Computer reduction of absorption and luminescence emission and excitation spectra in solids

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

- F. D. BLAIR -

OTTAWA

JANUARY 1970

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 XPLØT1 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 I1, 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 (Å)
E14.7	Maximum x coordinate in wavelength (Å)
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.

$$W_n = W_{\mathrm{Cmin}} + (W_{\mathrm{T}n} - W_{\mathrm{T\,min}}) \left[\frac{W_{\mathrm{C\,max}} - W_{\mathrm{C\,min}}}{W_{\mathrm{T\,max}} - W_{\mathrm{T\,min}}} \right]$$

$$I_n = \left[I_{\mathrm{C\,min}} + (I_{\mathrm{T}n} - I_{\mathrm{T\,min}}) \left\{ \frac{I_{\mathrm{C\,max}} - I_{\mathrm{C\,min}}}{I_{\mathrm{T\,max}} - I_{\mathrm{T\,min}}} \right\} \right] S_{\mathrm{K}} - D.C.$$

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 (I5) 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:

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

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,
ϵ 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, 1X, A4, 1X, 5E14.7	One plus continuation	I1 data, program 2	For program 1, spectrum data, See Section IIb.
9	I1, 1X, A4, 1X 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 XPLOT1 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 XPLOT 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 XPLOT 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 I5 position
2	I5, E14.7	Maximum of 15	Scale factors	See Section IId. 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	I1, lX, A4, 1X, 5E14.7	One plus any number of continuations	Data for spectrum	See Section IIb
9	I5	1	Scale factor origin	See Section IId
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	I1	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 IIb. 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.

Acknowledgments

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Appendix A

Absorption Spectra Program

```
C       *** CALCULATICN CF ABSORPTICN SPECTRA,
C            I1,I2 INPUT - OPTICAL DENSITY=LCG1C(I1/I2).
C            WRITTEN BY F.D.BLAIR,
C            RADIC AND ELECTRICAL ENGINEERING,
C            NATIONAL RESEARCH CCUNCIL CF CANADA,
C            CTTAWA, ONTARIC.
C              1969.
C
      DIMENSICN  TIL(20),XQ1(2C),XQ2(20),YQ(2C),MK(42),M1(20),M2(2C),
     1M3(20),SC(20),WL(1000),FI(1000),EV(1000),FN(1000),SI(1C0C),
     1WWK(4),WIN(4),YQ1(20),YQ2(20),SKK(1C00),SKQ(1000),
     2FIRW(10C0),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
      READ (IC,5C0) 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 FACTCRS')
      CALL EXIT
    9 READ (IC,1)TIL,XQ1,XQ2,YQ1,YQ2
    1 FORMAT (20A4)
  20C IIL=1
      ISC=I1
   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 INCORE (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(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 70
   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) 104,1C4,1C5
  104 WK=FIRW(I)
      IF (WK-WL(1)) 116,117,117
  117 DO 106 K=1,MQ
      IF (WK-WL(K)) 108,1C7,106
  107 S=SI(K)
      GO TO 109
  108 KW=K-2
  112 IF ((KW+3) -MQ) 11C,110,111
  111 KW=KW-1
      GO TC 112
  110 IF (KW) 113,113,114
  113 KW=KW+1
      GO TC 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=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 TC 118
  109 WZZ=FIRI(I)/S
      IF (WZZ) 6CC,600,601
  601 NN=NN+1
      FI(NN)=ALOG10(WZZ)
      SKI(NN)=S
      SKK(NN)=FIRI(I)
      SKQ(NN)=FIRW(I)
      IF (THICK) 6C4,605,604
  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,'IO',12X,
     1'OPT. DEN.  ',2X,'ABSCRP. 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,YOPD,YABS
      IF (ICON) 610,610,611
  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,
     1MZQ,Q,YSC)
      CALL NAME2 (TIL,80)
      CALL PAGE
      CALL XPLOT1(XS2,XC2,XS1,XC1,XC,YC,XL,YL,EV,FI,XQ2,XQ1,YQ,TR,
     1MZQ,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 BLOCK',I5)

      GO TO 17
      END
```

Appendix B

Luminescence Emission Spectra Program

```
C     *** CALCULATION OF LUMINESCENCE EMISSION SPECTA.
C          WRITTEN BY F.D.BLAIR,
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C          NATIONAL RESEARCH COUNCIL OF CANADA,
C          OTTAWA, ONTARIO.
C            1969.
C
C
      DIMENSION  TIL(20),XQ1(20),XQ2(20),YQ(20),MK(42),M1(20),M2(20),
     1M3(20),SC(15),WL(1000),FI(1000),EV(1000),FN(1000),SI(1000),
     2CWL(1000),CIN(1000),WWK(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, W1
    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
```

```
      IF (MZ-9) 17,5,17
   17 IF (UFREAD(MK,L )) 13,4,32
   13 IF (MK(1)-LQ) 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 (MZ-1) 71,311,71
  311 CALL UFREW (0)
      GO TO 70
   71 FX=0.0
      ISS=0
      DO 22 I=1,MQ
      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
```

```
 3004 CONTINUE
      CALL XPLOT (XS1,XC1,XS2,XC2,XC,YC,XL,YL,WX,FN,XQ1,XQ2,YQ,TR,MQ,Q)
      LX=MQ
      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
```

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
C
      DIMENSION MK(42),M1(20),M2(20),M3(20),FI(2000),EV(2000),FN(2000),
     1WWK(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),IQ(20)
      CALL SUNDER
      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
      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 (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
```

```
      NI=1
   16 I=2
      LS=(L-4)/8
      DO 301 K=1,LS
      CALL INCORE (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(1)-9999 ) 76,77,76
   77 WRITE (IP,78)M1(1),M2(1),M3(1)
   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)+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=I2
      IIL=2
      MZQ=MQ
      MS=LQ
      CALL UFREW (0)
```

```
      GO TO 31
  102 I=1
      IF (J1-1) 118,118,501
  501 CALL PAGE
      J1=1
  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)
      WIN(L)=SI(KW)
  115 KW=KW+1
      S=SINTP(WK,WWK,WIN,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 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 (1H1,1X,20A4,6X,'PAGE',2X,I5//)
      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) 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 BLOCK',I5)
   GO TO 17
   END
```

```
C      *** CALCULATION OF LUMINESCENCE EXITATION 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             1969.
C
C
      DIMENSION  TIL(20),XQ1(20),XQ2(20),YQ(20),MK(42),M1(20),M2(20),
     1M3(20),SC(20),WL(1000),FI(1000),EV(1000),FN(1000),SI(1000),
     1WWK(4),WIN(4),
     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
      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)
      READ (IC,72) BOW,UPW
      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 INCORE (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(1)-9999 ) 76,77,76
   77 WRITE (IP,78)M1(1),M2(1),M3(1)
   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 IF (WZ-BOW) 2001,300C,3000
 3000 IF (WZ-UPW) 3001,3001,2001
 3C01 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) 71,3C0,71
  300 CALL UFREW (0)
      GO TO 70
   71 GO TO (1C1,102), IIL
  101 DO 103 I=1,MQ
      FIRW(I)=WL(I)
  103 FIRI(I)=SI(I)
      ISC=I2
      IIL=2
```

```
      MZQ=MQ
      MS=LQ
      CALL UFREW (0)
      GO TO 31
  102 I=1
      IF (J1-1) 118,118,501
  501 CALL PAGE
      J1=1
  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)
      WIN(L)=SI(KW)
  115 KW=KW+1
      S=SINTP(WK,WWK,WIN,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 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)=G/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 (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,E12.5),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,XQ1,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,XQ1,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

```
C     *** SUBRCUTINE XPLOT.
C          PLCTTING CF NORMALIZED INTENSITY AGAINS WAVELENGTH AND ENERGY.
C          WRITTEN BY F.D.BLAIR,
C          RADIC AND ELECTRICAL ENGINEERING,
C          NATIONAL RESEARCH COUNCIL CF CANADA,
C          CTTAWA, ONTARIC.
C            1969.
C
C
      SUBRCUTINE XPLOT (STM,SCM,STS,SCS,XC,YC,XL,YL,X,Y,XQ1,XQ2,YQ,
     1TIT,N,Q)
      DIMENSICN  X(1000),Y(1CCC),XQ1(20),XQ2(2C),YQ(2C),TIT(20),YP(2),
     1XP(2),XPAR(9),YPAR(9),XXR(4,100),XXP(7,9),YXP(7,9),ISAV(3)
      DOUBLE PRECISION WK,WLQ(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)=C.0
      XPAR(9)=1.0
      IP=1
      CALL GRID2 (1,8.0,XPAR,YPAR)
      DO 1000 I=1,9
      XXP(7,I)=XPAR(I)
 1CCC 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)=C.C
      YPAR(6)=C.C
      XPAR(7)=-0.3
      YPAR(7)=-0.1
      XPAR(3)=C.0
      YPAR(3)=C.0
      XPAR(4)=1.0
      YPAR(4)=1.0
      XPAR(5)=3.0
      YPAR(5)=8.0
      XP(1)=C.0
      XP(2)=0.0
      YP(1)=0.0
      YP(2)=0.25
```

```
      ILQ=0
      DO 300 I=1,9
      XXP(2,I)=XPAR(I)
  300 YXP(2,I)=YPAR(I)
      DO 1 I=1,K
      CALL LINE2 (XP,YP,2,XPAR,YPAR)
      CALL INCCRE (WK,8)
      WRITE (IP,2) XS
      ILQ=ILQ+1
      WLQ(1,ILQ)=WK
      XXR(1,ILQ)=XPAR(7)
      XPAR(7)=XPAR(7)+1.0
      XP(1)=XP(1)+1.0
      XP(2)=XP(2)+1.0
      XS=XS+SCM
    1 CONTINUE
      ISAV(1)=ILQ
      XPAR(7)=0.5
      YPAR(7)=YPAR(2)+0.375
      XPAR(8)=0.1
      DO 302 I=1,9
      XXP(3,I)=XPAR(I)
  302 YXP(3,I)=YPAR(I)
      XS=STS
   13 XR=Q/XS
      IF (XR-STM) 16,15,14
   14 XS=XS+SCS
      GO TO 13
   16 XS=XS-SCS
      XR=Q/XS
      IF (XR-STM) 16,15,15
   15 YP(1)=YPAR(2)-0.25
      YP(2)=YPAR(2)-0.05
      XZ=SCM*XPAR(2)
      XPAR(7)=-0.3
      YPAR(7)=YPAR(2)+0.25
      XPAR(4)=SCM
      YPAR(4)=1.0
      ISK=0
      DO 303 I=1,9
      XXP(4,I)=XPAR(I)
  303 YXP(4,I)=YPAR(I)
      I=0
    4 XP(1)=(Q/XS)-STM
      XP(2)=XP(1)
      XPAR(7)=(XP(1)/XPAR(4))-0.3
      IF (ISK) 200,201,200
  200 ISK=0
      YPAR(7)=YPAR(7)+0.15
      GO TO 202
  201 ISK=1
      YPAR(7)=YPAR(7)-0.15
  202 CONTINUE
      IF (XP(1)-XZ) 12,12,5
   12 CALL LINE2 (XP,YP,2,XPAR,YPAR)
```

```
      CALL INCORE (WK,8)
      WRITE (IP,2) XS
    2 FORMAT (F8.2)
    3 FORMAT (F8.4)
      I=I+1
      XXR(2,I)=XPAR(7)
      XXR(3,I)=YPAR(7)
      WLQ(2,I)=WK
      XS=XS-SCS
      GO TO  4
    5 XPAR(7)=-.25
      ISAV(2)=I
      YPAR(7)=0.5
      YPAR(8)=0.1
      XPAR(8)=0.0
      XPAR(9)=2.0
      DO 304 I=1,9
      XXP(5,I)=XPAR(I)
  304 YXP(5,I)=YPAR(I)
      K=20
      XZ=YPAR(2)/20.0
      XPAR(7)=-0.1
      YPAR(7)= 0.0
      XS=0.0
      XPAR(3)=0.0
      YPAR(3)=0.0
      XPAR(4)=1.0
      YPAR(4)=1.0
      YPAR(8)=0.1
      XP(1)=0.0
      XP(2)=.25
      YP(1)=0.0
      YP(2)=0.0
      ISK=0
      DO 305 I=1,9
      XXP(6,I)=XPAR(I)
  305 YXP(6,I)=YPAR(I)
      ILQ=0
      DO 6 I=1,K
      IF (ISK) 204,205,204
  205 XP(2)=0.25
      GO TO 206
  204 XP(2)=0.15
  206 CONTINUE
      CALL LINE2 (XP,YP,2,XPAR,YPAR)
      IF (ISK) 207,208,207
  208 ISK=1
      CALL INCORE (WK,5)
      WRITE (IP,7) XS
    7 FORMAT (F5.2)
      ILQ=ILQ+1
      XXR(4,ILQ)=YPAR(7)
      WLQ(3,ILQ)=WK
      GO TO 209
  207 ISK=0
```

```
  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                                   XPL01600
      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 (3C8,309,311,312,314,315,1001), 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
 1C01 CALL PRINT2 (TIT,80,XPAR,YPAR)
  306 CONTINUE                                   XPL01910
   10 RETURN                                     XPL01990
      END                                        XPL02000
```

```
C      *** SUBROUTINE XPLOT1,
C          PLOTTING OF UNNORMALIZED INTENSITY AGAINST WAVELENGTH AND ENERGY.
C          WRITTEN BY F.D.BLAIR,
C          RADIC AND ELECTRICAL ENGINEERING,
C          NATIONAL RESEARCH COUNCIL OF CANADA,
C          OTTAWA, CNTARIC.
C            1969.
C
      SUBROUTINE XPLOT1(STM,SCM,STS,SCS,XC,YC,XL,YL,X,Y,XQ1,XQ2,YQ,
     1TIT,N,Q,YSC)
      CIMENSICN  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),WSX(6)
      DOUBLE PRECISION WK,WLQ(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(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
      ILQ=0
```

```
      DO 300 I=1,9
      XXP(2,I)=XPAR(I)
  300 YXP(2,I)=YPAR(I)
      DO 1 I=1,K
      CALL LINE2 (XP,YP,2,XPAR,YPAR)
      CALL INCORE (WK,8)
      WRITE (IP,2) XS
      ILQ=ILQ+1
      WLQ(1,ILQ)=WK
      XXR(1,ILQ)=XPAR(7)
      XPAR(7)=XPAR(7)+1.0
      XP(1)=XP(1)+1.0
      XP(2)=XP(2)+1.0
      XS=XS+SCM
    1 CONTINUE
      ISAV(1)=ILQ
      XPAR(7)=0.5
      YPAR(7)=YPAR(2)+0.375
      XPAR(8)=0.1
      DO 302 I=1,9
      XXP(3,I)=XPAR(I)
  302 YXP(3,I)=YPAR(I)
      XS=STS
   13 XR=Q/XS
      IF (XR-STM) 16,15,14
   14 XS=XS+SCS
      GO TO 13
   16 XS=XS-SCS
      XR=Q/XS
      IF (XR-STM) 16,15,15
   15 YP(1)=YPAR(2)-0.25
      YP(2)=YPAR(2)
      XZ=SCM*XPAR(2)
      XPAR(7)=-0.3
      YPAR(7)=YPAR(2)+0.25
      XPAR(4)=SCM
      YPAR(4)=1.0
      ISK=0
      DO 303 I=1,9
      XXP(4,I)=XPAR(I)
  303 YXP(4,I)=YPAR(I)
      I=0
    4 XP(1)=(Q/XS)-STM
      XP(2)=XP(1)
      XPAR(7)=(XP(1)/XPAR(4))-0.3
      IF (ISK) 200,201,200
  200 ISK=0
      YPAR(7)=YPAR(7)+0.15
      GO TO 202
  201 ISK=1
      YPAR(7)=YPAR(7)-0.15
  202 CONTINUE
      IF (XP(1)-XZ) 12,12,5
   12 CALL LINE2 (XP,YP,2,XPAR,YPAR)
      CALL INCORE (WK,8)
```

```
      WRITE (IP,2) XS
    2 FORMAT (F8.2)
    3 FORMAT (F8.4)
      I=I+1
      XXR(2,I)=XPAR(7)
      XXR(3,I)=YPAR(7)
      WLQ(2,I)=WK
      XS=XS-SCS
      GO TO  4
    5 XPAR(7)=-.25
      ISAV(2)=I
      YPAR(7)=0.5
      YPAR(8)=0.1
      XPAR(8)=0.0
      XPAR(9)=2.0
      DO 304 I=1,9
      XXP(5,I)=XPAR(I)
  304 YXP(5,I)=YPAR(I)
      K=20
      XZ=YPAR(2)/20.0
      XPAR(7)=-0.1
      YPAR(7)=-0.1
      XS=0.0
      DSN=(YSC*YPAR(2))/20.0
      XPAR(3)=0.0
      YPAR(3)=0.0
      XPAR(4)=1.0
      YPAR(4)=YPAR(2)/10.0
      YPAR(8)=0.1
      XP(1)=0.0
      XP(2)=.25
      YP(1)=0.0
      YP(2)=0.0
      ISK=0
      DO 305 I=1,9
      XXP(6,I)=XPAR(I)
  305 YXP(6,I)=YPAR(I)
      ILQ=0
      DSS=4
      DO 6 I=1,K
      IF (ISK) 204,205,204
  205 XP(2)=0.25
      ISK=1
      GO TO 206
  204 XP(2)=0.15
      ISK=0
  206 CONTINUE
      CALL LINE2 (XP,YP,2,XPAR,YPAR)
      IF (DSS-4) 207,208,207
  208 CONTINUE
      DSS=0
      CALL INCORE (WK,6)
      WRITE (IP,7) XS
    7 FORMAT (F6.2)
      ILQ=ILQ+1
```

```
      XXR(4,ILQ)=YPAR(7)                                                RRA03200
      WLQ(3,ILQ)=WK                                                     RRA03210
      GO TO 209                                                         RRA03220
  207 CONTINUE
  209 CONTINUE                                                          RRA03240
      DSS=DSS+1
      YPAR(7)=YPAR(7)+XZ                                                RRA03250
      YP(1)=YP(1)+XZ                                                    RRA03260
      YP(2)=YP(2)+XZ                                                    RRA03270
      XS=XS+DSN
    6 CONTINUE                                                          RRA03290
      ISAV(3)=ILQ                                                       RRA03300
      XPAR(3)=-STM/SCM                                                  RRA03610
      YPAR(3)=0.0                                                       RRA03620
      XPAR(4)=SCM                                                       RRA03630
      YPAR(4)=YSC
      XPAR(5)=17.0                                                      RRA03650
      YPAR(5)=13.0                                                      RRA03660
      CALL  PCINT (X,Y,N,XPAR,YPAR)                                     RRA03670
      DO 306 I=1,7
      DO 307 K=1,9                                                      RRA03320
      XPAR(K)=XXP(I,K)                                                  RRA03330
  307 YPAR(K)=YXP(I,K)                                                  RRA03340
      GO TO (308,309,311,312,314,315,1052), I
  308 CALL PRINT2 (XQ1,80,XPAR,YPAR)                                    RRA03360
      GO TO 306                                                         RRA03370
  309 J=ISAV(1)                                                         RRA03380
      DO 310 L=1,J                                                      RRA03390
      WK=WLQ(1,L)                                                       RRA03400
      XPAR(7)=XXR(1,L)                                                  RRA03410
  310 CALL PRINT2 (WK,8,XPAR,YPAR)                                      RRA03420
      GO TO 306                                                         RRA03430
  311 CALL PRINT2 (XQ2,80,XPAR,YPAR)                                    RRA03440
      GO TO 306                                                         RRA03450
  312 J=ISAV(2)                                                         RRA03460
      DO 313 L=1,J                                                      RRA03470
      XPAR(7)=XXR(2,L)                                                  RRA03480
      YPAR(7)=XXR(3,L)                                                  RRA03490
      WK=WLQ(2,L)                                                       RRA03500
  313 CALL PRINT2 (WK,8,XPAR,YPAR)                                      RRA03510
      GO TO 306                                                         RRA03520
  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                                                          RRA03600
   10 RETURN                                                            RRA03680
      END                                                               RRA03690
```

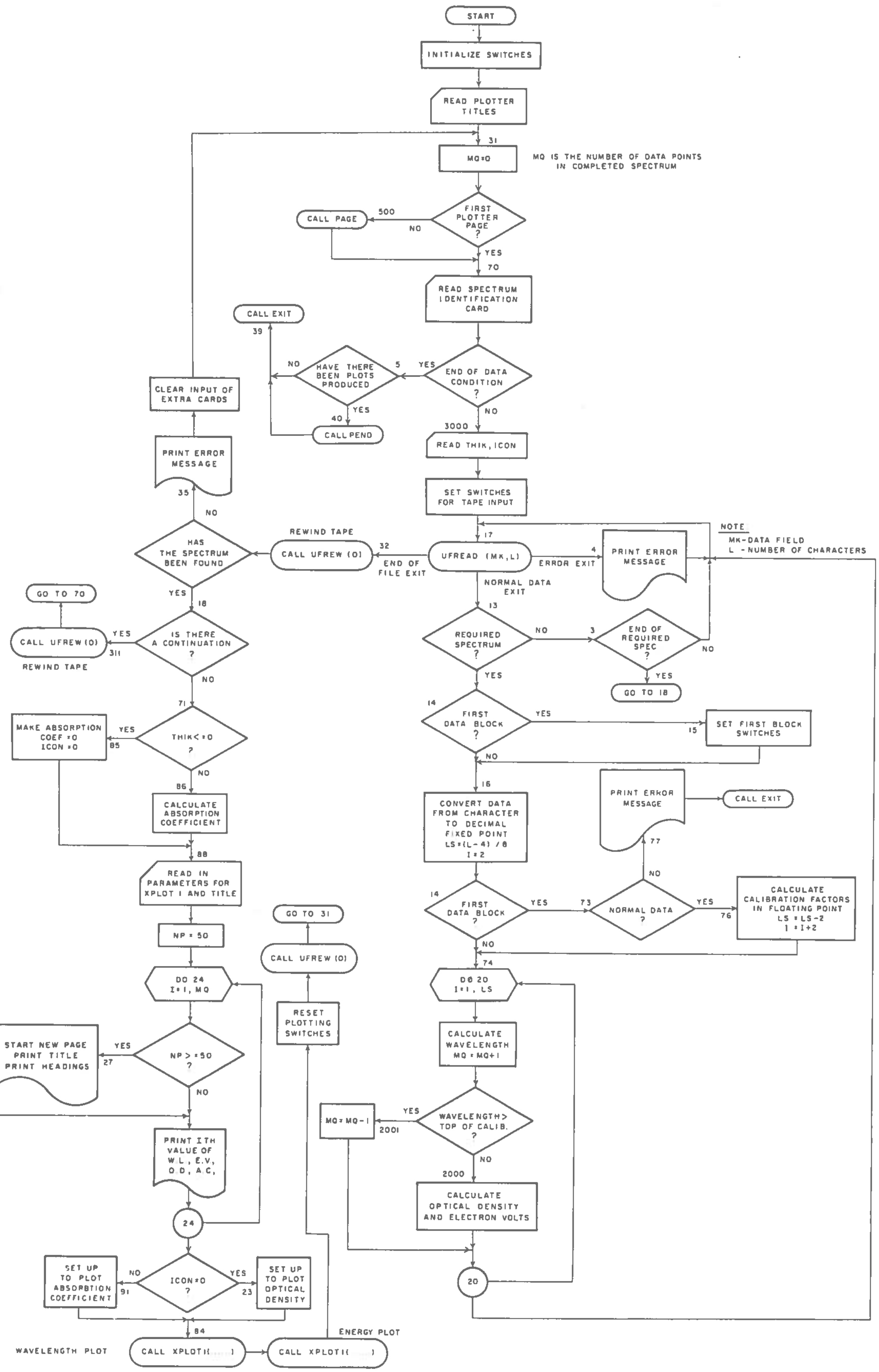


FIGURE 1 FLOW CHART FOR THE ABSORPTION PROGRAM, OPTICAL DENSITY INPUT

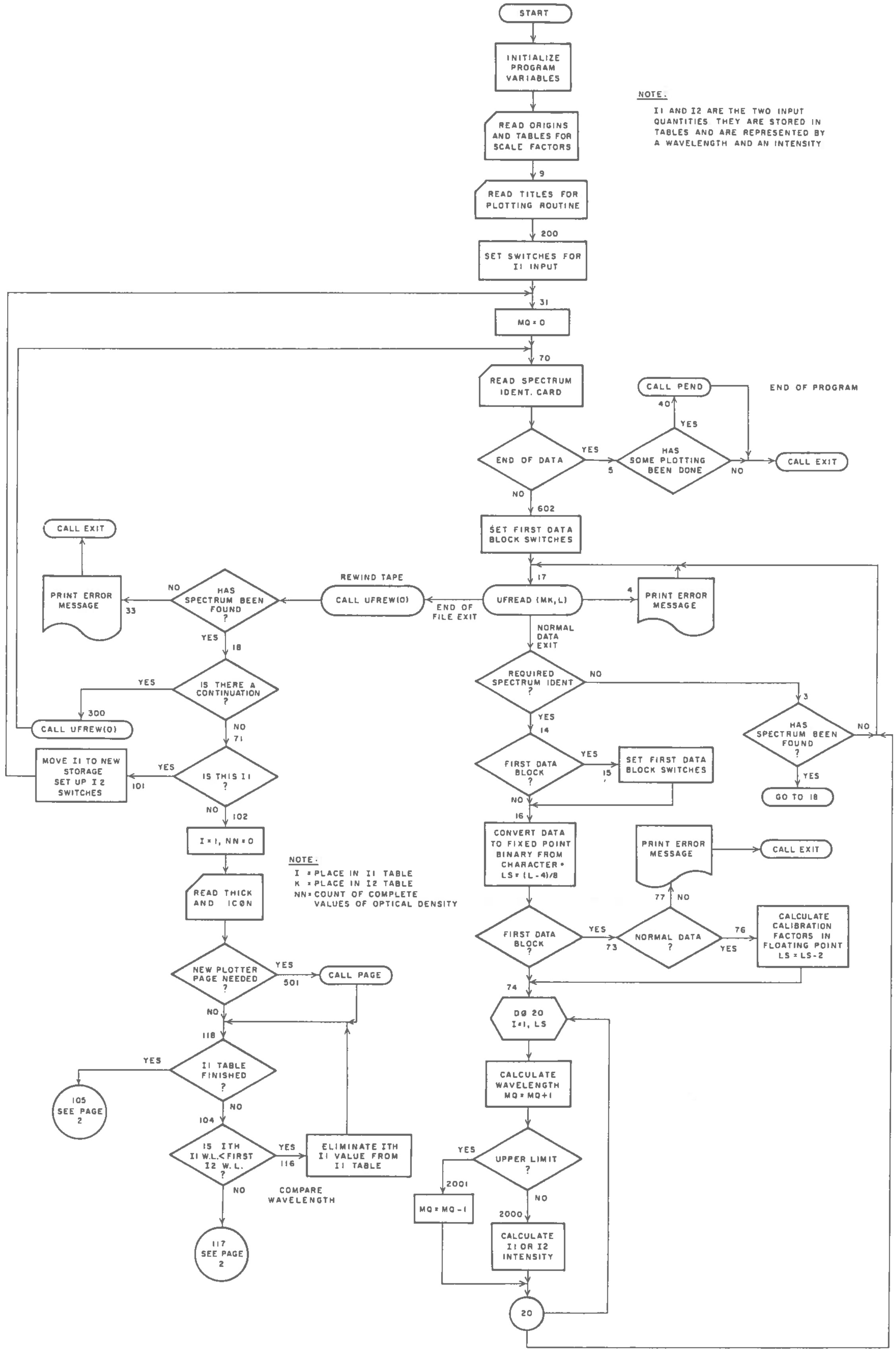


FIGURE 2 FLOW CHART FOR ABSORPTION SPECTRA PROGRAM, TWO INPUT QUANTITIES

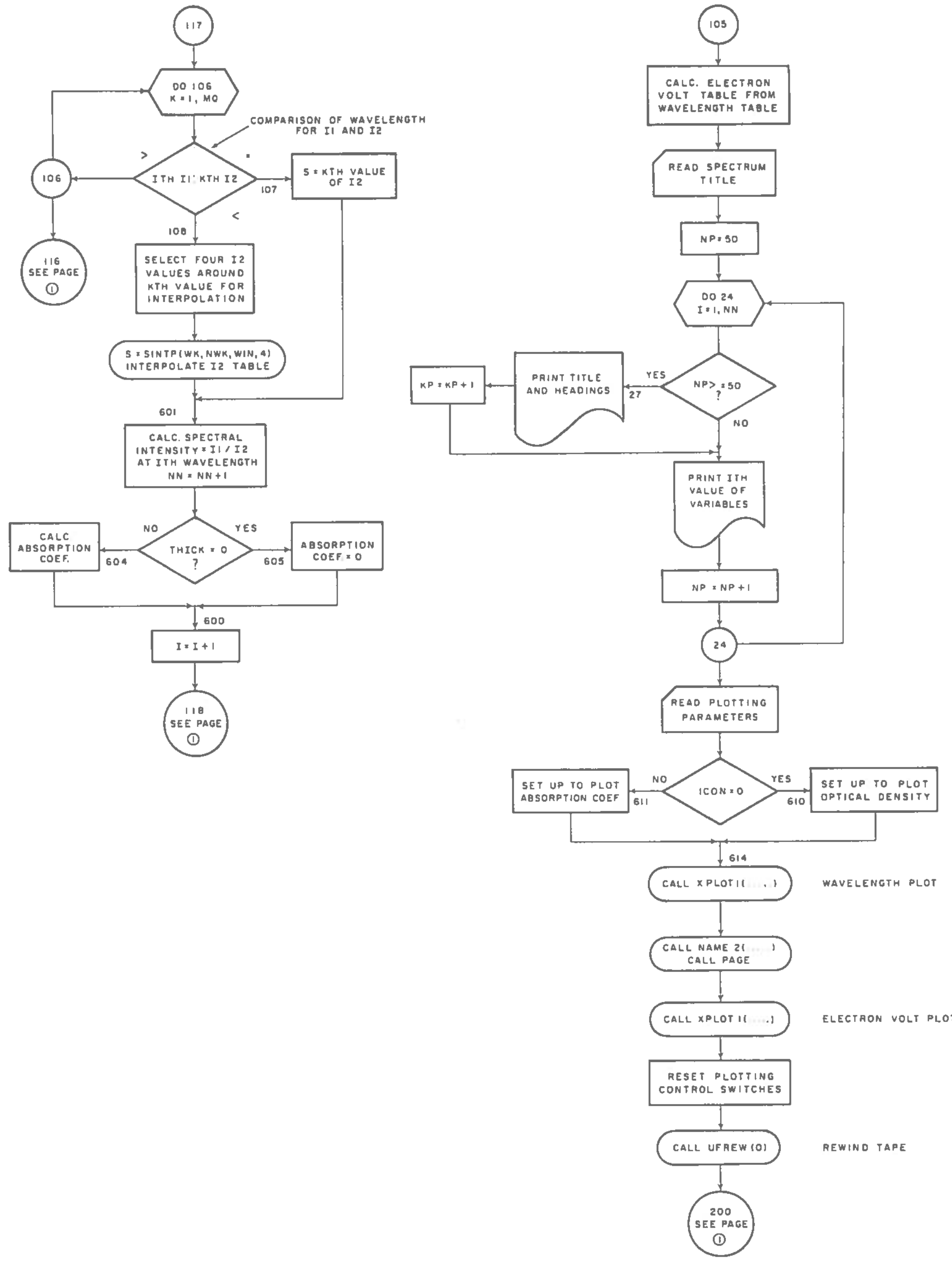


FIGURE 2 (CONT'D.)

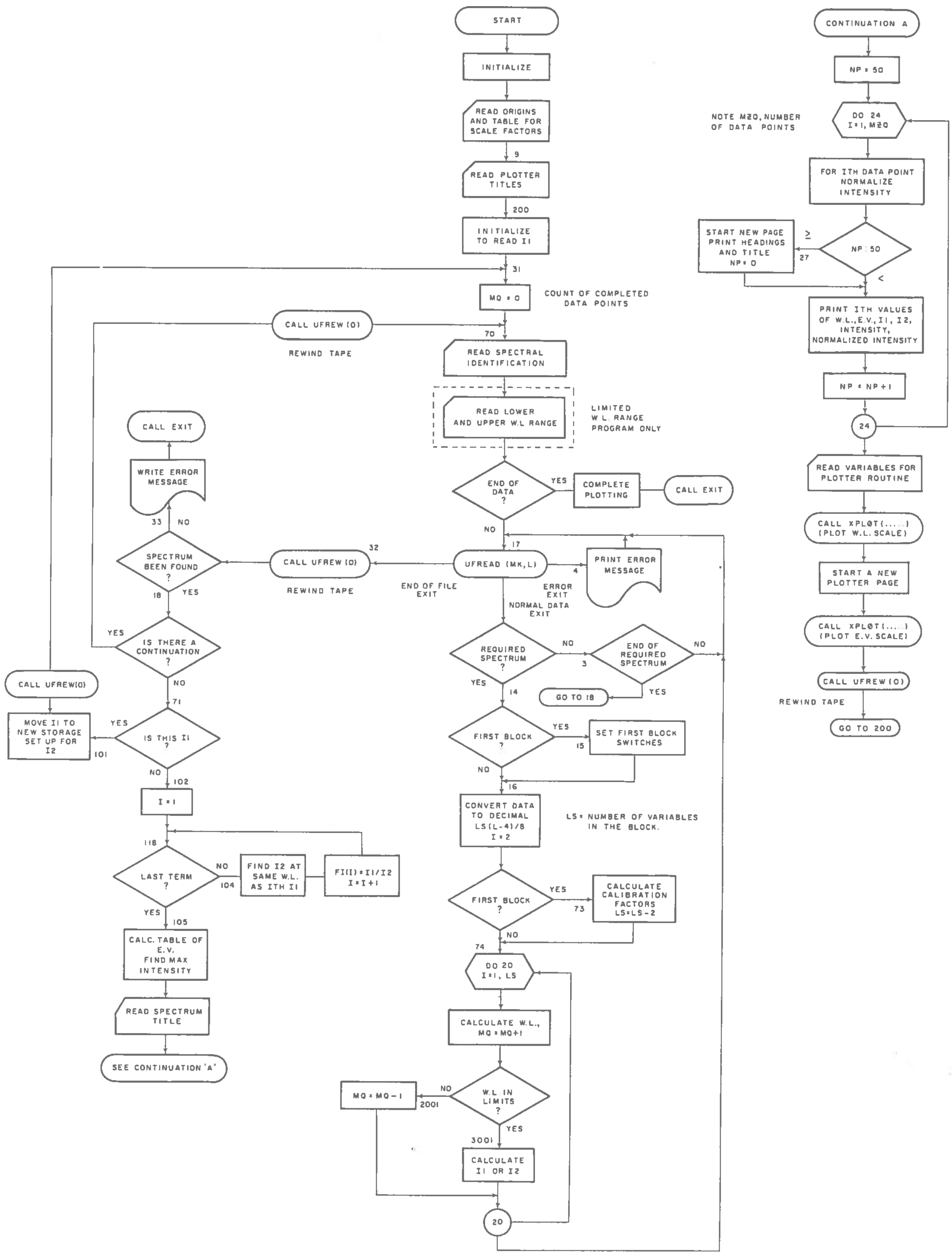
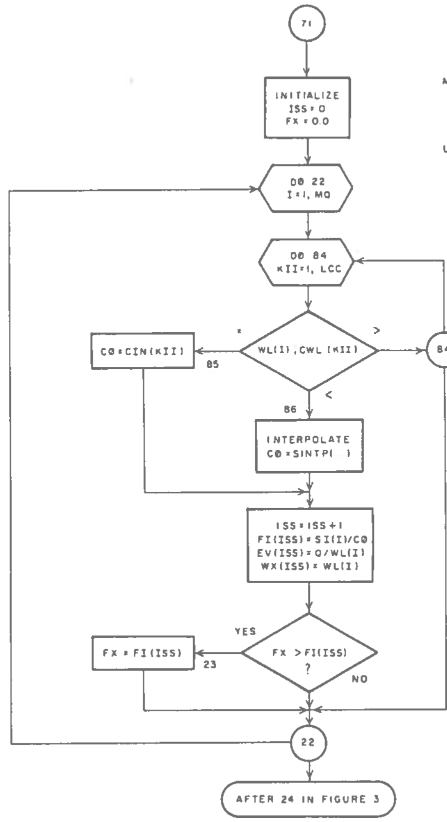


FIGURE 3 FLOW CHART FOR THE LUMINESCENCE EXCITATION PROGRAMS



MQ = NUMBER OF VARIABLES IN I1
TABLES ARE WL(I) = WAVELENGTH
SI(I) = INTENSITY

LCC = NUMBER OF VARIABLES IN THE RESPONSE FUNCTION TABLES (FROM CARDS).
TABLES ARE CWL(KII) = WAVELENGTH
CIN(KII) = INTENSITY

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 INSERTED AT THE INDICATED POINT (STATEMENT 71). ANOTHER DIFFERENCE IS THAT INSTEAD OF THE QUANTITY I2 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