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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 XPL $\backslash$ T and XPL $\backslash$ T1 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 ( $\text{\AA}$ )
E14.7	Maximum $x$ coordinate in wavelength ( $\text{\AA}$ )
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.

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

$$I_n = \left[ I_{C\min} + (I_{Tn} - I_{T\min}) \left\{ \frac{I_{C\max} - I_{C\min}}{I_{T\max} - I_{T\min}} \right\} \right] S_K - D.C.$$

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 (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 XPL0T 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 XPL0T called XPL0T1 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,  
 $\mu$  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 IIId.
2	I5, E14.7	13	Scale factors	Program 2 only, See Section IIId.
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 Coef- ficient 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 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	I1, 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	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 II d
2	I5, E14.7	Maximum of 15	Scale factors	See Section II d. Last card must be 99999 0.000000E 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 II b. 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 \*\*\* CALCULATION OF ABSORPTION SPECTRA,  
C I1,I2 INPUT - OPTICAL DENSITY=LCG1C(I1/I2).  
C WRITTEN BY F.D.BLAIR,  
C RADIC AND ELECTRICAL ENGINEERING,  
C NATIONAL RESEARCH COUNCIL OF CANADA,  
C OTTAWA, ONTARIO.  
C 1969.

```
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),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  
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,YC1,YC2  
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)  
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)
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 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
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 TO 112
    110 IF (KW) 113,113,114
    113 KW=KW+1
        GO TO 110
    114 DO 115 L=1,4
        WK(L)=WL(KW)
        WIN(L)=SI(KW)
    115 KW=KW+1
        S=SINTP(WK,WK,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 WZZ=FIRI(I)/S
        IF (WZZ) 6C0,600,601
    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,*PACE*,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'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,YCPD,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
614 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 XPLCT1(XS2,XC2,XS1,XC1,XC,YC,XL,YL,EV,FI,XC2,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)
35 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,  
C RADIO AND ELECTRICAL ENGINEERING,  
C NATIONAL RESEARCH COUNCIL OF CANADA,  
C OTTAWA, ONTARIO.  
C 1969.

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),WNK(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  
Q=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 DC 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 (5F14.7)  
READ (IC,8) TORG  
11  
10  
9  
8  
7  
6  
5  
4  
3

```
1 IF (MZ-9) 17,5,17
17 IF (UFREAD(MK,L)) 13,4,32
13 IF (MK(1)-1Q) 3,14,3
14 GO TO (15,16), IL
15 L=2
N1=1
16 I=2
LS=(L-4)/8
DO 300 K=1,LS
CALC 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(1)
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=M3(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)
12 GO TO 70
11 71 FX=0.0
10 ISS=0
9 DO 22 I=1,MQ
8 DO 84 KII=1,LCC
7
6
5
4
3
```

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 FURMAT (1H1,20A4 ,6X,'PAGE',2X,I5)  
WRITE (IP,1000) SUBT  
1000 FORMAT (1/10X,'DARK CURRENT=',E14.7/)  
WRITE (IP,26)  
26 FORMAT (2X,'W.L.',6X,'E.V.',5X,'EMISSION I',4X,'CORRECTION',4X ,  
'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 FFORMAT (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  
12 3003 CALL PAGE  
3002 JP=3  
10 GO TO 3004  
9 3001 YC=1.0  
8 JP=2  
7  
6  
5  
4  
3

```
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
```

12  
11  
10  
9  
8  
7  
6  
5  
4  
3  
2  
1

**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.

```
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),TQ(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  
12 17 IF (UREAD(MK,L)) 90,4,32  
11 90 IF (L-84) 17,13,17  
10 13 IF (MK(1)-LQ) 3,14,3  
9 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 (IX,'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 2C  
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 UREW (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 UREW (0)
```

30 TO 31  
102 I=1  
IF (J1=1) 118,118,501  
501 CALL PAGE  
J1=1  
118 IF (I-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=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,15//)  
KP=KP+1  
WRITE (IP,26)

```
26 FORMAT (2X,'W.L.',6X,'E.V.',5X,'I1',12X,'I2',12X,  
1'COPRECTED 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,Q1)  
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,Q1)  
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
```

\*\*\* CALCULATION OF LUMINESCENCE EXITATION SPECTRA,  
LIMITED RANGE OF SPECTRA.  
WRITTEN BY F.D.PLAIR,  
RADIO AND ELECTRICAL ENGINEERING,  
NATIONAL RESEARCH COUNCIL OF CANADA,  
OTTAWA, ONTARIO.  
1969.

```
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),  
1WVK(4),WIN(4),  
2FIRW(1000),FIRI(1000),SKI(1000)  
INTEGER*4 TR(20),TQ(20)  
CALL PSAVE (8000) FDB00010  
IP=3 FDB00020  
IC=1 FDB00030  
IT=99 FDB00040  
J1=1 FDB00050  
IZM=1 FDB00060  
J2=1 FDB00070  
Q=12395.0 FDB00080  
YC=1.0 FDB00090  
XL=19.0 FDB00100  
YL=11.0 FDB00110  
READ (IC,500) I1,I2 FDB00120  
500 FORMAT (2I5) FDB00130  
DO 45 I=1,20 FDB00140  
45 SC(I)=0.0 FDB00150  
DO 7 I=1,20 FDB00160  
READ (IC,8) N, W1 FDB00170  
8 FORMAT (I5,E14.7) FDB00180  
IF (N-99999) 7,9,7 FDB00190  
7 SC(I)=W1 FDB00200  
WRITE (IP,42) FDB00210  
42 FORMAT (1X,'TO MANY SCALE FACTORS') FDB00220  
CALL EXIT FDB00230  
9 READ (IC,1)TIL,XQ1,XC2,YG FDB00240  
1 FORMAT (20A4) FDB00250  
200 IIL=1 FDB00260  
ISC=I1 FDB00270  
31 MQ=0 FDB00280  
70 READ (IC,2) MZ,LQ,WLS,WLE,FIS,FIE,DCU FDB00290  
72 FORMAT (5E14.7) FDB00300  
READ (IC,72) BOW,UPW FDB00310  
INS=1 FDB00320  
XC=1.0 FDB00330  
IL=1 FDB00340  
IBL=0 FDB00350  
2 FORMAT (I1,1X,A4,1X,6(E14.7)) FDB00360  
IF (MZ-9) 17,5,17 FDB00370  
17 IF (UFREAD(MK,L )) 90,4,32 FDB00380  
90 IF (L-84) 17,13,17 FDB00390  
13 IF (MK(1)-LQ) 3,14,3 FDB00400  
14 GO TO (15,16),IL FDB00410  
FDB00420  
FDB00430  
FDB00440  
FDB00450
```

15 IL=2 FDB00460  
N1=1 FDB00470  
16 I=2 FDB00480  
LS=(L-4)/8 FDB00490  
DO 301 K=1,LS FDB00500  
CALL INCORE (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(1),M2(1),M3(1) FDB00570  
78 FORMAT (1X,'SCALE ERROR',3(5X,I5)) FDB00580  
CALL EXIT FDB00590  
76 WMS=M1(1) FDB00600  
FIMS=M2(1) 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-BOW) 2001,3000,3000  
3000 IF (WZ-UPW) 3001,3001,2001  
3C01 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  
17 GO TO (17,18),IL FDB00890  
18 IF (MZ-1) 71,3C0,71 FDB00900  
300 CALL UFREW (0) FDB00910  
GO TO 70 FDB00920  
71 GO TO (1C1,1C2), III FDB00930  
101 DO 103 I=1,MQ FDB00940  
FIRK(I)=WL(I) FDB00950  
103 FIRI(I)=SI(I) FDB00960  
ISC=I2 FDB00970  
III=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) 1C4,1C4,105 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)) 1C8,107,106 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 CGNTINUE FDB01270  
116 LK=I FDB01280  
119 IF (LK+1-MZQ) 12C,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 XPLQT and XPLQT1**

C \*\*\* SUBROUTINE XPLOT.

C PLOTTING OF NORMALIZED INTENSITY AGAINST WAVELENGTH AND ENERGY.  
C WRITTEN BY F.D.BLAIR,  
C RADICAL AND ELECTRICAL ENGINEERING,  
C NATIONAL RESEARCH COUNCIL OF CANADA,  
C OTTAWA, ONTARIO.  
C 1969.

SUBROUTINE XPLOT (STM,SCM,STS,SCS,XC,YC,XL,YL,X,Y,XQ1,XQ2,Y0,  
ITIT,N,Q) XPL00010  
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) XPL00020  
DOUBLE PRECISION WK,WLQ(3,100) XPL00030  
IF (N-2) 10,11,11 XPL00040  
11 XPAR(1)=XC XPL00050  
YPAR(1)=YC XPL00060  
XPAR(2)=XL XPL00070  
YPAR(2)=YL XPL00080  
XPAR(7)=0.1 XPL00090  
YPAR(7)=0.1 XPL00100  
XPAR(8)=0.1 XPL00110  
YPAR(8)=0.0 XPL00120  
XPAR(9)=1.0 XPL00130  
IP=1 XPL00140  
CALL GRID2 (1,8.0,XPAR,YPAR) XPL00150  
DO 1000 I=1,9 XPL00160  
XXP(7,I)=XPAR(I) XPL00170  
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 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

```
ILQ=0 XPL00450
DO 300 I=1,9 XPL00490
  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 INCRE (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 INCRE (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 INCORE (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 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 RADIO AND ELECTRICAL ENGINEERING,  
C NATIONAL RESEARCH COUNCIL OF CANADA,  
C OTTAWA, ONTARIO.  
C 1969.

SUBROUTINE XPLOT1(STM,SCM,STS,SCS,XC,YC,XL,YL,X,Y,XQ1,XQ2,YQ)  
1 TIT,N,Q,YSC) RRA01700  
DIMENSION X(1000),Y(1000),XQ1(20),XQ2(20),YQ(20),TIT(20),YP(2),  
1 XXP(2),XPAR(9),YPAR(9),XXR(4,100),XXP(7,9),YXP(7,9),ISAV(3),WSX(6) RRA01720  
DOUBLE PRECISION WK,WLQ(3,100) RRA01740  
IF (N-2) 10,11,11 RRA01750  
11 XPAR(1)=XC RRA01750  
YPAR(1)=YC RRA01760  
XPAR(2)=XL RRA01770  
YPAR(2)=YL RRA01780  
XPAR(7)=0.1 RRA01790  
YPAR(7)=0.1 RRA01800  
XPAR(8)=0.1 RRA01810  
YPAR(8)=0.0 RRA01820  
XPAR(9)=1.0 RRA01830  
IP=1 RRA01840  
CALL GRID2 (1,8.0,XPAR,YPAR) RRA01850  
DO 1051 I=1,9 RRA01860  
XXP(7,I)=XPAR(I)  
1051 YXP(7,I)=YPAR(I) RRA01870  
XPAR(1)=XPAR(1)+0.5 RRA01880  
YPAR(1)=YPAR(1)+0.5 RRA01890  
XPAR(2)=XPAR(2)-1.0 RRA01900  
YPAR(2)=YPAR(2)-1.0 KRA01910  
CALL GRID2 (1,8.0,XPAR,YPAR) RRA01920  
XPAR(7)=0.5 RRA01930  
YPAR(7)=-0.25 RRA01940  
DO 301 I=1,9 RRA01950  
XXP(1,I)=XPAR(I) RRA01960  
301 YXP(1,I)=YPAR(I) RRA01970  
K=XPAR(2) RRA01980  
XS=STM RRA01990  
XPAR(6)=0.0 RPA02000  
YPAR(5)=0.0 RPA02010  
XPAR(7)=-0.3 RPA02020  
YPAR(7)=-0.1 RPA02030  
XPAR(3)=0.0 RRA02040  
YPAR(3)=0.0 RRA02050  
XPAR(4)=1.0 RRA02060  
YPAR(4)=1.0 RRA02070  
XPAR(5)=3.0 RRA02080  
YPAR(5)=8.0 RRA02090  
XP(1)=0.0 RRA02100  
XP(2)=0.0 RPA02110  
YP(1)=0.0 RPA02120  
YP(2)=0.25 RRA02130  
ILQ=0 RRA02140

```
DO 300 I=1,9 RRA02150
XXP(2,I)=XPAR(I) RRA02160
300 YXP(2,I)=YPAR(I) RRA02170
DO 1 I=1,K RRA02180
CALL LINE2 (XP,YP,2,XPAR,YPAR) RRA02190
CALL INCORE (WK,8) RRA02200
WRITE (IP,2) XS RRA02210
ILQ=ILQ+1 RRA02220
WLQ(1,ILQ)=WK RRA02230
XXR(1,ILQ)=XPAR(7) RRA02240
XPAR(7)=XPAR(7)+1.0 RRA02250
XP(1)=XP(1)+1.0 RRA02260
XP(2)=XP(2)+1.0 RRA02270
XS=XS+SCM RRA02280
1 CCNTINUE RRA02290
ISAV(1)=ILQ RRA02300
XPAR(7)=0.5 RRA02310
YPAR(7)=YPAR(2)+0.375 RRA02320
XPAR(8)=0.1 RRA02330
DO 302 I=1,9 RRA02340
XXP(3,I)=XPAR(I) RRA02350
302 YXP(3,I)=YPAR(I) RRA02360
XS=STS RRA02370
13 XR=Q/XS RRA02380
IF (XR-STM) 16,15,14 RRA02390
14 XS=XS+SCS RRA02400
GO TO 13 RRA02410
16 XS=XS-SCS RRA02420
XR=Q/XS RRA02430
IF (XR-STM) 16,15,15 RRA02440
15 YP(1)=YPAR(2)-0.25 RRA02450
YP(2)=YPAR(2) RRA02460
XZ=SCM*XPAR(2) RRA02470
XPAR(7)=-0.3 RRA02480
YPAR(7)=YPAR(2)+0.25 RRA02490
XPAR(4)=SCM RRA02500
YPAR(4)=1.0 RRA02510
ISK=0 RRA02520
DO 303 I=1,9 RRA02530
XXP(4,I)=XPAR(I) RRA02540
303 YXP(4,I)=YPAR(I) RRA02550
I=0 RRA02560
4 XP(1)=(Q/XS)-STM RRA02570
XP(2)=XP(1) RRA02580
XPAR(7)=(XP(1)/XPAR(4))-0.3 RRA02590
IF (ISK) 200,201,200 RRA02600
200 ISK=0 RRA02610
YPAR(7)=YPAR(7)+0.15 RRA02620
GO TO 202 RRA02630
201 ISK=1 RRA02640
YPAR(7)=YPAR(7)-0.15 RRA02650
202 CCNTINUE RRA02660
IF (XP(1)-XZ) 12,12,5 RRA02670
12 CALL LINE2 (XP,YP,2,XPAR,YPAR) RRA02680
CALL INCORE (WK,8) RRA02690
```

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(12)/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

RRAC2700  
RRAC2710  
RRA02720  
RRAC2730  
RPAC2740  
RRAC2750  
RRA02760  
RRA02770  
RPAC2780  
RRAC2790  
RRA02800  
RPAC2810  
RRA02820  
RRA02830  
RRA02840  
RRA02850  
RRA02860  
RRA02870  
RPAC2880  
RRAC2890  
RRA02900  
RRAC2920  
RRA02930  
RRAC2940  
RRAC2950  
RRAC2960  
RRA02970  
RRA02980  
RPAC2990  
RRA03000  
RRA03010  
RRAC3020  
RRA03030  
RRA03040  
RRA03050  
RRAC3060  
RPAC3070  
RPAC3080  
RRAC3090  
RRA03100  
RRA03110  
RPA03120  
RPA03130  
RPA03170  
RRA03190

XXR(4,ILQ)=YPAR(7)	RRAC3200
WLQ(3,ILQ)=WK	RRA03210
GO TO 209	RRAC3220
207 CONTINUE	
209 CONTINUE	RRA03240
DSS=DSS+1	
YPAR(7)=YPAR(7)+XZ	RPA(3250
YP(1)=YP(1)+XZ	RRA03260
YP(2)=YP(2)+XZ	RRA03270
XS=XS+DSN	
6 CONTINUE	RRA03290
ISAV(3)=ILQ	RPA03300
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	RRA03650
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)	
GO TO 306	RRA03360
309 J=ISAV(1)	RRA03370
DO 310 L=1,J	RRA03380
WK=WLQ(1,L)	RRA03390
XPAR(7)=XXR(1,L)	RRA03400
310 CALL PRINT2 (WK,8,XPAR,YPAR)	RRA03410
GO TO 306	RRA03420
311 CALL PRINT2 (XQ2,80,XPAR,YPAR)	RRA03430
GO TO 306	RRA03440
312 J=ISAV(2)	RRA03450
DO 313 L=1,J	RRA03460
XPAR(7)=XXR(2,L)	RRA03470
YPAR(7)=XXR(3,L)	RRA03480
WK=WLQ(2,L)	RRA03490
313 CALL PRINT2 (WK,8,XPAR,YPAR)	RRA03500
GO TO 306	RRA03510
314 CALL PRINT2 (YQ,80,XPAR,YPAR)	RRA03520
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	RRAC3680
END	RRAD3690

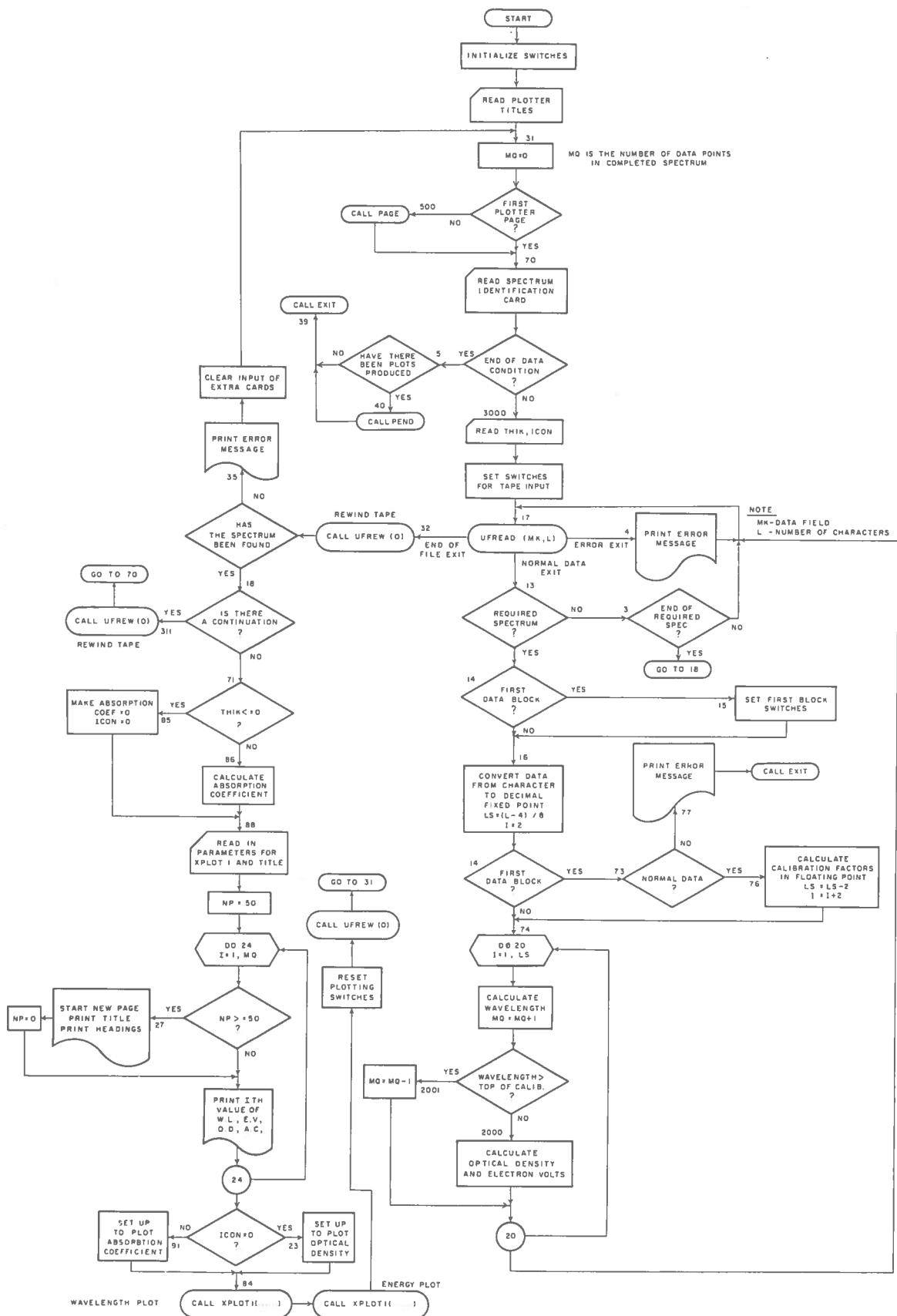


FIGURE 1 FLOW CHART FOR THE ABSORPTION PROGRAM, OPTICAL DENSITY INPUT

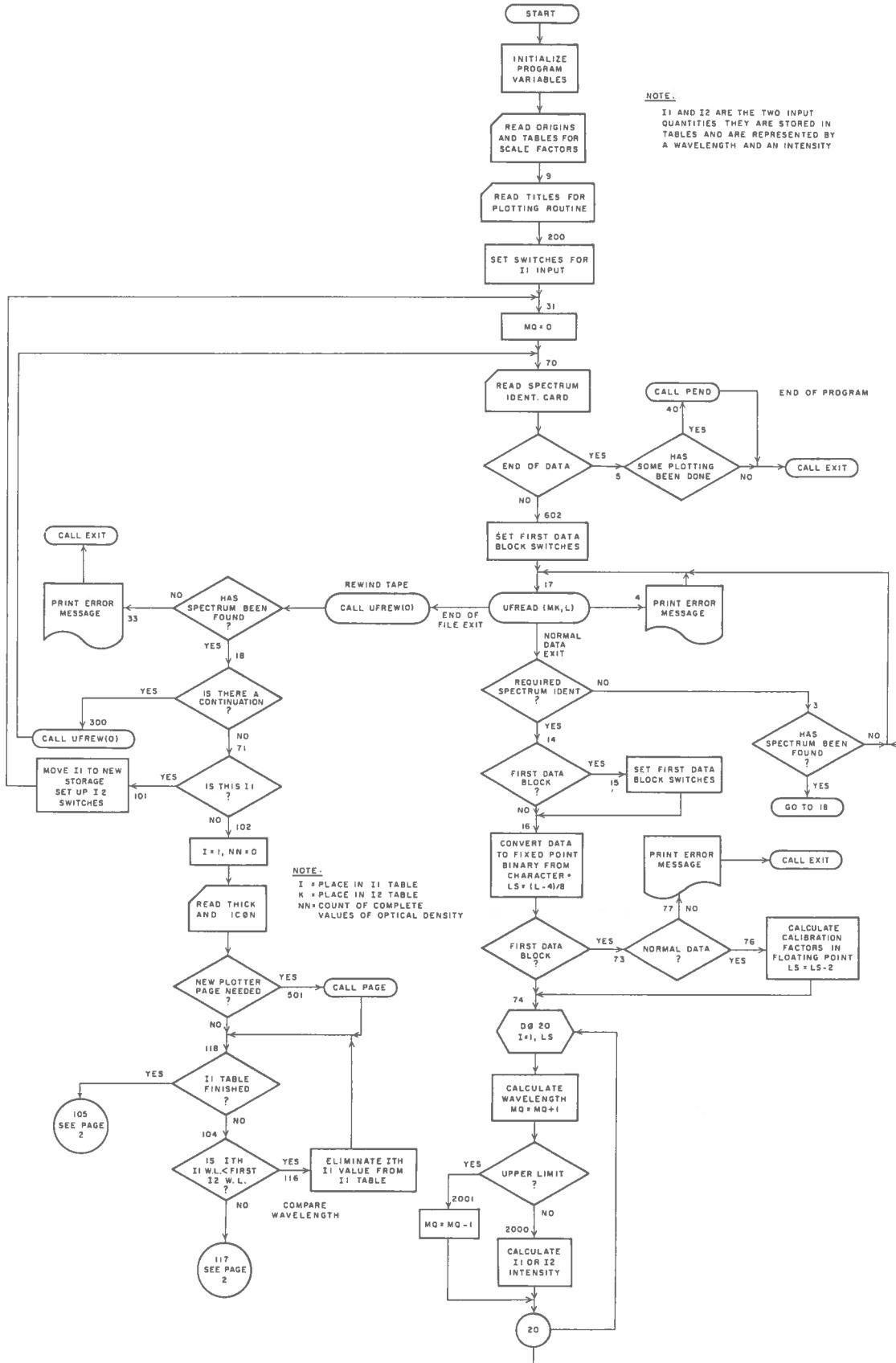


FIGURE 2 FLOW CHART FOR ABSORPTION SPECTRA PROGRAM, TWO INPUT QUANTITIES

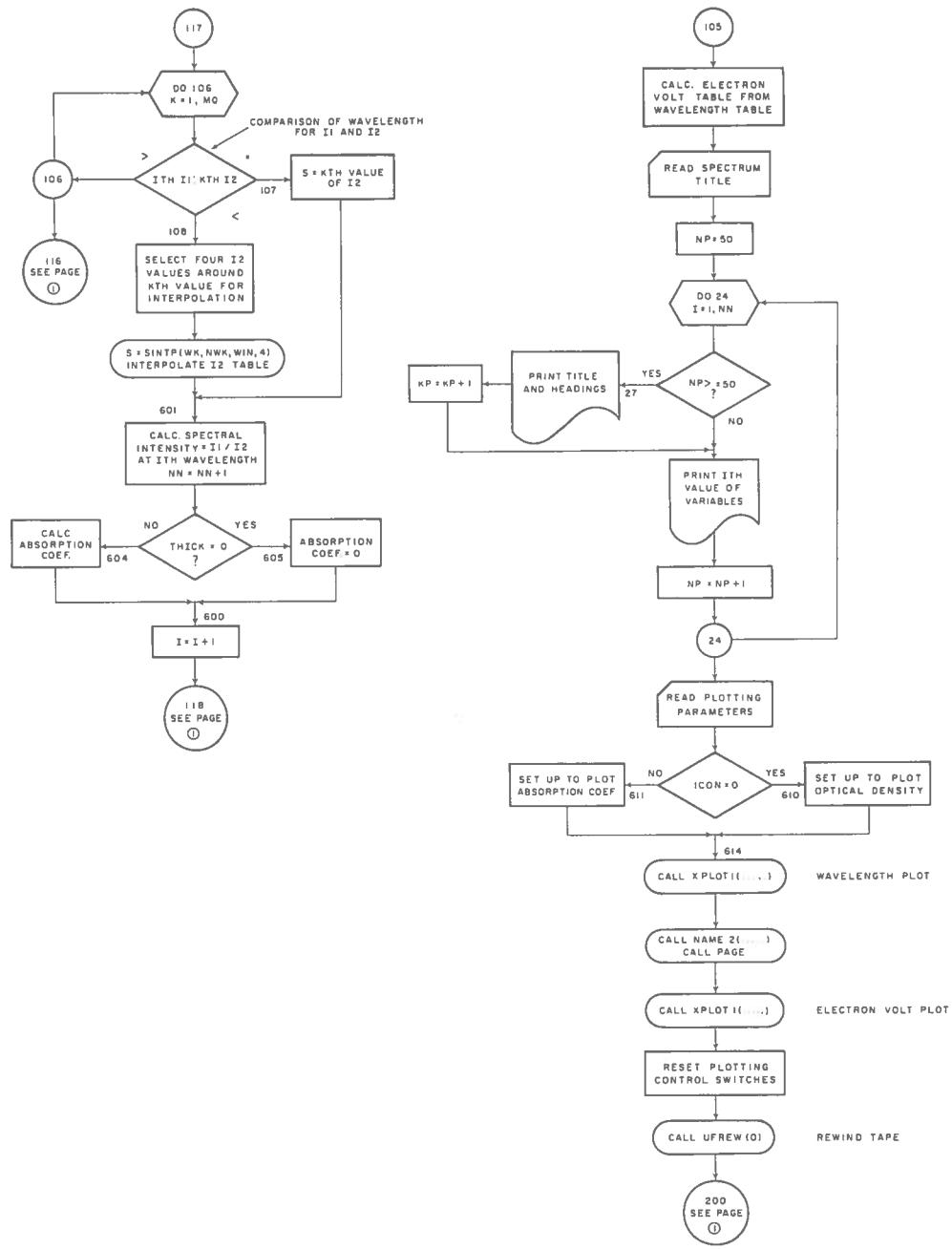


FIGURE 2 (CONT'D.)

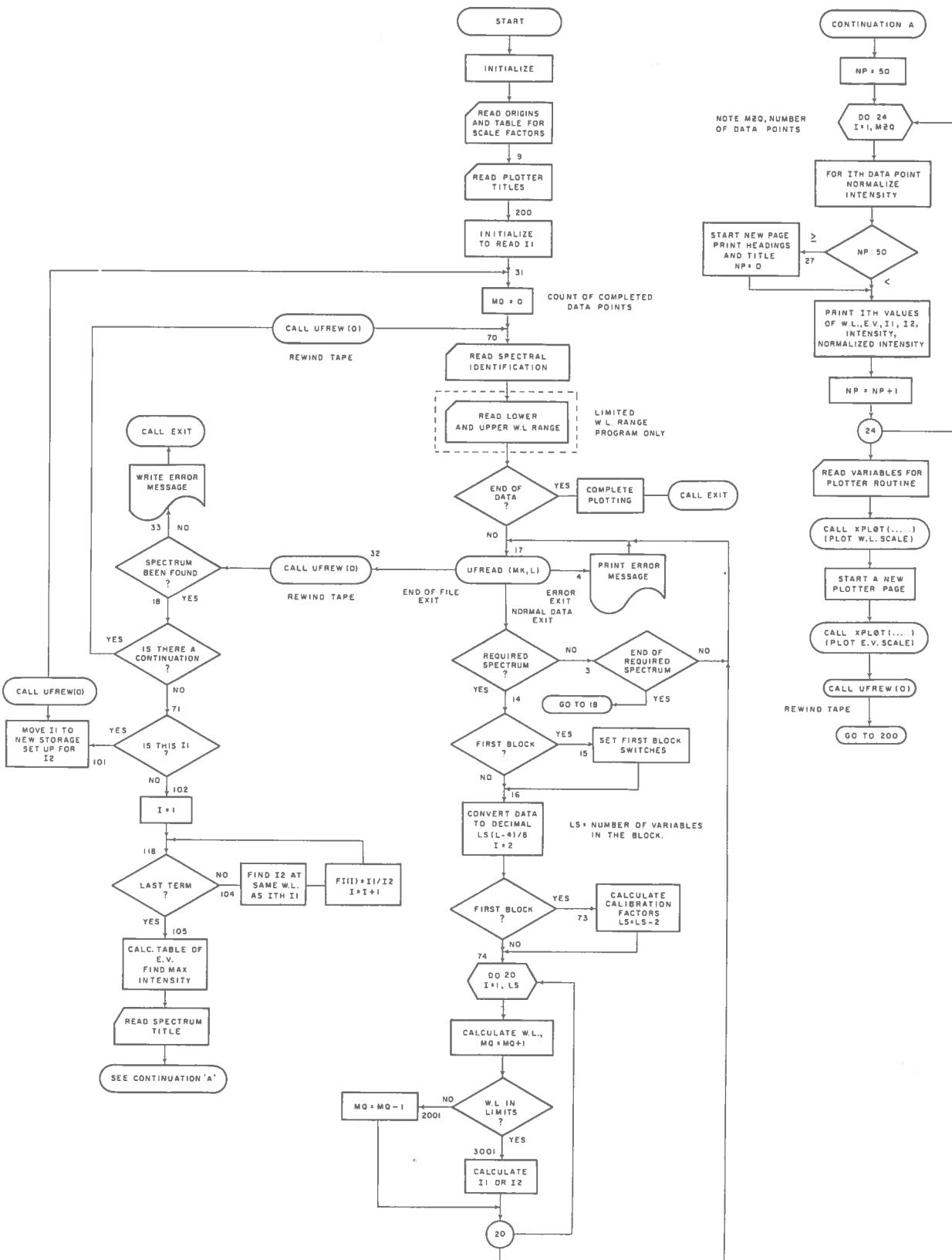
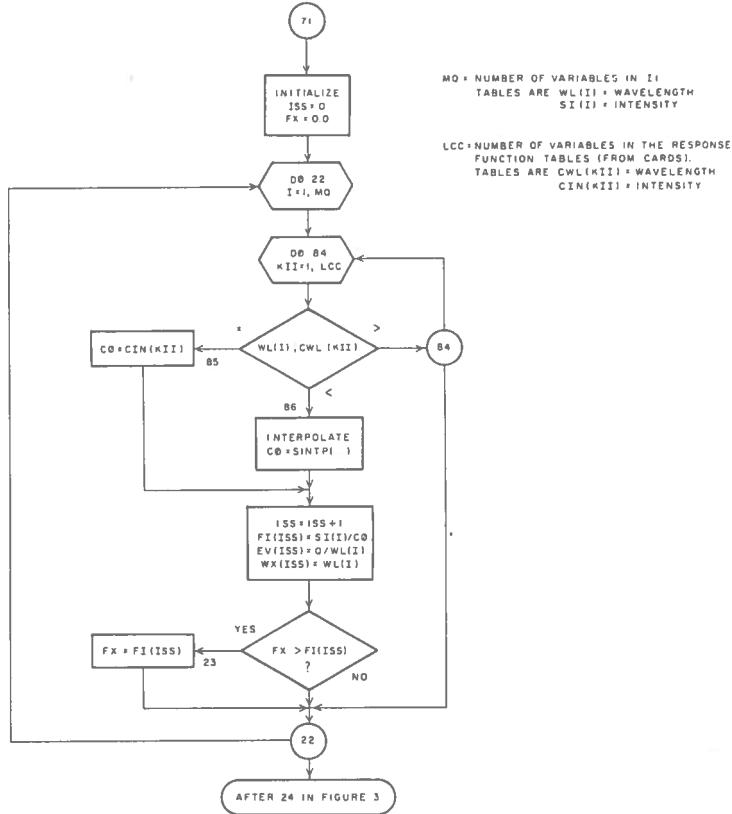


FIGURE 3 FLOW CHART FOR THE LUMINESCENCE EXCITATION PROGRAMS



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 I<sub>I</sub> 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