appear on the cards. These cards must be rejected, since they interfere with the plotting program. Sometimes this results in incomplete spectra.

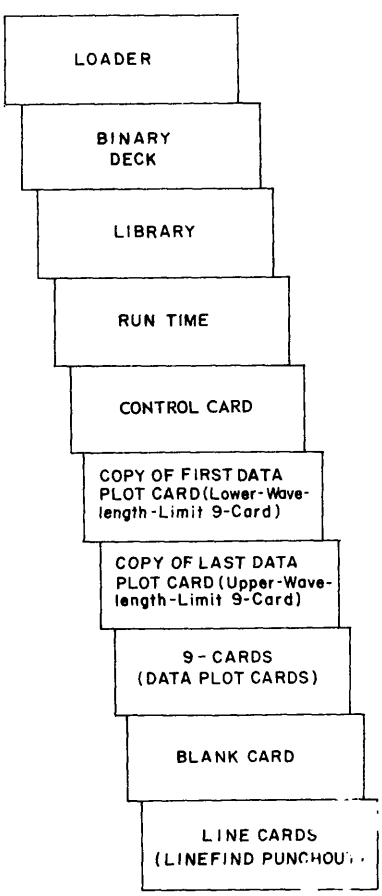


Fig. 18 - Loading sequence for plotting

Generally, it is worthwhile to print out all cards before plotting them; errors are apparent on the printed sheet. In particular, defects should be carefully sought after every parity error signal on the printed line-card list. The signal is given by the following printout statement:

"Tape error in partial record ...."

PLOTTING PROCEDURE

Plotting Data from the Computer Output Cards

For plotting, two programs are available, and both are compatible with the CDC 3100. These specialized programs, Plot Cubic and Plot Quadratic, exist in two versions, one for moderate-resolution spectra and the other for high-resolution spectra. The high-resolution plots (cubic and quadratic) are used for general absorption and emission spectra and for the echellegrams, while the low-resolution plots are used on coarse spectra like those from the plasma tube. Their printouts are given in Appendices B and C. The high and low resolution versions differ only in statements 11 through 20, and 35.

Plotting is most convenient in millimeters, at 1 mm to the inch. During plotting all sense switches are in the OFF position on the computer. The plotting deck is assembled as shown in Fig. 18.

After loading these cards into the read hopper of the CDC 3100 the master power switch is pressed, then

the STOP, MC, and AUTO LOAD switches are pressed. As the program and data begin to load, various messages will be written on the console typewriter. After the expression, "there are ... major divisions" is typed, there will be a pause (this also offers a check point for the proper operation of the program, since one can estimate if the number of major wavelength divisions typed is reasonably correct). The major divisions will be every 100Å for the low-resolution deck and every 1Å for the high-resolution deck.

The GO switch is pressed after the pause, so that the plotter can begin drawing the position or wavelength scale. Upon completing this grid there will be another pause. Pressing the GO switch will permit the data to be plotted. At the beginning of the line working routine another pause occurs, which permits changing the pen. Again the GO button must be pressed.

Restarting the Plotting Program

Under certain unfavorable conditions the plotting program will stop before completion. This will occur when the Calcomp plotter or the 3100 fails, or when defective data are present. In such cases the programmer may restart the plotting without replotting all the previous points.

When a failure occurs, the last card already read by the CDC 3100 must be removed and examined. If it is defective, it is discarded and several succeeding cards then examined for defects before proceeding.

To reinitiate the program, a new control card identical to the original one is made, but with spaces 21 through 35 blank. The plotter pen is lowered and then raised and the plotter carriage and pen are returned to their original positions, with the pen resting against the right limit of the plotter.

The cards previously plotted are set aside, the program decks, the new control card, the two limit cards, the remaining plot cards, etc., are replaced in the read hopper, and the programmer proceeds as originally. While the coarse grid is being drawn, any corrections necessary to bring the new grid base in line with the old one are made, by stopping the plotter and moving, the pen by single steps. Plotting will then proceed as before.

Format for the Plotting Control Card

The format for the control card is shown in Fig. 19. Spaces 1-10 contain SCALE X (F10.3), which is the number of intensity units

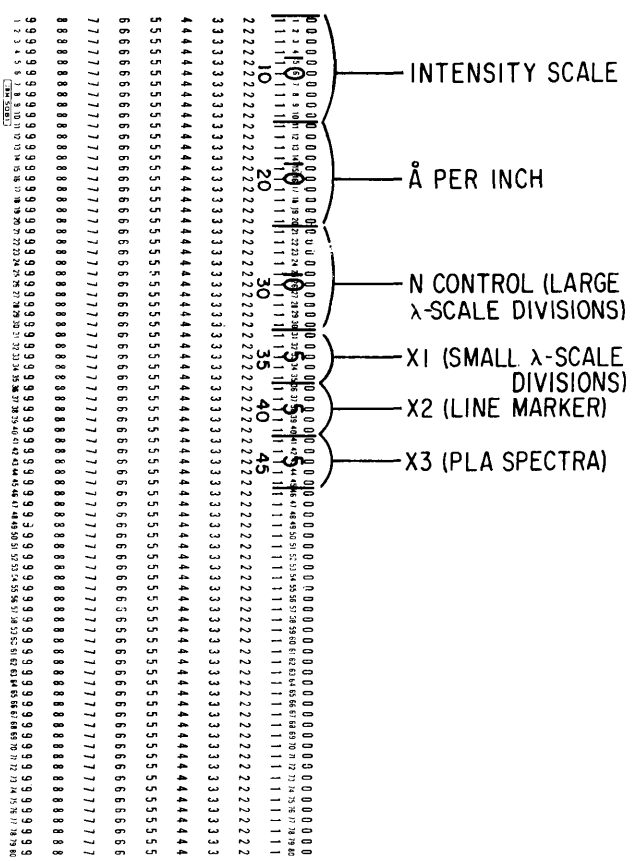


Fig. 19 - Control card for plotting

equivalent to 1 in. (density, spectral radiance, microwatts, etc.). Ten times this value is full scale. For density a convenient value is 0.35, which gives 3.5 density units full scale. (If X = 0.1, it will produce a scale factor ten times greater than X = 1.0.)

We note that SCALE X and SCALE Y are inverted in the plotting program, the former yielding the ordinate and the latter yielding the abscissa of the graph. Both SCALES are floating point fields, and the number entered requires a decimal point but no left or right justification.

Spaces 21-30 hold N CONTROL (I10). If a nonzero integer is placed here, subdivisions of one-tenth will be drawn on the wavelength axis. A negative number or zero produces only a coarse scale (one division for each angstrom for the high resolution and one division for each 100 angstroms for the low resolution plot). The numerical entry must be right-justified. For fast work, leave this entry blank.

Spaces 31-35 hold XI (F5.2). A positive number determines the spacing on the intensity axis. A zero, blank, or negative number causes the plotting pen to return to the zero level of the grid, and no grid is drawn. If it is a positive number X, a line will be drawn X units above the base, 2X units above the base, etc.

Spaces 36-40 hold X2 (F5.2). This is the signal for line-marking. Any negative number with a decimal point will cause the spectral peaks to be identified. Using this feature requires a blank card to be placed after the 9-cards, followed by the line cards, which are also ended with a blank card. The blank card stops the computer. Execution is then automatic.

Spaces 41-45 hold X3 (F5.2). If it is blank, the plotting pen will advance 10 in., and the program will repeat. If it is positive, the pen will move back to its starting position, and the program will restart.

Spaces 46-50 hold X4 (F5.2). A negative number modifies the line marker length for use in the plasma tube spectra; a blank or zero leaves it unchanged.

Spaces 51-55 hold X5 (F5.2), which is not presently used. In general N CONTROL, X1, and X2 control the wavelength scale.

Recycling Program, Replot Card – The normal end for a plot occurs when a blank card follows the 9-cards. To plot additional spectra on the same grid, a replot card is used. The replot card consists of spaces 3 through 8 filled with the entry -9999, and the rest of the card is blank.

The steps used are (a) end the first set of 9-cards with a replot card, (b) add the second set of cards without control or limit cards, (c) end these with a replot card, and (d) add the third set of data, etc. End them all with a blank.

Modifications on the Position Axis

The position scale can be converted from, say, millimeters to angstroms by a quadratic or cubic interpolation, if three or four wavelength standards are known, respectively. For quadratic conversions use Plot Quadratic, and for cubic conversions use Plot Cubic. (In all other respects these two programs are identical. They were not combined because of memory limitation of the CDC 3100.)

To use this conversion, sense switch 5 must be ON, and the three (or four for cubic) position-wavelength cards must directly follow the control card. These cards contain the wavelength in spaces 16 through 25 and the position in spaces 26 through 36.

For the echelle program it is necessary to convert the wavelengths of the University-of-Florida data to millimeters, the reverse of the normal conversion. For this case, the positions are typed in spaces 16 through 25 and the wavelengths are typed in spaces 26 through 36.

Modifications of the Intensity Axis

Various alterations can be made on the intensity axis. All were designed for the echelle project, but most are generally useful for other spectra.

The Ax Intensity + B Alteration – If sense switch 6 is ON, the console typewriter will ask for values of A and B to be applied to all intensity values (coded as GA and GB). By inserting a positive or negative value of B, the scale can be shifted up or down. By inserting a value for A greater than or less than 1.0, the relief of the plot can be magnified or diminished.

GA and GB are normally 1.0 and 0.0, unless altered. A new value for either is inserted by typing the numbers, with a decimal point, and pressing the FINISH button. The typewriter will repeat the number as a confirmation. If FINISH is pressed without a number being previously typed, a zero will be assumed. GA must never equal zero.

The Skew Correction – Simetimes it is necessary to tilt a spectrum. This occurs in the echellegrams, and it might occur when the background density of an emission spectrum rises or falls as a nearly linear function of wavelength.

Sense switch 3 is turned to ON. When the console typewriter asks for it, the positive or negative correction to be made at the 38-millimeter position is typed in assuming that there is no correction to the 10-millimeter position (which acts as the axis). A decimal point is needed. All intensities will be shifted proportionately.

The Polynomial Background Corrections – In the echelle project a large adjustment must be made for scattered light. For this purpose a fourth-degree polynomial is used to represent the density of the scattered light. This is evaluated at every point and is subtracted from the raw intensity.

Since the level of scattered light varies from side to side of an echelle order, polynomials are generated separately for each side. Polynomials represent density as a function of position, in millimeters, with the low-wavelength edge of each order arbitrarily set at 10.0 mm.

The coefficients FA, FB ..., FE of the expression

$$\text{density} = FA + (FB \times P) + (FC \times P^2) + (FD \times P^3) + (FE \times P^4),$$

where P is the position in mm, are punched in order, five to a card. The program therefore uses two such cards and averages the readings. The format of the punched cards is E16.8, while that of the printout portion is F15.3.

The Punch Order – If sense switch 1 is ON, the console typewriter will ask that identification be typed, and then cards containing all modifications will be punched. These may be used to convert the present 9-cards to new 9-cards, altered by all modifications listed above. With these cards and the Conversion of Densities to Intensities program, echelle density cards can be converted to intensity cards on the CDC 3800.

Defects of the Program

1. The overwhelming time consumer is the linetype subroutine. It is probable that many changes can be made to improve its efficiency.

2. The linetype subroutine does not adequately handle very dense lines which "bottom" in the transmission, i.e., lines with a peak transmission of less than about 1%. These lines have steps in the dark portions of their profiles which makes the second-derivative analysis erroneous. This problem can be corrected.

3. Shoulders and near-shoulders are not adequately analyzed in the linetype; at times, broad lines are typed as shoulders and are not analyzed.

SUPPLEMENTARY PROGRAMS

Blocked Gaussian Smoothing Designed for the CDC 3100 Computer

Data are smoothed by a Gaussian curve approximated by six weighted data blocks. During the reading of the program into the computer, there will be three pauses where the console typewriter will request information.

At the first pause an integer followed by a decimal point is typed in. The minimum value is 1.0, which gives minimum smoothing. Maximum values will depend upon the required degree of smoothing. The FINISH button is then pressed.

At the second pause the difference between the true fiducial and the actual position on the densitometer is typed in (in millimeters). The FINISH button is then pressed.

At the third pause some minimum density above background is typed in to eliminate background noise. The FINISH button is again pressed. Original 9-cards placed behind a binary deck of this program will be read, and the smoothed cards will be punched.

Polynomial Fit of Backgrounds Used in the CDC 3800 Computer

Using three subroutines (INCARDS, POLYFIT, and OUTCARDS) this program reads in 9-cards, obtains the least-squares polynomial of fourth degree that best fits these data, punches out the coefficients of the polynomial, and punches out 9-cards showing the data as calculated by the polynomial. It is designed to obtain the polynomial that best represents the backgrounds adjacent to the orders (scattered light). The card output allows trial plotting of the backgrounds in polynomial form.

A-Plot Conversion Used in the CDC 3800 Computer

The Plot Quadratic and Plot Cubic programs overflow the memory of the CDC 3100 when used with the versatile A-Plot subroutine of Douglas McNutt's library program. To conserve space, McNutt developed a conversion of A-Plot to Plot-F (Calcomp plotter) or Plot-G (Gerber plotter). These are generated by this program.

To execute the program, the A-Plot and the Plot-F decks are placed behind the binary Plot Quadratic or Plot Cubic programs. Note that the program must be recompiled for use with Plot G. (See program description for Plot F and Plot G.)

Programs Used for the Echellegrams

Conversion of the University of Florida Cards (3100) – The program for the echellegrams condenses the University of Florida cards to the 9-card format, scaling those that need to be scaled. Punchout can be intensity in either the microwatt – or photon-form.

Conversion to 1.000 + LOG_{10} Intensity – Using the decks of the subroutines Incards and Outcards, 9-cards are read, data are converted to log data + 1.000, and the converted data are punched. This program converts the University of Florida intensity data to log intensity, and adds 1.000 to avoid the inconvenience of negative numbers.

Conversion of Densities to Intensities (CDC 3800) – Control cards from the punch output of Plot Quadratic or Plot Cubic are read (title card; FA, FB, FC, FD, and FE; GA and GB; HA; and ZC, ZB, ZA, and ZD) and then a Plot Correction card is read. An Incards subroutine then reads the 9-cards to be converted. The conversion is made, and an Outcards routine punches the converted 9-cards. Operation is completely automatic.

OPERATING PROCEDURE FOR THE TAPE DENSITOMETER

Decide how many spools of magnetic tape will be needed. The maximum usable scan of the comparator is about 190 mm. At a scan rate of 1 mm/min, 1-1/2 scans will fit on the usual tape. If only one 10-in. plate is to be scanned (possible to do only in two sections) one tape will suffice.

Before using the densitometer, the light source should have been in the "Operation" position for several hours (not on "standby"); this helps to eliminate drift produced by the lamp. The following steps are used in operating the comparator.

1. Filters – The filters are located on the JACO unit. To operate this unit, turn the neutral-density filter knob to 7 or 8 to avoid damaging the phototube in the following steps. The normal filter position in a spectral scan is 4 or 5.

2. Spectral Plate, Carriage, and Slits – Insert the plate with the low wavelength to the right. Adjust the carriage angle so that the optics remain centered on the spectrum through an entire scan. Rotate the bottom table so that its slit is aligned to some compromise average line. Adjust the tilt of the light source slit to be parallel to this line. (The light source slit is unstable and changes direction unpredictably during operation of the densitometer.) Focus the optics on complex weak-line structure with the bottom lens (which lies above the bottom table) of the JACO unit.

3. Slit Length and Slit Width – Adjust the OCCULTER to the desired slit length (it is best to partially block the slit, watching the transmission on the digital voltmeter, to determine the precise limits of the occulter). The maximum possible length is usually best.

Back off the slit WIDTH knob, turn it back until light just registers on the digital voltmeter (this is presumably the zero point) then continue opening it to 15μ (or any desired value) above the apparent zero point (normal operation for a JACO slit).

4. Gain and Filter – Move the carriage manually to a point off the plate where there is only air. (Air is the first medium in this procedure. Any other medium may be used, such as glass or the unexposed emulsion.)

Adjust GAIN on the Datex unit for maximum amplification with a suitable noise level. Simultaneously adjust the neutral-density filter on the JACO lower table and the fine control on the Datex amplifier to read about 97% on the digital voltmeter, using the highest possible neutral-density filter position (97 on the voltmeter indicates 97%, etc.).

5. Noise Level Determination – Move the carriage so that a moderately dark portion of the plate can be measured. Observe the noise level from the variations on the digital voltmeter. If the transmission is, say, 10% and the plate is not moving, there should be no apparent noise. If noise is apparent, there is an electrical problem.

6. Parameters on the Datex Unit – The important input parameters to consider in conjunction with the Datex unit are those for absorption, emission, and solar echellegrams, and those for plasma-tube spectrograms. The formats for the parameter inputs is listed in Appendix M.

7a. Fiducial for Absorption, Emission, and Echellegrams – Adjust the carriage to the fiducial point. This is conveniently the low-wavelength edge of the plate, normally coded 10.000 mm, but it may be any other feature with a known nonnegative calibration.

To use the low-wavelength edge of the plate, move the carriage by rotating the hand wheel to an OFF-PLATE position adjacent to the low wavelength edge. Using the REVERSE DRIVE switch, advance the carriage until transmission decreases from 97% or so to, say, 40%. This value will be considered to represent the edge of the plate and will automatically assign 10.00 mm in the main program, if no value is specified by the operator.

Since the plate cannot be completely scanned in one pass, the high-wavelength edge must be used for the high-wavelength end of the plate. For this region the same operation is performed in reverse as for the low-wavelength edge. On the control card the high edge can be assigned a value 262.8 mm; this will maintain nearly constant values on a nominal 10-in. plate.

7b. Fiducial for Plasma Tube Spectrogram – The fiducial mark used here is the 4358.35-Å Hg line and falls at the 54.279-mm position on the JACO densitometer. This millimeter value is specified on the control card for the program input.

8. Mounting Tape – Clean the tape recording head and associated parts with Freon solvent. The capstan drive is wiped by placing the first switch in the LOAD position and turning the SLEW switch for a few seconds (holding this switch on for more than 2-1/2 min may cause the motor to burn out. The inner part of the capstan is reached by opening the front panel.

Mount the tape, and advance it to the starting position by pressing the LOAD POINT switch until the tape stops at the metal mirror, which is attached about 10 ft from the beginning of the tape (this switch also must not be held down for longer than 2-1/2 min).

Next, turn the left-hand switch to AUTOMATIC and press the PARAMETER button five times. This will write five parameter records on the tape, each containing the parameters dialed on the DATEX console.

9. Room Lights – Turn off any fluorescent lights in the densitometer cubicle. During the densitometer run, avoid turning on lights, since the switching introduces false data on the tape. (Keep a flashlight available.)

10. Fiducial and Record Length – Adjust the record length to 3000 on the Datex unit. The first data recorded are the "fiducial record." The carriage should be in the

fiducial position at this point (from operation 7a or 7b). Next write a partial record by turning the console switch to RECORD for 5 sec and then returning it to the OFF position. Even if the fiducial is bypassed in later processing, a record must appear in this position. Record the densitometer position; this is the first record.

10a. First-Medium Record – Back the carriage off manually to an OFF-PLATE position, and record another partial record (5 sec or less at a setting of 3000). The digital voltmeter should read about 97% from the last operation. If it has drifted to a higher value, readjust the Datex fine-gain control to the 97% value. This is the second record and is called the "first-medium record." It establishes the 100%-transmission point and converts all subsequent data by this factor. As an indication of noise level it measures root-mean-square deviation from the average. For the plasma-tube spectrograms the first-medium record is taken at a clear glass area on the plate.

10b. Second-Medium Record – The third record is the second-medium record. In grazing incidence spectra there is no second medium, such as unexposed emulsion, which one normally wishes to measure. This record must be filled, however, and one may record air transmission again as a check on the first-medium records. Transmission of the second medium is calculated and printed out, but no use is made of it in the program (a 5-sec reading at a record length of 3000).

In the plasma-tube case the second-medium record is made at an area on the emulsion, free from spectral lines. The plate should be scanned over this region while the measurement is taken.

11. Record Length – Turn the record-length switch to 15,000. For coarse spectra, as is the plasma-tube type, a record length of 7500 is appropriate. (See the section on N SEARCH in the Main Program.)

12. Main Scan – Move the carriage manually to just below the portion of the spectrum to be scanned, turn the scan speed knob to 1 mm/min, and turn the drive switch to REVERSE to begin the scan. Turn the Datex console knob, lying below the parameter switches, to RECORD after the carriage is visibly moving.

If the background is sufficiently opaque as indicated by a low voltmeter reading, turn the filter knob to the lowest position which does not yield more than about 95% in the lightest areas of the plate; make this change as soon as possible.

Allow the spectrum to record continuously for a maximum of about 3 hrs or 190 mm.

13. Finishing the Scan – When the scan is completed, turn the RECORD switch on the Datex console off. Also, turn the drive switch on the JACO unit off. After the tape stops running (up to 100 sec later) press the END OF FILE button on the Datex unit, thereby writing a file mark on the tape.

14. Not Last Scan – If another scan is to be made on the same tape, change the parameters to represent the next scan and press the PARAMETER button as before. Do not turn on the lights, nor turn off any portion of the Datex unit. Proceed to immediately adjust the plate carriage, the 97% clear transmission, locate the fiducial, and proceed with the next scan (steps 1 thru 13) to the end of the tape or experiment. It is not possible to record part of the tape, remove the tape, or turn off the Datex system, and later continue recording.

15. Final Scan – If no more data to be recorded, press the END OF FILE button four or five times. This completes the run.

Processing the Tape – Using the Main Program (Appendix A), process the tape on the CDC 3800. If the scan is to be plotted at 1 mm = 1 in., then NO CARDS = 10 is a convenient punched-card output. If lines are to be found, but no plotting is necessary, NO CARDS should be left blank. A card will be generated for each line found.

THE LEAST-SQUARES SOLUTION OF WAVELENGTHS (POLYFIT PROGRAM)

To convert the raw comparator-microphotometer data (plate position and transmission) from a spectrogram into useful wavelength and spectral-radiance (or energy or intensity) information, the following information must be known from previous calibration experiments:

1. The variation of wavelength with reciprocal dispersion, relative to a standard or fiducial spectrum line for the spectrograph.

2. Variation of spectral radiance (or relative exposure) for the photographic film or plate which is used. This may be determined from the standard H-D curve technique (density vs log exposure).

3. To change in the response of the photographic film or plate as a function of wavelength.

Each of these quantities can vary considerably, if the exact temperature, photographic development techniques, and emulsion characteristics are not rigorously maintained to some standard reference. In the following discussion, however, we will assume that these conditions have remained constant.

The usual method for determining wavelengths from a photographic record is to (a) identify a number of wavelengths with the respective emissions at given positions on a plate, (b) calculate the approximate positions of the wavelengths from some standard equation, such as the grating equation, a linear or quadratic equation, and (c) plot the differences between the true positions and the calculated positions to obtain a correction curve.

The correction curve has the property that for any position the true wavelength may be determined. Similar techniques are required to reduce the transmission data described previously in paragraphs 2 and 3.

A technique more easily adapted to computer methods, and perhaps even more accurate, has been applied in the present computer program to reduce the spectroscopic data. This technique employs a least-squares solution, which considers all observed data. A sufficient number of terms are included in the final solution so that the standard or root-mean-square deviation is less than some predetermined limit. Several such least-squares programs exist, and, in this program, a modified version of the IBM 1620 program 7.0.002 was used.

To determine the wavelengths by this approach, a least-squares solution of the equation $\lambda = f(d)$ is obtained, where λ is the wavelength and d is the position. The wavelength can be calculated from the expression

$$\lambda = A_1 + A_2 d + A_3 d^2 + \ldots + A_{n+1} d^n, \tag{1}$$

where the A's are the coefficients of the least-squares solution and n is the highest power used in the expansion.

Since spectral radiance is proportional to the inverse of the transmission, a similar least-squares solution of the type

$$SR = f(1/T), \tag{2}$$

where SR is the spectral radiance and T is the transmission, was solved to obtain absolute values of the intensity.

To obtain a better fit of the data to this type of expansion, the solution was divided into two separate solutions depending upon the value of T, i.e., if $T \leq T_x$ one solution was used, but if $T > T_x$ the other solution was applied. The predetermined value of the transmission used to separate the two solutions is T_x.

Using this method of separating the solutions, the two solutions may be calculated by using

$$SR = C_1 + C_2 \times (1/T) + C_3 \times (1/T)^2 + \ldots + C_{m+1} \times (1/T)^m \text{ for } T > T_x, \tag{3a}$$

and

$$SR = D_1 + D_2 \times (1/T) + D_3 \times (1/T)^2 + \ldots + D_{n+1} \times (1/T)^n \text{ for } T \leq T_x, \tag{3b}$$

where the C's and the D's are the coefficients and m and n are the highest powers in each of the respective solutions.

Similarly, the variation of the film response with wavelength may be determined as the solutions

$$V = B_1 + B_2 \lambda + B_3 \lambda^2 + \ldots + B_{q+1} \lambda^q \text{ for } \lambda > \lambda_y \tag{4a}$$

and

$$V = E_1 + E_2 \lambda + E_3 \lambda^2 + \ldots + E_{r+1} \lambda^r \text{ for } \lambda \leq \lambda_y , \tag{4b}$$

where V is the multiplication factor. (To be able to use the available least-squares programs, λ was divided by 10 to determine the above solutions, and it was corrected in the main program.)

With these solutions for each set of data, a wavelength is calculated from Eq. (1) and the final spectral radiance is calculated from Eqs. (3) and (4) as SP*V. These results are then printed out with the position and transmission, or they are plotted from the 9-cards as a computer trace.

The program used in the polynomial curve-fitting (POLYFIT) uses four "sense switches" on the console of the CDC 3100. Setting these switches to the ON position has specific effects on the program. (POLYFIT – Listed in Appendix J)

Sense switch 1 causes cards to be punched out, and it prints the coefficients A_0, A_1, ... A_n. The printout sequence is (a) order, (b) deviation, (c) rms deviation, and (d) number of points. These coefficients will be punched on the cards.

Sense switch 2 commands the program to go to the next higher order of the least-squares fit; it will continue to increase the order of the calculations until the switch is turned off.

Sense switch 3 uses the information contained in the preceding order of the least-squares fit and will cause the columns of information to be printed out in the order (a) position, (b) input data, (c) computed data, and (d) difference.

Sense switch 4 permits typing in the highest order used in the curve-fitting; i.e., it permits the tolerance to be determined. After the desired value is typed in, the switch is turned off, the FINISH button is pressed, and the GO button is pressed on the console.

To execute this program the cards are grouped in the following manner: (a) dumped binary deck, (b) runtime deck, (c) an identification card, (d) the data cards with wavelength in angstroms punched in columns (F10.4) 16 to 26 and position in mm punched in columns (F8-3) 30 to 38, and (e) a blank card.

THE WAVELENGTH COMPUTATION PROGRAM (λ CALC)

The wavelength computation program is given in Appendix K, and allows one to calculate the wavelengths found by the least-squares method (POLYFIT). The calculation is achieved by using the coefficients from each order obtained from the POLYFIT program.

To execute the program, the order to be used for the computer decks is (a) binary λ calc, (b) runtime, (c) identification card, (d) order coefficients, (e) blank card, (f) POLYFIT cards, and (g) blank card. In the λ calc program the sense switches used on the CDC 3100 are (a) switch 2, which when off gives the format λ only and when on given the format λ and frequency, (b) switch 3, which when on punches cards, and (c) switch 4, which when on prints on the console typewriter.

PROCEDURE FOR REDUCING ECHELLE DENSITIES TO INTENSITIES

Reducing echelle densities to intensities is complex and assumes some familiarity with the equipment and programs. A sound approach would be to go through all steps, including plotting, given previously. When this procedure is mastered, the additional complexities of the echelle project will be manageable.

Obtaining Coefficients of the Polynomials Representing Scattered Light

Most of the following steps can be performed in one operation for all the scattered light (backgrounds) on a given film. For example, the calculation in 6 below can be performed on many sets of data in one pass through the 3800. A reasonable method of naming backgrounds is by the orders surrounding them, for example, the background between orders 104 and 105 can be named 104-105. All plotting is in millimeters versus the density of intensity.

1. Trace the backgrounds surrounding all usable orders on a given film at 1 mm/min on the tape densitometer according to the previous directions and the checklist (Appendix N). The backgrounds can be traced on one standard spool of tape. The carriage will have to be moved laterally during a scan, since the orders are not straight. The fiducial record should be at the low-wavelength edge of the order.

2. Using the Main Program, obtain condensed data cards (9-cards) for plotting. This program uses the CDC 3800. Suppress linefind, use 10.000 mm as the fiducial representing the short-wavelength end of the scattered light, and punch every fifteenth datum (NO PUNCH - 15).

3. Plot the backgrounds on the Calcomp plotter of the CDC 3100.

4. Identify those features on the plots which arise from defects such as scratches, pinholes, dirt, and ghosts. Remove data encoding the defects by inserting blanks in the density and millimeter positions of the cards, or remove the cards if the defect covers data of an entire card. Smooth the remaining data with the Blocked Gaussian Smoothing program (Appendix D) on the CDC 3100. The mean deviation ($\sigma/2$) should be set to 25,

which results in a great reduction of cards. Other linear adjustments can be made to the data during processing by this program. Edge cards, that is, cards containing the transition from pure film-emulsion density to scattered light should be discarded before processing with this program, to give a curve which can reasonably be approximated by a polynomial.

5. Plot the cards from 4 to ensure that the smoothing proceeded as desired.

6. Obtain the polynomial equation representing each background using the Polynomial Fit of Backgrounds program on the CDC 3800 computer. The output will be (a) cards with the coefficients of the polynomial equation and (b) cards containing the data calculated by the polynomial in 9-card form for plotting. Preserve the coefficient cards and label each one.

7. (Optional) Plot the 9-cards from 6 to ensure that they are a satisfactory representation of the scattered light.

Preparing the Standard Spectrum in Useful Form

Data were received from Alex Green, Department of Physics, University of Florida, on cards containing wavelength, intensity in $\mu W/cm^2$-Å, and intensity in photons/cm^2-sec-Å. The microwatts form was chosen for this project. See Ref. 9 for a tabulation of the data.

1. The number of cards had to be reduced to a reasonable quantity. They were condensed to 9-card form using the Compress Solar Spectrum Cards program (Appendix I).

2. The log of the intensity is necessary for subsequent operations. Conversion is made by using the program in Appendix G the CDC 3800 computer.

3. The arbitrary 1.000 added to log intensity to eliminate troublesome negative values must be corrected for in all subsequent calculations.

4. It should be remembered that there are discrepancies in these cards which are not present in the original NRL reduction of the data. Step discontinuities can be seen at 2499 Å and 2519 Å, for example.

Preliminary Preparation of an Order

1. Trace an order of the echelle, from low to high wavelength, on the tape densitometer at 0.5 mm/min. A mask made from two IBM cards can conveniently isolate an order, allowing about 3/4 of the order to show. It will be necessary to constantly adjust the stage laterally during a scan. Make certain that the slit is tilted properly to match the average line tilt, usually about 3 degrees. The upper (scattered-light) mask must be in place. Parameters should be precisely set and recorded five times, and the fiduciary record (the first record) should be on the short-wavelength edge. Adjust the filter setting to its constant setting in the order during the fourth record, to avoid bottoming and stopping in dense portions and changing settings during the scan.

2. Process the tape using the Main Program. The output will be about 3000 cards (9-cards). The following are suggested parameter settings for the control card:

SPECTRUM:	ECH
N SEARCH:	24
N SMOOTH:	1

N SKIP:	blank (1) if first file on tape
N FILES:	blank (1)
N RECORDS:	blank (0)
NO LINES:	blank
NO CARDS:	3
NO PRINT:	blank
NO WL STD:	blank
N PUNCH WL:	blank
NO REFINE:	blank
N PRNT SKP:	blank
MAX PRINT:	blank

DIF 2 MIN:	blank (.021)
DENS MIN:	blank
WIDTH MIN:	blank
FIDUCIAL:	blank (10.000 mm)

3. Separate the linefind cards from the 9-cards by sorting on column 2. (However, with the above entry for NO LINES, no linefind cards will be punched.)

4. To verify that there are no missing gaps, bottoming, step areas, or other defects in the data, plot the cards on the Calcomp plotter of the CDC 3100 using either the Plot Quadratic or Plot Cubic programs. This will give a standard high-resolution densitometer trace of density vs position in mm, similar to that previously used for line identification.

The above control card might have consisted of the four entries: 0.35 (for a dense order), 1, 0.25, and -1 (the latter only if it is wished to mark the lines identified by the linefind feature of the Main Program.

5. Next, the spectrum must be deresolved to match the standard spectrum. It will be necessary to deresolve it to varying degrees to find the proper resolution match to the standard spectrum. For this the Blocked Gaussian Smoothing (Appendix D) program should be used on the CDC 3100. The proper value for the 1961 spectrum is generally $\sigma/2 = 75$, but it would be appropriate to test several values, say, 60, 75, and 90 to assure the best possible resolution match between the deresolved order and the standard spectrum.

6. Preserve the cards produced from 2.

Determining the Coefficients for Converting Echelle Densities to Intensities

The critical phase in converting echelle densities to intensities is generating the coefficients used in the final reduction of the spectrum.

All plotting is done with the Plot Quadratic or Plot Cubic program on the CDC 3100. Although previous plotting could have been done on the 3800 and plotter, this phase must be performed on the CDC 3100, because of the many adjustments in this trial-and-error procedure.

1. Abstract the cards for the proper wavelength range from the logarithmic cards of the standard spectrum obtained from the program in Appendix G. Prepare three wavelength standard cards for the quadratic plot, or four for the cubic program, relating the millimeter position to wavelength. Since the beginning point of each spectrum is coded as 10 mm, the middle is 24 mm, and the end is 38 mm, the tabulated begin, middle, and

end values for the various orders may be used here (found in the data section of the Main Program). They must be used backward, to convert wavelengths to millimeters, for the greatest convenience in the phase of the project.

The entire project may be performed on a wavelength instead of a millimeter basis if corrections are made in the "background correction" portion of the plotting programs. Such a change would be intricate and might tax the small memory of this computer.

2. A convenient set of plot parameters should be found for scaling the standard spectrum, including constant upward or downward shifts (i.e., a number to be subtracted from the 1.000 + $\log_{10}$ intensity, without multiplicative corrections). The standard spectrum is then plotted with the constant corrections entered from sense switch 6, using sense switch 4 and the standard cards, to make the long intensity-vs-mm plot.

3. The deresolved order cards from the Blocked Gaussian Smoothing program are plotted on the same scale using the two surrounding background cards from the Polynomial Fit of Backgrounds program (Appendix E) with sense switch 4 on.

4. Consider the constant value that should be added to the order plot to bring it vertically to the same position as the standard plot. Replot as before with background cards and sense switch 4 on) with sense switch 6 on, typing this constant correction when asked for by the console typewriter and typing 1.0 when asked for the linear correction.

5. Examine the resulting plot. If the order plot needs more relief to match the standard, replot with a greater linear correction. Continue to replot the order until it matches the standard plot as well as possible. It will probably be necessary to replot the standard on fresh paper after three or four plots of the order have been made.

6. After obtaining the best possible fit by adjusting the linear and constant factors, there may remain a slight tilt of the order plot relative to the standard plot. The skew correction, activated by sense switch 3, allows the right edge of the order spectrum to be raised or lowered to correct such a tilt.

7. When all corrections have been made, replot the standard on fresh paper, turn sense switch 1 on, and replot the order with all final corrections. Besides the graphs, output will consist of punched cards preserving all the corrections for later use (it will be necessary to type some information for identifications when requested by the typewriter). Preserve this final graph as a record of the closeness of fit of the order to the standard spectrum.

8. Determine the plot correction by considering the constant corrections applied to the standard spectrum (in the log-intensity form). The standard cards used in steps 3 through 7 of this section are log intensity + 1.000, and a constant correction is normally used to plot these cards on a convenient scale. If such a correction is -0.6, for example, the net plot correction is -0.4, from - (1.000-0.6).

9. Using the Conversion of Densities to Intensities program with the card output from 7 and another card specifying the plot correction from 8, convert the deresolved order cards to intensities. Save the cards for reference.

10. The output of 9 should then be plotted on the same scale as the same wavelength range of the standard cards in microwatt form (9-cards, output from Appendix F). Wavelength standard cards and sense switch 4 should be used to convert the standard cards to millimeters.

11. If the two spectra from 10 are very similar, the coefficients may be accepted. In all cases, the edges of the order will not be satisfactory and will have to be discarded – the acceptable portion of all spectra will include at most the range from 15 mm to 35 mm. In some cases it may even be necessary to determine several sets of coefficients for different sections of the order.

Final Preparation of Wavelength – Intensity Curves

The reader who has followed the previous four sections should have a good comprehension of the capabilities of the available equipment and the significance and limitations of the data.

After the preceding steps have been followed for several orders, several decisions must be made concerning the final preparation of the wavelength-intensity curves. The following are some important ones.

1. The original echelle wavelength table was made by a cubic-least-squares polynomial fit within each order. Since four data pairs will uniquely determine a cubic equation relating wavelength and millimeter position, the calculated wavelength from the table and the position of four lines on the present scan will precisely reproduce the calibration used in the echelle wavelength table. Therefore, the Plot Cubic program can be used with some form of the order cards (not deresolved) to obtain the spectrums calibrated by wavelength. There are several alternatives.

After obtaining and testing the calibration in the last section, convert the millimeter-density cards (not deresolved) from the order to millimeter-position cards with the Conversion of Densities to Intensities program (as was done with the deresolved order cards). These can then be used with the Plot Cubic program with four wavelength standard cards to generate the finished wavelength-intensity spectrum on the Calcomp plotter.

Since the Calcomp plotter yields a "stepped" plot generally unsuitable for publication, the same steps can be performed with the Plot Cubic program and the A Plot to Plot G subroutine to yield paper tape for the ESD Gerber plotter. (Plot Quadratic and Plot Cubic both use a two-card binary subroutine, which is A Plot to Plot F for the Calcomp plotter and A Plot to Plot G for the Gerber plotter. In addition, for the Gerber plotter, the programs must be recompiled with a "Call A Plot (dummy, dummy, 5)" order (this card is included in the Fortran statements as a comment card). This complicated procedure must be followed because of the small memory of the CDC 3100.

The Plot Quadratic and Plot Cubic programs may be altered so that all conversions listed in the last section are performed on a wavelength scale instead of a millimeter scale. This would probably only involve conversion of the background correction to a wavelength form. There may not be room in the computer's memory for such a change. The background correction cards themselves must be in millimeters instead of wavelengths, since each card refers to two adjacent orders (background card 94-95 is used to correct order 94 and order 95, and the only common scale for both orders is in millimeters).

2. Decisions must be made on the form of presentation of the final curve. If it is to be in, say, 20-in. sections at 0.3 A/in., it would be most reasonable to plot the data directly in this form, that is, in the appropriate sections to be directly reproduced rather than alter the final plot by scissors and pen before reproduction. Decisions must be made concerning (a) publication format - length and width of plot, (b) the scale markers for the intensity scale as well as the wavelength scale, and (c) modifications of the scaling of both axes.

See Appendix N for the checklist necessary for densitometer operation in processing the echellegrams. Also, refer to the section on supplementary programs.

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Appendix A

THE MAIN PROGRAM FOR SPECTROSCOPIC ANALYSIS

```
'JOB,73N0111,220EFD,5
'EQUIP,1=SV,RO,LO,**,DA
'FTN, L,X
      PROGRAM MAIN
COMMENT     SPECTRA FROM A TAPE DENSITOMETER
      TYPE INTEGER TYPE, MESSAGE, INTEGERS, SPECTRUM, OPTION 1,OPTION 5
      DIMENSION INDATA (2000), POSN (3000), TRANSM (3000), WL (3000),
     1 TRANSM1(3000),  DENSITY1(3000), WLS (125,3), LINEFIND (3000),
     1 FILDENS (9), FILDEN (9), NTITLE (8), ITITLE(10), DIF (3000),
     1 DIF 2 (3000), Y OUT (3000), INTEGERS (24) , SPEC RAD (3000)
      EQUIVALENCE (N FILTER, Y OUT)
      COMMON/BLOCK/DENSITY (3000), N FILTER (3000)
C  INPUT DATA STATEMENTS . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .
C   WAVELENGTH DATA FOR ESTABLISHING STANDARD LINES BY A QUADRATIC CURVE FITTING
      DATA ( ( WLS(I,1),I = 80, 120)  =
     13027.861, 2990.533, 2954.010, 2918.423, 2883.770,
     12849.773, 2816.871, 2784.286, 2752.709, 2721.783,
     12691.588, 2661.983, 2633.093, 2604.779, 2577.123,
     12549.987, 2523.451, 2497.555, 2472.095, 2447.178,
     12422.747, 2398.753, 2375.240, 2352.249, 2329.645,
     12307.597, 2285.788,    0.   ,    0.   , 2264.045,
     12243.624, 2223.393, 2203.545, 2184.077, 2164.992,
     12146.295, 2127.766, 2109.716, 2091.905,    0.   )
      DATA ( ( WLS(I,2),I = 80, 120)  =
     13049.477, 3011.811, 2975.093, 2939.250, 2904.289,
     12870.101, 2836.733, 2804.109, 2772.252, 2741.107,
     12710.636, 2680.844, 2651.708, 2623.211, 2595.296,
     12567.988, 2541.221, 2515.087, 2489.419, 2464.288,
     12439.633, 2415.469, 2391.775, 2368.559, 2345.771,
     12323.430, 2301.493,    0.   ,    0.   , 2278.075,
     12257.426, 2237.059, 2217.079, 2197.455, 2178.131,
     12159.203, 2140.556, 2122.245, 2104.226,    0.   )
      DATA ( ( WLS(I,3),I = 80, 120)=
     13069.606,  3031.751,  2994.729,  2958.672,  2923.435,
     12889.055, 2855.414, 2822.590, 2790.494, 2759.187,
     12728.438, 2698.456, 2669.125, 2640.441, 2612.289,
     12584.829, 2557.875, 2531.516, 2505.628, 2480.295,
     12455.409, 2431.147, 2407.289, 2383.814, 2360.907,
     12338.334, 2316.252,    0.   ,    0.   , 2291.224,
     12270.448, 2249.881, 2229.703, 2209.962, 2190.500,
     12171.335, 2152.573, 2134.072, 2115.883,    0.   )
C   JACO FILTER DENSITIES.....................................................
      DATA (FILDEN  = .479,.425,.420,.413,.380,.378,.376,.378,.352 )
    1 FORMAT (1H0)
    2 FORMAT (1H1)
C  SPACE FOR CONTROL CARD PARAMETERS . . . . . . . . . . . . . . . . . . . . . . . .
    3 FORMAT (A3, I2, 5I5, 6I2, I3, 3I5, F5.3, F5.2, F4.3, F6.3)
    4 FORMAT (*0CONTROL CARD WAS *,A5,I2, 5I7, 6I3, I4, 3I7, F7.3, F7.2,
     1 F7.3, F8.3, / )
    5 FORMAT (*     EFFECTIVELY *,A5,I2, 5I7, 6I3, I4, 3I7, F7.3, F7.2 ,
     1 F7.3, F8.3, / )
    6 FORMAT(* LINECARD IS*,I3,* N SEARCH IS*,I5,* N SMOOTH IS*,I3,* N
     1SKIP IS*,I5,*, N FILES IS*,I5,*, N RECORDS IS*,I5,*, NO LINES IS*,
     1 I3, *, NO CARDS IS*I3,*,*/*0NO PRINT IS*, I3, *, NO WL STD IS*,
     1 I3,*, N PUNCH WL IS*, I3,*, NO REFINE IS *,I3,*, N PRNT SKP IS *,
     1 I4, *, MAX PRINT IS*,I7, *,*,/,*0MIN WIDTH IS*, I5,*, N DUMMY IS*
     1 I5,     *, DIF 2 MIN IS*, F7.3, *, DENS MIN IS*, F7.2, *, WIDTH M
```

```
     1IN IS*, F7.3, *, AND FIDUCIAL IS AT*, F8.3, * MM.*)
    7 FORMAT ( 2X, I10, 3F10.3)
    8 FORMAT ( 7( 3PF4.0, 3PF7.0) )
    9 FORMAT (I1, *0*, F6.0, 18( 3P F4.0) )
   10 FORMAT ( I1     ,I7, 18I4 )
C SIGNAL FOR PARITY ERRORS IS.................................................
   11 FORMAT ( I1, F7.0, 18F4.3 )
   12 FORMAT (*0*, I4, * RECORDS WERE BYPASSED AT THIS POINT.*, /)
   13 FORMAT (*0THERE IS A TAPE ERROR IN THE FIRST RECORD.  THE FIDUCIAL
     1 CONVERSION MAY BE COMPROMISED.  X X X X X X X X X X X X X X X X*,/)
   14 FORMAT (*0THERE IS A TAPE ERROR IN THE RECORD AFTER*,I5,*    X X X
     1 X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X X
     1 X X X X X*,/)
   15 FORMAT ( 6X, 9X, F9.3, 3X, F9.3)
   16 FORMAT (*0WAVELENGTH STANDARDS ARE *, 8F10.3)
C SPECTRAL TYPES AND COMPENSATION FOR AN UNSPECIFIED CONTROL CARD..............
   17 FORMAT ( 38X, *PROCESSING SPECTRA FROM A TAPE DENSITOMETER*, ///)
   18 FORMAT ( 30X, *ABSORPTION SPECTRUM FROM 1961 OR 1964 NRL ECHELLE F
     1LIGHT*, //)
   19 FORMAT ( 48X, *AN EMISSION SPECTRUM*, //)
   20 FORMAT (49X, *AN ABSORPTION SPECTRUM*, //)
   21 FORMAT ( 50X, *A PLASMATUBE SPECTRUM*, //)
   22 FORMAT (25X, *SPECTRUM ASSUMED TO BE EMISSION, ALTHOUGH THE CONTRO
     1L CARD DID NOT SO STATE*, //)
   23 FORMAT (*0(*, 12F8.3, * IS THE EFFECTIVE FILTER TABLE)*, /)
   24 FORMAT (I1,X, 2PF4.0,0P, 1X,9X,11X,F9.3 , 31X, A8, I3, I2)
   25 FORMAT (24H0SMOOTHING PARAMETER IS      , I6 , 22H, SEARCH PARAMETE
     1R IS      , I6, /  )
   26 FORMAT ( 22H0STARTING POSITION IS     , F8.3, 13H MILLIMETERS    )
C  PRINTOUT FOR PLASMATUBE DATA...............................................
   27 FORMAT (*      POS   TRANS  WL      SP RAD     POS  TRANS  WL     SP
     1RAD     POS   TRANS  WL      SP RAD      POS   TRANS  WL      SP RAD*)
   28 FORMAT (I6, I3, I1, I1, I2, 2I2, I1)
C   FORMAT FOR NTITLE(8) PARAMETRIC DATA.....................................
   29 FORMAT(*0IDEN NUM*,2X,I6,3X,*SCAN SPEED(MM/MIN)*,1X,I3,2X,*JA GAIN
     1*,1X,I1, 2X,*DATEX GAIN*,1X,I1, 2X,*RECORDING CYCLE-SEE PLASMA COD
     2E*,1X,I2,2X, *DATE IS*,2X,I2,*/*,1X,I2,*/*,1X,*/6*,I1)
C      CODE FOR RECORDING CYCLE  FOR PLASMA SPECTRUM ............................
C      DIGITS /CYCLE = 1500  DATA SETS PER CYCLE = 125 PARAMETER =  1
C      DIGITS/CYCLE = 3000  DATA SETS /CYCLE = 250  PARAMETER =  2
C      DIGITS/CYCLE = 7500  DATA SETS /CYCLE = 625  PARAMETER =  5
C      DIGITS/CYCLE = 15,000  DATA SETS/CYCLE = 1250  PARAMETER = 10
C PRINT OUTPUT FORMAT FOR ALL SPECTRA BUT PLASMA TYPE ........................
   30 FORMAT ( *0      INDICES   POSITION DENSITY   WL   LINEFIND WIDTH
     1 PEAK NCODE   FIRST DIFFERENCES      SECOND DIFFERENCES    JJ1   T
     1YPE   REC  NO*)
C  TITLES INDICATING METHOD OF CORRECTION TO 100 PERCENT TRANSMISSION . . . . .
   31 FORMAT (X, 4I4, F8.3, F6.3, F9.3, 2I2, I3,
     1 F7.3, F8.3, I3, 6F8.3, I5, X, A8, I3, I5)
   32 FORMAT (  5H0FROM, I4, * DATA, AVERAGE TRANSMISSION OF FIRST MEDIU
     1M IS *, F5.1, * PERCENT, RMS DEVIATION OF *, F5.3, * AT FILTER SET
     1TING *, I1/)
   33 FORMAT (  5H0FROM, I4, * DATA, AVERAGE TRANSMISSION OF SECOND MEDI
     1UM IS *, F5.1, * PERCENT, RMS DEVIATION *, F5.3, * AT FILTER SE
     1TTING *, I1, /)
   34 FORMAT ( 78H ALL FOLLOWING DATA CORRECTED TO 100 PERCENT GLASS TRA
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     1NSMISSION BY THE FACTOR      , F5.3, / )
   35 FORMAT (11CHOBECAUSE OF SOME PROBLEM THE FACTOR WAS SET TO ZERO.
     1TO ALLOW FURTHER CALCULATIONS, IT IS RESET HERE TO 1.      )
   36 FORMAT (* MESSAGE IS *, A8 )
   37 FORMAT(2I8, 12F8.3)
   38 FORMAT (15F8.3)
   39 FORMAT (15I8)
   40 FORMAT ( I3, I1, I3, I2, 3I1, 3I2 )
C    1TITLE(10) PARAMETRIC DATA FOR EMI, ABS, ECH.................................
  41  FORMAT(* ORDER-PLATE*,2X,I3,2X,* EXPOSURE-TRIAL*,2X,I1,2X,
     1* TAPE NUMBER*,2X,I3,2X,* BAND*,2X,I2,2X,* CODE*2X,I1,2X,* DATEX G
     2AIN*,2X,I1,2X,* SCREW SPEED IS*,2X,I2,2X,* DATE IS*,2X,I2,*/*,I2,*
     3/*,I2)
C  TIMING OF LOADING AND OTHER OPERATIONS . . . . . . . . . . . . . . . . . . .
   42 FORMAT (22H0TIME SINCE START IS                ,F8.3,10H MINUTES    )
   43 FORMAT (33H0TIME SINCE LAST MEASUREMENT IS    ,F8.3,10H SECONDS    )
   44 FORMAT (    F6.3, F3.1, I1, 2X, F6.3, F3.1, I1, I2 )
   45 FORMAT (24A1)
   46 FORMAT ( *0(*, 7(F7.1, I3),* FILTER CHANGE CAUSED SOME DATA TO BE
     1REJECTED)*, /)
   47 FORMAT (*0(*, 10A10, * CONTAINS A DEFECTIVE INPUT DATUM)*, /)
C  REJECTION OF BAD DATA . . . . . . . . . . . . . . . . . . . . . . . . . . . .
   48 FORMAT (  X, 5H  K =     , I5 , I10, 15H DATA IN RECORD            ,
     1 I5, 5X, I10,25H BAD DATA WERE REJECTED,     ,I5,  20H OTHERS THROW
     1N OUT.       )
   49 FORMAT ( 4( X, F8.3, F6.1, F8.2, F7.3          ) )
   50 FORMAT (10F8.3)
C...............BEGINNING OF EXECUTABLE PART OF PROGRAM.......................
C     READING AND INTERPRETING THE CONTROL CARD...............................
       READ 3,SPECTRUM, LINECARD,
     1N SEARCH,            N SMOOTH, N SKIP, N FILES, N RECORDS,NO LINES,
     1 NO CARDS, NO PRINT, NO WL STD, N PUNCH WL, NO REFINE,
     1                     N PRNT SKP, MAX PRINT, MIN WIDTH, N DUMMY,
     1 DIF 2 MIN, DENS MIN, WIDTH MIN, FIDUCIAL
       PRINT  17
   51 IF(SPECTRUM.NE.3HECH) GO TO 52 $PRINT 18 $SIGN=-1. $ GO TO 56
   52 IF(SPECTRUM.NE.3HEMI) GO TO 53 $PRINT 19 $SIGN=1. $ GO TO 56
   53 IF(SPECTRUM.NE.3HABS) GO TO 54 $ PRINT 20 $SIGN=-1. $GO TO 56
   54 IF(SPECTRUM.NE.3HPLA)  GO TO 55 $PRINT 21 $SIGN=1. $ GO TO 56
   55 PRINT 22  $ SPECTRUM = 3HEMI  $  SIGN = 1.  $  GO TO 56
   56  CONTINUE
       PRINT 4, SPECTRUM , LINECARD,
     1          N SEARCH, N SMOOTH, N SKIP, N FILES, N RECORDS,NO LINES,
     1 NO CARDS, NO PRINT, NO WL STD, N PUNCH WL, NO REFINE,
     1                     N PRNT SKP, MAX PRINT, MIN WIDTH, N DUMMY,
     1 DIF 2 MIN, DENS MIN, WIDTH MIN, FIDUCIAL
C    INTERNAL ALTERATIONS TO BE READ AUTOMATICALLY INTO THE PROGRAM WHEN THE
C     CONTROL CARD IS LEFT UNSPECIFIED........................................
       IF (LINECARD .LE. 0) LINECARD = 0
       IF (N SEARCH .EQ. 0) N SEARCH = 12
       IF ( N PRNT SKP .EQ. 0) N PRNT SKP = 1
       IF ( N FILES .EQ. 0 )  N FILES = 1
       IF ( MAX PRINT .EQ. 0 )  MAX PRINT = 50000
C    ASSIGNING  OPTION 1.....................................................
       ASSIGN 111 TO OPTION 1 $ IF(N PUNCH WL.NE.0) ASSIGN 120TO OPTION 1
       IF (DIF 2 MIN .EQ. 0.)  DIF 2 MIN = .021
       IF (FIDUCIAL .EQ. 0.)  FIDUCIAL = 10.
```

```
      PRINT 5, SPECTRUM,  , LINECARD,
     1          N SEARCH, N SMOOTH, N SKIP, N FILES, N RECORDS,NO LINES,
     1 NO CARDS, NO PRINT, NO WL STD, N PUNCH WL, NO REFINE,
     1                     N PRNT SKP, MAX PRINT, MIN WIDTH, N DUMMY,
     1 DIF 2 MIN, DENS MIN, WIDTH MIN, FIDUCIAL
      PRINT 6, LINECARD, N SEARCH, N SMOOTH, N SKIP, N FILES, N RECORDS,
     1NO LINES, NO CARDS, NO PRINT, NO WL STD, N PUNCH WL, NO REFINE,
     1                     N PRNT SKP, MAX PRINT, MIN WIDTH, N DUMMY,
     1 DIF 2 MIN, DENS MIN, WIDTH MIN, FIDUCIAL
      ASSIGN 83  TO N OPTION
C    DESCRIPTION OF THE DATA INPUT TABLE.....................................
C          LL0 IS 1, THE BOTTOM OF THE TABLE.  LL1 = BOTTOM OF THE LOWER
C          SET OF DATA, N OVERLAP + 1.  LL2 = LL1 + NSEARCH.
C          LL4 IS THE TOP OF THE BOTTOM SET OF DATA, AND LL3 = LL4 - NOVERLAP + 1
C          LL5 = LL4 + 1, THE BOTTOM OF THE TOP SET OF DATA.  LL6 = LL5 + NSEARCH
C          LL7 IS THE TOP OF THE TOP SET OF DATA.
COMMENT    LL8 IS LL4 - N SEARCH, AND LL9 IS LL7 - NSEARCH
      TIME A = TIMEF (ZZ)    $   STARTIME = TIME A
       DO 57 MMMMMMM = 1, N SKIP
C  FINDING THE FILES THAT WILL BE PROCESSED . . . . . . . . . . . . . . . . . .
   57  CALL SKIP FILE (1)
      DO 141 MMMMMMMM = 1, N FILES
   58  CONTINUE
C  SETTING INITIAL VALUES OF SOME VARIABLES . . . . . . . . . . . . . . . . . .
      LINE = 0
      LL1 = LL2 = LL3 = LL4 = LL5 = LL6 = LL7 = LL8 = LL9 = LL10 = 0
      N OVERLAP = 5*NSEARCH + 1 $ FACTOR = 1. $ JJ=AAA=BBB=CCC=0.
      LL0=1 $ LL1=NOVERLAP + 1 $   LL2 = LL1 + NSEARCH   $   LL7 = 246
      N NFILTER = -1     $  FACTRLOG = 0.
C  READING IN AND INTERPRETING THE PARAMETERS.....................................
      BUFFER IN (1, 0) (INDATA (1), INDATA (1000) )
   59  IF (UNIT,1) 59, 60, 58
   60  CONTINUE
       TIME = (TIMEF(ZZ) - TIMEA)/60000.$PRINT 42,TIME $TIMEA=TIMEF(ZZ)
C  KAY IS DEFINED AS THE LENGTH FUNCTION...........................................
      KAY = LENGTHF(1)
      IF (KAY .GT. 4 )  GO TO  65
      IF  (SPECTRUM  .EQ. 3HPLA)  GO TO 61
C   DECODING PARAMETRIC DATA FOR EMI, ECH, ABS.....................................
      DECODE (18,  40, INDATA)  ITITLE
      IF ( ITITLE (7) .EQ. 5  )  ITITLE(7) = 50
       PRINT 2
       PRINT 41, ITITLE
      NNTRI = ITITLE (2)  $  N ORDER = I TITLE (1)  $  ID = I TITLE (1)
COMMENT   ITITLE (5) IS THE CODE FOR ORDER OR ITS PRECEDING BACKGROUND
C  DECODING PARAMETRIC DATA FOR PLASMATUBE SPECTRUM...............................
       GO TO 62
   61  DECODE (18,  28, INDATA)  N TITLE
      PRINT 2
       PRINT 29,  NTITLE
      ID = N TITLE(1)/100
      NN TRI = N TITLE (1)
   62  CONTINUE
C    FILLING IN AND DECODING THE MIDDLE DATA ZONE(DONE ONLY ONCE)................
      BUFFER IN (1, 0) (INDATA (1), INDATA (2000) )
   63   IF (UNIT,1)  63,  65, 140 , 64
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   64  CONTINUE  $ PRINT 13
   65   CONTINUE
   66  CONTINUE
C  PARAMETER RECORDS ONLY ARE LESS THAN OR EQUAL TO FOUR WORDS IN LENGTH........
C   KAY FINDS THE OF 8-DIGIT WORDS READ IN STORAGE UNIT 1. L IS SO
C   DEFINED SINCE THE RATIO OF COMPUTER SPACE TO DATEX SPACE IS 8/12............
      KAY = LENGTHF(1)  $   L = 2 * KAY / 3
      IF ( KAY .LE. 4 )      GO TO 62
      IF ( L .GT. 1500) L = 1500  $   KAY = 3 * L / 2   $   L = 1
      DO 67 N = 1, KAY, 3
      M = L + 1
C  DECODING DATA AND STORING IN PROPER ARRAYS . . . . . . . . . . . . . . . . . .
       DECODE (24, 44, INDATA(N))
     1 POSN(L), TRANSM(L), NFILTER(L), POSN(M), TRANSM(M),NFILTER(M)
      L = L + 2 $ GO TO 67
   67  CONTINUE
      L = L - 2
   68 K1  = NFILTER (1)     $  STARTPOS = POSN (1)
C  COMPENSATING FOR FIRST RECORD FIDUCIALS (START POS) WHICH ARE LESS
C  THAN ZERO , BUT NOT ENCODED NEGATIVELY BY THE DATEX UNIT.....................
      IF(STARTPOS .GT. 900.) STARTPOS = STARTPOS - 1000.
      PRINT  26, STARTPOS $ IF (FIDUCIAL.LT.0.)FIDUCIAL = STARTPOS = 0.
C....THIS SECTION GENERATES COEFFICIENTS FOR THE QUADRATIC EXTRAPOLATION
C          OF WAVELENGTHS, ASSUMING THE SPECTRUM TO BE 28.0 MM WIDE, AND GIVEN
C          THE BEGINNING, MIDDLE, AND END WAVELENGTHS OF EACH ORDER FROM PREVIOUS
C          WORK.  START POSITION (STARTPOS) IS THE FIRST POSITION READING OF THE
C          FIRST RECORD LONGER THAN A TITLE RECORD.
      X1 = 10.   $   X2 = 24.   $   X3 = 38.   $   X4 = 28.67 $ X5=19.33
      IF (SPECTRUM .EQ. 3HECH )  GO TO 69
      IF ( NO WL STD .EQ. 0 )  GO TO 70
      N ORDER = 1
       READ 15, WLS (1,1), X1
      READ 15,  WLS (1,2), X2
      READ 15,  WLS (1,3), X3
      PRINT 16,  WLS(1,1), X1, WLS(1,2), X2, WLS(1,3), X3
   69 IF (N ORDER .GT. 120)  GO TO 70
C   SOLVING A QUADRATIC EQUATION TO OBTAIN CONSTANTS.............................
      AY 1 =(WLS (NORDER, 1) - WLS (NORDER, 2))/ (X1 - X2)
      AY 2 =(WLS (NORDER, 2) - WLS (NORDER, 3))/ (X2 - X3)
      AAA= (AY1 - AY2) / (X1 - X3)
      BBB= (AY1 -AAA*(X1 + X2) )
      CCC=  WLS (NORDER, 1) -AAA*X1*X1 -BBB*X1
   70   CONTINUE
       DO 71 K = 1, 9
C  PREPARING THE FILDENS TABLE ON THE BASIS OF THE FILTER NUMBER IN RECORD 1 . .
   71   FILDENS (K) = 0
      K2 = K1 - 1
       DO 72 K= 1, K2
       DO 72 KK = K, K2
C  FILDENS DATA IS FIRST INTRODUCED INTO THE PROGRAM AT THIS POINT..............
      FILDENS (K) = FILDENS (K) + FILDEN (KK)
   72   CONTINUE
       PRINT 23, FILDENS
       PRINT 25, NSMOOTH, NSEARCH
COMMENT   BECAUSE OF A FALSE SWITCHING PROBLEM IN THE DENSITOMETER OR TAPE
C  OUTPUT UNIT,DATA WHERE ADJACENT NFILTER VALUES DIFFER ARE
C   ELIMINATED FROM  THE TABLE...................................................
```

```
      N = LL1 - 1
      DO 74 I = 3, L
      IF ( N FILTER (I-1) .NE.N FILTER (I) ) GO TO 73
      IF ( N FILTER (I+1) .NE.N FILTER (I) ) GO TO 73
      IF ( N FILTER (I) .EQ. 0 )  GO TO 73
      IF ( TRANSM (I) .EQ. 99.9)   GO TO 73
      IF ( TRANSM (I) .LT.  .2 )   GO TO 73
      N = N + 1
C   REDIFINING POSITION, TRANSMISSION, AND NFILTER FOR USE IN PLASMATUBE
C SPECTRA.  I IMPLIES ABS, ECH, EMI.  N IS THE RUNNING INDEX FOR PLA.............
      POSN(N) = POSN(I) $ TRANSM(N) = TRANSM(I) $ NFILTER(N) =NFILTER(I)
       GO TO 74
   73  CONTINUE
      N N FILTER = N N FILTER + 1
      IF ( N N FILTER .NE. 1 )  GO TO  74
C   SETS UPPER AND LOWER LIMITS ON NFILTER AND TRANSM...........................
      J1 = I - 3   $   J2 = I + 3
      PRINT  46, ( TRANSM (I1), NFILTER (I1), I1 = J1, J2 )
C     DEFINING THE PARAMETERS WHICH LOCATE THE DATA IN STORAGE...................
   74 CONTINUE  $  L=N $ LL4=N $ LL3=LL4-NOVERLAP+1 $ LL5=LL4+1
      LL6=LL4+NSEARCH $ JJ1=1
      LL8 = LL4 - N SEARCH
C  CONVERTING THE DATA TO USABLE FORM, APPLYING THE FILTER NUMBER CORRECTION,
C  CONVERTING TO WAVELENGTH, AND OBTAINING VALUES FOR DENSITY, POSITION, AND
C     TRANSMISSION . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .
C  CALCULATING DENSITY(I), WL(I) AND TRANSM, DEFINED AS X.......................
      DO 75 I =LL1,LL4 $ J1 = NFILTER(I) $ X = FACTOR*TRANSM(I)/100.
      DENSITY (I) = - ALOG10 (X)  + FILDENS (J1)
      WL (I) =AAA*POSN(I)*POSN(I) +BBB*POSN(I) + CCC
      X = - 2.303 * DENSITY (I)   $   TRANSM (I) =          EXPF(X)*100.
   75  CONTINUE
   76  CONTINUE
C    READING IN RECORDS TO FILL THE TOP ZONE OF DATA AND DECODING,  THIS
C     IS DONE REPETITIVELY.......................................................
      BUFFER IN (1, 0) (INDATA (1), INDATA (2000) )
   77  IF (UNIT, 1) 77, 79,140 ,78
   78  PRINT 14,JJ  $ ASSIGN 81 TO N OPTION
   79  CONTINUE
   80  CONTINUE
C    DEFINING KAY AND LL.  LL IMPLIES SEARCH OF THE DATA TABLE...................
      KAY = LENGTHF(1)  $  LL = 2 * KAY / 3
      IF ( KAY .LE. 4 )      GO TO  76
      IF (LL .GT.3000 )LL =3000   $   KAY = 3 *LL / 2   $  LL = LL5
       DO 85  N = 1, KAY, 3
      GO TO N OPTION
C  IF A PARITY ERROR IS FOUND, THIS SECTION IS USED TO RECOVER AS MUCH DATA AS
C    POSSIBLE . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .
   81  DECODE(24, 45, INDATA(N) ) INTEGERS  $ DO 82 NN = 1, 24
   82 IF (INTEGERS (NN) .GT. 1H9 )  GO TO 84
   83 M = LL + 1
C   NORMAL DECODING WHEN NO PARITY ERROR IS IN DATA.............................
      DECODE  (24, 44, INDATA(N) )
     1 POSN(LL),TRANSM(LL),NFILTER(LL),POSN(M), TRANSM(M),NFILTER(M),
     1 IN PHASE   $   IF (IN PHASE .NE. 0)  GO TO 84
      LL = LL + 2
       GO TO  85
```

```
   84 N BAD DATA = N BAD DATA + 1
      IF ( N BAD DATA .GT. 3 )  GO TO 85
      J1 = N - 3  $  J2 = N + 5  $  PRINT 47, (INDATA(I), I = J1, J2 )
   85   CONTINUE
       ASSIGN 83 TO N OPTION
C    READING IN THE NEXT RECORD WHILE THE CALCULATIONS ARE CONTINUING.............
      BUFFER IN (1, 0) (INDATA (1), INDATA (2000) )
      LL = LL - 2   $   LL7 = LL
C     BECAUSE OF FALSE FILTER SWITCHING SOME DATA ATE ELIMINATED...................
      JJ = JJ + 1   $   L1 = LL5        $   N = LL4
      DO 87 I = LL5,  LL7
      IF (NFILTER(I).EQ.0)GO TO 86  $ IF(TRANSM(I).GT.99.7)GO TO 86
      IF ( N FILTER (I-1) .NE.N FILTER (I) ) GO TO 86
      IF ( N FILTER (I+1) .NE.N FILTER (I) ) GO TO 86
      IF ( TRANSM (I) .LT.  .2 )GO TO 86  $  N=N+1  $  X=TRANSM(I)/100.
C  N OPTION--OBTAINING EXPRESSIONS FOR DENSITY, POSITION, AND TRANSMISSION IN
C  TERMS OF N. USED FOR MAKING CALCULATIONS IN PLASMA SPECTRA....................
      POSN(N)=POSN(I)-STARTPOS+ FIDUCIAL
      NFILTER(N)  =  NFILTER(I)   $  J1 = NFILTER(I)
      DENSITY(N)=-ALOG10(X)+FILDENS(J1)-FACTRLOG
      X  =  -2.303 * DENSITY(N)
      TRANSM(N)=EXPF(X)*100.
      WL(N) = AAA * POSN(N) * POSN(N) + BBB * POSN(N) + CCC
C  D(FINING TRANSM 1 AND DENSITY1...............................................
      TRANSM1(N) = TRANSM(N)  $  DENSITY1(N) = DENSITY (N) $ GO TO 87
   86 CONTINUE
C    IN CASE OF IMPROPER DENSITY FILTER SWITCHING..............................
      NN FILTER = NN FILTER + 1
      IF ( N N FILTER .NE. 1 )  GO TO 87
      J1 = I - 3   $   J2 = I + 3
      PRINT  46, ( TRANSM (I1), NFILTER (I1), I1 = J1, J2 )
   87   CONTINUE
C  REPRESENT THE TOP OF THE UPPER DATA ZONE BY N, AND THE RUNNING INDEX LL......
      LL = N  $   LL7 = N
      LL9 = LL7 - N SEARCH
   88 CONTINUE
      LL10 = LL7 - LL5
C  PRINTS TITLE ONLY IF THERE ARE BAD DATA . . . . . . . . . . . . . . . . . . .
      IF ( N BAD DATA .NE. 0 )
     1PRINT 48, KAY,LL10,JJ, N BAD DATA, NNFILTER
      N BAD DATA = 0   $   N N FILTER = -1
C  REFERS TO THE PARAMETERIC RECORDS............................................
      IF ( JJ .LE. 3 )  GO TO  131
   89 CONTINUE
COMMENT......SMOOTHING TRANSMISSION AND DENSITY DATA...........................
C   0 INDICATES NO SMOOTHING, 1 AN AVERAGE OF 3 POINTS,ETC.(2N +1)..............
      IF (NSMOOTH .EQ. 0) GO TO 93   $  L1 = NSMOOTH + 1  $  L2 = LL3+L1
   90 DO 92 I = LL1, LL4  $  AA = BB = 0.
      J1 = I - NSMOOTH   $   J2 = I + NSMOOTH   $   J3 = 2 * NSMOOTH + 1
      DO  91 J = J1, J2  $  BB = BB + DENSITY1(J) $  AA = AA +TRANSM1(J)
   91 CONTINUE
      TRANSM  (I) = AA/J3   $   DENSITY   (I) = BB / J3
   92 CONTINUE
   93 CONTINUE
      IF (SPECTRUM .NE.  3HPLA)  GO TO 94
C   CALLING PLASMA SUBROUTINE...................................................
       CALL PLASMA   (LL5, LL7, TRANSM, POSN, SPEC RAD, WL)
```

```
   94 CONTINUE
COMMENT   PRINTING OF RECORDS IF PERMITTED BY CONTROL CARD.......................
      IF (NO PRINT .EQ. 0 )  GO TO 96
      IF (SPECTRUM .EQ. 3HPLA ) PRINT 27
      IF (SPECTRUM .EQ. 3HPLA)  GO TO 95
      IF (JJ.LE. MAX PRINT) PRINT 49 , (POSN(N), TRANSM(N), WL(N),
     1DENSITY(N)            , N = LL1, LL4, N PRNT SKP)
      GO TO 96
   95 IF(JJ.LE.MAX PRINT) PRINT 49,  (POSN(N), TRANSM(N), WL(N),
     1SPEC RAD(N), N = LL5, LL7, N PRNT SKP)
   96 CONTINUE
C ................LINEFIND PART OF PROGRAM.....................................
      IF ( NO LINES .EQ.  0)  GO TO 110
      IF(JJ.LT.4)GO TO 110
C    AN INTEGER LESS OR EQUAL TO ZERO PERMITS THE LINEFIND ANALYSIS TO OPERATE
C   BUT THE LINETYPE ASSIGNMENT IS NOT MADE. . . . . . . . . . . . . . . . . . .
C. . . . N SEARCH IS THE INTERVAL USED FOR SCANNING IN THE LINEFIND PORTION
C. . . (N SEARCH  = 2N +  1  DATA POINTS). . . . . . . . . . . . . . . . . . . .
      IF (NO REFINE .LE. 0)  ASSIGN 106 TO OPTION 5
      IF  (NO REFINE .GT.  0) ASSIGN 104 TO OPTION 5
      DO 97  N =LL8,LL9    $   J1 = N - N SEARCH   $   J2 = N + N SEARCH
   97 DIF (N) = DENSITY (J2) - DENSITY (J1)
      DO 98  N =LL8,LL9    $   J1 = N - N SEARCH   $   J2 = N + N SEARCH
      DIF 2 (N) = SIGN * (DIF (J1) - DIF (J2) )
C   DIF 2 TABLE IS NOW EXAMINED FOR CRITICAL POINTS..........................
      LINEFIND(N)=-1.*SIGNF (1., DIF 2 (N) )
C  CODE (+) TO (-) POINTS AS -, (-) TO (+) AS +,ETC. ALONG THE LINES............
   98 IF (LINEFIND(N) .EQ. LINEFIND(N-1)) LINEFIND(N-1) = 0
      IF (JJ .LT. 5 )  GO TO 110
      IF ( POSN (LL1) .GT. 900.)  GO TO  110
COMMENT     NOW GO THROUGH THE TABLE AGAIN TO FIND MAXIMA BETWEEN ZERO POINTS.
       DO 110 I = JJ1, LL4
COMMENT   FIND THE FIRST - TO + POINT (THE FIRST +1 POINT IN LINEFIND)
      IF ( LINEFIND (I) .NE. +1 )  GO TO 110  $  J1 = I
   99 I1=I+1 $ DO 100 J=I1,LL9
C   FIND THE FIRST SUCCEEDING + TO - POINT, IE, THE FIRST SUCCEEDING
C           -1 POINT IN LINEFIND
      IF (LINEFIND (J) .NE.-1 )  GO TO  100
      J2 = J   $   GO TO 101
  100 CONTINUE  $ GO TO 110
  101 CONTINUE  $ C = D = 0.
COMMENT      FIND THE  MAXIMUM BETWEEN J1 AND J2, THE TWO ZERO POINTS OF DIF 2
      DO 103 J = J1, J2
      IF(DIF2(J).LE.C)GO TO 102 $ MAX=J $ C=DIF2(J) $ GO TO 103
  102 IF(DIF2(J).GE. D)GO TO 103 $ MIN = J $ D = DIF2(J)
  103 CONTINUE $ X = ABSF(D) $ Y = ABSF(C)
      WIDTH = POSN(J2) - POSN(J1)
      IF (MAX - J1 .LE. 1) GO TO 109  $  IF (J2 - MAX .LE. 1) GO TO 109
      IF ( DIF 2 (MAX) .LT. DIF 2 MIN )  GO TO 109
      IF ( WIDTH .LT. WIDTH MIN) GO TO 109
      IF (DENSITY(MAX) .LT. DENS MIN)  GO TO 109
      GO TO OPTION   5
C   STATEMENT 104 IS USED WHEN THE ANALYTICAL PART OF THE LINETYPE SUBROUTINE
C    IS BYPASSED BY   NO REFINE........... . . . . . . . . . . . . . . . . . . .
  104 MAXI  =  MAX   $   PEAK  =  0   $   N CODE  =  6
      TYPE   =    17HLINE NOT ANALYZED
```

```
      GO TO   105
  105 LINE  =  LINE  +  1
  106       CALL  LINETYPE (          J1,J2,MAX,WIDTH,PEAK,MAXI,NCODE,TYPE)
      PRINT 31,  J1, MAX, MAXI, J2, POSN(MAXI), DENSITY(MAXI), WL(MAXI),
     1 LINEFIND(J1), LINEFIND(MAXI), LINEFIND(J2),WIDTH, PEAK, NCODE,
     1   DIF (J1), DIF (MAXI),DIF (J2), DIF 2 (J1), DIF2(MAXI),DIF2(J2)
     1 , JJ1, TYPE, JJ, LINE
C  DETERMINES IF LINECARDS WILL BE PUNCHED. . . . . . . . . . . . . . . . . . .
      IF (LINECARD .GT. 0) GO TO 1061
      IF (LINECARD .LE. 0) GO TO 108
C  AN ALTERNATIVE IS GIVEN TO PUNCH LINECARDS IN WL OR MM. . . . . . . . . . .
 1061   IF (NPUNCH WL .GT.0) GO TO 107
      PUNCH 24,NCODE,DENSITY(MAXI),          POSN(MAXI),TYPE,ID,NNTRI
      GO TO 108
  107  PUNCH 24 , NCODE, DENSITY(MAXI), WL(MAXI), TYPE, ID, NNTRI
  108 CONTINUE
      JJ1 = J2
  109 CONTINUE
  110 CONTINUE
COMMENT     PUNCH   CONDENSED DATA CARDS(9-CARDS)..............................
      IF (NO CARDS.EQ.0) GO TO 129  $  IF (JJ.LE.3) GO TO 129
      IF ( POSN (LL1) .GT. 900.)  GO TO 129
C  J12 IS A VARIABLE REPRESENTING  NO CARDS.....................................
      J12 = 9 * NO CARDS  $  L = LL4 - J12
C  OPTION 1 IS INTRODUCED.......................................................
      GO TO OPTION 1
C  PUNCH POSITION CARDS INSTEAD OF WAVELENGTH CARDS .  . . . . . . . . . . . . H
  111 DO 115 I = LL1, L, J12   $   NY = POSN(I)   $   FNY = NY
      J2 = I + J12   $   J3 = I + J12+ 1
      J5 = I + 1+8*NO CARDS      $   J6 = LL4 - NO CARDS +1
      DO 112 J = I, J2, NO CARDS
  112 Y OUT(J) = POSN(J) - FNY
      JKL = 0 $ DO 113  I1 = I, J5, NO CARDS
C  JKL IS A SCALING VARIABLE USED IN SPEC RAD, JKL = 0 IMPLIES A SCALE FACTOR
C  OF 1, JKL = 1 GIVES A SCALE FACTOR 10, ETC. (EFFECTS 9-CARDS)................
  113  IF ( DENSITY (I1) .GT. 9.9994)  JKL=1 $ IF(JKL.EQ.0) GO TO115
      DO 114  I1 = 1, J5, NO CARDS
  114  DENSITY (I1) = DENSITY (I1)/10.
C    FNY IS THE CONSTANT PART OF THE POSITION.................................
  115 PUNCH  9 ,JKL,FNY,(YOUT (I1), DENSITY (I1), I1 = I, J5, NO CARDS )
      L = L+1 $ NY = POSN(L) $ FNY=NY $ DO 116, J = J3, J6, NO CARDS
  116 Y OUT (J) = POSN(J) - FNY $ IF (J3 .GE. J6)  GO TO 129
      JKL = 0  $  DO 117  I1 = J3, J6,   NO CARDS
C  JKL = 1 IN 9-CARDS IMPLIES MULTIPLY ALL SPEC RAD DATUM BY 10
  117 IF ( DENSITY (I1) .GT. 9.9994) JKL = 1$ IF (JKL.EQ.0) GO TO 119
      DO 118 I1 = J3, J6, NO CARDS
  118 DENSITY (I1) = DENSITY (I1)/10.
  119 PUNCH 9,  JKL,FNY,(YOUT (I1) , DENSITY(I1), I1 = J3, J6, NO CARDS)
C)))))))) BY-PASSES THE PUNCHING OF WL 9-CARDS. . . . . . . . . . . . . . . . .
      GO TO 129
C  PUNCH WAVELENGTH CARDS INSTEAD OF POSITION CARDS (NOT YET TESTED) . . . . . .
  120 DO 124 I = LL1, L, J12   $   NY =  WL (I)   $   FNY = NY
      J2=I+J12 $ J3=I+J12+1 $ J5=I+1+8*NOCARDS $ J6=LL4-NOCARDS+1
      DO 121 J = I, J2, NO CARDS
C  DEFINE Y OUT.................................................................
  121 Y OUT(J) =  WL (J) - FNY
      JKL = 0  $ DO 122  I1 = I,  J5,   NO CARDS
```

```
  122  IF( DENSITY (I1) .GT. 9.9994 ) JKL = 1 $ IF(JKL.EQ.0) GO TO 124
       DO123   I1 = I, J5, NO CARDS
  123  DENSITY (I1) = DENSITY (I1)/10.
  124 PUNCH 9,  JKL,FNY,(Y OUT (I1), DENSITY (I1), I1 = I, J5, NO CARDS)
      L = L+1 $ NY =  WL (L) $ FNY=NY $ DO 125, J = J3, J6, NO CARDS
  125 Y OUT (J) =  WL (J) - FNY $ IF (J3 .GE. J6)  GO TO 129
       JKL = 0       $ DO 126     I1 = J3, J6,  NO CARDS
  126  IF ( DENSITY (I1) .GT. 9.9994 )  JKL = 1 $ IF(JKL.EQ.0) GO TO 128
      DO 127  I1 = J3, J6, NO CARDS
  127   DENSITY (I1) = DENSITY (I1)/10.
  128 PUNCH 9,  JKL,FNY,(YOUT (I1), DENSITY (I1), I1 = J3, J6, NO CARDS)
  129 CONTINUE
C. . . THE TOP ZONE OF DATA IS NOW MOVED DOWN, FILLING THE MIDDLE AND BOTTOM
C ZONES. GIVES TWO NEW LOWER ZONES OF DATA. . . . . .
      N = 0
      DO 130 I=LL3,LL7 $ N = N+1 $ WL(N) = WL(I)$DENSITY(N)=DENSITY(I)
C   DEFINES N OPTION IN TERMS OF I OPTION.....................................
      POSN(N) = POSN(I) $ TRANSM(N) = TRANSM(I) $ TRANSM1 (N)=TRANSM1(I)
      DENSITY1(N) = DENSITY1(I)
      LINEFIND(N)=LINEFIND(I) $ DIF2(N)=DIF2(I)          $ DIF(N)=DIF(I)
  130 CONTINUE
C   REDEFINE THE INDICES WHICH SPECIFY THE ZONES IN THE TABLE. HERE THE INDICES
C  L AND  N ARE GIVEN.........................................................
      LL4 = N   $   L = N  $  LL3 = LL4 - N OVERLAP + 1 $ LL5 = LL4   1
      LL6 = LL4 + NSEARCH $  JJ1 = JJ1 - LL4 + NOVERLAP + 1
      LL8 = LL4 - N SEARCH
      IF (JJ1 .LT. 1 )  JJ1 = 1
C   GOING BACK TO 77 FOR RECYCLING TO BRING IN A NEW TOP ZONE OF DATA...........
      GO TO 77
C TREATING THE THIRD AND SECOND DATA RECORDS WHERE JJ REFERS TO THE FIRST
C  THREE PARAMETER RECORDS.....................................................
  131 IF ( JJ .LE. 1 )  GO TO 93
COMMENT    CALCULATING AVERAGE TRANSMISSION.....................................
C  J IS DEFINED AS THE FILTER NUMBER
      SUMSQ = SUMTRANS = NUM = 0   $   J = NFILTER (LL1)
      DO 132 I = LL1, LL4
      NUM = NUM + 1   $   SUMTRANS = SUMTRANS + TRANSM(I)
  132 CONTINUE
      SUMTRANS = SUMTRANS / NUM
COMMENT    CALCULATING ROOT MEAN SQUARE DEVIATION, A MEASURE OF THE NOISE LEVEL.
      DO 133 I = LL1, LL4
      SUMSQ = (TRANSM(I) - SUMTRANS)**2 + SUMSQ
  133 CONTINUE
      SUMSQ = SUMSQ / NUM   $   SUMSQ = SQRTF (SUMSQ)
      GO TO  (93, 134, 135) JJ
  134 PRINT 32, NUM, SUMTRANS, SUMSQ, J
COMMENT...FACTOR(VARIABLE) CONVERTS ALL TRANSMISSION TO CONFORM TO FIRST MEDIUM
      FACTOR = 100. / SUMTRANS   $   PRINT 34 , FACTOR
C DEFINE X AS FACTOR.......................................................
      X = FACTOR   $   FACTRLOG = ALOG10 (X)
      IF ( FACTOR .LE. .10  )  GO TO 139   $   GO TO 93
C  DURING THE THIRD RECORD, RECORRDS OTHER THAN THIS ARE SKIPPED IF THE CONTROL
C CARD SO SPECIFIES........................................................
  135 PRINT 33,  NUM, SUMTRANS, SUMSQ, J
      PRINT 30
      DO 138 NNNNNNNN = 1, N RECORDS
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      BUFFER IN (1, 0) (INDATA (1), INDATA (2000) )
  136 IF (UNIT,1) 136, 137, 140, 138
  137 KAY = LENGTHF (1)  $  IF (KAY  .LE.  4)  GO TO 138
      JJ = JJ + 1
  138 CONTINUE
      N RECORDS = 0
      IF (N RECORDS .NE. 0 )  PRINT 12,  N RECORDS
      GO TO 93
  139 PRINT 35    $   FACTOR = 1.   $  FACTRLOG = 0.   $   GO TO 93
  140 CONTINUE
       TIME = (TIMEF(Z)-STARTIME)/60000.$PRINT 42,TIME $TIMEA=TIMEF(ZZ)
      PRINT 2
  141 CONTINUE
      END
      SUBROUTINE LINETYPE (J1, J2, MAX, WIDTH, PEAK, MAXI, NCODF, TYPE)
C.............LINETYPE PART OF PROGRAM.........................................
      DIMENSION                A(11,11),SUMX(31),SUMY(15)
      COMMON/BLOCK/DENSITY(3000),X(1500),Y(1500)
C   ASSIGNS NUMBER TYPE TO THE VARIABLES.......................................
      TYPE DOUBLE        A, SUMX, SUMY, S1, S2, S3
      TYPE DOUBLE FA, FB, FC, FD, FFA, FFB, FFC, DISCR
      TYPE INTEGER TYPE
C   DEFINES THE PEAK DENSITY FUNCTION .........................................
      PEAKF(MAXI,J1,J2) = DENSITY(MAXI) - (DENSITY(J1) + DENSITY(J2))/2.
  150 FORMAT (1H0)
  151 FORMAT ( X, 8E16.8, /,X6I4, 3F8.4, 2I4)
  152 FORMAT (X10( F6.0, F7.3) )
  153 FORMAT (* MESSAGE IS *, A8 )
      MAXI = MAX
C  DEFINES THE VARIABLES Z AND B IN TERMS OF DENSITY...........................
 1153 N=0$LAST=3$Z=DENSITY(MAX)-DENSITY(J1)$B=DENSITY(MAX)-DENSITY(J2)
      TYPE = 8H  PEAK
      IF (Z .LT. 0.)   TYPE = 8H VALLEY
      IF (Z*B .EQ. 0.)   GO TO 176
      DO  154  I=J1,J2 $ N=N+1 $ X(N) = I $ Y(N) = DENSITY(I)
  154 CONTINUE $ IF(N.LT. 3)GO TO 176 $ W=1.
C   SETTING INITIAL VALUES OF SUMX AND SUMY AND CALCULATING THEIR VALUES AS A
C   PRODUCT OF W, X, AND Y.....................................................
  155 SUMX (1) = SUMX (2) = SUMX (3) = SUMY (1) = SUMY (2) = 0.
      DO156I=1,N$ SUMX(1)=SUMX(1)+W $ SUMX(2)=SUMX(2)+W*X(I)
      SUMX(3)=SUMX(3)+W*X(I)*X(I) $ SUMY(1)=SUMY(1)+W*Y(I)
  156 SUMY(2)=SUMY(2)+W*X(I)*Y(I) $ NORD=1
C   DEFINITION OF L, KK, IK, ANDRANGES OF J AND I..............................
  157 L=NORD+1 $ KK=L+1 $ DO159 I=1,L $ DO158 J=1,L $ IK=J-1+I
  158 A(I,J)=SUMX(IK)
  159 A(I,KK)=SUMY(I) $ DO 162 I=1,L $ A(KK,I)=-1.$KKK=I+1$DO160J=KKK,KK
  160 A(KK,J)=0. $ C=1./A(1,I) $ DO161 II=2,KK $ DO161 J=KKK,KK
  161 A(II,J)=A(II,J)-A(1,J)*A(II,I)*C $ DO162 II=1,L $ DO162 J=KKK,KK
  162 A(II,J)=A(II+1,J) $ S2=0. $ DO164 J=1,N $ S1=0. $ S1=S1+A(1,KK)
      DO 163 I = 1, NORD
  163 S1 = S1 + A(I+1,KK)*X(J)**I
  164 S2=S2+(S1-Y(J))*(S1-Y(J)) $ B=N-L $ S2=(S2/B)**.5
      IF (NORD .NE. LAST )  GO TO 165
COMMENT  A CUBIC EXTRAPOLATION IS NOW DONE..A + BX + CX*X + DX*X*X..............
      FA = A(1,KK)   $   FB = A(2,KK)   $   FC = A(3,KK) $ FD = A(4,KK)
      GO TO 167
  165 NORD=NORD+1 $ J=2*NORD $ SUMX(J)=0. $ SUMX(J+1)=0.$SUMY(NORD+1)=0.
```

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      DO166 I=1,N $ SUMX(J)=SUMX(J)+X(I)**(J-1)*W
      SUMX(J+1) = SUMX(J+1)+X(I)**J*W
  166 SUMY(NORD+1)=SUMY(NORD+1)+Y(I)*X(I)**NORD*W $ GO TO 157
  167 CONTINUE
COMMENT   TAKING FIRST DERIVATIVE AND SETTING IT TO ZERO--
      FFC = FB   $   FFB =2.*FC   $   FFA =3.*FD
      DISCR = FFB*FFB - 4.*FFA*FFC
      IF ( DISCR .LT. 0. )  GO TO 175
      DISCR =DSQRT  (DISCR)
C    MAX1 AND MAX2 ARE OBTAINED AND THE PEAK IS SET TO ZERO
       MAX1=(-FFB+DISCR)/(2.*FFA)$ MAX2=(-FFB-DISCR)/(2.*FFA)
      PEAK =          NCODE = NCODE 1 = NCODE 2 = 0
      IF ( MAX 1 .GT. J1 .AND. MAX 1 .LT. J2 )  NCODE 1 = 1
      IF ( MAX 2 .GT. J1 .AND. MAX 2 .LT. J2 )  NCODE 2 = 1
      IF (N CODE 1 + N CODE 2 - 1) 168,  169,  176
  168 IF (Z*B  .LT.  0. )   GO TO 174  $  GO TO  175
  169 MAXI=MAX1 $ IF(NCODE2.EQ.1)MAXI=MAX2 $ FJ5=J2-J1 $ J6=MAXI-J1
      J7=J2-MAXI $ PEAK=PEAKF(MAXI,J1,J2) $ ASYM=(J6*J6+J7*J7)/FJ5-.5
      NCODE=0$IF(ASYM.LE..04)GOTO177$NCODE=1$IF(J7.GT.J6)NCODE=2$GOTO177
C    LINE CODE IS AFTER STEINHAUS.............................................
C    0 COMPLETELY ACCEPTABLE, SYMMETRIC       5
C    1 ASYMMETRIC, SHADED TO RED, ACCEPTABLE 6
C    2 ASYMMETRIC, SHADED TO BLUE, ACCEPTABLE 7 SHOULDER
C    3                                        8 POOR LINE, FIT OUT OF RANGE
C    4 WIDE LINE                              9 NOTHING
  170 NCODE=3 $ TYPE=8H          $                                GOTO177
  171 NCODE=4 $ TYPE=8H  WIDE    $                                GOTO177
  172 NCODE=5 $ TYPE=8H          $                                GOTO177
  173 NCODE=6 $ TYPE=8H          $                                GOTO177
  174 NCODE=7 $ TYPE=8HSHOULDER $ PEAK=PEAKF(MAX,J1,J2) $         GOTO177
  175 NCODE=8 $ TYPE=8H  POOR    $ PEAK=PEAKF(MAX,J1,J2) $         GOTO177
  176 NCODE=9 $ TYPE=8HNOTHING   $ PEAK=0.                $         GOTO177
  177 CONTINUE
      RETURN $ END
C.............SUBROUTINE FOR PLASMATUBE SPECTRUM.............................
      SUBROUTINE PLASMA (LL5,  LL7,  TRANSM,  POSN,  SPEC RAD,  WL)
C...FOR DATA CARDS FROM 'PLASMA',MUST INSERT  A POSITIVE INTEGER IN 'NO WL'
      DIMENSION TRANSM (3000), WL (3000), POSN (3000), SPEC RAD (3000)
      DIMENSION A(12), B(12), C(12), D(12), E(12)
      DATA (A = +.32545008E+04, +.20079624E+02,  +.71875617E-03, +.15231
     1070E-03, -.18274754E-05, +.71617321E-08  ), (B= -.11640708E+03, +
     2.15520201E+01, -.51678338E-02, +.51082205E-05), (C=-.10515427E+02,
     3+.10643331E+02, -.39589637E+01, +.79004647E+00, -.74864830E-01,
     4+.27394308E-02), (D=-.15769239E+01, +.75482312E+00, +.11277031E+00
     5, -.66193739E-02, +.17440403E-03, -.16853878E-05), (E=-.37899022E+
     604, +.34280211E+02, -.79662748E-01, -.10138259E-03, +.52796105E-06
     7, -.18945425E-11,-.15991413E-11, +.14448870E-14)
      DATA (II=6), (JJJJ=4), (KKKK=6), (MM=8), (LLLL=6)
C  PERFORMING WAVELENGTH AND SPECTRAL RADIANCE CALCULATIONS FOR PLASMA SPECTRA..
      DO 315  N  =  LL5,  LL7
      T = TRANSM(N) * 0.01
      DIST = POSN(N)
      DD = DIST
      WVL = A(1)
      DO 300 III = 2,II
      WVL = WVL + A(III) * DD
```

```
  300 DD = DD*DIST
      IF (WVL - 4475. )  303,  303,  301
  301 TIMES = B(1)
      WW = WVL/10.
      DO 302 JJJ = 2,JJJJ
      TIMES = TIMES + B(JJJ) * WW
  302 WW = WW*(WVL/10.)
      GO TO 305
  303 TIMES = E(1)
      WW = WVL/10.
      DO 304 MMM = 2,MM
      TIMES = TIMES + E(MMM)*WW
  304 WW = WW*(WVL/10.)
  305 IF  (TRANSM(N) -  50.)  307,  307,  306
  306 SPEC RAD(N) = 0.0   $   TIMES = 0.0
      GO TO 314
  307 IF (T) 308,  314,   308
  308 IF  ((1./T)  -  7.95) 309,  309,  311
  309 SPFRD = C(1)
      TRANS = 1./T
      DO 310 KKK = 2,KKKK
      SPFRD = SPFRD + C(KKK)*TRANS
  310 TRANS = TRANS*(1./T)
      GO TO 313
  311 SPFRD = D(1)
      TRANS = 1./T
      DO 312 LLL = 2,LLLL
      SPFRD = SPFRD + D(LLL)*TRANS
  312 TRANS = TRANS * (1./T)
  313 SPEC RAD(N) = SPFRD * TIMES
  314  WL(N) = WVL
  315 CONTINUE  $ RETURN  $  END
        SCOPE
'LOAD
'RUN,20,1000
PLA 1   24   20                1 10 1   1 1 20                                54.279
''GG
```

Appendix B

PLOT QUADRATIC

```
      PROGRAM PLTQUAD
C  PLTQUA1----LOW RESOLUTION SPECTRA(1 DIVISION /100 ANGSTROM
C PLOT 9-CARDS, ALL OPTIONS, Y = WL, X = DENSITY
      DIMENSION X (9), Y (9)
  200 FORMAT (/)
  201 FORMAT (1H1)
  202 FORMAT (//)
  203 FORMAT (///)
  205 FORMAT (62H1 PUNCH  , 2 INTERVAL, 3 SKEW COR 4 SUBTR BASE, 5 WL,6
     1AX + B )
  206 FORMAT (66HCARD ORDER= 1 CONTROL, 3 WL STDS (5), 2 BASE (4), 1 STA
     1RT, 1 END  )
  207 FORMAT  (18HCONTROL CARD IS      )
  208 FORMAT (21HSTANDARD LINES ARE      )
  209 FORMAT (30H COEFFICIENTS OF QUADRATIC ARE , 3F10.3 )
  210 FORMAT  ( 7( F4.3, F7.3) )
  211 FORMAT (8F10.3)
  212 FORMAT ( 3I10)
  213 FORMAT (I1, 1X, F6.0, 18F4.3)
  214 FORMAT (2F10.3, I10, 10F5.2 )
  215 FORMAT ( 8F10.3)
  216 FORMAT (I1)
  217 FORMAT (55HTURN SS2 OFF, THEN TYPE INTERVAL.  PREVIOUS VALUE WAS
     1     , I2 )
  219 FORMAT ( 40HTYPE CONSTANT CORRECTION GB, PREVIOUSLY     , F10.3 )
  220 FORMAT ( 39HTYPE LINEAR CORRECTION GA, PREVIOUSLY    , F10.3 )
  221 FORMAT (    37HCOEFFICIENTS FOR WL CALIBRATION ARE        )
  222 FORMAT (26HINPUT CARDS FOR BASE ARE       )
  223 FORMAT (32HRESULTANT BASE PARAMETERS ARE      )
  224 FORMAT (15HGA AND GB ARE        ,   F8.3  , 4H AND    , F8.3  )
  225 FORMAT (32HBOTTOM OF SCALE IS ZERO, TOP IS     , F10.3 )
  226 FORMAT (17HSTART OF SCALE IS  ,F10.3,  8H, END IS      ,
     1F10.3, 12H. THERE ARE     , I5, 18H MAJOR DIVISIONS.              )
  230 FORMAT (70HTYPE SKEW CORRN AT 38 MM, ASSUMED ZERO AT 10 MM.  PREVI
     1OUS VALUE WAS      , F10.5 )
  231 FORMAT (27HMAXIMUM SKEW CORRECTION IS      , F10.5,  8H UNITS.  )
  232 FORMAT (E16.8, 24H IS THE SKEW CORRECTION    )
  250 FORMAT (I1,1H0,  F4.2,   1X,F9.3,11X,F9.3)
  252 FORMAT ( 7H GRAPH       , 2F10.3 )
  254 FORMAT (20H PREVIOUS VALUE WAS    , E20.10 )
  255 FORMAT ( E16.8 )
  256 FORMAT ( 35H TURN SS3 OFF, THEN TYPE SCALE X       )
  257 FORMAT (5E16.8 )
  260 FORMAT (15X, F10.4, F11.3 )
  269 FORMAT(2X,F3.2,25X, F8.3 )
  280 FORMAT (80H
     1                                                  )
  290 FORMAT (25HREADY PUNCH, TYPE TITLE      )
      COMMON X, Y
  501 READ(3, 214) SCALE X, SCALE Y, N CONTROL, X1, X2, X3, X4, X5
      WRITE(1,203 )
      WRITE(1,205  )
      WRITE(1,206  )
      AGA = 1.
      AGB = 0.
      AHA = 0.
```

```
  1 CONTINUE
    WRITE(1,203  )
    WRITE(1,207  )
    WRITE(1,214) SCALE X, SCALE Y, N CONTROL, X1, X2, X3, X4, X5
    FA = 0.
    FB = 0.
    FC = 0.
    FD = 0.
    FE = 0.
    GA = 1.
    GB = 0.
    HA = 0.
    INTERVAL = 1
    ZA = 0.
    ZB = 1.
    ZC = 0.
    IF ( SENSE SWITCH 5 )  310, 2
310 READ(3, 260) WLS 1, ZY1
    READ(3, 260) WLS 2, ZY2
    READ(3, 260) WLS 3, ZY3
    WRITE(1,208  )
    WRITE(1,215) WLS1, ZY1, WLS2, ZY2, WLS3, ZY3
    AY1 = (WLS 1 - WLS 2) / (ZY1 - ZY2)
    AY2 = (WLS 2 - WLS 3) / (ZY2 - ZY3)
    ZA = (AY1 - AY2) / (ZY1 - ZY3)
    ZB = (AY1 - ZA * (ZY1 + ZY2) )
    ZC = WLS 1 - ZA * ZY1 * ZY1 - ZB * ZY1
  2 WRITE(1,221  )
    WRITE(1,257) ZA, ZB, ZC
    IF (SENSE SWITCH 4) 3, 10
  3 READ(3, 257) FA1, FB1, FC1, FD1, FE1
    WRITE(1,222  )
    WRITE(1,257) FA1, FB1, FC1, FD1, FE1
    READ(3, 257) FA2, FB2, FC2, FD2, FE2
    WRITE(1,257) FA2, FB2, FC2, FD2, FE2
    FA = (FA1 + FA2)/2.
    FB = (FB1 + FB2)/2.
    FC = (FC1 + FC2)/2.
    FD = (FD1 + FD2)/2.
    FE = (FE1 + FE2)/2.
 10 CONTINUE
    WRITE(1,223  )
    WRITE(1,257) FA, FB, FC, FD, FE
    IF (SENSE SWITCH 6) 12, 20
 12 WRITE(1,219) AGB
    READ (9, 255) GB
    WRITE(1,255) GB
    WRITE(1,220) AGA
    READ (9, 255) GA
    WRITE(1,255) GA
    AGA = GA
    AGB = GB
 20 CONTINUE
    WRITE(1,224) GA, GB
    IF (SENSE SWITCH 3) 25, 30
 25 WRITE(1,230) AHA
    READ (9, 255) HA
```

```
      WRITE(1,231) HA
      AHA = HA
   30 CONTINUE
      IF ( SENSE SWITCH 1 )  31, 35
   31 WRITE(1,290  )
      READ (9, 280)
      WRITE(4,280  )
      WRITE(4,257) ZA, ZB, ZC
      WRITE(4,257) FA, FB, FC, FD, FE
      WRITE(4,257) GA, GB
      WRITE(4,232) HA
   35 TOP = 10. * SCALE X
      CALL APLOT ( SCALE X, SCALE Y, 1)
      READ(3, 213) LL,      STARTPOS
      READ(3, 213) LL,      ENDPOS
      ENDPOS = ENDPOS + 100 .
      STARTPOS = ZA*STARTPOS*STARTPOS + ZB*STARTPOS + ZC
      ENDPOS = ZA*ENDPOS*ENDPOS + ZB*ENDPOS + ZC
      NSTART = STARTPOS
      NSTART  = NSTART /100
      NSTART = NSTART * 100
      STARTPOS = NSTART
      NENDPOS = ENDPOS
      NENDPOS = NENDPOS/100
      NENDPOS = NEND POS * 100
      ENDPOS = NENDPOS
      FLIMIT = (ENDPOS - STARTPOS)/100.
      LIMIT = FLIMIT
      FLIMIT = 100*FLIMIT
      GRAPH 0 = TOP
      GRAPH 1 = TOP - .2 * SCALE X
      GRAPH 2 = TOP - .05* SCALE X
      ATOP = TOP + .5*SCALEX
      CALL APLOT (ATOP, STARTPOS, 2)
      CALL APLOT (ATOP, STARTPOS, 3)
      IF (X1) 58, 43, 43
   43 CONTINUE
      WRITE(1,226) STARTPOS, ENDPOS,  LIMIT
      PAUSE
      DO 47 N = 1, LIMIT
      CALL APLOT ( GRAPH 1, STARTPOS, 3 )
      CALL APLOT ( GRAPH 1, STARTPOS, 4 )
      CALL APLOT ( GRAPH 0, STARTPOS, 4 )
      DO 46 I = 1, 10
      IF ( N CONTROL ) 44, 45, 44
   44 CONTINUE
      CALL APLOT ( GRAPH 2, STARTPOS, 3 )
      CALL APLOT ( GRAPH 2, STARTPOS, 4 )
      CALL APLOT ( GRAPH 0, STARTPOS, 4 )
   45 CONTINUE
      STARTPOS = STARTPOS + 10.
   46 CONTINUE
   47 CONTINUE
      STARTPOS = STARTPOS - FLIMIT
   50 XX = TOP
   51 CALL APLOT ( XX,   ENDPOS, 3 )
```

```
      CALL APLOT ( XX,    ENDPOS, 4 )
      CALL APLOT ( XX, STARTPOS, 4 )
      XX = XX - X1
      IF (X1) 58, 58, 52
   52 IF (XX) 55, 53, 53
   53 CALL APLOT ( XX, STARTPOS, 3 )
      CALL APLOT ( XX, STARTPOS, 4 )
      CALL APLOT ( XX,    ENDPOS, 4 )
      XX = XX - X1
      IF (XX) 55, 51, 51
   55 CALL APLOT ( TOP,    ENDPOS, 3 )
      CALL APLOT ( TOP,    ENDPOS, 4 )
      CALL APLOT (  0.,    ENDPOS, 4 )
      CALL APLOT (  0., STARTPOS, 4 )
      CALL APLOT ( TOP, STARTPOS, 4 )
   58 CONTINUE
      PAUSE
  158 READ(3, 213) LL, FNY, ( Y(N), X(N), N = 1, 9 )
      WRITE(1,202  )
      U = Y(1)
      W     = Y(1) + FNY
      V = X(1)
      WW    = GB + GA*(V - FA - FB*W - FC*W*W - FD*W*W*W - FE*W*W*W*W)
      X(1) = WW    + ( W - 10. ) * HA / 28.
      Y(1) = ZA*W*W + ZB*W + ZC
      X (1) = TOP - X (1)
      CALL APLOT (X(1), Y(1), 3)
      Y(1) = U
      X(1) = V
      GO TO 60
   59 CONTINUE
      READ(3, 213) LL, FNY, ( Y(N), X(N), N = 1, 9 )
      IF ( FNY + X(1) ) 158, 90, 60
   60 CONTINUE
      DO 70 N = 1, 9, INTERVAL
      IF ( X(N) + Y (N) ) 70, 70, 65
   65 CONTINUE
      W     = Y(N) + FNY
      V = X(N)
      Y(N) = ZA*W*W + ZB*W + ZC
      IF (LL) 66, 67, 66
   66 V = 10. * V
   67 CONTINUE
      V = V - FA - FB*W - FC*W*W - FD*W*W*W - FE*W*W*W*W
      X(N) = GA*V + GB  + (W - 10.) * HA / 28.
      IF ( X(N) ) 80, 80, 68
   68 IF ( TOP - X(N)) 82, 69, 69
   69 IF ( Y(N) )  70, 70, 169
  169 X(N) = TOP - X(N)
      CALL APLOT (X(N), Y(N), 4)
      GO TO 70
   80 X(N) = 0.
      GO TO 169
   82 X(N) = TOP
      GO TO 169
   70 CONTINUE
      IF ( SENSE SWITCH 2 )  88, 59
```

```
   88 WRITE(1,217) INTERVAL                                          0091803
      READ (9, 216) INTERVAL                                         0091804
      WRITE(1,216) INTERVAL                                          0091805
      GO TO 59                                                       0091806
   90 CONTINUE                                                       0091807
  REMOVING THIS CARD AND THE FOLLOWING TWO COMMENT CARDS PERMITS A   0091808
   COMPILATION FOR THE GERBER PLOTTING--GIVES A DIFFERENT BINARY DECK 0091809
      CALL APLOT ( DUMMY, DUMMY, 5 )                                 0091810
      LINEMARKING PORTION OF PROGRAM.....................................,.......
      IF(X2) 109,110,110                                             0091812
  109 PAUSE                                                          0091813
  110 CONTINUE                                                       0091814
      ADD  = .05                                                     0091815
      IF (X2) 111, 95, 95                                            0091816
  111 CONTINUE                                                       0091817
      READ(3, 250) NCODE, XX, YYYY, YY                               0091818
          IF ( YY + XX)  120, 95, 120                                0091819
  120 XX = TOP - XX + ADD                                            0091820
      CALL APLOT ( XX, YY, 3)                                        0091821
      CALL APLOT ( XX, YY, 4)                                        0091822
      IF(X4) 108,107,107                                             0091823
  108 XX = XX - 5. * ADD                                             0091824
      GO TO 1071                                                     0091825
  107 XX = XX - 2. * ADD                                             0091826
 1071 CALL APLOT ( XX, YY, 4)                                        0091827
      GO TO 111                                                      0091828
   95 IF (X3) 97, 97, 96                                             0091829
   96 CALL APLOT(ATOP, STARTPOS, 3)                                  0091830
      GO TO 98                                                       0091831
   97 END POS = END POS + 10.                                        0091832
      CALLAPLOT( ATOP, END POS, 3)                                   0091833
   98 READ(3, 214) SCALE X, SCALE Y, N CONTROL, X1, X2, X3, X4, X5   0091834
      GO TO 1                                                        0091835
  100 CONTINUE                                                       0091836
      END                                                            0091837
                                                                     0091838
```

Appendix C

PLOT CUBIC

```
      PROGRAM PLTCUB2
CPLT CUB2 ----HIGH RESOLUTION SPECTRA (1 DIVISION / 1 ANGSTROM)
CPLOT CUBIC - HIGH RESOLUTION (REVISED 8/17/67)
CPLOT 9-CARDS, ALL OPTIONS, Y = WL,  X = DENSITY, CUBIC WL OPTION
      DIMENSION X (9), Y (9)
  200 FORMAT (/)
  201 FORMAT (1H1)
  202 FORMAT (//)
  203 FORMAT (///)
  205 FORMAT (62H1 PUNCH  , 2 INTERVAL, 3 SKEW COR 4 SUBTR BASE, 5 WL,6
     1AX + B )
  206 FORMAT (66HCARD ORDER= 1 CONTROL, 3 WL STDS (5), 2 BASE (4), 1 STA
     1RT, 1 END  )
  207 FORMAT  (18HCONTROL CARD IS      )
  208 FORMAT (21HSTANDARD LINES ARE      )
  209 FORMAT (30H COEFFICIENTS OF QUADRATIC ARE , 3F10.3 )
  210 FORMAT  ( 7( F4.3, F7.3) )
  211 FORMAT (8F10.3)
  212 FORMAT ( 3I10)
  213 FORMAT (I1,X,F6.0, 18F4.3 )
  214 FORMAT (2F10.3, I10, 10F5.2 )
  215 FORMAT ( 8F10.3)
  216 FORMAT (I1)
  217 FORMAT (55HTURN SS2 OFF, THEN TYPE INTERVAL.  PREVIOUS VALUE WAS
     1     , I2 )
  219 FORMAT ( 40HTYPE CONSTANT CORRECTION GB, PREVIOUSLY     , F10.3 )
  220 FORMAT ( 39HTYPE LINEAR CORRECTION GA, PREVIOUSLY    , F10.3 )
  221 FORMAT (    37HCOEFFICIENTS FOR WL CALIBRATION ARE        )
  222 FORMAT (26HINPUT CARDS FOR BASE ARE       )
  223 FORMAT (32HRESULTANT BASE PARAMETERS ARE      )
  224 FORMAT (15HGA AND GB ARE        ,    F8.3  , 4H AND    , F8.3  )
  225 FORMAT (32HBOTTOM OF SCALE IS ZERO, TOP IS     , F10.3 )
  226 FORMAT (17HSTART OF SCALE IS  ,F10.3,  8H, END IS      ,
     1F10.3, 12H. THERE ARE     , I5, 18H MAJOR DIVISIONS.              )
  230 FORMAT (70HTYPE SKEW CORRN AT 38 MM, ASSUMED ZERO AT 10 MM.  PREVI
     1OUS VALUE WAS      , F10.5 )
  231 FORMAT (27HMAXIMUM SKEW CORRECTION IS      , F10.5,  8H UNITS.  )
  232 FORMAT (E16.8, 24H IS THE SKEW CORRECTION    )
  250 FORMAT (I1,1H0,  F3.2,   2X,F9.3,11X,F9.3)
  252 FORMAT ( 7H GRAPH       , 2F10.3 )
  254 FORMAT (20H PREVIOUS VALUE WAS    , E20.10 )
  255 FORMAT ( E16.8 )
  256 FORMAT ( 35H TURN SS3 OFF, THEN TYPE SCALE X       )
  257 FORMAT (5E16.8 )
  260 FORMAT (15X, F10.4, F11.3 )
  269 FORMAT(2X,F3.2,25X, F8.3 )
  280 FORMAT (80H
     1                                                        )
  290 FORMAT (25HREADY PUNCH, TYPE TITLE      )
      COMMON X, Y
  501 READ(3, 214) SCALE X, SCALE Y, N CONTROL, X1, X2, X3, X4, X5
      WRITE(1,203)
      WRITE(1,205  )
      WRITE(1,206   )
      AGA = 1.
      AGB = 0.
```

```
      AHA = 0.
    1 CONTINUE
      WRITE(1,203  )
      WRITE(1,207  )
      WRITE(1,214) SCALE X, SCALE Y, N CONTROL, X1, X2, X3, X4, X5
      FA = 0.
      FB = 0.
      FC = 0.
      FD = 0.
      FE = 0.
      GA = 1.
      GB = 0.
      HA = 0.
      INTERVAL = 1
      ZA = 0.
      ZB = 1.
      ZC = 0.
      ZD = 0.
      IF ( SENSE SWITCH 5 )  310, 2
  310 READ(3, 260)   Y 1,  X1
      READ(3, 260)   Y 2,  X2
      READ(3, 260)   Y 3, X 3
      READ(3, 260)   Y 4, X 4
      WRITE(1,208  )
      WRITE(1,215) Y1, X1, Y2, X2, Y3, X3, Y4, X4
      C11 = (Y2 - Y1) / ((X2 - X1)*(X2- X3) * (X2 - X4))
      C12 = (Y3 - Y1)/((X3 - X1) * (X3 - X2) *(X3 - X4))
      C13 = (Y4 - Y1) / ((X4 - X1)*(X4 - X2) * (X4 - X3))
      ZD = C11 + C12 + C13
      C21 = (Y2 -Y1)/((X2 - X1) *(X2 - X3))
      C22 = (Y3 - Y1)/((X3 - X1) * (X3 - X2))
      C23 = (X1 + X2 + X3)* ZD
      ZA = C21 + C22 - C23
      C31 = (Y2 - Y1) /(X2 - X1)
      C32 = (X1 + X2) * ZA
      C33 = (X2*X2 + X2 *X1 + X1*X1) * ZA
      ZB = C31 - C32 - C33
      ZC = Y1 - ZB*X1 - ZA*X1*X1 - ZD* X1* X1 *X1
    2 WRITE(1,221   )
      WRITE(1,257) ZC, ZB, ZA, ZD
      IF (SENSE SWITCH 4) 3, 10
    3 READ(3, 257) FA1, FB1, FC1, FD1, FE1
      WRITE(1,222  )
      WRITE(1,257) FA1, FB1, FC1, FD1, FE1
      READ(3, 257) FA2, FB2, FC2, FD2, FE2
      WRITE(1,257) FA2, FB2, FC2, FD2, FE2
      FA = (FA1 + FA2)/2.
      FB = (FB1 + FB2)/2.
      FC = (FC1 + FC2)/2.
      FD = (FD1 + FD2)/2.
      FE = (FE1 + FE2)/2.
   10 CONTINUE
      WRITE(1,223  )
      WRITE(1,257) FA, FB, FC, FD, FE
      IF (SENSE SWITCH 6) 12, 20
   12 WRITE(1,219) AGB
      READ (9, 255) GB
```

```
      WRITE(1,255) GB                                                   7082180
      WRITE(1,220) AGA                                                  7082181
      READ (9, 255) GA                                                  7082182
      WRITE(1,255) GA                                                   7082183
      AGA = GA                                                          7082184
      AGB = GB                                                          7082185
   20 CONTINUE                                                          7082186
      WRITE(1,224) GA, GB                                               7082187
      IF (SENSE SWITCH 3) 25, 30                                        7082188
   25 WRITE(1,230) AHA                                                  7082189
      READ (9, 255) HA                                                  7082190
      WRITE(1,231) HA                                                   7082191
      AHA = HA                                                          7082192
   30 CONTINUE                                                          7082193
      IF ( SENSE SWITCH 1 )  31, 35                                     7082194
   31 WRITE(1,290  )                                                    7082195)
      READ (9, 280)                                                     7082196
      WRITE(4,280  )                                                    7082197)
      WRITE(4,257) ZC, ZB, ZA, ZD                                       7082198
      WRITE(4,257) FA, FB, FC, FD, FE                                   7082199
      WRITE(4,257) GA, GB                                               7082200
      WRITE(4,232) HA                                                   7082201
   35 TOP = 10. * SCALE X                                               7082202
      CALL APLOT ( SCALE X, SCALE Y, 1)                                 7082203
      READ(3, 213) LL,       STARTPOS                                   7082204
      READ(3, 213) LL,       ENDPOS                                     7082205
      STARTPOS = ZA*STARTPOS*STARTPOS + ZB*STARTPOS + ZC                7082206
     1 + ZD * STARTPOS * STARTPOS * STARTPOS                            7082207
      ENDPOS = ZA*ENDPOS*ENDPOS + ZB*ENDPOS + ZC                        7082208
     1 + ZD * ENDPOS * ENDPOS * ENDPOS                                  7082209
      NSTART = STARTPOS                                                 7082211
      STARTPOS = NSTART
      NENDPOS = ENDPOS                                                  7082214
      ENDPOS = NENDPOS
      FLIMIT = ENDPOS - STARTPOS                                        7082216
      LIMIT =  FLIMIT                                                   7082217
      GRAPH 0 = TOP                                                     7082218
      GRAPH 1 = TOP - .2 * SCALE X                                      7082219
      GRAPH 2 = TOP - .05* SCALE X                                      7082220
      ATOP = TOP + .5*SCALEX                                            7082221
      CALL APLOT (ATOP, STARTPOS, 2)                                    7082222
      CALL APLOT (ATOP, STARTPOS, 3)
      IF (X1) 58, 43, 43                                                7082223
   43 CONTINUE                                                          7082224
      WRITE(1,226) STARTPOS, ENDPOS,  LIMIT                             7082225
      PAUSE                                                             7082226
      DO 47 N = 1, LIMIT                                                7082227
      CALL APLOT ( GRAPH 1, STARTPOS, 3 )                               7082228
      CALL APLOT ( GRAPH 1, STARTPOS, 4 )                               7082229
      DO 46 I = 1, 10                                                   7082230
      IF ( N CONTROL ) 44, 45, 44                                       7082231
   44 CONTINUE                                                          7082232
      CALL APLOT ( GRAPH 2, STARTPOS, 3 )                               7082233
      CALL APLOT ( GRAPH 2, STARTPOS, 4 )                               7082234
   45 CONTINUE                                                          7082235
      STARTPOS = STARTPOS + .1                                          7082236
```

```
 46 CONTINUE
 47 CONTINUE
    STARTPOS = STARTPOS - FLIMIT
 50 XX = TOP
 51 CALL APLOT ( XX,   ENDPOS, 3 )
    CALL APLOT ( XX,   ENDPOS, 4 )
    CALL APLOT ( XX, STARTPOS, 4 )
    XX = XX - X1
    IF (X1) 58, 58, 52
 52 IF (XX) 55, 53, 53
 53 CALL APLOT ( XX, STARTPOS, 3 )
    CALL APLOT ( XX, STARTPOS, 4 )
    CALL APLOT ( XX,   ENDPOS, 4 )
    XX = XX - X1
    IF (XX) 55, 51, 51
 55 CALL APLOT ( TOP,   ENDPOS, 3 )
    CALL APLOT ( TOP,   ENDPOS, 4 )
    CALL APLOT (  0.,   ENDPOS, 4 )
    CALL APLOT (  0., STARTPOS, 4 )
    CALL APLOT ( TOP, STARTPOS, 4 )
 58 CONTINUE
    PAUSE
158 READ(3, 213) LL, FNY, ( Y(N), X(N), N = 1, 9 )
    WRITE(1,202  )
    U = Y(1)
    W    = Y(1) + FNY
    V = X(1)
    WW   = GB + GA*(V - FA - FB*W - FC*W*W - FD*W*W*W - FE*W*W*W*W)
    X(1) = WW   + ( W - 10. ) * HA / 28.
    Y(1) = ZA*W*W + ZB*W + ZC + ZD * W * W * W
    X (1) = TOP - X (1)
    CALL APLOT (X(1), Y(1), 3)
    Y(1) = U
    X(1) = V
    GO TO 60
 59 CONTINUE
    READ(3, 213) LL, FNY, ( Y(N), X(N), N = 1, 9 )
    IF ( FNY + X(1) ) 158, 90, 60
 60 CONTINUE
    DO 70 N = 1, 9, INTERVAL
    IF ( X(N) + Y (N) ) 70, 70, 65
 65 CONTINUE
    W    = Y(N) + FNY
    V = X(N)
    Y(N) = ZA*W*W + ZB*W + ZC + ZD * W * W * W
    IF (LL) 66, 67, 66
 66 V = 10. * V
 67 CONTINUE
    V = V - FA - FB*W - FC*W*W - FD*W*W*W - FE*W*W*W*W
    X(N) = GA*V + GB  + (W - 10.) * HA / 28.
    IF ( X(N) ) 80, 80, 68
 68 IF ( TOP - X(N)) 82, 69, 69
 69 IF ( Y(N) )  70, 70, 169
169 X(N) = TOP - X(N)
    CALL APLOT (X(N), Y(N), 4)
    GO TO 70
 80 X(N) = 0.
```

```
      GO TO 169
   82 X(N) = TOP
      GO TO 169
   70 CONTINUE
      IF ( SENSE SWITCH 2 )  88, 59
   88 WRITE(1,217) INTERVAL
      READ (9, 216) INTERVAL
      WRITE(1,216) INTERVAL
      GO TO 59
   90 CONTINUE
   THE OMITTING OF THIS COMMENT AND THE FOLLOWING TWO COMMENT CARDS WILL
      A NEW BINARY DECK FOR PLOTTING ON THE GERBER
      CALL APLOT ( DUMMY, DUMMY, 5 )
      ADD = .05
      IF (X2) 111, 94, 95
  111 CONTINUE
      READ(3, 250) NCODE, XX, YYYY, YY
          IF ( YY + XX)  120, 95, 120
  120 XX = TOP - XX + ADD
      CALL APLOT ( XX, YY, 3)
      XX = XX - 2. * ADD
      CALL APLOT ( XX, YY, 4)
      GO TO 111
   94  CONTINUE
   95  CONTINUE
       IF (X3) 97, 97, 96
   96  CALL APLOT (ATOP, STARTPOS ,3)
       GO TO  98
   97 ENDPOS = ENDPOS + 10
       CALL APLOT (ATOP, ENDPOS, 3)
   98 READ(3, 214) SCALE X, SCALE Y, NCONTROL, X1, X2, X3, X4, X5
      GO TO 1
  100 CONTINUE
      END
```

Appendix D

GAUSSIAN SMOOTHING

```
*       SMOOTH DATA BY BLOCKED GAUSSIAN METHOD,
C       'BLOCKED GAUSSIAN SMOOTHING'
        DIMENSION X (9), Y (9), X1 (9), Y1 (9), NX1 (9), NY1(9)
        DIMENSION WEIGHT (10), STEP X (10), STEP Y (10)
  212 FORMAT (I1, 1X, I6, 18I4)
  213 FORMAT ( I1, 1X, F6.0, 18F4.3)
  257 FORMAT ( 35H T                    ,,PE N AV          )
  258 FORMAT (I3)
  259 FORMAT ( I8, 4F8.3)
  260 FORMAT ( 14H PUNCH ORDER          )
  261 FORMAT ( 9F8.2 )
  265 FORMAT (12H TYPE Y ADD    )
  266 FORMAT (12H TYPE X ADD    )
  267 FORMAT ( E20.10)
  268 FORMAT ( F20.10 )
        WEIGHT (1) = .0167
        WEIGHT (10)= .0167
        WEIGHT ( 2)= .0446
        WEIGHT ( 9)= .0446
        WEIGHT ( 3)= .0930
        WEIGHT ( 8)= .0930
        WEIGHT ( 4)= .1517
        WEIGHT ( 7)= .1517
        WEIGHT ( 5)= .1940
        WEIGHT ( 6)= .1940
        JJ = 0
        JJJ = 0
    1 CONTINUE
        I = 0
        J = 0
        X AV = 0.
        Y AV = 0.
        NY = 0
        FFNY = 0.
        PRINT 257
        READ (9, 258) N AV
        AV = N AV
        PRINT 258, N AV
        PRINT 265
        READ (9, 267) Y ADD
        PRINT 268, Y ADD
        PRINT 266
        READ (9, 267) X ADD
        PRINT 268, X ADD
   59 CONTINUE
        READ 213, LL, FNY, ( Y(N), X(N), N = 1, 9 )
        IF ( FNY + X(1) )  90, 90, 60
   60 CONTINUE
        DO 70 N = 1, 9
        IF ( X(N) + Y (N) ) 70, 70, 65
   65 CONTINUE
        Y(N) = Y(N) + FNY + Y ADD
        IF (LL) 66, 67, 66
   66 X(N) = 10. * X(N)
   67 CONTINUE
        IF ( X(N) )  70, 70, 169
  169 CONTINUE
        X(N) = X(N) + X ADD
        I = I + 1
        X AV = X AV + X (N)
        Y AV = Y AV + Y(N)
        IF (N AV - I )  320, 320, 70
```

```
320 I = 0
    JJ = JJ + 1
    STEP X (JJ) = X AV / AV
    STEP Y (JJ) = Y AV / AV
    X AV = 0.
    Y AV = 0.
    IF (10 - JJ )  330, 330, 70
330 JJ = 9
    DO 335 JJJ = 1, 10
    X AV = X AV + WEIGHT (JJJ) * STEP X (JJJ)
    Y AV = Y AV + WEIGHT (JJJ) * STEP Y (JJJ)
335 CONTINUE
    STEP X (1) = STEP X (2)
    STEP X (2) = STEP X (3)
    STEP X (3) = STEP X (4)
    STEP X (4) = STEP X (5)
    STEP X (5) = STEP X (6)
    STEP X (6) = STEP X (7)
    STEP X (7) = STEP X (8)
    STEP X (8) = STEP X (9)
    STEP X (9) = STEP X (10)
    STEP Y (1) = STEP Y (2)
    STEP Y (2) = STEP Y (3)
    STEP Y (3) = STEP Y (4)
    STEP Y (4) = STEP Y (5)
    STEP Y (5) = STEP Y (6)
    STEP Y (6) = STEP Y (7)
    STEP Y (7) = STEP Y (8)
    STEP Y (8) = STEP Y (9)
    STEP Y (9) = STEP Y (10)
    J = J + 1
    X1 (J) = X AV
    Y 1 (J) = Y AV
    X AV = 0.
    Y AV = 0.
    IF ( 9 - J )  340, 340, 70
340 J = 0
    N1 = 0
    NY = Y1 (1)
    FFNY = NY
    DO 20 I = 1, 9
    X1 (I) = 1000. * X1 (I)
    Y1 (I) = Y1 (I) - FFNY
    Y1 (I) = 1000. * Y1 (I)
    NX1 (I) = X1 (I)
    NY1(I) = Y1 (I)
    IF ( 9999 - NX1 (I) ) 16, 17, 17
 16 N1 = 1
 17 CONTINUE
 20 CONTINUE
    IF ( N1 )  28, 28, 25
 25 DO 26 I = 1, 9
 26 NX1 (I) = NX1 (I) / 10
 28 CONTINUE
    PUNCH 212, N1, NY, ( NY1(M), NX1 (M), M = 1, 9 )
    I = 0
    J = 0
    Y1 (1) = 0.
    Y1 (2) = 0.
    Y1 (3) = 0.
     Y1(4) = 0.
     Y1 (5) = 0.
     Y1 (6) = 0.
    Y1 (7) = 0.
    Y1 (8) = 0.
    Y1 (9) = 0.
 70 CONTINUE
    GO TO 59
 90 CONTINUE
    GO TO 1
    END
```

Appendix E

POLYNOMIAL FIT OF BACKGROUNDS

```
C       'POLYNOMIAL FIT OF BACKGROUNDS'
C       THIS PROGRAM  MUST BE ACCOMPANIED BY A JOB CARD. . . . . . . . . . . . . .
'FTN, L,X
        PROGRAM MAIN
        DIMENSION WL(2000), DENSITY (2000), DENSTEST(2000)
  220 FORMAT (8F15.3)
  260 FORMAT ( 6(F8.2, 2F6.2 )   )
    1 CONTINUE
        L1 = L2 = L3 = N = 0
        CALL INCARDS (DENSITY, WL, L1, L2, L3, N)
        N FIT = 4
        CALL POLYFIT (DENSITY, WL, N, NFIT, FA, FB, FC, FD, FE)
        PRINT 220, FA, FB, FC, FD, FE
        DO 5 L = 1, N   $   Z = WL(L)
    5 DENS TEST (L) = FA + FB*Z + FC*Z*Z + FD*Z*Z*Z + FE*Z*Z*Z*Z
        PRINT 260, (WL(L), DENSITY(L), DENS TEST(L), L= 1, N)
        L1 = 1   $   L2 = N    $   L3 = 0
        CALL OUTCARDS(DENSTEST, WL, L1, L2, L3, N)
        GO TO 1
        END
        SUBROUTINE POLYFIT (Y, X, N, LAST, FA, FB, FC, FD, FE )
        DIMENSION X(2000), Y(2000), A(11,11), SUMX(31), SUMY(15)
        TYPE DOUBLE X, Y, A, SUMX, SUMY, S1, S2, S3
  255 FORMAT (* RMS ERROR =*, F10.3 ,* WHEN DEGREE OF EQUATION IS*,I3)
  257 FORMAT ( 5 E16.8 )
   50 CONTINUE $ IF(N.GT.2000)N=2000 $ W=1.
        SUMX(1) = SUMX(2) = SUMX(3) = SUMY(1) = SUMY(2) =FA=FB=FC=FD=FE=0.
        DO90I=1,N $ SUMX(1)=SUMX(1)+W $ SUMX(2)=SUMX(2)+W*X(I)
        SUMX(3)=SUMX(3)+W*X(I)*X(I) $ SUMY(1)=SUMY(1)+W*Y(I)
   90 SUMY(2)=SUMY(2)+W*X(I)*Y(I) $ NORD=1
   93 L=NORD+1 $ KK=L+1 $ DO101 I=1,L $ DO100 J=1,L $ IK=J-1+I
  100 A(I,J)=SUMX(IK)
  101 A(I,KK)=SUMY(I) $ DO 140 I=1,L $ A(KK,I)=-1.$KKK=I+1$DO110J=KKK,KK
  110 A(KK,J)=0. $ C=1./A(1,I) $ DO120 II=2,KK $ DO120 J=KKK,KK
  120 A(II,J)=A(II,J)-A(1,J)*A(II,I)*C $ DO140 II=1,L $ DO140 J=KKK,KK
  140 A(II,J)=A(II+1,J) $ S2=0.
                                        DO160 J=1,N $ S1=0. $ S1=S1+A(1,KK)
        DO 150 I = 1, NORD
  150 S1 = S1 + A(I+1,KK)*X(J)**I
  160 S2=S2+(S1-Y(J))*(S1-Y(J)) $ B=N-L $ S2=S2/B $ S2 = SQRT(S2)
        PRINT 255, S2, NORD
        IF (NORD .NE. LAST )  GO TO 171
COMMENT   A + BX + CX2 + DX3 + FX4
        FA=A(1,KK) $ FB=A(2,KK) $ FC=A(3,KK) $ FD=A(4,KK) $ FF=A(5,KK)
        PUNCH 257, (A (MM,KK), MM = 1, 5 )
        PRINT 257, (A (MM,KK), MM = 1, 5 )
        GO TO 173
  171 NORD=NORD+1 $ J=2*NORD $ SUMX(J)=0. $ SUMX(J+1)=0.$SUMY(NORD+1)=0.
        DO172 I=1,N $ SUMX(J)=SUMX(J)+X(I)**(J-1)*W
        SUMX(J+1) = SUMX(J+1)+X(I)**J*W
  172 SUMY(NORD+1)=SUMY(NORD+1)+Y(I)*X(I)**NORD*W $ GO TO 93
  173 CONTINUE $ RETURN $ END
        SUBROUTINE INCARDS (X1, Y1, L1, L2, L3, N)
COMMENT   USED TO READ 9-CARD CONDENSED DECKS.  IF N IS ZERO, THE NORMAL CASE,
C         CARDS ARE READ UNTIL A BLANK ONE IS ENCOUNTERED.  IF N IS NOT ZERO,
C         CARDS ARE READ UNTIL N DATA PAIRS HAVE BEEN ACCUMULATED, THEN THE
```

```
C          REMAINDER OF THE DATA ON THE LAST CARD IS IGNORED, AND SUBSEQUENT
C          CALLS START ON THE SUCCEEDING CARD.
CAUTION    DOES NOT YET WORK PROPERLY IF L2 AND N ARE NOT ZERO
      DIMENSION X(9), Y(9), X1(2000), Y1(2000)
  213 FORMAT (I1, F7.0, 18F4.3)
      IF (L1.EQ.0) L1=1  $ IF(L3.EQ.0) L3=1
      IF(N.LE.0.AND.L2.LE.0)GO TO 50
      IF(L2.EQ.0)L2=L1+N-1 $ IF(N.EQ.0)N=L2-L1+1
      DO40 I=L1,L2,9 $ J1=I $ J2=J1+8
   30 READ213,LL,FNY,(X1(J),Y1(J),J=J1,J2) $ IF(FNY+X1(J1).EQ.0)GO TO 30
      DO35 J=J1,J2 $ IF(X1(J).EQ.0.)GO TO 35 $ Y1(J)=Y1(J)+FNY
      IF(LL.EQ.0)GO TO 35 $ X(J)=X(J)*10**LL
   35 CONTINUE
   40 CONTINUE $ IF(J1.LE.L2)GO TO 90 $ J1=L2+1 $ DO45 J=J1,J2
   45 X1(J)=Y1(J)=0. $ GO TO 90
   50 READ 213, LL, FNY, (Y(I),X(I),I=1,9)  $ IF(FNY+X(1).EQ.0.)GO TO 90
      DO70 I=1,9 $ IF(X(I)+Y(I).EQ.0.)GOTO90 $ IF(X(I).EQ.0.)GOTO 70
      Y(I)=Y(I)+FNY $ N=N+1 $ Y1(N)=Y(I) $ X1(N)=X(I)
      IF(LL.EQ.0)GO TO 70 $ X1(N)=X1(N)*10**LL
   70 CONTINUE  $  IF (N .GT. 1991 )  GO TO 90   $   GO TO 50
   90 RETURN $ END
      SUBROUTINE OUTCARDS (X, Y, L1, L2, L3, N)
      DIMENSION X(2000), Y(2000), NX(2000), NY(2000)
  212 FORMAT (I1, I7, 18I4)
      IF (L1.EQ.0) L1=1  $ IF(L3.EQ.0) L3=1
      J1 = L2 + 1   $   J2 = L2 + 8   $   DO 5 I = J1, J2
    5 X(I) = Y(I) = 0.
      DO50I=L1,L2,9  $  N1=0  $  NNY=Y(I)  $  J1=I  $  J2=I+8 $ FNY=NNY
      DO30 J=J1,J2 $ NX(J)=1000.*X(J) $ NY(J)=1000.*(Y(J)-FNY)
      NN=NX(J) $ NN1=N1+1 $ IF(J.GT.L2)GO TO 60$GO TO(14,15,16,17,18)NN1
   14 IF (NN .LE. 9999     ) GO TO 30   $   N1 = 1
   15 IF (NN .LE. 99999    ) GO TO 30   $   N1 = 2
   16 IF (NN .LE. 999999   ) GO TO 30   $   N1 = 3
   17 IF (NN .LE. 9999999  ) GO TO 30   $   N1 = 4
   18 IF (NN .LE.99999999) GO TO 30   $   N1 = 5
   30 CONTINUE $ IF(N1.EQ.0)GO TO 40 $ NDIVIDE=10.**N1 $ DO35 J=J1,J2
   35 NX(J) = NX(J)/N DIVIDE
   40 PUNCH 212, N1, NNY, (NY(K),NX(K),K=J1,J2)
   41 PRINT 212, N1, NNY, (NY(K),NX(K),K=J1,J2)
   50 CONTINUE   $   GO TO 80
   60 NDIVIDE = 10.**N1   $   DO 70 I=J1, L2
   70 X(I) = X(I)/NDIVIDE  $  PRINT212,N1,NNY,(NY(I),NX(I),I=J1,L2)
                              PUNCH 212,N1,NNY,(NY(I),NX(I),I=J1,L2)
   80 RETURN   $   END
        SCOPE
'LOAD
'RUN,2,1000
```

Appendix F

CONVERSION OF DENSITIES TO INTENSITIES

```
C       'CONVERT DENSITIES TO INTENSITIES'
COMMENT   CONVERT DENSITIES TO INTENSITIES, USING OUTPUT OF ADJUSTED PLOT
C. . . CONVERTER PROGRAM MUST BE  PREFIXED BY 1), 'PLOT F'(2 CARDS) AND BY 2),
C     A 'JOB CARD' FOR USE IN THE CDC 3800. . . . . . . . . . . . . . . . . . . . .
'FTN, L,X
      PROGRAM MAIN
      DIMENSION POSN(2000), DENSITY (2000)
  220 FORMAT (8F15.3)
  257 FORMAT ( 5 E16.8 )
  260 FORMAT ( 6(F8.2, 2F6.2 )  )
  277 FORMAT (8I10)
  278 FORMAT (* MESSAGE IS *, A8 )
  281 FORMAT (10A8)
  282 FORMAT (X10A8)
      DIMENSION TITLE (10)
      TYPE INTEGER TITLE
      READ 281, TITLE  $  PRINT 282, TITLE   $   PUNCH 281, TITLE
      READ 257, FA, FB, FC, FD, FE
      READ 257, GA, GB   $   READ 257, HA
      READ 257, ZC, ZB, ZA, ZD
      READ 257, PLOT CORR
    1 CONTINUE
      L1 = L2 = L3 = N = 0
      MESSAGE = 8HINCARDS      $   PRINT 278, MESSAGE
      PRINT 277, L1, L2, L3, N
      CALL INCARDS (DENSITY,POSN,L1, L2, L3, N)
      DO 10 J = L1, L2
COMMENT   PLACE ALTERATION CARDS FROM HERE TO 10, IN A DISTINCTIVE COLOR.
C         ALTER IN NAME OF POSN (Y) OR DENSITY (X) WITH PARAMETER J.
      W = POSN (J)   $   V = DENSITY (J)
      POSN (J) = ZC + ZB*W + ZA*W*W + ZD*W*W*W
      WW = GB + GA * (V - FA - FB*W - FC*W*W - FD*W*W*W - FE*W*W*W*W)
                X = WW + (W - 10.) * HA / 28.
      X = 2.303 * (X + PLOT CORR )
COMMENT   INTENSITY IS HERE CODED AS DENSITY
      DENSITY (J) = EXPF (X)
   10 CONTINUE
      CALL OUTCARDS (DENSITY,POSN,L1, L2, L3, N)
      PRINT 277, L1, L2, L3, N
      GO TO 1   $   END
      SUBROUTINE INCARDS (X1, Y1, L1, L2, L3, N)
COMMENT   USED TO READ 9-CARD CONDENSED DECKS.  IF N IS ZERO, THE NORMAL CASE,
C         CARDS ARE READ UNTIL A BLANK ONE IS ENCOUNTERED.  IF N IS NOT ZERO,
C         CARDS ARE READ UNTIL N DATA PAIRS HAVE BEEN ACCUMULATED, THEN THE
C         REMAINDER OF THE DATA ON THE LAST CARD IS IGNORED, AND SUBSEQUENT
C         CALLS START ON THE SUCCEEDING CARD.
CAUTION   DOES NOT YET WORK PROPERLY IF L2 AND N ARE NOT ZERO
      DIMENSION X(9), Y(9), X1(2000), Y1(2000)
  213 FORMAT (I1, F7.0, 18F4.3)
      IF (L1.EQ.0) L1=1  $ IF(L3.EQ.0) L3=1
      IF(N.LE.0.AND.L2.LE.0)GO TO 50
      IF(L2.EQ.0)L2=L1+N-1 $ IF(N.EQ.0)N=L2-L1+1
      DO40 I=L1,L2,9 $ J1=I $ J2=J1+8
   30 READ213,LL,FNY,(X1(J),Y1(J),J=J1,J2) $ IF(FNY+X1(J1).EQ.0)GO TO 30
      DO35 J=J1,J2 $ IF(X1(J).EQ.0.)GO TO 35 $ Y1(J)=Y1(J)+FNY
      IF(LL.EQ.0)GO TO 35 $ X(J)=X(J)*10**LL
```

```
   35 CONTINUE
   40 CONTINUE $ IF(J1.LE.L2)GO TO 90 $ J1=L2+1 $ DO45 J=J1,J2
   45 X1(J)=Y1(J)=0. $ GO TO 90
   50 READ 213, LL, FNY, (Y(I),X(I),I=1,9)  $ IF(FNY+X(I).EQ.0.)GO TO 89
      DO70 I=1,9 $ IF(X(I)+Y(I).EQ.0.)GOTO70 $ IF(X(I).EQ.0.)GOTO 70
      Y(I)=Y(I)+FNY $ N=N+1 $ Y1(N)=Y(I) $ X1(N)=X(I)
      IF(LL.EQ.0)GO TO 70 $ X1(N)=X1(N)*10**LL
   70 CONTINUE  $  IF (N .GT. 1991 )  GO TO 89   $   GO TO 50
   89 L2 = L1 + N - 1
   90 RETURN $ END
      SUBROUTINE OUTCARDS (X, Y, L1, L2, L3, N)
      DIMENSION X(2000), Y(2000), NX(2000), NY(2000)
  212 FORMAT (I1, I7, 18I4)
      IF (L1.EQ.0) L1=1  $ IF(L3.EQ.0) L3=1
      J1 = L2 + 1   $   J2 = L2 + 8   $   DO 5 I = J1, J2
    5 X(I) = Y(I) = 0.
      DO50I=L1,L2,9  $  N1=0  $  NNY=Y(I)  $  J1=I  $  J2=I+8 $ FNY=NNY
      DO30 J=J1,J2 $ NX(J)=1000.*X(J) $ NY(J)=1000.*(Y(J)-FNY)
      NN=NX(J) $ NN1=N1+1 $ IF(J.GT.L2)GO TO 60$GO TO(14,15,16,17,18)NN1
   14 IF (NN .LE. 9999     ) GO TO 30   $   N1 = 1
   15 IF (NN .LE. 99999    ) GO TO 30   $   N1 = 2
   16 IF (NN .LE. 999999   ) GO TO 30   $   N1 = 3
   17 IF (NN .LE. 9999999  ) GO TO 30   $   N1 = 4
   18 IF (NN .LE.99999999) GO TO 30   $   N1 = 5
   30 CONTINUE $ IF(N1.EQ.0)GO TO 40 $ NDIVIDE=10.**N1 $ DO35 J=J1,J2
   35 NX(J) = NX(J)/N DIVIDE
   40 PUNCH 212, N1, NNY, (NY(K),NX(K),K=J1,J2)
   50 CONTINUE   $   GO TO 80
   60 NDIVIDE = 10.**N1   $   DO 70 I=J1, L2
   70 X(I) = X(I)/NDIVIDE  $  PRINT212,N1,NNY,(NY(I),NX(I),I=J1,L2)
   80 RETURN   $   END
        SCOPE
'LOAD
'RUN,2,1000
ORDER 97  SIGMA/2 = 75, THE BEST OVERALL COMPROMISE    FILM 2
 -0.13050888-003  0.57252245-001  0.20386514-002 -0.14985304-003  0.18745418-005
  0.97000000+000 -0.35000000-001
 -0.50000000-001 IS THE SKEW CORRECTION
  0.00000000+000  0.10000000+001  0.00000000+000
-.5                IS THE PLOT CORRECTION
0      10 312 958 3981000 4841031 5701057 6561077 7431081 8291069 915104610011030
0      11  881033 1741057 2611091 3471124 4331148 5191166 6061179 6921189 7781199
0      11 8641202 9511198103711871123117512101161129611481382113614691121155511 04
0      12 6411084 7271068 8131061 9001068 986108810721117115911521245119313311236
0      13 4181275 5041298 5901299 6761280 7621248 848122 0 935121410211235110 71272
0      14 1941309 2801334 3671344 4531344 5391338 6251341 7111356 7971380 8841406
0      14 9701428105614441143145512291461131514641402146614881467157414661660145 8
0      15 7461440 8331414 919138710051368109213581178135512641359135113691437137 9
0      16 5231386 6091383 6951371 7821354 8681336 954131810401302112712891213127 9
0      17 3001273 3861276 4721292 5581317 6441344 7301366 8171376 9031376 9891371
0      18  761373 1621391 2491429 3351476 4211517 5071540 5931548 6801541 7661522
0      18 8521505 938149710251501111115141197153112841551137015741456159515421613
0      19 6291624 7151627 8011623 8881615 975160110641581115215511240151413281470
0      20 4151428 5021398 5881391 6741411 7601452 8461499 933154010191569110 61579
0      21 1921574 2781561 3651549 4511543 5371536 6231529 7091527 7961535 8821550
0      21 968156810541579114115791227157113141556140015411486152715721516165815 09
0      22 7441504 8311497 917148610051469109514461187141812811392137513761468137 7
0      23 5591392 6471417 7341442 8211466 9071485 994150010801509116615101253150 1
0      24 3391485 4251459 5111426 5971391 6831359 7701337 8561331 942134110291361
0      25 1151386 2011411 2881434 3741454 4601467 5461473 6321473 7181471 8051470
0      25 8911469 977146710641460115014511236144013231427140914171495141415811420
0      26 6671429 7531436 8401436 926143210121425109914141185139712711377135813 62
0      27 4441360 5301366 6161381 7021396 7881413 8751435 961146310471497113415 30
0      28 2201556 3061573 3931580 4791573 5651554 6511528 7371503 8231481 9101470
0      28 996147010821476116914851255149013411491142814851514147316001461168614 56
0      29 7721453 8581448 945143710311413111713801204134312901310137612881462128 2
0      30 5491293 6351317 7211343 8071361 8931367 979136110661348115213341239132 0
0      31 3251304 4111286 4971271 5841264 6701272 7561292 8421318 928134210151363
0      32 1011376 1871380 2741377 3601372 4461367 5321361 6191356 7051357 7911368
0      32 8771385 963140010491406113614021222139013091379139513741481137615671379
0      33 6531377 7391365 8261348 9121332 998131410841292117112671257124013441222
0      34 4301217 5161227 6021247 6881266 7741277 8601275 947126010331236111912 07
0      35 2061178 2921157 3781148 4651151 5511156 6371156 7231147 8091133 8951120
0      35 982111510711119116611241271112713861128151111341638114717591166186911 84
0      36 968119710601200114812011234120813201228140612551493128115791296166512 79

''GO
```

Appendix G

CONVERSION TO 1.000 + LOG 10 INTENSITY

```
C     'CONVERSION TO 1.000 + LOG 10 INTENSITY'
CC  THIS PROGRAM IS FOR THE CDC 3800 AND MUST BE PRECEDED BY A JOB CARD. . . . .
'FTN, L,X
      PROGRAM MAIN
COMMENT   CONVERT TO 10 BASE LOG AND ADD 1.0
      DIMENSION POSN(2000), DENSITY (2000)
  220 FORMAT (8F15.3)
  257 FORMAT ( 5 E16.8 )
  260 FORMAT ( 6(F8.2, 2F6.2 )  )
  277 FORMAT (8I10)
  278 FORMAT (* MESSAGE IS *, A8 )
    1 CONTINUE
      L1 = L2 = L3 = N = 0
      MESSAGE = 8HINCARDS      $   PRINT 278, MESSAGE
      PRINT 277, L1, L2, L3, N
      CALL INCARDS (DENSITY,POSN,L1, L2, L3, N)
      PRINT 277, L1, L2, L3, N
      DO 10 J = L1, L2
COMMENT   PLACE ALTERATION CARDS FROM HERE TO 10, IN A DISTINCTIVE COLOR.
C         ALTER IN NAME OF POSN (Y) OR DENSITY (X) WITH PARAMETER J.
      DENSITY (J) = A LOG 10 (DENSITY(J))  + 1.
   10 CONTINUE
      PRINT 277, L1, L2, L3, N
      CALL OUTCARDS (DENSITY,POSN,L1, L2, L3, N)
      PRINT 277, L1, L2, L3, N
      GO TO 1   $   END
      SUBROUTINE INCARDS (X1, Y1, L1, L2, L3, N)
COMMENT   USED TO READ 9-CARD CONDENSED DECKS.  IF N IS ZERO, THE NORMAL CASE,
C         CARDS ARE READ UNTIL A BLANK ONE IS ENCOUNTERED.  IF N IS NOT ZERO,
C         CARDS ARE READ UNTIL N DATA PAIRS HAVE BEEN ACCUMULATED, THEN THE
C         REMAINDER OF THE DATA ON THE LAST CARD IS IGNORED, AND SUBSEQUENT
C         CALLS START ON THE SUCCEEDING CARD.
CAUTION   DOES NOT YET WORK PROPERLY IF L2 AND N ARE NOT ZERO
      DIMENSION X(9), Y(9), X1(2000), Y1(2000)
  213 FORMAT (I1, F7.0, 18F4.3)
      IF (L1.EQ.0) L1=1  $ IF(L3.EQ.0) L3=1
      IF(N.LE.0.AND.L2.LE.0)GO TO 90
      IF(L2.EQ.0)L2=L1+N-1 $ IF(N.EQ.0)N=L2-L1+1
      DO40 I=L1,L2,9 $ J1=I $ J2=J1+8
   30 READ213,LL,FNY,(X1(J),Y1(J),J=J1,J2) $ IF(FNY+X1(J1).EQ.0)GO TO 30
      DO35 J=J1,J2 $ IF(X1(J).EQ.0.)GO TO 35 $ Y1(J)=Y1(J)+FNY
      IF(LL.EQ.0)GO TO 35 $ X(J)=X(J)*10**LL
   35 CONTINUE
   40 CONTINUE $ IF(J1.LE.L2)GO TO 90 $ J1=L2+1 $ DO45 J=J1,J2
   45 X1(J)=Y1(J)=0. $ GO TO 90
   50 READ 213, LL, FNY, (Y(I),X(I),I=1,9)  $ IF(FNY+X(1).EQ.0.)GO TO 89
      DO70 I=1,9 $ IF(X(I)+Y(I).EQ.0.)GOTO70 $ IF(X(I).EQ.0.)GOTO 70
      Y(I)=Y(I)+FNY $ N=N+1 $ Y1(N)=Y(I) $ X1(N)=X(I)
      IF(LL.EQ.0)GO TO 70 $ X1(N)=X1(N)*10**LL
   70 CONTINUE  $  IF (N .GT. 1991 )  GO TO 89   $   GO TO 50
   89 L2 = L1 + N - 1
   90 RETURN $ END
      SUBROUTINE OUTCARDS (X, Y, L1, L2, L3, N)
      DIMENSION X(2000), Y(2000), NX(2000), NY(2000)
  212 FORMAT (I1, I7, 18I4)
      IF (L1.EQ.0) L1=1  $ IF(L3.EQ.0) L3=1
      J1 = L2 + 1   $   J2 = L2 + 8   $   DO 5 I = J1, J2
```

```
    5 X(I) = Y(I) = 0.
      DO50I=L1,L2,9  $  N1=0  $  NNY=Y(I)  $  J1=I  $  J2=I+8 $ FNY=NNY
      DO30 J=J1,J2 $ NX(J)=1000.*X(J) $ NY(J)=1000.*(Y(J)-FNY)
      NN=NX(J) $ NN1=N1+1 $ IF(J.GT.L2)GO TO 60$GO TO(14,15,16,17,18)NN1
   14 IF (NN .LE. 9999     ) GO TO 30   $   N1 = 1
   15 IF (NN .LE. 99999    ) GO TO 30   $   N1 = 2
   16 IF (NN .LE. 999999   ) GO TO 30   $   N1 = 3
   17 IF (NN .LE. 9999999  ) GO TO 30   $   N1 = 4
   18 IF (NN .LE.99999999) GO TO 30   $   N1 = 5
   30 CONTINUE $ IF(N1.EQ.0)GO TO 40 $ NDIVIDE=10.**N1 $ DO35 J=J1,J2
   35 NX(J) = NX(J)/N DIVIDE
   40 PUNCH 212, N1, NNY, (NY(K),NX(K),K=J1,J2)
   50 CONTINUE   $   GO TO 80
   60 NDIVIDE = 10.**N1   $   DO 70 I=J1, L2
   70 X(I) = X(I)/NDIVIDE  $  PRINT212,N1,NNY,(NY(I),NX(I),I=J1,L2)
   80 RETURN   $   END
        SCOPE
'LOAD
'RUN,2,1000
```

Appendix H

A-PLOT CONVERSION

```
C       'APLOT CONVERSION'
C             THE FOLLOWING CARDS GENERATE BINARY CARDS WHICH ALLOW THE PLOT CUBIC
C        AND PLOT QUADRATIC PROGRAMS TO GENERATE CONVERSIONS FOR THE STANDARD
C        PLOT F OR PLOT G SUBROUTINES.  THIS ALLOWS THESE PROGRAMS TO PLOT ON THE
C        CALCOMP PLOTTER FOR THE 3100 OR THE GERBER PLOTTER IN ESD.  SEE MCNUTT
C        FOR DETAILS ON ITS USE.
C
C
C
C
C
*
      SUBROUTINE APLOT (X, Y, N)
      CALL PLOTF (X, Y, N)
      RETURN
      END
      SUBROUTINE APLOT (X, Y, N)
      CALL PLOTG (X, Y, N)
      RETURN
      END
'
) + GXC *)PP  73(+ 9(+GZ(1GY(HGZ7-X X X P+7077((      9))PP    7    = 7 ' 7
)92'(' '
```

Appendix I

COMPRESS SOLAR SPECTRUM CARDS

```
*       PROGRAM TO COMPRESS SOLAR SPECTRUM CARDS FROM THE UNIVERSITY OF FLORIDA
C       CONVERSION OF THE UNIVERSITY OF FLORIDA CARDS'
  211 FORMAT ( F8.0, 18F4.0)
  212 FORMAT ( I1     ,I7, 18I4 )
  215 FORMAT ( 3F10.3, 4I10 )
  275 FORMAT ( 13X, F8.3, 2F7.4, I10 )
      DIMENSION WL (9), X1 (9), X2 (9), NX1 (9), NX2 (9), NWL (9)
   10 CONTINUE
      N = 0
      DO 11 N = 1, 9
      READ 275,   WL(N), X1(N), X2(N)
   11 CONTINUE
      N1 = 0
      N2 = 0
      NY = WL(1)
      FNY = NY
      DO 20 I = 1, 9
      X1 (I) = 1000. * X1 (I)
      X2 (I) = 1000. * X2 (I)
      WL (I) = WL (I) - FNY
      WL (I) = 1000. * WL (I)
      NX1 (I) = X1 (I)
      NX2 (I) = X2 (I)
      NWL (I) = WL (I)
      IF ( 9999 - NX1 (I) ) 16, 17, 17
   16 N1 = 1
   17 CONTINUE
      IF ( 9999 - NX2 (I) ) 18, 19, 19
   18 N2 = 1
   19 CONTINUE
   20 CONTINUE
      IF ( N1 )  28, 28, 25
   25 DO 26 I = 1, 9
   26 NX1 (I) = NX1 (I) / 10
   28 CONTINUE
      IF ( N2 ) 38, 38, 35
   35 DO 36 I = 1, 9
   36 NX2 (I) = NX2 (I) / 10
   38 CONTINUE
      PUNCH 212, N1, NY, ( NWL(I), NX1 (I), I = 1, 9 )
      GO TO 10
      END
'
C
C
C
C
C
C
C       TO ABSTRACT OTHER DATA FROM THE U OF FLORIDA CARDS, SUBSTITUTE
C           THE FOLLOWING CARD FOR THE PUNCH ORDER IN THE PROGRAM ABOVE.
      PUNCH 212, N2, NY, ( NWL(I), NX2 (I), I = 1, 9 )
```

Appendix J

LEAST-SQUARES SOLUTION OF WAVELENGTHS (POLYFIT)

```
*       POLYNOMIAL CURVE FITTING   NRL       REV 3/15/67
C       Y(I)=STD WL ON ITH CARD    /     X(I)=LINE POSITION ON ITH CARD
C       MAX NO. ANCR PTS=100       /     MAX ORDER OF POLY=10
C       INPUT=TITLE CARD/DATA CARDS/BLANK CARD
C       SW 1 ON=PUNCH AND PRINT OUTPUT COEFS / OFF=PRINT ONLY
C       SW 2 ON=COEF READOUT FOR EACH ORDER / OFF=HIGHEST ORDER ONLY
C       SW 3 ON=LINE POS,STD WL, COMP WL AND DIFF TYPEOUT FOR EACH ORDER/
C            OFF=HIGHEST ORDER ONLY
        DIMENSION X(100),Y(100),A(12,12),SUMX(31),SUMY(15)
        COMMON X,Y
  250   FORMAT(80H
       1
  201    FORMAT(15X, F10.4, 3X, F8.3)
  204   FORMAT (1X)
  205   FORMAT(///I3,F10.4,1X,F10.4,1X,I3)
  206   FORMAT(I3, 2X, E16.8)
  207   FORMAT(F8.3, 2F13.4, F10.5)
  202   FORMAT(/45H       X          ANCR      YCOMP      ANCR-YCOMP/)
    1   READ 250
        PRINT 250
        IF(SENSE SWITCH 1)4,5
    4   PUNCH 250
    5   TOL = 0.001
        LAST=10
        N = 0
        I = 1
   11   READ 201, Y(I), X(I)
        IF(X(I) + Y(I) ) 20,70,20
   20   IF(Y(I) ) 21,11,21
   21   N = N + 1
         I = I + 1
        GO TO 11
   70   SUMX(1)=0.
        SUMX(2)=0.
        SUMX(3)=0.
        SUMY(1)=0.
        SUMY(2)=0.
        DO 90 I=1,N
        SUMX(1)=SUMX(1)+1.0
        SUMX(2)=SUMX(2)+X(I)
        SUMX(3)=SUMX(3)+X(I)*X(I)
        SUMY(1)=SUMY(1)+Y(I)
   90   SUMY(2)=SUMY(2)+X(I)*Y(I)
        NORD=1
   91   CONTINUE
   93   L=NORD+1
        KK=L+1
        DO 101 I=1,L
        DO 100 J=1,L
        IK=J-1+I
  100   A(I,J)=SUMX(IK)
  101   A(I,KK)=SUMY(I)
        DO 140 I=1,L
        A(KK,I)=-1.
        KKK=I+1
        DO 110 J=KKK,KK
  110   A(KK,J)=0.
        C=1./A(1,I)
        DO 120 II=2,KK
        DO 120 J=KKK,KK
```

```
120 A(II,J)=A(II,J)-A(1,J)*A(II,I)*C
    DO 140 II=1,L
    DO 140 J=KKK,KK
140 A(II,J)=A(II+1,J)
    S2=0.
    DO 160 J=1,N
    S1=0.
    S1=S1+A(1,KK)
    DO 150 I=1,NORD
    Q=1.0
    DO 9 K=1,I
  9 Q=Q*X(J)
150 S1=S1+A(I+1,KK)*Q
160 S2=S2+(S1-Y(J))*(S1-Y(J))
    B = N
    S2=SQRT(S2/B)
    IF(SENSE SWITCH 2)163,161
161 IF(NORD-LAST)162,163,162
162 IF(S2-TOL)163,163,171
163 PRINT 205, NORD, TOL, S2, N
    DO 164 I=1,L
    J=I-1
    IF(SENSE SWITCH 1) 7, 164
  7 PUNCH 206, J, A(I,KK)
164 PRINT 206, J, A(I,KK)
    IF(SENSE SWITCH 3)167,165
165 IF(NORD-LAST)166,167,166
166 IF(S2-TOL)167,167,171
167 PRINT 202
    DO 169 I=1,N
    S1=0.
    S1=A(1,KK)
    DO 168 J=1,NORD
    Q=1.0
    DO 6 K=1,J
  6 Q=Q*X(I)
168 S1=S1+A(J+1,KK)*Q
    S3=Y(I)-S1
169  PRINT 207, X(I), Y(I), S1, S3
    IF(NORD-LAST)170,173,173
170 IF(S2-TOL)173,173,171
171 NORD=NORD+1
    J=2*NORD
    SUMX(J)=0.
    SUMX(J+1)=0.
    SUMY(NORD+1)=0.
    DO 172 I=1,N
    MR=J-1
    Q=1.0
    DO 8 K=1,MR
  8 Q=Q*X(I)
    SUMX(J)=SUMX(J)+Q
    Q=1.0
    DO 10 K=1,J
 10 Q=Q*X(I)
    SUMX(J+1)=SUMX(J+1)+Q
    Q=1.0
    DO 12 K=1,NORD
 12 Q=Q*X(I)
172 SUMY(NORD+1)=SUMY(NORD+1)+Y(I)*Q
    GO TO 91
173 PAUSE
    IF(SENSE SWITCH 4)171,1
    END
```

Appendix K

WAVELENGTH COMPUTATION (λ CALC)

```
*       WAVELENGTH COMPUTATION PROGRAM          REV 3/24/67
C       COMPUTES WAVELENGTHS USING COEFS  OUTPUT FROM POLY CRVE FTG PROG
C       TILFORD - MICHELS  11/3/66
C       Y = A(1) + SUM(A(I)*X**(I-1))
C       K(I) = ORDER OF TERM                A(I) = VALUE OF COEF
C       Y = COMPUTED WAVELENGTH             X = MEASURED LINE POS
C       VAR = LINE IDENT                    ANCR = STD WL
C       COMM = COMMENTS                     M1,M2= MEASUREMENT IDENT
C       INPUT=TITLE CARD/COEFS (FORMAT 3)/BLANK CARD/DATA CARDS/BLANK CARD
C       SW 2 ON=OUTPUT FORMAT 17 / OFF=OUTPUT 18 (INCLUDES FREQ.)
C       SW 3 ON=PUNCH OUTPUT / OFF=NO PUNCH
C       SW 4 ON=PRINT OUTPUT / OFF=NO PRINT
        DIMENSION K(12),A(12)
      2 FORMAT( 80H
       1
      3 FORMAT(I3, 2X, E16.8)
      4 FORMAT(A6,7X,F10.4,5X,F8.3,27X,A6,A1)
     17 FORMAT(/50HLINE   POSITION      CALC WL  COMM STD    IDENT
     18 FORMAT(/70HLINE   POSITION      CALC WL      FREQ    COMM STD
       1IDENT
    117 FORMAT(A6,F8.3,4X,F10.4,2X,A6,A1)
    217 FORMAT(A6,F8.3,4X,F10.4,2X,A6,A1,2X,F10.4)
    118 FORMAT(A6,F8.3,4X,F10.4,1X,F11.3,2X,A6,A1)
    218 FORMAT(A6,F8.3,4X,F10.4,1X,F11.3,2X,A6,A1,2X,F10.4)
     99 FORMAT(1X)
      1 READ 2
        IF(SENSE SWITCH 3)20,21
     20 PUNCH 99
        PUNCH 99
        PUNCH 99
        PUNCH 2
        PUNCH 99
     21 IF(SENSE SWITCH 4)22,23
     22 CONTINUE
        PRINT 99
        PRINT 99
        PRINT 99
        PRINT 2
        PRINT 99
     23 CONTINUE
        I = 1
     24 READ 3, K(I), A(I)
        IF(A(I) ) 25,26,25
     25 IF(SENSE SWITCH 3) 27,28
     27 PUNCH 3, K(I), A(I)
     28 IF(SENSE SWITCH 4)29,30
     29 PRINT 3, K(I), A(I)
     30 I = I + 1
        GO TO 24
     26  I = I - 1
        IF(SENSE SWITCH 2) 51,52
     51 IF(SENSE SWITCH 3) 53,54
     53 PUNCH 17
     54 IF(SENSE SWITCH 4) 55,58
     55 PRINT 17
        GO TO 58
```

```
52 IF(SENSE SWITCH 3) 60,61
60 PUNCH 18
61 IF(SENSE SWITCH 4) 57,58
57 PRINT 18
58 L = 1
31 READ 4, VAR, ANCR, X, COMM,N
   IF(X+ANCR)32,1,32
32 WL = A(1)
   XI=X
   DO 36 J = 2,I
   WL = WL + A(J)*X
36 X = X*XI
   FREQ = (1.1F+8/WL)
   X = XI
37 IF(SENSE SWITCH 2) 38,39
38 IF (SENSE SWITCH 3)4 ,41
40 IF(ANCR)80,81,80
80 PUNCH 217,VAR, X,WL,COMM,N,ANCR
   GO TO 41
81 PUNCH 117,VAR,X,WL,COMM,N
41 IF(SENSE SWITCH 4)82,31
82 IF (ANCR)83,84,83
83 PRINT 217,VAR,X,WL,COMM,N,ANCR
   GO TO 31
84 PRINT 117,VAR,X,WL,COMM,N
   GO TO 31
39 IF(SENSE SWITCH 3)42,43
42 IF(ANCR)90,91,90
90 PUNCH 218,VAR,X,WL,FREQ,COMM,N,ANCR
   GO TO 43
91 PUNCH 118,VAR,X,WL,FREQ,COMM,N
43 IF(SENSE SWITCH 4)92,31
92 IF(ANCR)93,94,93
93 PRINT 218,VAR,X,WL,FREQ,COMM,N,ANCR
   GO TO 31
94 PRINT 118,VAR,X,WL,FREQ,COMM,N
   GO TO 31
   END
''
```

Appendix L

USEFUL RECORDING INFORMATION

Number of Words Contained in Various DATEX Record Lengths

Record Length (Digits)	Number of Eight-Digit Words	Number of Twelve-Digit Words	Approximate Time to Write One Record (Sec)
1,500	188	125	5
3,000	375	250	10
7,500	938	625	25
15,000	1875	1250	50
30,000*	3750	2500	100
60,000*	7500	5000	200

*Not usable with the Main Program.

Data Readings Produced by Various JACO Scan Speeds for Plasma Tube Spectra*

Scan Speed (mm/min)	Readings/mm	Length of One Reading (mm)	Readings/Å	Length of One Reading Å	Spacing Between Data Points at a Given Reading (Å)							
					2nd	3rd	4th	5th	10th	15th	20th	25th
0.5	3000	0.00033	144.70	0.007	0.014	0.020	0.028	0.035	0.069	0.104	0.138	0.173
1	1500†	0.00067	72.35‡	0.013	0.028	0.041	0.055	0.069	0.138	0.207	0.276	0.346
2	750	0.00133	36.17	0.027	0.055	0.083	0.110	0.138	0.276	0.415	0.553	0.691
3	500	0.00200	24.11	0.041	0.083	0.124	0.166	0.207	0.415	0.622	0.829	1.037
5	300	0.00333	14.47	0.069	0.138	0.207	0.276	0.346	0.691	1.037	1.382	1.728

*Meinel Spectrograph.
†25 readings/sec; Datex (60 sec) = 1500 in a 1-mm scan of JACO at 1 mm/min.
‡Average reciprocal linear dispersion = 20.736 Å/mm; average linear dispersion = 0.04823 mm/Å; 0.04823/0.00067 = 72.35 readings/Å.

Total Readings and Main Program Output Card Data vs JACO Scan Speed

Scan Speed (mm/min)	Scan Time* (min)	Every Data Point Recorded Total Readings	Readings	Total No. Cards for a Given Reading†			
				2nd	3rd	4th	5th
0.5	52	78000	8667	4334	2889	2167	1734
1	26	39000	4334	2167	1445	1084	867
2	13	19500	2167	1084	723	542	434
3	8.67	13000	1445	723	482	362	289
5	5.2	7800	867	434	289	217	174

*Distanced scanned on spectrogram is 26 mm (41 mm to 67 mm wavelength region, ~4100 Å to 4500 Å).
†There are nine data points per card.

Appendix M

PARAMETERS ON THE DATEX CONSOLE

Type of Spectrum	Switch Number*									
	1 2 3	4	5 6 7	8 9	10	11	12	13 14	15 16	17 18
Absorption or Emission	Plate	Exposure	Tape	Band	Code	Datex Gain	JACO Speed	Month	Day	Year
	Identification									

*Each number represents one of the rotary switches on the parameter panel.

Type of Spectrum	Switch Number									
	1 2 3	4	5 6 7	8 9	10	11	12	13 14	15 16	17 18
Echelle	Order Plate	Trial	Tape	Band	Code	Datex Gain	JACO Speed	Month	Day	Year
	Identification									

Type of Spectrum	Switch Number									
	1	2 3	4 5 6	7 8 9	10	11	12 13	14 15	16 17	18
Plasma	Operator	Tape	Plate No.	JACO Speed	J-A Gain	Datex Gain	Recording Cycle	Month	Day	Year
	Identification									

Appendix N

CHECKLIST FOR DENSITOMETER OPERATION FOR ECHELLEGRAMS

1. Before Scan

   Scan speed – 0.5 mm/min

   Slit width – 15μ

   Bottom mask in place – record the mask number (thickness in IBM cards)

   Slit tilted – record the number of degrees net tilt

   Travel of carriage – adjusted to match endpoints

   Upper mask, for scattered light, in place

   Datex gain at 2, densitometer sensitivity at 8, neutral density filters as needed

   Parameters set to order, film number, tape number, date, etc.

   Film mounted with low-wavelength edge at right.

2. During Scan

   First record the fiducial on the low-wavelength edge, with the neutral-density filter at the base (100% transmission) setting. Record for 5 sec at the 3000 record length.

   Next record on glass, carriage not moving, for 5 sec at record length 3000 (nearly 100% transmission).

   Then record on the emulsion adjacent to the spectrum, carriage moving, for 5 sec at record length 3000.

   Change the record length to 15,000. Adjust the carriage to the low-wavelength edge of the spectrum on the emulsion.

   Begin scan, adjust the neutral-density filter to the permanent value as soon as possible, preferably in the next record.

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4. DESCRIPTIVE NOTES *(Type of report and inclusive dates)*
A final report on one phase of the problem; work on other phases continues.

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13. ABSTRACT

A computer program, for use with an associated spectral comparator, has been developed at the Naval Research Laboratory for automatically reducing spectroscopic data. A Datex digitizing magnetic-tape recorder, in conjunction with a Jarrel-Ash microphotometer, allows wavelength and intensity information to be read from a photographic plate at 25 data pairs per second. A computer program written in Fortran IV was designed to facilitate processing the information into a usable form.

The computer program permits analysis of spectroscopic data by making simple specifications on a control card. Spectra of local interest are (a) absorption, (b) emission, (c) plasma type, obtained from time-resolved spectroscopic techniques, and (d) solar echellegrams obtained from rocket probings of the upper atmosphere.

Markedly useful features of the program are its capabilities of (a) recognizing spectral peaks from a background of variable density and (b) obtaining absolute values for the radiance or irradiance. The program's essential characteristic is the significant amount of time saved in reducing photographic spectroscopic data. As a rough estimate of the time-saving advantage, one may obtain thirty times the information in 1/100 of the time, as compared to manual reduction of spectroscopic data.

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Absorption spectra						
Emission spectra						
Plasma spectra						
CDC 3800 computer						
CDC 3100 computer						

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