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RADIO AND ELECTRICAL ENGINEERING DIVISION



ANALYZED

COMPUTER REDUCTION OF ABSORPTION AND LUMINESCENCE
EMISSION AND EXCITATION SPECTRA IN SOLIDS

- F. D. BLAIR -

OTTAWA
JANUARY 1970

ANALYZED

ABSTRACT

This report describes a series of programs used for processing data from luminescence experiments and an accompanying technique for transferring the data from strip charts to magnetic tapes for input to a digital computer.

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COMPUTER REDUCTION OF ABSORPTION AND LUMINESCENCE EMISSION AND EXCITATION SPECTRA IN SOLIDS

— F.D. Blair —

I. Introduction

The programs to be described were developed to assist in the reduction of data from a series of experiments on the luminescence of alkali halides. When the experiments were set up, the results were taken on a strip chart recorder and no provision was made for automatically recording the data for later processing by digital computer. This system of recording the results was dictated by the cost of the associated digital recording equipment.

The manual operations required to produce corrected spectra from the strip charts proved to be laborious and time consuming. With a large number of experiments already on strip charts and more experiments to be run, it was decided to find some simple but reasonably efficient method to put the results into a form suitable for processing on a digital computer. The main restrictions placed on the method to be used included:

- a) previously recorded data had to be salvaged,
- b) the method had to be easily and quickly applied to new results being produced,
- c) the recording medium had to be suitable for use as an input to a digital computer, and
- d) some simple method had to be built into the data recording to indicate to the computer the necessary conversions to wavelength and intensity from the original graph readings.

Several methods of conversion were possible but most of these neglected one or more of the above mentioned requirements. The method finally chosen was to use a curve tracer to magnetic tape system which not only satisfied all the restrictions, but also offered a saving in manual labour over the other methods.

For the present system of programs, the data are transferred from the strip chart to a seven-track low-density magnetic tape by use of an Auto-trol Corporation 3400 curve tracer and the magnetic tapes are then processed on an IBM 360/50 computer. Data for the conversion of units is in part included on the tape. A simple linear relation is used for the conversion of the various units. Tests on the data have shown that the accuracy of the method of conversion is within the experimental error.

Since most of the programs to be described require the same form of input data conversion and similar output representation, these features will be outlined in several common sections. Variations of each program from the general form will be described in separate sections for each program. It should be noted that the main programs have been kept independent of the NRC plotting routines as much as possible. All references to these plotting routines, used at the NRC Computation Centre, are contained in XPLØT and XPLØTI with the exception of the control subroutines NAME, PAGE, and PEND.

II. General System Description

a) Magnetic Tape Format

The data on the magnetic tape are blocked at 84 characters per block, with the first four characters giving the spectrum number taken from positions 11, 12, 13, and 14 of the thumb wheels on the console of the curve tracer. In the processing programs, the first block of the desired experiment is found using the four-digit spectrum identification, and each following block is accepted until a different identification is found.

The remaining 80 characters of each block after the spectrum identification contain ten data points of eight characters each. Positions 1, 2, 3, and 4 of each point make up the X value taken from the left four positions of the X register as displayed on the console of the curve tracer. Positions 5, 6, and 7 give the Y value taken from the middle three digits of the Y register. The eighth position of the data point is taken from digit fifteen of the thumb wheels on the console and it is used to represent the scale factor of the recording instrument.

In the first block of each spectrum, the first two data points contain the calibration data. The first point is the minimum ($x-y$) coordinate taken at the lowest value on the chart being recorded and the second point contains the maximum ($x-y$) coordinate taken at the highest point on the chart for both the x and y readings. At run time, these two points are used to form factors which multiply each ($x-y$) pair to give the readings in wavelength and source graph divisions (see Section IIc).

At the end of each spectrum being transferred to magnetic tape, the last block must be filled with nines by pressing the final button on the console of the curve tracer. When the tape has been completed, an end-of-file must be put on the tape.

b) General Card Format

Each spectrum to be processed by any of the processing programs must be indicated by a card with the format shown in Table I. The general format is II, 1X, A4, 1X, 5E14.7.

The continuation indicator must be one of the following:

- 0 No continuation to follow,
- 1 Next spectrum card contains information about a spectrum which is to be considered as a continuation of the present spectrum, and
- 9 No more spectra, terminate the program. This must be the last data card to avoid an end-of-file indication.

The identification (A4) is a four-digit number which must be equal to one of the identifications on the tape.

The four maximum—minimum values are in angstroms and divisions on the graph and must correspond to the two first experimental points on the tape from the curve tracer.

TABLE I

Format of spectrum identification card

Format	Purpose
I1	Continuation indicator
A4	Spectrum identification
E14.7	Minimum x coordinate in wavelength (\AA)
E14.7	Maximum x coordinate in wavelength (\AA)
E14.7	Minimum y coordinate in source graph divisions
E14.7	Maximum y coordinate in source graph divisions
E14.7	Dark current in nanoamperes

The final variable on the card is the dark current and must be in units of nanoamperes to agree with the final experimental data points after processing.

c) Conversion of Raw Data

The first step in processing the raw data is to convert each data point to known units from the relative representation produced by the digital converter. The conversion equations are as follows.

$$W_n = W_{Cmin} + (W_{Tn} - W_{Tmin}) \left[\frac{W_{Cmax} - W_{Cmin}}{W_{Tmax} - W_{Tmin}} \right]$$

$$I_n = \left[I_{Cmin} + (I_{Tn} - I_{Tmin}) \left\{ \frac{I_{Cmax} - I_{Cmin}}{I_{Tmax} - I_{Tmin}} \right\} \right] S_K - D.C.$$

where W is the wavelength,
 I is the intensity,
 n is the n th point,
 C is the value from the card,
 T is the value from the magnetic tape,
 S_K is the scale factor, and
 $D.C.$ is the dark current.

d) Scale Factors

The scale factors are the appropriate ranges of the Keithly micromicroammeter in use for the present experimental setup. At input time in the program these factors are fed into the computer, one factor per card with format I5, E14.7. The fixed point

number (15) which appears first on the card represents the number of the factor and its location in the storage array. This number should be between 1 and 15 and should be unique for each card.

Since the digit on the magnetic tape which selects the scale factor can only vary from one to nine and since the table of factors can contain fifteen values, it was necessary to define a table origin for the set of scale factors to be used. The location of the scale factor in the table which is to be selected is calculated as

$$L = T + N - 1,$$

where L is the factor location in the storage array,

T is the digit from the tape and

N is the origin from the input card.

e) Output Requirements

In each of the processing programs, the final data are both printed in table form and output on magnetic tape for the plotter. Since each program requires different printer formats, the description of the output printing will be deferred until the individual programs are described.

Two graphs per spectrum are required. The first is the normalized intensity plotted against wavelength in angstroms and the second is the normalized intensity plotted against the energy in electron volts. In each case, the alternate independent variable scale is given at the top of the graph as a reference (i.e., an electron volt scale is given at the top of the angstrom plot and vice versa).

Four additional requirements placed on the output graphs are as follows:

- a) the values of the variables are printed on the graphs at convenient intervals along each scale,
- b) descriptive titles are included along each scale,
- c) the dimensions of the graphs are variable, and
- d) the scale factors and starting values are variable.

To satisfy the above requirements, a subroutine called XPLOT was written and it is used by all of the processing programs except the absorption spectra program. In the case of the absorption spectra program, a variation of XPLOT called XPLOT1 was written.

III. Absorption Spectra

The absorption of a material at a given wavelength is proportional to the optical density of the material at the same wavelength. The optical density can be calculated using the following relationship:

$$\text{Optical density} = \log_{10} \frac{I_1}{I_2} = \mu x \log e$$

where I_1 is the light incident on the sample,
 I_2 is the light transmitted through the sample,
 μ is the absorption coefficient of the material,
 x is the thickness of the sample,
 e is the base of natural logarithms.

Two programs have been written to process the absorption data. The choice of program is determined by the form of the source data. In both cases, either the optical density or the absorption coefficient may be plotted as a function of wavelength in angstroms and energy in electron volts. The input data for both programs are in the form described in Section II.

The input to the first program is the optical density taken from the graph of a Cary spectrophotometer. In this case only, the scale factors are accepted according to the following scheme.

Range (from tape)	Optical density range
1	0 to 1
2	1 to 2
3	0 to .1

The second program uses the quantities I_1 and I_2 to calculate the optical density. Both programs use the optical density to calculate the absorption coefficient as;

$$\text{Absorption coefficient} = \frac{\text{Optical density} \times 2.303}{\text{Thickness of the sample}}$$

Input Card Format

The input card format for both programs is shown in Table II. Differences in the card layout between the programs is indicated in the comments column.

Output Results

The final printout of results from the two programs is as follows.

1. Wavelength in angstroms (F7.1),
2. Electron volts (F7.4),
3. I_1 (E12.5) (program 2 only),
4. I_2 (E12.5) (program 2 only),
5. Optical density (E12.5) and
6. Absorption coefficient (E12.5).

Two plots are given for each spectrum processed. In the first the x axis is in wavelength, and in the second the x axis is in electron volts. For the y axis, either optical density or absorption coefficient may be chosen (see Table III item 11).

TABLE II
Card input to optical density - Absorption coefficient program

Item	Format	Number of cards	Use	Comments
1	2I5	1	Origin for scale factors	Program 2 only, See Section IId.
2	I5, E14.7	13	Scale factors	Program 2 only, See Section IId.
3	20A4	1	Overall page title-plotter	
4	20A4	1	Wavelength scale title-plotter	
5	20A4	1	Electron volt scale title-plotter	
6	20A4	1	Optical density scale title-plotter	
7	20A4	1	Absorption Coefficient scale title-plotter	
8	I1, IX, A4, IX, 5E14.7	One plus continuation	I1 data, program 2	For program 1, spectrum data, See Section IIb.
9	I1, IX, A4, IX, 5E14.7	One plus continuation	I2	Program 2 only
10	E14.7	1	Thickness of specimen	If not used must be zero.
11	I5	1	Selection of quantity for plotting	If equal to zero, the program plots the optical density, otherwise it plots the absorption coefficient.
12	20A4	1	Spectrum title	In this position for program 2 only.
13	8E14.7	2	Plotting information (1) Start wavelength (2) Wavelength scale (3) Start electron volt (4) Electron volt scale (5) x length (6) y length (7) Optical density scale (8) Absorption Coefficient scale.	
14	20A4	1	Spectrum title	In this position for program 1 only
15	I1	1	End of data card	

NOTE:- For each set of absorption coefficient and optical density values to be processed, items 8 to 14 must be repeated.

Subroutines Used

Both programs described use the XPLOTT subroutine for setting up and formatting the graphs. The SINTP function subroutine is used to interpolate where required.

IV. Luminescence Emission Spectra

The uncorrected luminescence emission intensity I_1 is read into the machine on magnetic tape and converted to the appropriate units as described in Section II, a) and c). The emission intensity is then corrected at each wavelength by the response function of the measuring equipment with the relationship

$$\text{Corrected emission intensity} = \frac{I_1}{\text{Response function}}$$

The response function is the product of the quantum efficiency of the photomultiplier tube and the transmission function of the monochromator.

Input Card Formats

The order, number and formats of the input cards are given in Table III. It should be noted that for each spectrum to be processed, the group of cards starting at item 8 and ending at 12, inclusive, must be repeated. The card in item 13 must be placed after the last group and before the end-of-file card.

Output Data

The processed data are printed in the following format.

1X, F7.1, 2X, F8.4, 3(2X, E12.5), F8.5

These format items correspond to:

1. wavelength in angstroms (F7.1),
2. electron volts (F8.4),
3. uncorrected intensity (E12.5),
4. value of the response function used (E12.5),
5. corrected intensity (E12.5) and
6. the normalized intensity (F8.5).

As well as the printer output, the normalized intensity was plotted against both angstroms and electron volts by use of the XPLOTT subroutine. It should be noted that the program at present is designed to plot four graphs per page and that the size of the page described under 'Input Card Formats' must be kept within limits to avoid overlapping.

Subroutines Used

All plotting was carried out using the XPLOTT subroutine. The subroutine SINTP was required to interpolate the response function when required.

TABLE III

Input cards for emission spectrum program

Item	Format	Number of cards	Use	Comments
1	I5, 2E14.7	As required	Response function	Last card must have 99999 in 15 position
2	I5, E14.7	Maximum of 15	Scale factors	See Section II d. Last card = 99999 0.0 0E00
3	20A4	1	Overall page title for plotter	
4	20A4	1	Heading for wavelength scale on plotter	
5	20A4	1	Heading for electron volt scale on plotter	
6	20A4	1	Heading for intensity scale on plotter	
7	20A4	1	Heading for spectrum on plotter	
8	II, IX, A4, 1X, 5E14.7	One plus any number of continuations	Data for spectrum	See Section II b
9	I5	1	Scale factor origin	See Section II d
10			Data for the plotting routine: (1) Start of wavelength (2) Wavelength scale (3) Start of e.v. plot (4) e.v. scale factor	
11	2E14.7	1	Page size for plotter (1) x direction (2) y direction	Actual plotting surface will be one inch smaller
12	20A4	1	Individual spectrum title	
13	II	1	end card	This must contain a nine in column one and be the last card

V. Luminescence Excitation Spectra

The excitation spectrum is calculated at each given wavelength by the relationship

$$I_c = \frac{I_1}{I_2}$$

where I_1 is the uncorrected intensity of luminescence and I_2 is the intensity of the source causing the excitation.

Both I_1 and I_2 vary in intensity as a function of wavelength.

In the processing program, both I_1 and I_2 are selected, converted to the appropriate units, and stored in temporary tables. The wavelengths associated with I_1 are selected one at a time and used as the reference in selecting I_2 . If the I_2 table does not contain a wavelength identical with the wavelength being used from I_1 , the I_2 table is interpolated at the nearest wavelength by use of the SINTP subroutine. When the excitation spectrum has been completely calculated, the program normalizes the spectrum to one at the peak value.

Two programs have been written to process the excitation spectra. The first program calculates the spectrum as it is given over its entire range. The second program has the ability to select a given range of each spectrum and to give results for this limited range only. In all other ways, the two programs are identical.

Input Card Format

The details of the input data cards are shown in Table IV.

Output Data

The completed data output is both printed and plotted. The following variables are printed with the Fortran format items indicated in brackets:

1. wavelength (F7.1),
2. electron volts (F8.4),
3. I_1 in nanoamperes (E12.5),
4. I_2 in nanoamperes (E12.5),
5. excitation intensity (E12.5) and
6. normalized intensity of excitation (E12.5).

The normalized intensity is plotted against angstroms and electron volts. Both graphs are plotted on the same page with the angstrom plot in the upper half of the page. The size of the graphs is fixed at 19 X 11 inches (18 X 10 inch plotting surface).

TABLE IV

Input cards for excitation spectrum program

Item	Format	Number of cards	Use	Comments
1	2I5	1	Table origins for scale factors	See Section IId
2	I5, E14.7	Maximum of 15	Scale factors	See Section IId. Last card must be 99999 0.0000000E 00
3	20A4	1	Main page title for plotter	
4	20A4	1	Wavelength scale title for plotter	
5	20A4	1	Electron volt scale title	
6	20A4	1	Intensity scale title	
7	I1, 1X, A4, 1X, 5E14.7	One plus continuation	Data for I_1	See Section IId. In the case of the 'limited range' program, a second card must follow with a format of 2E14.7 where the last two fields are the lower and upper limits in angstroms of the range to be processed. This applies to the continuation cards as well.
8	I1, 1X, A4, 1X, 5E14.7	One plus continuation	Data for I_2	Same as item 7 above.
9	20A4	1	Title for the specific spectrum	
10	4E14.7	1	Data for plotting (1) Start of wavelength (2) Wavelength scale (3) Start of e.v. plot (4) e.v. scale factor	
11	I_1	1	End of data card	

NOTE:- For each spectrum to be processed, the group of cards from item 7 to item 10 must be repeated.

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Appendix A

Absorption Spectra Program

C *** CALCULATION OF ABSORPTION SPECTRA,
C I1,I2 INPUT - OPTICAL DENSITY=LCGIC(I1/I2).
C WRITTEN BY F.D.BLAIR,
C RADIO AND ELECTRICAL ENGINEERING,
C NATIONAL RESEARCH COUNCIL OF CANADA,
C OTTAWA, ONTARIO.
C 1969.
C

DIMENSION TIL(20),XQ1(20),XQ2(20),YQ(20),MK(42),M1(20),M2(20),
IM3(20),SC(20),WL(1000),FI(1000),EV(1000),FN(1000),SI(1000),
1WK(4),WIN(4),YQ1(20),YQ2(20),SKK(1000),SKQ(1000),
2FIRW(1000),FIRI(1000),SKI(1000)
INTEGER*4 TR(20),TQ(20)
CALL PSAVE (8000)

IP=3

IC=1

IT=99

J1=1

IZM=1

J2=1

Q=12395.0

YC=1.0

XL=19.0

YL=11.0

500 READ (IC,500) I1,I2

DO 45 I=1,20

45 SC(I)=0.0

DO 7 I=1,20

READ (IC,8) N, W1

8 FORMAT (I5,E14.7)

IF (N-99999) 7,9,7

7 SC(I)=W1

WRITE (IP,42)

42 FORMAT (1X,'TO MANY SCALE FACTORS')

CALL EXIT

9 READ (IC,1)TIL,XQ1,XQ2,YC1,YC2

1 FORMAT (20A4)

200 IIL=1

ISC=11

31 MQ=0

70 READ (IC,2) MZ,LQ,WLS,WLE,FIS,FIE,DCU

72 FORMAT (5E14.7)

IF (MZ-9) 602,5,602

602 INS=1

XC=1.0

IL=1

IBL=0

2 FORMAT (I1,1X,A4,1X,6(E14.7))

IF (MZ-9) 17,5,17

17 IF (UFREAD(MK,L)) 90,4,32

90 IF (L-84) 17,13,17

13 IF (MK(1)-LQ) 3,14,3

14 GO TO (15,16),IL

15 IL=2

```

      N1=1
16  I=2
      LS=(L-4)/8
      DO 301 K=1,LS
      CALL INCCRE (MK(I),8)
      REAC (IT,6) M1(K),M2(K),M3(K)
      6  FORMAT (I4,I3,I1)
301  I=I+2
      GO TO (73,74) , INS
      73 IF (M1(1)-9999 ) 76,77,76
      77 WRITE (IP,78)M1(1),M2(1),M3(1)
      78 FORMAT (1X,'SCALE ERRCR',3(5X,I5))
      CALL EXIT
      76 WMS=M1(1)
      FIMS=M2(1)
      WMB=M1(2)
      FIMB=M2(2)
      INS=2
      LS=LS-2
      DO 75 I=1,LS
      M1(I)=M1(I+2)
      M2(I)=M2(I+2)
      75 M3(I)=M3(I+2)
      WMA=ABS(WMB-WMS)
      FIMA=(FIMB-FIMS)
      WLM=(WLE-WLS)/WMA
      FIX=(FIE-FIS)/FIMA
      74 DO 20 I=1,LS
      IF (M1(I)-9999 ) 21,20,21
      21 MQ=MQ+1
      WK=M1(I)
      WZ =WLS+((WK-WMS)*WLM)
      IF (WZ-WLE) 2000,2001,2001
2001 MQ=MQ-1
      GO TO 20
2000 WL(MQ)=WZ
      WK=M2(I)
      WK=FIS+((WK-FIMS)*FIX)
      LX=M3(I)+ISC-1
      SI(MQ)=(WK*SC(LX))-DCU
      20 CONTINUE
      GO TO 17
      3  GO TO (17,18),IL
      18 IF (MZ-1) 71,300,71
300  CALL UFREW (0)
      GO TO 7C
      71 GO TO (101,102), IIL
101  DO 103 I=1,MQ
      FIRW(I)=WL(I)
103  FIRI(I)=SI(I)
      ISC=I2
      IIL=2
      MZQ=MQ
      MS=LQ
      FIDC=DCU

```

```
CALL UFREW (0)
GO TO 31
102 I=1
    READ (IC,72) THICK
    READ (IC,81) ICON
    81 FORMAT (5I5)
    NN=0
    IF (J1-1) 118,118,501
501 CALL PAGE
    J1=I
118 IF (I-MZQ) 104,104,105
104 WK=FIRW(I)
    IF (WK-WL(1)) 116,117,117
117 DO 106 K=1,MQ
    IF (WK-WL(K)) 108,107,106
107 S=SI(K)
    GO TO 109
108 Kw=K-2
112 IF ((Kw+3) -MQ) 110,110,111
111 Kw=Kw-1
    GO TO 112
110 IF (Kw) 113,113,114
113 Kw=Kw+1
    GO TO 110
114 DO 115 L=1,4
    WwK(L)=WL(Kw)
    WwIN(L)=SI(Kw)
115 Kw=Kw+1
    S=SINTP(WwK,WwK,WwIN,4)
    GO TO 109
106 CONTINUE
116 LK=I
119 IF (LK+1-MZQ) 120,120,123
120 FIRW(LK)=FIRW(LK+1)
    FIRI(LK)=FIRI(LK+1)
    LK=LK+1
    GO TO 119
123 MZQ=MZQ-1
    GO TO 118
109 WZZ=FIRI(I)/S
    IF (WZZ) 600,600,601
601 NN=NN+1
    FI(NN)=ALOG10(WZZ)
    SKI(NN)=S
    SKK(NN)=FIRI(I)
    SKQ(NN)=FIRW(I)
    IF (THICK) 604,605,604
604 FN(NN)=(FI(NN)*2.303)/THICK
    GO TO 606
605 FN(NN)=C.0
    ICON=0
606 CONTINUE
600 I=I+1
    GO TO 118
105 FX=C.0
```

```
MZQ=NN
DO 121 I=1,MZQ
EV(I)=Q/SKQ(I)
121 CONTINUE
READ (IC,1) TR
NP=50
KP=1
DO 24 I=1,MZQ
IF (NP-50) 28,27,27
27 WRITE (IP,25) TR,KP
25 FORMAT (1H1,1X,20A4,6X,'PAGE',2X,I5//)
KP=KP+1
WRITE (IP,608) THICK,FIDC,DCU
608 FORMAT (5X,'THICKNESS=',E14.7/5X,'DARK CURRENT FOR I=',E14.7/
15X,'DARK CURRENT FOR IO=',E14.7)
WRITE (IP,26)
26 FORMAT (2X,'W.L.',6X,'E.V.',5X,'I ',12X,'IC',12X,
1'DPT. DEN. ',2X,'ABSCR. COEF.'/)
NP=0
28 WRITE (IP,29) SKQ(I),EV(I),SKK(I),SKI(I),FI(I),FN(I)
29 FORMAT (1X,F7.1,2X,F8.4,4(2X,E12.5))
24 NP=NP+1
READ (IC,72) XS1,XC1,XS2,XC2,XL,YL,YCPD,YABS
IF (ICON) 61C,610,611
611 DO 612 I=1,MZQ
612 FI(I)=FN(I)
YSC=YABS
DO 613 I=1,20
613 YQ(I)=YQ2(I)
GO TO 614
610 DO 615 I=1,20
615 YQ(I)=YQ1(I)
YSC=YOPD
614 CONTINUE
CALL XPLOT1(XS1,XC1,XS2,XC2,XC,YC,XL,YL,SKQ,FI,XQ1,XQ2,YQ,TR,
IMZQ,Q,YSC)
CALL NAME2 (TIL,80)
CALL PAGE
CALL XPLOT1(XS2,XC2,XS1,XC1,XC,YC,XL,YL,EV,FI,XC2,XC1,YQ,TR,
IMZQ,Q,YSC)
J1=2
J2=2
CALL NAME2 (TIL,80)
IZM=2
CALL UFREW(0)
GO TO 200
32 CALL UFREW (0)
GO TO (33,18),IL
33 WRITE (IP,35) LQ
35 FORMAT (//1X,'CAN NOT FIND EXP. NO.',A4)
5 GO TO (39,40),J2
40 CALL PEND
39 CALL EXIT
4 WRITE (IP,41) IBL
41 FORMAT (//1X,'ERROR IN BLCK',I5)

GO TO 17
END
```

Appendix B

Luminescence Emission Spectra Program

```

C   *** CALCULATION OF LUMINESCENCE EMISSION SPECTRA.
C   WRITTEN BY F.D.BLAIR,
C   RADIO AND ELECTRICAL ENGINEERING,
C   NATIONAL RESEARCH COUNCIL OF CANADA,
C   OTTAWA, ONTARIO.
C   1969.
C

```

```

DIMENSION TIL(20),XQ1(20),XQ2(20),YQ(20),MK(42),M1(20),M2(20),
IM3(20),SC(15),WL(1000),FI(1000),EV(1000),FN(1000),SI(1000),
2CWL(1000),CIN(1000),WVK(4),WIN(4),CORE(1000),WX(1000)
INTEGER*4 TR(20),TQ(20)

```

```

CALL SUNDER
CALL PSAVE (8000)

```

```

IP=3

```

```

IC=1

```

```

IT=99

```

```

J1=1

```

```

J2=1

```

```

G=12395.0

```

```

IZM=1

```

```

XL=8.5

```

```

YC=11.0

```

```

JP=1

```

```

LCC=0

```

```

DO 80 I=1,1000

```

```

READ (IC,81) KI,CWL(I),CIN(I)

```

```

81 FORMAT (I5,2E14.7)

```

```

LCC=LCC+1

```

```

IF (KI-99999) 80,82,80

```

```

80 CONTINUE

```

```

WRITE (IP,83)

```

```

83 FORMAT (1X,'TO MANY CORRECTIONS')

```

```

CALL EXIT

```

```

82 DO 45 I=1,15

```

```

45 SC(I)=0.0

```

```

DO 7 I=1,15

```

```

READ (IC,8) N, WI

```

```

8 FORMAT (I5,E14.7)

```

```

IF (N-99999) 7,9,7

```

```

7 SC(N)=W1

```

```

WRITE (IP,42)

```

```

42 FORMAT (1X,'TO MANY SCALE FACTORS')

```

```

CALL EXIT

```

```

9 READ (IC,1)TIL,XQ1,XQ2,YQ,TQ

```

```

1 FORMAT (20A4)

```

```

31 MQ=0

```

```

70 READ (IC,2) MZ,LQ, WLS,WLE,FIS,FIE,SUBT

```

```

2 FORMAT (I1,1X,A4,1X,5(E14.7))

```

```

72 FORMAT (5E14.7)

```

```

READ (IC,8) IORG

```

```

INS=1

```

```

XC=1.0

```

```

IL=1

```

```

IBL=0

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```
IF (M2-9) 17,5,17
17 IF (UFREAD(MK,L)) 13,4,32
13 IF (MK(1)-10) 3,14,3
14 GO TO (15,16),IL
15 IL=2
    NI=1
16 I=2
    LS=(L-4)/8
    DO 300 K=1,LS
        CALL INCORE (MK(I),8)
        READ (IT,6) M1(K),M2(K),M3(K)
    6 FORMAT (I4,I3,I1)
300 I=I+2
    GO TO (73,74),INS
73 IF (M1(2)-9999) 76,77,76
77 WRITE (IP,78)M1(2),M2(2),M3(2)
78 FORMAT (1X,'SCALE ERROR',3(5X,I5))
    CALL EXIT
76 WMS=M1(1)
    FIMS=M2(1)
    WMB=M1(2)
    FIMB=M2(2)
    INS=2
    LS=LS-2
    DO 75 I=1,LS
        M1(I)=M1(I+2)
        M2(I)=M2(I+2)
75 M3(I)=M3(I+2)
        WMA=ABS(WMB-WMS)
        FIMA=(FIMB-FIMS)
        WLM=(WLE-WLS)/WMA
        FIX=(FIE-FIS)/FIMA
74 DO 20 I=1,LS
    IF (M1(I)-9999) 21,20,21
21 MQ=MQ+1
    WK=M1(I)
    WZ=WLS+((WK-WMS)*WLM)
    IF (WZ-WLE) 2000,2001,2001
2001 MQ=MQ-1
    GO TO 20
2000 WL(MQ)=WZ
    WK=M2(I)
    WK=FIS+((WK-FIMS)*FIX)
    LX=M3(I)+IORG-1
    SI(MQ)=WK*SC(LX)-SUBT
20 CONTINUE
    GO TO 17
3 GO TO (17,18),IL
18 IF (M2-1) 71,311,71
311 CALL UFEW (0)
    GO TO 70
71 FX=0.0
    ISS=0
    DO 22 I=1,MQ
72 DO 84 KII=1,LCC
```

```
IF (WL(I)-CWL(KII)) 86,85,84
85 CO=CIN(KII)
GO TO 93
86 KW=KII-2
89 IF ((KW+3)-LCC) 87,87,88
88 KW=KW-1
GO TO 89
87 IF (KW) 90,90,91
90 KW=KW+1
GO TO 87
84 CONTINUE
GO TO 22
91 DO 92 KKK=1,4
WWK(KKK)=CWL(KW)
WIN(KKK)=CIN(KW)
92 KW=KW+1
WSZ=WL(I)
CO=SINTP(WSZ,WWK,WIN,4)
93 ISS=ISS+1
FI(ISS)=SI(I)/CO
CORE(ISS)=CO
EV(ISS)=Q/WL(I)
WX(ISS)=WL(I)
IF (FX-FI(ISS)) 23,22,22
23 FX=FI(ISS)
22 CONTINUE
MQ=ISS
READ (IC,72) XS1,XC1,XS2,XC2
READ (IC,72) XL,YL
READ (IC,1) TR
NP=50
KP=1
DO 24 I=1,MQ
FN(I)=FI(I)/FX
IF (NP-50) 28,27,27
27 WRITE (IP,25) TR,KP
25 FORMAT (1H1,20A4,6X,'PAGE',2X,I5)
WRITE (IP,1000) SUBT
1000 FORMAT (/10X,'DARK CURRENT=',E14.7/)
WRITE (IP,26)
26 FORMAT (2X,'W.L.',6X,'E.V.',5X,'EMISSION I',4X,'CORRECTION',4X,
1 'CORRECTED I',2X,'NORMALIZED I'/)
NP=0
KP=KP+1
28 WRITE (IP,29) WX(I),EV(I),SI(I),CORE(I),FI(I),FN(I)
29 FORMAT (1X,F7.1,2X,F8.4,3(2X,E12.5),2X,F8.5)
24 NP=NP+1
IF (JP-2) 3000,3000,3001
3000 YC=11.0
IF (JP-1) 3002,3002,3003
3003 CALL PAGE
3002 JP=3
GO TO 3004
3001 YC=1.0
JP=2
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```
3004 CONTINUE
CALL XPLOT (XS1,XC1,XS2,XC2,XC,YC,XL,YL,WX,FX,XQ1,XQ2,YQ,TR,MQ,Q)
LX=XC
DO 30 I=1,MQ
WL(I)=EV(LX)
SI(I)=FN(LX)
30 LX=LX-1
XC=11.0
CALL XPLOT (XS2,XC2,XS1,XC1,XC,YC,XL,YL,WL,SI,XQ2,XQ1,YQ,TR,MQ,Q)
CALL NAME2(TIL,80)
J1=2
J2=2
IZM=2
CALL UFREW (0)
GO TO 31
32 CALL UFREW (0)
GO TO (33,34),IL
33 WRITE (IP,35) LQ
35 FORMAT (//1X,'CAN NOT FIND EXP. NO.',A4)
READ (IC,72) XS1,XC1,XS2,XC2
READ (IC,1) TR
IZM=1
GO TO 31
34 GO TO 18
5 GO TO (39,40),J2
40 CALL PEND
39 CALL EXIT
4 WRITE (IP,41) IBL
41 FORMAT (//1X,'ERROR IN BLOCK',I5)
GO TO 17
END
```

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Appendix C

Luminescence Excitation Spectra Program

C *** CALCULATION OF LUMINESCENCE EXITATION SPECTRA,
C COMPLETE SPECTRA.
C WRITTEN BY F.D.BLAIR,
C RADIO AND ELECTRICAL ENGINEERING,
C NATIONAL RESEARCH COUNCIL OF CANADA,
C OTTAWA, ONTARIO.
C 1969.
C

DIMENS(CN MK(42),M1(20),M2(20),M3(20),FI(2000),EV(2000),FN(2000),
1WVK(4),WIN(4),SKI(2000),TIL(20),XQ1(20),XQ2(20),YQ(20),SC(20),
2WL(2000),SI(2000),FIRW(2000),FIRI(2000)
INTEGER*4 TR(20),TQ(20)
CALL SUNDER
CALL PSAVE (800)

IP=3
IC=1
IT=99
J1=1
IZM=1
J2=1

Q=12395.0
YC=1.0
XL=19.0
YL=11.0

READ (IC,500) I1,I2

500 FORMAT (2I5)

DO 45 I=1,20

45 SC(I)=0.0

DO 7 I=1,20

READ (IC,8) N, W1

8 FORMAT (I5,E14.7)

IF (N-99999) 7,9,7

7 SC(I)=W1

WRITE (IP,42)

42 FORMAT (1X,'TO MANY SCALE FACTORS')

CALL EXIT

9 READ (IC,1)TIL,XQ1,XQ2,YQ

1 FORMAT (20A4)

200 IIL=1

ISC=I1

31 MQ=0

70 READ (IC,2) MZ,LQ,WLS,WLE,FIS,FIE,DCU

72 FORMAT (5E14.7)

INS=1

XC=1.0

IL=1

IBL=0

2 FORMAT (I1,1X,A4,1X,6(E14.7))

IF (MZ-9) 17,5,17

17 IF (N)EREAD(MK,1) 90,4,32

90 IF (L-84) 17,13,17

13 IF (MK(1)-LQ) 3,14,3

14 GO TO (15,16),IL

15 IL=2

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```
      NI=J
16  I=7
      LS=(IL-4)/8
      DO 301 K=1,LS
      CALL INCDRE (MK(I),8)
      READ (IT,6) M1(K),M2(K),M3(K)
6    FORMAT (I4,I3,I1)
301  I=I+2
      GO TO (73,74) , INS
73  IF (M1(I)-9999) 76,77,76
77  WRITE (IP,78)M1(I),M2(I),M3(I)
78  FORMAT (IX,'SCALE ERROR',3(5X,I5))
      CALL EXIT
76  WMS=M1(I)
      FIMS=M2(I)
      WMB=M1(2)
      FIMB=M2(2)
      INS=2
      LS=LS-2
      DO 75 I=1,LS
      M1(I)=M1(I+2)
      M2(I)=M2(I+2)
75  M3(I)=M3(I+2)
      WMA=ABS(WMB-WMS)
      FIMA=(FIMB-FIMS)
      WLM=(WLE-WLS)/WMA
      FIX=(FIE-FIS)/FIMA
74  DO 20 I=1,LS
      IF (M1(I)-9999) 21,20,21
21  MQ=MQ+1
      WK=M1(I)
      WZ      =WLS+((WK-WMS)*WLM)
      IF (WZ-WLE) 2000,2001,2001
2001 MQ=MQ-1
      GO TO 20
2000 WL(MQ)=WZ
      WK=M2(I)
      WK=FIS+((WK-FIMS)*FIX)
      LX=M3(I)+ISC-1
      SI(MQ)=(WK*SC(LX))-DCU
20  CONTINUE
      GO TO 17
3    GO TO (17,18),IL
18  IF (MZ-1) 71,300,71
300  CALL UFREW (0)
      GO TO 70
71  GO TO (101,102) , IIL
101  DO 103 I=1,MQ
      FIRW(I)=WL(I)
103  FIRI(I)=SI(I)
      ISC=12
      IIL=2
      MZQ=MQ
      MS=LQ
      CALL UFREW (0)
```

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```
GO TO 31
102 I=1
IF (LJ1=1) 118,118,501
501 CALL PAGE
J1=1
118 IF (1-M7Q) 104,104,105
104 WK=FIRW(I)
IF (WK-WL(1)) 116,117,117
117 DO 106 K=1,MQ
IF (WK-WL(K)) 108,107,106
107 S=SI(K)
GO TO 109
108 KW=K-2
112 IF ((KW+3) -MQ) 110,110,111
111 KW=KW-1
GO TO 112
110 IF (KW) 113,113,114
113 KW=KW+1
GO TO 110
114 DO 115 L=1,4
WWK(L)=WL(KW)
WIN(L)=SI(KW)
115 KW=KW+1
S=SINTP(WK,WWK,WIN,4)
GO TO 109
106 CONTINUE
116 LK=1
119 IF (LK+1-MZQ) 120,120,123
120 FIRW(LK)=FIRW(LK+1)
FIRI(LK)=FIRI(LK+1)
LK=LK+1
GO TO 119
123 MZQ=MZQ-1
GO TO 118
109 FI(I)=FIRI(I)/S
SKI(I)=S
I=I+1
GO TO 118
105 FX=0.0
DO 121 I=1,MZQ
EV(I)=Q/FIRW(I)
IF (FX-FI(I)) 122,121,121
122 FX=FI(I)
121 CONTINUE
READ (IC,1) TR
NP=50
KP=1
WK=1.0/FX
DO 24 I=1,MZQ
FN(I)=FI(I)*WK
IF (NP=50) 28,27,27
27 WRITE (IP,25) TR,KP
25 FORMAT (11H1,1X,20A4,6X,'PAGE',2X,15//)
KP=KP+1
WRITE (IP,26)
```

```
26 FORMAT (2X,'W.L.',6X,'E.V.',5X,'I1',12X,'I2',12X,  
1'CORRECTED I',2X,'NORMALIZED I'/)  
NP=0  
28 WRITE (IP,29) FIRW(I),EV(I),FIRI(I),SKI(I),FI(I),FN(I)  
29 FORMAT (1X,F7.1,2X,F8.4,3(2X,E12.5),2X,F8.5)  
24 NP=NP+1  
READ (IC,72) XS1,XC1,XS2,XC2  
CALL XPLOT (XS1,XC1,XS2,XC2,XC,YC,XL,YL,FIRW,FN,XQ1,XQ2,YQ,TR,  
1MZQ,Q)  
CALL NAME2 (TIL,80)  
CALL PAGE  
LX=MZQ  
DO 30 I=1,MZQ  
WL(I)=EV(LX)  
SI(I)=FN(LX)  
30 LX=LX-1  
CALL XPLOT (XS2,XC2,XS1,XC1,XC,YC,XL,YL,WL,SI,XQ2,XQ1,YQ,TR,  
1MZQ,Q)  
J1=2  
J2=2  
CALL NAME2 (TIL,80)  
IZM=2  
CALL UFREW(0)  
GO TO 200  
32 CALL UFREW (0)  
GO TO (33,18),IL  
33 WRITE (IP,35) IQ  
35 FORMAT (//1X,'CAN NOT FIND EXP. NO.',A4)  
5 GO TO (39,40),J2  
40 CALL PEND  
39 CALL EXIT  
4 WRITE (IP,41) IBL  
41 FORMAT (//1X,'ERROR IN BLOCK',I5)  
GO TO 17  
END
```

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```
C *** CALCULATION OF LUMINESCENCE EXCITATION SPECTRA,  
C LIMITED RANGE OF SPECTRA.  
C WRITTEN BY F.D. BLAIR,  
C RADIO AND ELECTRICAL ENGINEERING,  
C NATIONAL RESEARCH COUNCIL OF CANADA,  
C OTTAWA, ONTARIO.  
C 1965.  
C  
C DIMENSION TIL(20),XQ1(20),XQ2(20),YQ(20),MK(42),M1(20),M2(20), FDB00010  
1M3(20),SC(20),WL(1000),FI(1000),EV(1000),FN(1000),SI(1000), FDB00020  
1MK(4),WIN(4), FDB00030  
2FIRW(1000),FIRI(1000),SKI(1000) FDB00040  
INTEGER*4 TR(20),TQ(20) FDB00050  
CALL PSAVE (8000) FDB00060  
IP=3 FDB00070  
IC=1 FDB00080  
IT=99 FDB00090  
J1=1 FDB00100  
IZM=1 FDB00110  
J2=1 FDB00120  
Q=12395.0 FDB00130  
YC=1.0 FDB00140  
XL=19.0 FDB00150  
YL=11.0 FDB00160  
READ (IC,500) I1,I2 FDB00170  
500 FORMAT (2I5) FDB00180  
DO 45 I=1,20 FDB00190  
45 SC(I)=0.0 FDB00200  
DO 7 I=1,20 FDB00210  
READ (IC,8) N, W1 FDB00220  
8 FORMAT (I5,E14.7) FDB00230  
IF (N-99999) 7,9,7 FDB00240  
7 SC(I)=W1 FDB00250  
WRITE (IP,42) FDB00260  
42 FORMAT (1X,'TO MANY SCALE FACTORS') FDB00270  
CALL EXIT FDB00280  
9 READ (IC,1)TIL,XQ1,XQ2,YQ FDB00290  
1 FORMAT (20A4) FDB00300  
200 IIL=1 FDB00310  
ISC=I1 FDB00320  
31 MQ=C FDB00330  
70 READ (IC,2) MZ,LQ,WLS,WLE,FIS,FIE,DCU FDB00340  
72 FORMAT (5E14.7) FDB00350  
READ (IC,72) BOW,UPW FDB00360  
INS=1 FDB00370  
XC=1.0 FDB00380  
IL=1 FDB00390  
IBL=0 FDB00400  
2 FORMAT (I1,1X,A4,1X,6(E14.7)) FDB00410  
IF (MZ-9) 17,5,17 FDB00420  
17 IF (UFREAD(MK,L )) 90,4,32 FDB00430  
90 IF (L-84) 17,13,17 FDB00440  
13 IF (MK(1)-LQ) 3,14,3 FDB00450  
14 GO TO (15,16),IL
```

15	IL=2	FDB00460
	N1=1	FDB00470
16	I=2	FDB00480
	LS=(L-4)/8	FDB00490
	DO 301 K=1,LS	FDB00500
	CALL INCRE (MK(I),8)	FDB00510
	READ (IT,6) M1(K),M2(K),M3(K)	FDB00520
6	FORMAT (I4,I3,I1)	FDB00530
301	I=I+2	FDB00540
	GO TO (73,74) , INS	FDB00550
73	IF (M1(I)-9999) 76,77,76	FDB00560
77	WRITE (IP,78)M1(I),M2(I),M3(I)	FDB00570
78	FORMAT (1X,'SCALE ERROR',3(5X,I5))	FDB00580
	CALL EXIT	FDB00590
76	WMS=M1(I)	FDB00600
	FIMS=M2(I)	FDB00610
	WMB=M1(2)	FDB00620
	FIMB=M2(2)	FDB00630
	INS=?	FDB00640
	LS=LS-2	FDB00650
	DO 75 I=1,LS	FDB00660
	M1(I)=M1(I+2)	FDB00670
	M2(I)=M2(I+2)	FDB00680
75	M3(I)=M3(I+2)	FDB00690
	WMA=ABS(WMB-WMS)	FDB00700
	FIMA=(FIMB-FIMS)	FDB00710
	WLM=(WLE-WLS)/WMA	FDB00720
	FIX=(FIE-FIS)/FIMA	FDB00730
74	DO 20 I=1,LS	FDB00740
	IF (M1(I)-9999) 21,20,21	FDB00750
21	MQ=MQ+1	FDB00760
	WK=M1(I)	FDB00770
	WZ =WLS+((WK-WMS)*WLM)	FDB00780
	IF (WZ-WLE) 2000,2001,2001	FDB00790
2001	MQ=MQ-1	FDB00800
	GO TO 20	FDB00810
2000	IF (WZ-80W) 2001,3000,3000	
3000	IF (WZ-UPW) 3001,3001,2001	
3001	WL(MQ)=WZ	FDB00820
	WK=M2(I)	FDB00830
	WK=FIS+((WK-FIMS)*FIX)	FDB00840
	LX=M3(I)*ISC-1	FDB00850
	SI(MQ)=(WK*SC(LX))-DCU	FDB00860
20	CONTINUE	FDB00870
	GO TO 17	FDB00880
3	GO TO (17,18),IL	FDB00890
18	IF (MZ-1) 71,300,71	FDB00900
300	CALL UFREW (0)	FDB00910
	GO TO 70	FDB00920
71	GO TO (IC1,IC2), IIL	FDB00930
101	DO 103 I=1,MQ	FDB00940
	FIRW(I)=WL(I)	FDB00950
103	FIRI(I)=SI(I)	FDB00960
	ISC=I2	FDB00970
	IIL=2	FDB00980

MZQ=MQ	FDB00990
MS=LQ	FDB01000
CALL UFREW (0)	FDB01010
GO TO 31	FDB01020
102 I=1	FDB01030
IF (J1-1) 118,118,501	FDB01040
501 CALL PAGE	FDB01050
J1=1	FDB01060
118 IF (I-MZQ) 104,104,105	FDB01070
104 WK=FIRW(I)	FDB01080
IF (WK-WL(1)) 116,117,117	FDB01090
117 DO 106 K=1,MQ	FDB01100
IF (WK-WL(K)) 108,107,106	FDB01110
107 S=SI(K)	FDB01120
GO TO 109	FDB01130
108 KW=K-2	FDB01140
112 IF ((KW+3) -MQ) 110,110,111	FDB01150
111 KW=KW-1	FDB01160
GO TO 112	FDB01170
110 IF (KW) 113,113,114	FDB01180
113 KW=KW+1	FDB01190
GO TO 110	FDB01200
114 DO 115 L=1,4	FDB01210
WWK(L)=WL(KW)	FDB01220
WIN(L)=SI(KW)	FDB01230
115 KW=KW+1	FDB01240
S=SINTP(WK,WWK,WIN,4)	FDB01250
GO TO 109	FDB01260
106 CONTINUE	FDB01270
116 LK=I	FDB01280
119 IF (LK+1-MZQ) 120,120,123	FDB01290
120 FIRW(LK)=FIRW(LK+1)	FDB01300
FIRI(LK)=FIRI(LK+1)	FDB01310
LK=LK+1	FDB01320
GO TO 119	FDB01330
123 MZQ=MZQ-1	FDB01340
GO TO 118	FDB01350
109 FI(I)=FIRI(I)/S	FDB01360
SKI(I)=S	FDB01370
I=I+1	FDB01380
GO TO 118	FDB01390
105 FX=0.0	FDB01400
DO 121 I=1,MZQ	FDB01410
EV(I)=G/FIRW(I)	FDB01420
IF (FX-FI(I)) 122,121,121	FDB01430
122 FX=FI(I)	FDB01440
121 CONTINUE	FDB01450
READ (IC,1) TR	FDB01460
NP=50	FDB01470
KP=1	FDB01480
WK=1.0/FX	FDB01490
DO 24 I=1,MZQ	FDB01500
FN(I)=FI(I)*WK	FDB01510
IF (NP-50) 28,27,27	FDB01520
27 WRITE (IP,25) TR,KP	FDB01530

25	FORMAT (1H1,1X,20A4,6X,'PAGE',2X,I5//)	FDB01540
	KP=KP+1	FDB01550
	WRITE (IP,26)	FDB01560
26	FORMAT (2X,'W.L.',6X,'E.V.',5X,'I1',12X,'I2',12X,	FDB01570
	1'CORRECTED I',2X,'NORMALIZED I'//)	FDB01580
	NP=0	FDB01590
28	WRITE (IP,29) FIRW(I),EV(I),FIRI(I),SKI(I),FI(I),FN(I)	FDB01600
29	FORMAT (1X,F7.1,2X,F8.4,3(2X,F12.5),2X,F8.5)	FDB01610
24	NP=NP+1	FDB01620
	READ (IC,72) XS1,XC1,XS2,XC2	FDB01630
	CALL XPLOT (XS1,XC1,XS2,XC2,XC,YC,XL,YL,FIRW,FN,XC1,XQ2,YQ,TR,	FDB01640
	1MZQ,Q)	FDB01650
	CALL NAME2 (TIL,80)	FDB01660
	CALL PAGE	FDB01670
	LX=MZQ	FDB01680
	DO 30 I=1,MZQ	FDB01690
	WL(I)=EV(LX)	FDB01700
	SI(I)=FN(LX)	FDB01710
30	LX=LX-1	FDB01720
	CALL XPLOT (XS2,XC2,XS1,XC1,XC,YC,XL,YL,WL,SI,XQ2,XC1,YQ,TR,	FDB01730
	1MZQ,Q)	FDB01740
	J1=2	FDB01750
	J2=2	FDB01760
	CALL NAME2 (TIL,80)	FDB01770
	IZM=2	FDB01780
	CALL UFREW(0)	FDB01790
	GO TO 200	FDB01800
32	CALL UFREW (0)	FDB01810
	GO TO (33,18),IL	FDB01820
33	WRITE (IP,35) LQ	FDB01830
35	FORMAT (//1X,'CAN NOT FIND EXP. NO.',A4)	FDB01840
	5 GO TO (39,40),J2	FDB01850
40	CALL PEND	FDB01860
39	CALL EXIT	FDB01870
	4 WRITE (IP,41) IBL	FDB01880
41	FORMAT (//1X,'ERROR IN BLOCK',I5)	FDB01890
	GO TO 17	FDB01900
	END	FDB01910

Appendix D

Subroutines XPLØT and XPLØT1

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C   *** SUBROUTINE XPLOT.
C   PLOTTING OF NORMALIZED INTENSITY AGAINST WAVELENGTH AND ENERGY.
C   WRITTEN BY F.O. BLAIR,
C   RADIO AND ELECTRICAL ENGINEERING,
C   NATIONAL RESEARCH COUNCIL OF CANADA,
C   OTTAWA, ONTARIO.
C   1969.

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C   SUBROUTINE XPLOT (STM,SCM,STS,SCS,XC,YC,XL,YL,X,Y,XQ1,XQ2,YQ,
1TIT,N,Q)
C   DIMENSION X(1000),Y(1000),XQ1(20),XQ2(20),YQ(20),TIT(20),YP(2),
1XP(2),XPAR(9),YPAR(9),XXR(4,100),XXP(7,9),YXP(7,9),ISAV(3)
C   DOUBLE PRECISION WK,WLQ(3,100)
C   IF (N-2) 10,11,11
11  XPAR(1)=XC
   YPAR(1)=YC
   XPAR(2)=XL
   YPAR(2)=YL
   XPAR(7)=0.1
   YPAR(7)=0.1
   XPAR(8)=0.1
   YPAR(8)=0.0
   XPAR(9)=1.0
   IP=1
   CALL GRID2 (1,8.0,XPAR,YPAR)
   DO 1000 I=1,9
   XXP(7,I)=XPAR(I)
1000 YXP(7,I)=YPAR(I)
   XPAR(1)=XPAR(1)+0.5
   YPAR(1)=YPAR(1)+0.5
   XPAR(2)=XPAR(2)-1.0
   YPAR(2)=YPAR(2)-1.0
   CALL GRID2 (1,8.0,XPAR,YPAR)
   XPAR(7)=0.5
   YPAR(7)=-0.25
   DO 301 I=1,9
   XXP(1,I)=XPAR(I)
301  YXP(1,I)=YPAR(I)
   K=XPAR(2)
   XS=STM
   XPAR(6)=0.0
   YPAR(6)=0.0
   XPAR(7)=-0.3
   YPAR(7)=-0.1
   XPAR(3)=0.0
   YPAR(3)=0.0
   XPAR(4)=1.0
   YPAR(4)=1.0
   XPAR(5)=3.0
   YPAR(5)=8.0
   XP(1)=0.0
   XP(2)=0.0
   YP(1)=0.0
   YP(2)=0.25

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XPL00010
XPL00020
XPL00030
XPL00040
XPL00050
XPL00060
XPL00070
XPL00080
XPL00090
XPL00100
XPL00110
XPL00120
XPL00130
XPL00140
XPL00150
XPL00160
XPL00170
XPL00190
XPL00200
XPL00210
XPL00220
XPL00230
XPL00240
XPL00250
XPL00260
XPL00270
XPL00280
XPL00290
XPL00300
XPL00310
XPL00320
XPL00330
XPL00340
XPL00350
XPL00360
XPL00370
XPL00380
XPL00390
XPL00400
XPL00410
XPL00420
XPL00430
XPL00440

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	ILQ=0		XPL00450
	DO 300 I=1,9		XPL00450
	XXP(2,I)=XPAR(I)		XPL00470
300	YXP(2,I)=YPAR(I)		XPL00480
	DO 1 I=1,K		XPL00490
	CALL LINE2 (XP,YP,2,XPAR,YPAR)		XPL00500
	CALL INCCRE (WK,8)		XPL00510
	WRITE (IP,2) XS		XPL00520
	ILC=ILC+1		XPL00530
	WLQ(1,ILQ)=WK		XPL00540
	XXR(1,ILQ)=XPAR(7)		XPL00550
	XPAR(7)=XPAR(7)+1.0		XPL00560
	XP(1)=XP(1)+1.0		XPL00570
	XP(2)=XP(2)+1.0		XPL00580
	XS=XS+SCM		XPL00590
1	CONTINUE		XPL00600
	ISAV(1)=ILQ		XPL00610
	XPAR(7)=0.5		XPL00620
	YPAR(7)=YPAR(2)+0.375		XPL00630
	XPAR(8)=0.1		XPL00640
	DO 302 I=1,9		XPL00650
	XXP(3,I)=XPAR(I)		XPL00660
302	YXP(3,I)=YPAR(I)		XPL00670
	XS=STS		XPL00680
13	XR=Q/XS		XPL00690
	IF (XR-STM) 16,15,14		XPL00700
14	XS=XS+SCS		XPL00710
	GO TO 13		XPL00720
16	XS=XS-SCS		XPL00730
	XR=Q/XS		XPL00740
	IF (XR-STM) 16,15,15		XPL00750
15	YP(1)=YPAR(2)-0.25		XPL00760
	YP(2)=YPAR(2)-0.05		XPL00770
	XZ=SCM*XPAR(2)		XPL00780
	XPAR(7)=-0.3		XPL00790
	YPAR(7)=YPAR(2)+0.25		XPL00800
	XPAR(4)=SCM		XPL00810
	YPAR(4)=1.0		XPL00820
	ISK=0		XPL00830
	DO 303 I=1,9		XPL00840
	XXP(4,I)=XPAR(I)		XPL00850
303	YXP(4,I)=YPAR(I)		XPL00860
	I=0		XPL00870
4	XP(1)=(Q/XS)-STM		XPL00880
	XP(2)=XP(1)		XPL00890
	XPAR(7)=(XP(1)/XPAR(4))-0.3		XPL00900
	IF (ISK) 200,201,200		XPL00910
200	ISK=0		XPL00920
	YPAR(7)=YPAR(7)+0.15		XPL00930
	GO TO 202		XPL00940
201	ISK=1		XPL00950
	YPAR(7)=YPAR(7)-0.15		XPL00960
202	CONTINUE		XPL00970
	IF (XP(1)-XZ) 12,12,5		XPL00980
12	CALL LINE2 (XP,YP,2,XPAR,YPAR)		XPL00990

	CALL INCCRE (WK,8)	XPL01000
	WRITE (IP,2) XS	XPL01010
2	FORMAT (F8.2)	XPL01020
3	FORMAT (F8.4)	XPL01030
	I=I+1	XPL01040
	XXR(2,I)=XPAR(7)	XPL01050
	XXR(3,I)=YPAR(7)	XPL01060
	WLQ(2,I)=WK	XPL01070
	XS=XS-SCS	XPL01080
	GO TO 4	XPL01090
5	XPAR(7)=-.25	XPL01100
	ISAV(2)=I	XPL01110
	YPAR(7)=0.5	XPL01120
	YPAR(8)=0.1	XPL01130
	XPAR(8)=0.0	XPL01140
	XPAR(9)=2.0	XPL01150
	DO 304 I=1,9	XPL01160
	XXP(5,I)=XPAR(I)	XPL01170
304	YXP(5,I)=YPAR(I)	XPL01180
	K=20	XPL01190
	XZ=YPAR(2)/20.0	XPL01200
	XPAR(7)=-0.1	XPL01210
	YPAR(7)=C.0	XPL01220
	XS=0.0	XPL01230
	XPAR(3)=0.0	XPL01240
	YPAR(3)=C.0	XPL01250
	XPAR(4)=1.0	XPL01260
	YPAR(4)=1.0	XPL01270
	YPAR(8)=0.1	XPL01280
	XP(1)=0.0	XPL01290
	XP(2)=.25	XPL01300
	YP(1)=0.0	XPL01310
	YP(2)=0.0	XPL01320
	ISK=0	XPL01330
	DO 305 I=1,9	XPL01340
	XXP(6,I)=XPAR(I)	XPL01350
305	YXP(6,I)=YPAR(I)	XPL01360
	ILQ=0	XPL01370
	DO 6 I=1,K	XPL01380
	IF (ISK) 204,205,204	XPL01390
205	XP(2)=0.25	XPL01400
	GO TO 206	XPL01410
204	XP(2)=0.15	XPL01420
206	CONTINUE	XPL01430
	CALL LINE2 (XP,YP,2,XPAR,YPAR)	XPL01440
	IF (ISK) 207,208,207	XPL01450
208	ISK=1	XPL01460
	CALL INCCRE (WK,5)	XPL01470
	WRITE (IP,7) XS	XPL01480
7	FORMAT (F5.2)	XPL01490
	ILQ=ILQ+1	XPL01500
	XXR(4,ILQ)=YPAR(7)	XPL01510
	WLQ(3,ILQ)=WK	XPL01520
	GO TO 209	XPL01530
207	ISK=0	XPL01540

209	CONTINUE	XPL01550
	YPAR(7)=YPAR(7)+XZ	XPL01560
	YP(1)=YP(1)+XZ	XPL01570
	YP(2)=YP(2)+XZ	XPL01580
	XS=XS+0.05	XPL01590
6	CONTINUE	YPL01600
	ISAV(3)=ILQ	XPL01610
	XPAR(3)=-STM/SCM	XPL01920
	YPAR(3)=0.0	XPL01930
	XPAR(4)=SCM	XPL01940
	YPAR(4)=1.0/YPAR(2)	XPL01950
	XPAR(5)=17.0	XPL01960
	YPAR(5)=13.0	XPL01970
	CALL PCINT (X,Y,N,XPAR,YPAR)	XPL01980
	DO 306 I=1,7	
	DO 307 K=1,9	XPL01630
	XPAR(K)=XXP(I,K)	XPL01640
307	YPAR(K)=YXP(I,K)	XPL01650
	GO TO (308,309,311,312,314,315,1001), I	
308	CALL PRINT2 (XQ1,80,XPAR,YPAR)	XPL01670
	GO TO 306	XPL01680
309	J=ISAV(1)	XPL01690
	DO 310 L=1,J	XPL01700
	WK=WLQ(1,L)	XPL01710
	XPAR(7)=XXR(1,L)	XPL01720
310	CALL PRINT2 (WK,8,XPAR,YPAR)	XPL01730
	GO TO 306	XPL01740
311	CALL PRINT2 (XQ2,80,XPAR,YPAR)	XPL01750
	GO TO 306	XPL01760
312	J=ISAV(2)	XPL01770
	DO 313 L=1,J	XPL01780
	XPAR(7)=XXR(2,L)	XPL01790
	YPAR(7)=XXR(3,L)	XPL01800
	WK=WLQ(2,L)	XPL01810
313	CALL PRINT2 (WK,8,XPAR,YPAR)	XPL01820
	GO TO 306	XPL01830
314	CALL PRINT2 (YQ,80,XPAR,YPAR)	XPL01840
	GO TO 306	XPL01850
315	J=ISAV(3)	XPL01860
	DO 316 L=1,J	XPL01870
	YPAR(7)=XXR(4,L)	XPL01880
	WK=WLQ(3,L)	XPL01890
316	CALL PRINT2 (WK,5,XPAR,YPAR)	XPL01900
	GO TO 306	
1001	CALL PRINT2 (TIT,80,XPAR,YPAR)	
306	CONTINUE	XPL01910
10	RETURN	XPL01990
	END	XPL02000

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C      *** SUBROUTINE XPLOT1,
C      PLOTTING OF UNNORMALIZED INTENSITY AGAINST WAVELENGTH AND ENERGY,
C      WRITTEN BY F.D.BLAIR,
C      RADIO AND ELECTRICAL ENGINEERING,
C      NATIONAL RESEARCH COUNCIL OF CANADA,
C      OTTAWA, ONTARIO.
C      1969.
C
SUBROUTINE XPLOT1(STM,SCM,STS,SCS,XC,YC,XL,YL,X,Y,XC1,XC2,YQ,      RRA01700
1TIT,N,Q,YSC)
DIMENSION X(1000),Y(1000),XC1(20),XC2(20),YQ(20),TIT(20),YP(2),      RRA01720
1XP(2),XPAR(9),YPAR(9),XXR(4,100),XXP(7,9),YXP(7,9),ISAV(3),WSX(6)
DOUBLE PRECISION WK,HLQ(3,100)
IF (N-2) 10,11,11
11 XPAR(1)=XC
   YPAR(1)=YC
   XPAR(2)=XL
   YPAR(2)=YL
   XPAR(7)=0.1
   YPAR(7)=0.1
   XPAR(8)=0.1
   YPAR(8)=0.0
   XPAR(9)=1.0
   IP=1
   CALL GRID2 (1,8.0,XPAR,YPAR)
   DO 1051 I=1,9
   XXP(7,I)=XPAR(I)
1051 YXP(7,I)=YPAR(I)
   XPAR(1)=XPAR(1)+0.5
   YPAR(1)=YPAR(1)+0.5
   XPAR(2)=XPAR(2)-1.0
   YPAR(2)=YPAR(2)-1.0
   CALL GRID2 (1,8.0,XPAR,YPAR)
   XPAR(7)=0.5
   YPAR(7)=-0.25
   DO 301 I=1,9
   XXP(I,I)=XPAR(I)
301 YXP(I,I)=YPAR(I)
   K=XPAR(2)
   XS=STM
   XPAR(6)=0.0
   YPAR(5)=0.0
   XPAR(7)=-0.3
   YPAR(7)=-0.1
   XPAR(3)=0.0
   YPAR(3)=0.0
   XPAR(4)=1.0
   YPAR(4)=1.0
   XPAR(5)=3.0
   YPAR(5)=8.0
   XP(1)=0.0
   XP(2)=0.0
   YP(1)=0.0
   YP(2)=0.25
   ILQ=0
   RRA01740
   RRA01750
   RRA01760
   RRA01770
   RRA01780
   RRA01790
   RRA01800
   RRA01810
   RRA01820
   RRA01830
   RRA01840
   RRA01850
   RRA01860
   RRA01880
   RRA01890
   RRA01900
   RRA01910
   RRA01920
   RRA01930
   RRA01940
   RRA01950
   RRA01960
   RRA01970
   RRA01980
   RRA01990
   RRA02000
   RRA02010
   RRA02020
   RRA02030
   RRA02040
   RRA02050
   RRA02060
   RRA02070
   RRA02080
   RRA02090
   RRA02100
   RRA02110
   RRA02120
   RRA02130
   RRA02140

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	DO 300 I=1,9	RAA02150
	XXP(2,I)=XPAR(I)	RAA02160
300	YXP(2,I)=YPAR(I)	RAA02170
	DO 1 I=1,K	RAA02180
	CALL LINE2 (XP,YP,2,XPAR,YPAR)	RAA02190
	CALL INCORE (WK,8)	RAA02200
	WRITE (IP,2) XS	RAA02210
	ILQ=ILQ+1	RAA02220
	WLQ(1,ILQ)=WK	RAA02230
	XXR(1,ILQ)=XPAR(7)	RAA02240
	XPAR(7)=XPAR(7)+1.0	RAA02250
	XP(1)=XP(1)+1.0	RAA02260
	XP(2)=XP(2)+1.0	RAA02270
	XS=XS+SCM	RAA02280
1	CONTINUE	RAA02290
	ISAV(1)=ILQ	RAA02300
	XPAR(7)=0.5	RAA02310
	YPAR(7)=YPAR(2)+0.375	RAA02320
	XPAR(8)=0.1	RAA02330
	DO 302 I=1,9	RAA02340
	XXP(3,I)=XPAR(I)	RAA02350
302	YXP(3,I)=YPAR(I)	RAA02360
	XS=STS	RAA02370
13	XR=Q/XS	RAA02380
	IF (XR-STM) 16,15,14	RAA02390
14	XS=XS+SCS	RAA02400
	GO TO 13	RAA02410
16	XS=XS-SCS	RAA02420
	XR=Q/XS	RAA02430
	IF (XR-STM) 16,15,15	RAA02440
15	YP(1)=YPAR(2)-0.25	RAA02450
	YP(2)=YPAR(2)	RAA02460
	XZ=SCM*XPAR(2)	RAA02470
	XPAR(7)=-0.3	RAA02480
	YPAR(7)=YPAR(2)+0.25	RAA02490
	XPAR(4)=SCM	RAA02500
	YPAR(4)=1.0	RAA02510
	ISK=0	RAA02520
	DO 303 I=1,9	RAA02530
	XXP(4,I)=XPAR(I)	RAA02540
303	YXP(4,I)=YPAR(I)	RAA02550
	I=0	RAA02560
4	XP(1)=(Q/XS)-STM	RAA02570
	XP(2)=XP(1)	RAA02580
	XPAR(7)=(XP(1)/XPAR(4))-0.3	RAA02590
	IF (ISK) 200,201,200	RAA02600
200	ISK=0	RAA02610
	YPAR(7)=YPAR(7)+0.15	RAA02620
	GO TO 202	RAA02630
201	ISK=1	RAA02640
	YPAR(7)=YPAR(7)-0.15	RAA02650
202	CONTINUE	RAA02660
	IF (XP(1)-XZ) 12,12,5	RAA02670
12	CALL LINE2 (XP,YP,2,XPAR,YPAR)	RAA02680
	CALL INCORE (WK,8)	RAA02690

WRITE (IP,2) XS	RPA02700
2 FORMAT (F8.2)	RRA02710
3 FORMAT (F8.4)	RRA02720
I=I+1	RRA02730
XXR(2,I)=XPAR(7)	RPA02740
XXR(3,I)=YPAR(7)	RRA02750
WLQ(2,I)=WK	RRA02760
XS=XS-SCS	RRA02770
GO TO 4	RPA02780
5 XPAR(7)=-.25	RRA02790
ISAV(2)=I	RRA02800
YPAR(7)=0.5	RPA02810
YPAR(8)=0.1	RRA02820
XPAR(8)=0.0	RRA02830
XPAR(9)=2.0	RRA02840
DO 304 I=1,9	RRA02850
XXP(5,I)=XPAR(I)	RRA02860
304 YXP(5,I)=YPAR(I)	RRA02870
K=20	RPA02880
XZ=YPAR(2)/20.0	RPA02890
XPAR(7)=-0.1	RRA02900
YPAR(7)=-0.1	
XS=0.0	RPA02920
DSN=(YSC*YPAR(2))/20.0	
XPAR(3)=0.0	RRA02930
YPAR(3)=0.0	RRA02940
XPAR(4)=1.0	RPA02950
YPAR(4)=YPAR(2)/10.0	RRA02960
YPAR(8)=0.1	RRA02970
XP(1)=0.0	RRA02980
XP(2)=.25	RPA02990
YP(1)=0.0	RRA03000
YP(2)=0.0	RPA03010
ISK=0	RRA03020
DO 305 I=1,9	RRA03030
XXP(6,I)=XPAR(I)	RRA03040
305 YXP(6,I)=YPAR(I)	RRA03050
ILQ=0	RRA03060
DSS=4	
DO 6 I=1,K	RPA03070
IF (ISK) 204,205,204	RPA03080
205 XP(2)=0.25	RRA03090
ISK=1	
GO TO 206	
204 XP(2)=0.15	RPA03100
ISK=0	RRA03110
206 CONTINUE	
CALL LINE2 (XP,YP,2,XPAR,YPAR)	RPA03120
IF (DSS-4) 207,208,207	RRA03130
208 CONTINUE	
DSS=0	
CALL INCCRE (WK,6)	
WRITE (IP,7) XS	RPA03170
7 FORMAT (F6.2)	
ILQ=ILQ+1	RRA03190

	XXR(4,ILQ)=YPAR(7)	RRAC3200
	WLQ(3,ILQ)=WK	RRAC3210
	GO TO 209	RRAC3220
207	CONTINUE	
209	CONTINUE	RRAC3240
	DSS=DSS+1	
	YPAR(7)=YPAR(7)+XZ	RRAC3250
	YP(1)=YP(1)+XZ	RRAC3260
	YP(2)=YP(2)+XZ	RRAC3270
	XS=XS+DSN	
6	CONTINUE	RRAC3290
	ISAV(3)=ILQ	RRAC3300
	XPAR(3)=-STM/SCM	RRAC3610
	YPAR(3)=0.0	RRAC3620
	XPAR(4)=SCM	RRAC3630
	YPAR(4)=YSC	
	XPAR(5)=17.0	RRAC3650
	YPAR(5)=13.0	RRAC3660
	CALL PCINT (X,Y,N,XPAR,YPAR)	RRAC3670
	DO 306 I=1,7	
	DO 307 K=1,9	RRAC3320
	XPAR(K)=XXP(I,K)	RRAC3330
307	YPAR(K)=YXP(I,K)	RRAC3340
	GO TO (308,309,311,312,314,315,1052), I	
308	CALL PRINT2 (XQ1,80,XPAR,YPAR)	RRAC3360
	GO TO 306	RRAC3370
309	J=ISAV(1)	RRAC3380
	DO 310 L=1,J	RRAC3390
	WK=WLQ(1,L)	RRAC3400
	XPAR(7)=XXR(1,L)	RRAC3410
310	CALL PRINT2 (WK,8,XPAR,YPAR)	RRAC3420
	GO TO 306	RRAC3430
311	CALL PRINT2 (XQ2,80,XPAR,YPAR)	RRAC3440
	GO TO 306	RRAC3450
312	J=ISAV(2)	RRAC3460
	DO 313 L=1,J	RRAC3470
	XPAR(7)=XXR(2,L)	RRAC3480
	YPAR(7)=XXR(3,L)	RRAC3490
	WK=WLQ(2,L)	RRAC3500
313	CALL PRINT2 (WK,8,XPAR,YPAR)	RRAC3510
	GO TO 306	RRAC3520
314	CALL PRINT2 (YQ,80,XPAR,YPAR)	
	GO TO 306	
315	J=ISAV(3)	
	DO 1050 L=1,J	
	YPAR(7)=XXR(4,L)	
	WK=WLQ(3,L)	
1050	CALL PRINT2 (WK,6,XPAR,YPAR)	
	GO TO 306	
1052	CALL PRINT2 (TIT,80,XPAR,YPAR)	
306	CONTINUE	RRAC3600
10	RETURN	RRAC3690
	END	RRAC3690

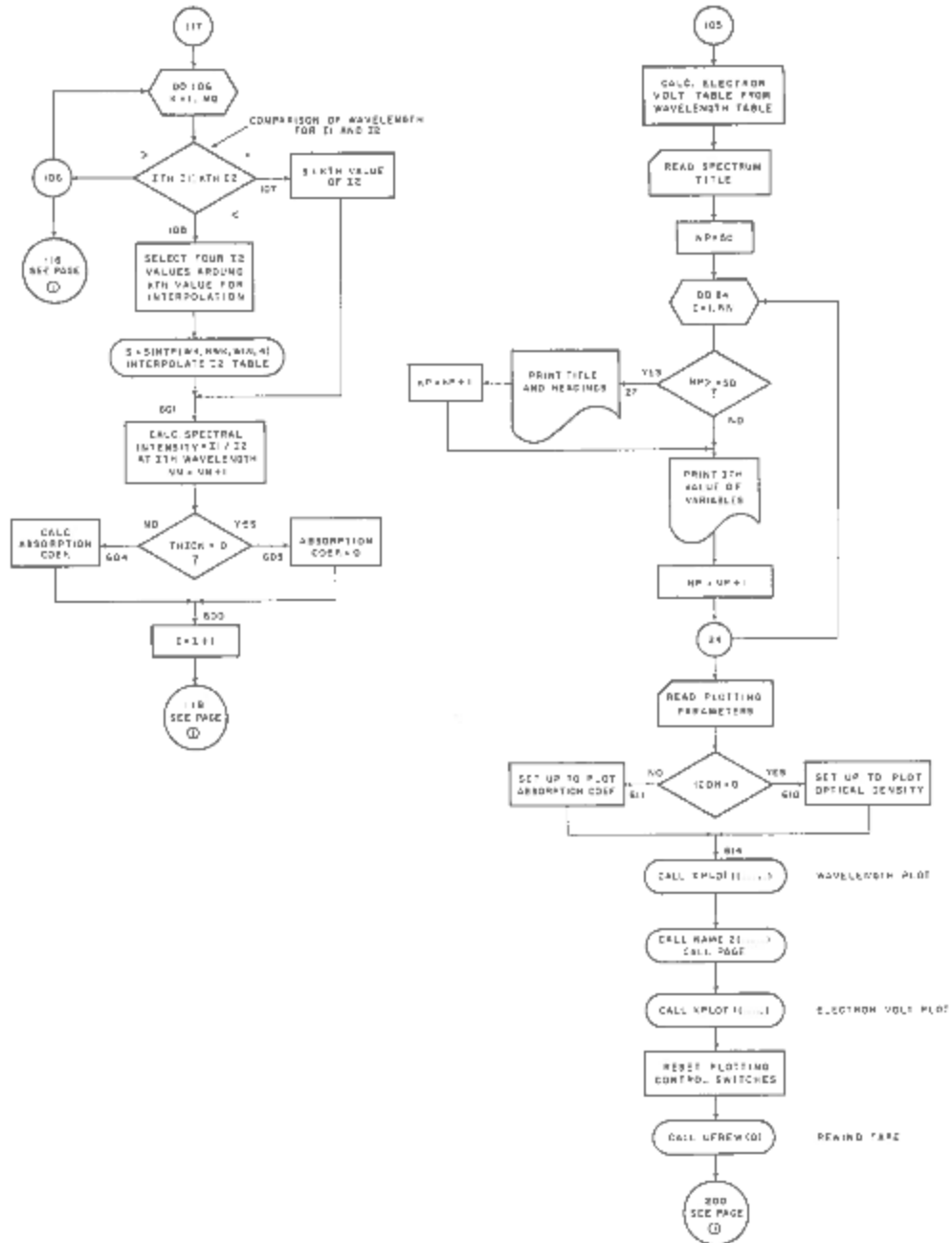
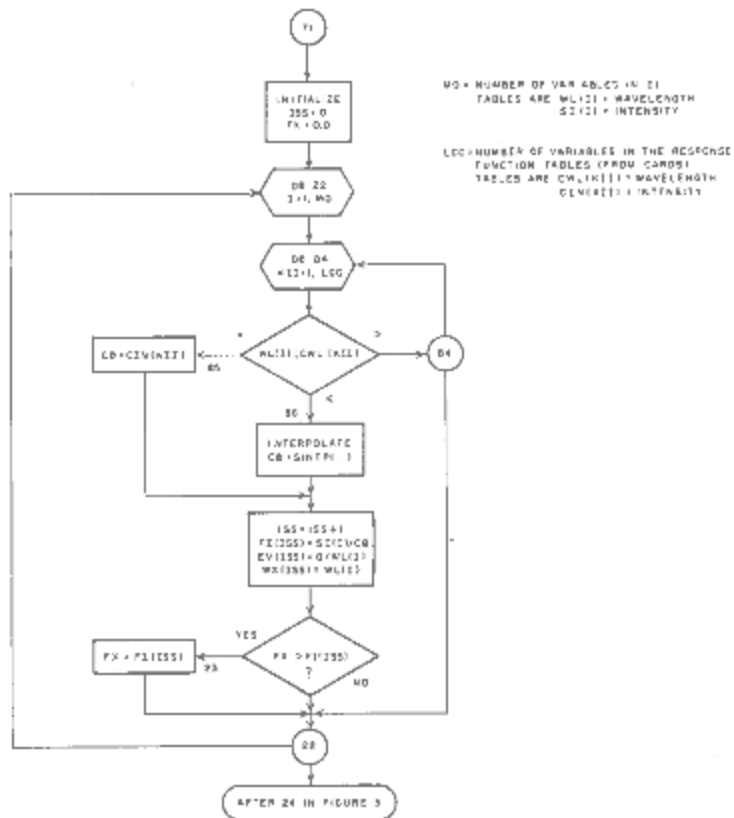


FIGURE 2 (CONT'D.)



NOTE: THE FLOW CHART FOR THE EMISSION SPECTRUM PROGRAM IS THE SAME AS THE EXCITATION SPECTRUM PROGRAM (FIGURE 3) EXCEPT FOR THE ABOVE SECTION OF LOGIC WHICH SHOULD BE IMPRINTED AT THE INDICATED POINT (STATEMENT 11). ANOTHER DIFFERENCE IS THAT INSTEAD OF THE QUANTITY BEING READ FROM THE INPUT TAPE AS IN THE EXCITATION PROGRAM, THE EMISSION PROGRAM USES THE SYSTEM RESPONSE FUNCTION WHICH IS READ INTO THE MACHINE ON CARDS.

FIGURE 4 PARTIAL FLOW CHART OF EMISSION PROGRAMS