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TECHNICAL REPORT

72-62-CE

COMPUTER CORRECTION OF SPECTROPHOTOMETRIC DATA

by

M. L. Herz

May 1972

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UNITED STATES ARMY
NATICK LABORATORIES
Natick, Massachusetts 01760

US ARMY MATERIEL COMMAND

Clothing & Personal Life Support Equipment Laboratory
C&PLSEL-97

UNCLASSIFIED

Security Classification

DOCUMENT CONTROL DATA - R & D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY (Corporate author)

US Army Natick Laboratories
Natick, MA 01760

2a. REPORT SECURITY CLASSIFICATION

UNCLASSIFIED

2b. GROUP

3. REPORT TITLE

Computer
Correction of Spectrophotometric Data

4. DESCRIPTIVE NOTES (Type of report and inclusive dates)

5. AUTHOR(S) (First name, middle initial, last name)

Matthew L. Herz

6. REPORT DATE	7a. TOTAL NO. OF PAGES	7b. NO. OF REFS
May 1972	38	2

8a. CONTRACT OR GRANT NO.

b. PROJECT NO. 1T062105A349

c.

d.

9a. ORIGINATOR'S REPORT NUMBER(S)

72-62-CE (C&PLSEL-97)

9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report)

10. DISTRIBUTION STATEMENT

Approved for public release; distribution unlimited.

11. SUPPLEMENTARY NOTES

12. SPONSORING MILITARY ACTIVITY

US Army Natick Laboratories
Natick, MA 01760

13. ABSTRACT

A program was designed for correction of spectral emission data to produce the true emission spectrum. The computer output from data processed by the program consists of a tabular presentation of intensity versus wavelength or wavenumber as well as a graphical plot of the spectrum with resolution up to 2.5 nm. The computation of quantum efficiency of emission can be carried out when a reference spectrum is included in the input.

This program was written in Fortran IV for use on GS 200 Series machines. Details of use, input form, output form, and program limitations are described.

DD FORM 1 NOV 65 1473 REPLACES DD FORM 1473, 1 JAN 64, WHICH IS OBSOLETE FOR ARMY USE.

UNCLASSIFIED

Security Classification

A

14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
Computer Programming	8		10			
Data Analysis	4					
Fortran IV	10		10			
Emission Spectra	9		1,2			
Correction	4		8			
Fluorescence	4	•				
Calculation	4					
Information Retrieval	8,4					
Quantum Efficiency	4					
Spectrophotometry	9					
Data			1			

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FOREWORD

The utilization of computers has been widely adopted as a means of maximizing research effort in the laboratory. Many methods of calculation that are unduly complex or tedious when done by hand can be carried out with ease on a high speed computer.

The computer program presented here provides a ready method of correcting spectrophotometric data for the optical and electrical characteristics of any suitable instrument. It was prepared and utilized in the characterization of compounds in the eye protection program, but its applicability is not limited to this area. The work was carried out in the Flame and Thermal Protection Section of the Chemical Modification of Textiles Branch of the Clothing and Personal Life Support Equipment Laboratory under Materials for Flashblindness Protection Project 1T062105A349 Task 05 during the period February to July 1971.

CONTENTS

ABSTRACT

A program was designed for correction of spectral emission data to produce the true emission spectrum. The computer output from data processed by the program consists of a tabular presentation of intensity versus wavelength or wavenumber as well as a graphical plot of the spectrum with resolution up to 2.5 nm. The computation of quantum efficiency of emission can be carried out when a reference spectrum is included in the input.

This program was written in Fortran IV for use on GE 200 Series machines. Details of use, input form, output form, and program limitations are described.

I. INTRODUCTION

The common fluorescence spectrophotometer used for the study of fluorescence and phosphorescence records "apparent emission spectra" or "relative spectral emission." Because of the non-linear response characteristics of the detector system, (Appendix B), the spectra obtained directly from the instrument are grossly distorted versions of the true spectrum. For use in such studies as fluorescence quenching, intermolecular energy transfer, fluorescence efficiencies, and fluorescence analysis, the data obtained must be expressed in terms of the actual, or true spectra. When this has been done, data from different instruments may be compared directly.

II. OBJECTIVE

The techniques used in the laboratory to calibrate spectrophotometers for source, monochromator, and detector system characteristics are described in a number of references(1). The objective of the present work is to provide a computer program which applies the overall calibration curve for the detector system to the uncorrected spectral data from a spectrofluorimeter to give the true values of the emission across the entire spectral range of the instrument. In addition, the program is designed to provide for calculation and presentation of the integrated area of the emission spectrum, a plot of the true spectrum versus wavelength or wavenumber, and the quantum efficiency of the emission.

III. DISCUSSION

Once a calibration curve, which gives the relative spectral response characteristics of the detector system for a particular instrument, is found, the adjustment of raw data to give the true spectrum involves simple calculations. The many required manipulations, being extremely tedious and repetitious, are ideal for electronic data processing.

A single computer program is presented here, which uses a given set of experimental (raw) data to compute and present the values for a number of quantities derived from emission spectra.

The computer program, (Appendix A), is written in Fortran IV in two forms, one for use with a Baird Atomic SF-1 spectrofluorimeter equipped with an RCA-Type 1P28 phototube for use in the ultraviolet and visible spectral region, and one for use in the same instrument equipped with an RCA Type 7102, used in the near infrared region. The calibration data for these detectors are given in Appendix B.

Although the programs were written for the Baird Atomic SF-1 for its two regions of spectral sensitivity (i.e., its two detectors), the program may be used in any fluorescence spectrophotometer.

The program treats the data in four steps (Appendix C). First, the uncorrected intensity of luminescence at definite wavelength increments (the input data) is corrected and normalized. The data are first corrected by dividing the observed intensity at each wavelength of interest by the normalized spectral response at that wavelength. The corrected intensity values are then normalized by dividing by the maximum corrected intensity value found in the spectrum being measured. The normalized and corrected intensity is then known at each wavelength increment. In the second part of the program, the relative area under the corrected curve is obtained using the fourth Newton-Cotes Quadrature Formula of the closed type which gives accuracy to the fifth degree[2].

The program also provides for the calculation of the quantum efficiency of the luminescence process being studied. The luminescence intensity of a standard of known optical density (Ds) and efficiency of luminescence (Qs) is used as input along with the measured optical density of the unknown. This uncorrected spectrum of the standard is then measured under exactly the same experimental conditions (source intensity, wavelength of excitation, recorder setting, etc.) as the unknown. The intensity data of the referenced compound is then treated in the same way as the intensity data for the unknown. It is corrected, normalized, and the relative area (As) under the resulting curve is found. From this, the quantum efficiency of luminescence of the unknown (Qu) is found using the standard equation:

$$Qu = \frac{AuDs}{AsDu} Qs$$

where Qu = Quantum Efficiency of Unknown
Ds = Optical Density of Std.
Du = Optical Density of the Unknown (1)
Au = Area under the corrected curve of the Unknown
As = Area under the corrected curve of the Std.
Qs = Efficiency of luminescence of Std.

Finally, by means of an appropriate subroutine, the corrected spectrum is plotted against wavelength, or, if desired, wavenumber. Since the data are stored as wavelength versus corrected intensity a plot against wavenumber necessitates the generation of a new table which lists corrected intensity against wavenumber.

The wavelengths in the original data list are converted to a precise wavenumber, and this wavenumber is then compared to many available, uniformly incremented wavenumbers on the newly generated list. The intensity associated with the wavelength is stored with the wavenumber which is closest in value to the precise wavenumber without loss of resolution. In this way the corrected data will be listed and plotted at discrete points as intensity versus wavenumber.

In the present work, separate programs, similar except for plotting subroutines, provide different printouts of the calculated values; one program plots intensity versus wavelength; the other, intensity versus wavenumber.

Program Limitations

The Fortran IV programs can treat data for either the spectral region 300-650 nm (1P28 response) or 650-1000 nm (7102 response) with a maximum resolution of 2.5 nm. The input must be in increments of 2.5 nm or multiples thereof.

The maximum number of points in the spectral range cannot exceed 140 (350 nm spectral width). The spectral output can be plotted against wavenumber and/or wavelength depending on the subroutine used.

Input Format - from punched cards

1. Detector Calibration Curve (141 values) - FORMAT (16F5.2)

Columns

1-5, 6-10, 11-15, etc.	WLA(2,I), I = 1, 141
2. Number of spectra	FORMAT (I3)
1-3	NRUNS (right justified-rj)
3. Run Specification Card	FORMAT (6A5,5X,4I5)
1-30	RUN(J), J=1,6 Run name
36-40	ISWL(rj) Initial λ (Å)

	41-45	N (rj)	No. of points in spectral range
	46-50	INC (rj)	Incrementation
	51-55	IND	Quantum yield option 0=No
4.	Intensity Data	FORMAT (16F5.2)	
	1-5,6-10,11-15, etc.	ADTA(I), I=1SWL,1SWL+N,INC	

5. Quantum efficiency standard specification card

FORMAT (6A5,5X,4I5,2F5.3)

1-30	STAND(I), I=1,6		Name of reference
36-40	IQY (rj)		Reference quantum yield
41-45	IS (rj)		Initial λ (Å)
46-50	NPTS (rj)		No. of points in spectral range
51-55	INC (rj)		Incrementation
56-60	ODS	Optional	Optical density std.
61-65	ODU		Optical density unknown

Output - on printer

MAIN PROGRAM

MEASUREMENT OF -----------------------------

GAVE THE FOLLOWING

WAVELENGTH	RESPONSE	ADJ. RESPONSE
XXX.X	XXXXX.XX	XXX.XXX

THE AREA UNDER THE ADJUSTED CURVE IS 0.XXXXE+XX RELATIVE UNITS.

If the quantum yield calculation is indicated, then:

THE QUANTUM YIELD CALCULATED FROM THIS RUN USING A QUANTUM YIELD OF

O.XX WITH

AS A STANDARD.

THE SPECTRUM OF THE STANDARD

WAVELENGTH	RESPONSE	ADJ. RESPONSE
XXXX.X	XXXXX.XX	XXX.XXX

THE ADJUSTED STANDARD GIVES A RELATIVE AREA OF XO.XXXXE+XX AND THE UNKNOWN A QY OF X.XXXX.

Output Plotting Subroutines

SUBROUTINE PAWN - Wavenumber plot prints

WAVENUMBER	ADJUSTED I
XXXXX.	XXX.XX

A horizontal plot of wavenumber in increments of 50 cm^{-1} (or 25 cm^{-1} in the near IR) vs. adjusted intensity.

Subroutine SPLOT - Wavelength plot prints

A vertical plot of the table printed in the main program excluding the last 50 nm.

GLOSSARY OF TERMS

Variable	Description
WLA (1,I), I = 1,141	Wavelengths
WLA (2,I), I = 1,141	Detector calibration curve
RUN (I), I = 1,6	Name of spectrum
ADTA (I)	Spectral intensities
ADJ (I)	Adjusted intensities

GLOSSARY OF TERMS (Cont'd)

STAND (I), I = 1,6	Name of reference standard
SDTA (I)	Standard spectral intensities
AI	An index for generating WLA (1,I)
I	A general index
NI	A general index (equals N + 1 SWL)
IQ	A general index
J	A general index
NRUNS	No. of spectra
ISWL	Initial wavelength
RSPEC	Subroutine to adjust and normalize intensities
REL	Value for largest intensity of spectrum
UREA	Area under the adjusted curve of the unknown
SAREA	Area under the adjusted curve of reference std.
AREA	Subroutine to find the area under curve
IQY	Integer value for reference quantum efficiency
IS	Initial wavelength of reference spectrum
NPTS	Number of points in range of reference spectrum
ODS	Optical density of reference
ODU	Optical density of unknown
NNI	General index (equals IS + NPTS)
L	General index
UQY	Unknown quantum yield

IV. References

1. R. J. Argauer and C. E. White, Anal. Chem. 36, 368 (1964) and references cited therein.

2. Kaiser, K. S., "Numerical Analysis", p. 145, McGraw Hill Book Co., New York, 1957.

APPENDIX A

FORTRAN IV PROGRAMS
AND
SPECIMEN OUTPUT

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```
$JOB
$ZERO
$FORTRAN
C       SPECTRUM ADJUST PROGRAM FOR AN 1P28 PHOTOTUBE WITH OPTION OF
C       CALCULATING QUANTUM YIELDS DIRECTLY.  INPUT CONSISTS OF UNADUST-
C       ED SPECTRUM INTENSITIES EVERY 2,5 OR 5 NM, FROM 300 TO 650 NM.
        COMMON WLA
        DIMENSION WLA(2,141),RUN(6),ADTA(141),ADJ(141),STAND(141),SDTA(141
       4)
      1 FORMAT(I3)
      2 FORMAT(16F5,2)
      3 FORMAT(6A5,5X,4I5,2F5,3)
      4 FORMAT(1H1,15HMEASUREMENT OF ,6A5/19HGAVE THE FOLLOWING-/)
      5 FORMAT(20X,10HWAVELENGTH,7X,8HRESPONSE,7X,13HADJ. RESPONSE/)
      6 FORMAT (22X,F5,1,9X,F8,2,11X,F7,3)
      7 FORMAT(1H0,37HTHE AREA UNDER THE ADJUSTED CURVE IS ,E11,4,15H RELA
       1TIVE UNITS)
      8 FORMAT(70HTHE QUANTUM YIELD CALCULATED FROM THIS RUN USING A QUANT
       2UM YIELD OF 0,,I2,1X,5HWITH ,6A5/14HAS A STANDARD./26X,28HTHE SPEC
       8TRUM OF THE STANDARD)
      9 FORMAT(47HTHE ADJUSTED STANDARD GIVES A RELATIVE AREA OF ,E11.4,1X
       3,24HAND THE UNKNOWN A QY OF ,F6,4)
        AI=0,
        DO 20 I=1,141
        WLA(1,I)=300.+AI
        AI=AI+2,5
     20 CONTINUE
        READ 2,(WLA(2,I),I=1,141)
        READ 1, NRUNS
        DO 10 IQ=1,NRUNS
        READ 3,(RUN(J),J=1,6),ISWL,N,INC,IND
        PRINT 4, (RUN(J),J=1,6)
        ISWL=(ISWL-3000)/25+1
        NI=ISWL+N
        READ 2,(ADTA(I),I=ISWL,NI,INC)
        CALL RSPEC(ADTA,ISWL,N,ADJ,INC,REL)
        PRINT 5
        PRINT6,(WLA(1,I),ADTA(I),ADJ(I),I=ISWL,NI,INC)
        UAREA=AREA(ADJ,ISWL,N,INC,REL)
        PRINT 7,UAREA
        CALL SPLOT(ADJ,ISWL,NI,INC)
        IF(IND.EQ,0)GO TO 10
        READ 3,(STAND(I),I=1,6),IQY,IS,NPTS,INC,ODS,ODU
        QY=FLOAT(IQY)*0.01
        IS=(IS-3000)/25+1
        NNI=IS+NPTS
        READ 2,(SDTA(L),L=IS,NNI,INC)
        CALL RSPEC(SDTA,IS,NPTS,ADJ,INC,REL)
        PRINT 8,IQY,(STAND(I),I=1,6)
        PRINT 5
        PRINT 6,(WLA(1,I),SDTA(I),ADJ(I),I=IS,NNI,INC)
        SAREA=AREA(ADJ,IS,NPTS,INC,REL)
        UQY=UAREA*QY/SAREA
        IF(ODU.NE,0,.AND,ODS,NE,0,)UQY=UQY*ODS/ODU
```

```
      PRINT 9, SAREA,UQY
      DO 30 I=1,141
   30 ADJ(I)=0.
   10 CONTINUE
      STOP
      END


$FORTRAN
      SUBROUTINE SPLOT(Y,ISWL,NI,INC)
      DIMENSION Y(141),IW(15),PLOT(120)
      REAL LOWER
      DATA BLANK, PLOT, POINT/121*1H ,1HX/
   98 FORMAT(1H0,119H I + I + I + I + I + I + I + I + I + I + I + I + I + I + I
     8+ I + I + I + I + I + I + I + I + I + I + I + I + I + I + I + I +
     8I //)
   99 FORMAT(1H1,119H I +    + I + I + I + I + I + I + I + I + I + I + I + I
     9+ I + I + I + I + ' , I + I + I + I + I + I + I + I + I + I + I +
     9I ////)
  100 FORMAT(120A1)
  101 FORMAT(I3,4X,I3,13(5X,I3))
  102 FORMAT(51X,15HWAVELENGTH (NM)///)
      UPPER=100.
      LOWER=98.
      PRINT 99
      IF(NI.GT.120) NI=120
      DO 10 K=1,50
      DO 20 I=ISWL,NI,INC
      IF(Y(I).LE.UPPER.AND.Y(I).GT.LOWER) PLOT(I)=POINT
   20 CONTINUE
      PRINT 100,(PLOT(I),I=1,NI)
      DO 30 I=1,120
   30 PLOT(I)=BLANK
      UPPER=UPPER-2.
      LOWER=LOWER-2.
   10 CONTINUE
      DO 40 I=1,120,INC
   40 IF(Y(I).EQ.0.)PLOT(I)=POINT
      PRINT 100,(PLOT(I),I=1,120)
      DO 45 I=1,120
   45 PLOT(I)=BLANK
      IA=0
      DO 50 I=1,15
      IW(I)=300+IA
      IA=IA+20
   50 CONTINUE
      PRINT 101,(IW(I),I=1,15)
      PRINT 102
      PRINT  98
      RETURN
      END


$FORTRAN
```

```
      REAL FUNCTION AREA[T,ISWL,M,INC,REL]
      DIMENSION Z[141],T[141]
      NI=ISWL+M-1
      N=0
      DO 10 J=ISWL,NI,INC
      N=N+1
      Z[N]=T[J]
   10 CONTINUE
      H=INC
      S=0.
C
C   NEWTON-COTES QUADRATURE FORMULA,  CLOSED TYPE
C
      IF[N .LT. 5]  GO TO 840
C           FIVE POINT FORMULA
      DO 830  I=5,N,4
      S=S+7.*Z[I-4]+32.*Z[I-3]+12.*Z[I-2]+32.*Z[I-1]+7.*Z[I]
  830 CONTINUE
      S=S*2./45.
  840 J=N-[[N/4]*4]+1
      GO TO [845,850,847,848],J
C           FOUR POINT FORMULA
  845 S=S+.375*[Z[N-3]+3.*Z[N-2]+3.*Z[N-1]+Z[N]]
      GO TO 850
C           TWO POINT FORMULA
  847 S=S+[Z[N-1]+Z[N]]/2.
      GO TO 850
C           THREE POINT FORMULA
  848 S=S+[Z[N-2]+4.*Z[N-1]+Z[N]]/3.
  850 S=S*H
      AREA=S*REL
      RETURN
      END


$FORTRAN
      SUBROUTINE RSPEC[ADTA,ISWL,N,ADJ,INC,REL]
      COMMON WLA
      DIMENSION ADTA[141],WLA[2,141],ADJ[141]
      REL=0.
      NI=ISWL+N
      DO 200 I=ISWL,NI,INC
      ADJ[I]=ADTA[I]/WLA[2,I]
      TEST=ADJ[I]
      IF[TEST.GT.REL] REL=TEST
  200 CONTINUE
      DO 210 I=ISWL,NI,INC
      ADJ[I]=ADJ[I]*100./REL
  210 CONTINUE
      RETURN
      END


$LOAD
```

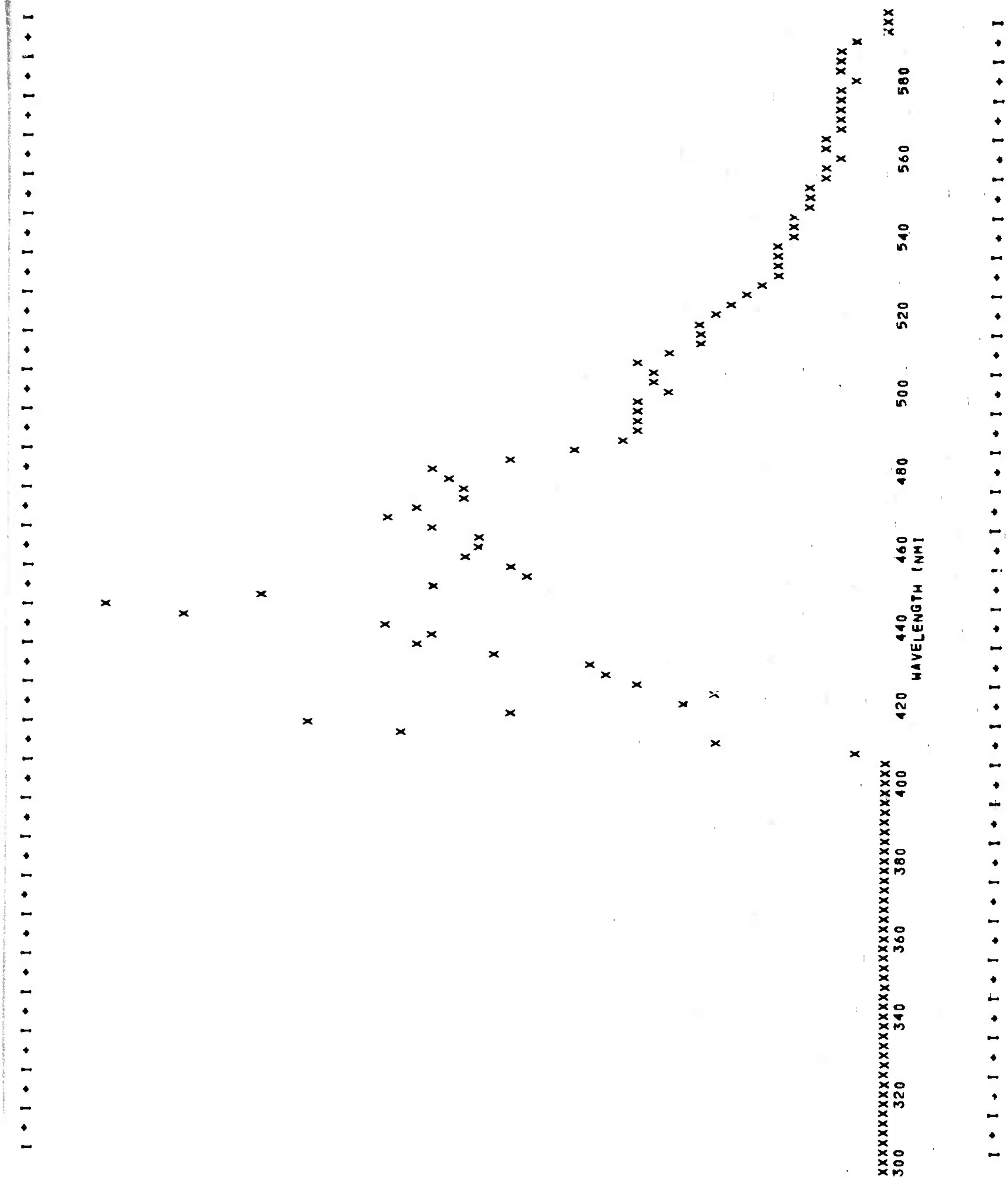
```
10.9114.3017.  20.5 22.   27.8 31.   34.5 39.6341.   43.2 49.6 53.2 55.5 59.   62.4
66.0568.7 70.2 72.7 74.   76.   77.2 78.5 79.9 82.   82.6 83.4 84.4 85.9 86.8 87.6
88.4488.7 89.1 90.3 90.8 91.4 92.1 92.4693.5 94.3 95.   95.2 94.4 93.6 92.5 90.81
90.  89.   88.4 86.0785.   83.8 82.2 80.3379.1 78.   77.2 75.8174.5 73.   71.7 70.19
69.  67.2 65.8 64.1662.8 61.   59.6 58.9656.7 55.3 54.1 51.8651.3 50.2 49.3 47.62
46.8 45.9 44.6 43.3 41.9 40.8 39.8 38.7 37.7 36.7 35.6 34.3933.6 33.   31.9 30.81
30.  28.9 28.1 26.9 25.9 24.9 24.1 22.3821.6 20.7 19.8 18.9 18.2 17.6 16.4 15.69
14.9 14.   13.4 12.3 11.7 11.1 10.5 9.5769.4   9.1  8.4  8.   7.6  7.2  6.7  6.37
6.   5.4  5.1  4.8  4.3  3.9  3.6  3.2  2.9  2.7  2.4  2.1  1.9  1.7
  2
CARBAZOLYLACETALDEHYDE PHOS           3950   79    1
                              3.   32.  90.   107.267.  35.5 30.   41.9 47.8 48.5 64.
76.  71.  78.5 109. 121.294.   67.   51.7 54.   57.4 56.   52.9 58.  62.8 59.   51.5
49.5 51.5 50.9 41.   32.7 26.6 24.5 24.6 24.   23.4 20.   20.9 20.  20.5 17.7 15.2
14.  13.4 13.  11.1 9.   8.2  7.   6.6  6.4  5.9  5.5  5.   4.5  4.   3.5  3.3
3.   2.8  2.   2.   1.9  1.7  1.4  1.4  1.1  1.   .9   .9   .9   .8   .5
 MGLN QUANTUM YIELD AT 28 16=1        3200  114    2    1
0.   1.5  9.9  11.3 17.1 21.5 23.9 23.8 23.1 22.1 20.4 19.1 17.2 15.3 13.5 12.
10.2 8.   7.6  6.9  6.2  5.8  5.9  5.9  6.   6.5  7.1  7.2  7.3  7.5  7.6  7.3
7.   6.9  6.3  5.9  5.6  5.   4.6  4.1  3.8  3.5  3.1  2.9  2.6  2.5  2.1  1.9
1.7  1.4  1.2  1.1  1.   .9   .9   .9   .6
QUININE SULFATE                        55 3750   92    2.102 .044
     1.   11.  25.  51.  90.  154. 203. 290. 360. 432. 528. 595. 666. 736. 770.
784. 772. 747. 710. 661. 610. 556. 501. 450. 408. 342. 302. 259. 230. 194. 167.
142. 121. 102. 87.  64.  42.  34.  31.  26.  17.  10.  9.   8.   6.
$EOJ
```

MEASUREMENT OF CARBAZOLYLACETALDEHYDE PHOS
GAVE THE FOLLOWING-

WAVELENGTH	RESPONSE	ADJ. RESPONSE
395,0	0,00	0.000
397.5	0,00	0.000
400,0	0,00	0.000
402,5	0,00	0.000
405,0	0,00	0.000
407,5	3,00	2.007
410,0	32,00	21.592
412,5	90,00	61.247
415,0	107,20	73.819
417,5	67,00	46.995
420,0	35,50	25.125
422,5	30,00	21.471
425,0	41,90	30.191
427,5	47,80	35.375
430,0	48,50	36.344
432,5	64,00	48.646
435,0	76,00	58.892
437,5	71,00	56.298
440,0	78,50	63.213
442,5	109,00	89.012
445,0	121,20	100.000
447,5	94,00	78.980
450,0	67,00	57.284
452,5	51,70	45.111
455,0	54,00	47.972
457,5	57,40	52.090
460,0	56,00	51.696
462,5	52,90	50.142
465,0	58,00	56.146
467,5	62,80	62.346
470,0	59,00	59.842
472,5	51,50	53.776
475,0	49,50	52.902
477.5	51,50	55.637
480,0	50,90	57.181
482,5	41,00	47.225
485,0	32,70	38.500
487,5	26,60	32.671
490,0	24,50	30.420
492,5	24,60	31.214
495,0	24,00	31.008
497,5	23,40	31.300
500,0	20,00	27.221
502,5	20,90	29.003
505,0	20,00	28.563
507,5	20,50	30.156
510,0	17,70	26.908
512,5	15,20	23.730
515,0	14,00	22.406
517,5	13,40	22.055
520,0	13,00	21.964
522,5	11,10	19.265
525,0	9,00	16.103
527,5	8,20	15.188
530,0	7,00	13.270
532,5	6,60	12.739
535,0	6,40	12.779
537,5	5,90	12.198
540,0	5,50	11.678

542,5	5,00	11.020
545,0	4,50	10.200
547,5	4,00	9.472
550,0	3,50	8.608
552,5	3,30	8.442
555,0	3,00	7.929
557,5	2,80	7.969
560,0	2,00	5.898
562,5	2,00	6.154
565,0	1,90	6.112
567,5	1,70	5.729
570,0	1,40	4.900
572,5	1,40	5.067
575,0	1,10	4.272
577,5	1,00	4.060
580,0	0,90	3.847
582,5	0,90	4.095
585,0	0,90	4.278
587,5	0,80	4.143
590,0	0,50	2.722
592,5	0,00	0.000

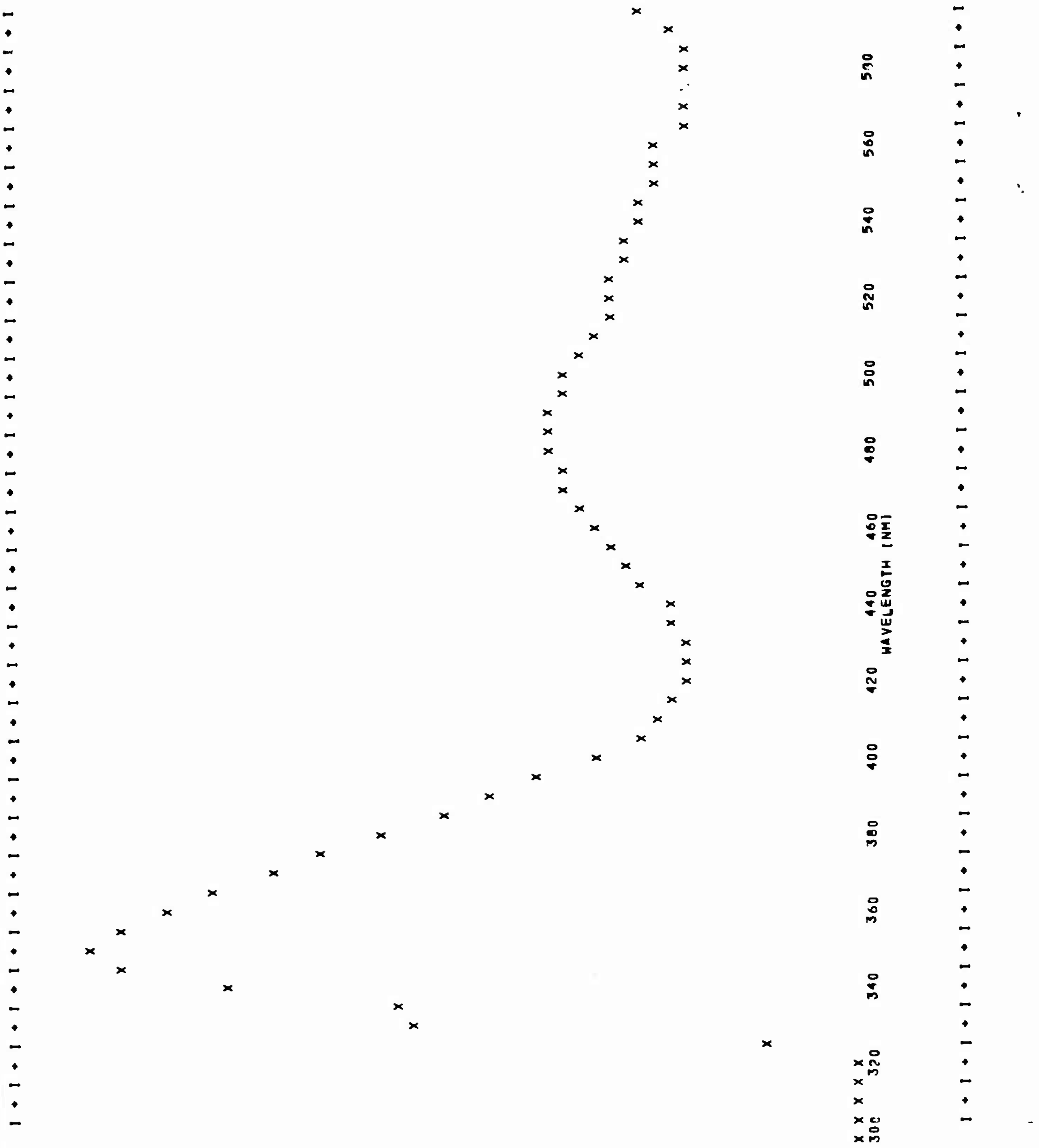
THE AREA UNDER THE ADJUSTED CURVE IS 0,3558E+04 RELATIVE UNITS


300 320 340 360 380 400 420 440 460 480 500 520 540 560 580
WAVELENGTH (NM)

MEASUREMENT OF MGLN QUANTUM YIELD AT 28 16-1
GAVE THE FOLLOWING-

WAVELENGTH	RESPONSE	ADJ. RESPONSE
320,0	0,00	0.000
325,0	1,50	10.751
330,0	9,90	57.618
335,0	11,30	59.301
340,0	17,10	80.160
345,0	21,50	94.828
350,0	23,90	100.000
355,0	23,80	95.454
360,0	23,10	89.516
365,0	22,10	82.841
370,0	20,40	74.838
375,0	19,10	68.131
380,0	17,20	60.216
385,0	15,30	53.168
390,0	13,50	46.034
395,0	12,00	40.342
400,0	10,20	33.777
405,0	8,00	26.074
410,0	7,60	24.927
415,0	6,90	23.096
420,0	6,20	21.330
425,0	5,80	20.315
430,0	5,90	21.492
435,0	5,90	22.224
440,0	6,00	23.486
445,0	6,50	26.069
450,0	7,10	29.508
455,0	7,20	31.092
460,0	7,30	32.757
465,0	7,50	35.291
470,0	7,60	37.470
475,0	7,30	37.924
480,0	7,00	38.225
485,0	6,90	39.490
490,0	6,30	38.024
495,0	5,90	37.054
500,0	5,60	37.049
505,0	5,00	34.711
510,0	4,60	33.992
515,0	4,10	31.896
520,0	3,80	31.209
525,0	3,50	30.441
530,0	3,10	28.566
535,0	2,90	28.148
540,0	2,60	26.834
545,0	2,50	27.347
550,0	2,10	25.105
555,0	1,90	24.410
560,0	1,70	24.369
565,0	1,40	21.893
570,0	1,20	20.415
575,0	1,10	20.767
580,0	1,00	20.780
585,0	0,90	20.796
590,0	0,90	23.817
595,0	0,90	26.539
600,0	0,60	19.763
605,0	0,00	0.000

THE AREA UNDER THE ADJUSTED CURVE IS 0,1390E+04 RELATIVE UNITS



WAVELENGTH (NM)
300
320
340
360
380
400
420
440
460
480
500
520
540
560

THE QUANTUM YIELD CALCULATED FROM THIS RUN USING A QUANTUM YIELD OF 0.55 WITH QUININE SULFATE AS A STANDARD.

THE SPECTRUM OF THE STANDARD

WAVELENGTH	RESPONSE	ADJ. RESPONSE
375.0	0.00	0.000
380.0	1.00	0.100
385.0	11.00	1.087
390.0	25.00	2.425
395.0	51.00	4.878
400.0	90.00	8.479
405.0	154.00	14.279
410.0	203.00	18.942
415.0	290.00	27.616
420.0	360.00	35.234
425.0	432.00	43.046
430.0	528.00	54.717
435.0	595.00	63.760
440.0	666.00	74.166
445.0	736.00	83.978
450.0	770.00	91.042
455.0	784.00	96.317
460.0	772.00	98.554
465.0	747.00	100.000
470.0	710.00	99.587
475.0	661.00	97.692
480.0	610.00	94.766
485.0	556.00	90.528
490.0	501.00	86.025
495.0	450.00	80.403
500.0	408.00	76.793
505.0	342.00	67.546
510.0	302.00	63.489
515.0	259.00	57.322
520.0	230.00	53.739
525.0	194.00	48.002
530.0	167.00	43.781
535.0	142.00	39.211
540.0	121.00	35.528
545.0	102.00	31.974
550.0	87.00	29.589
555.0	64.00	23.392
560.0	42.00	17.128
565.0	34.00	15.126
570.0	31.00	15.004
575.0	26.00	13.965
580.0	17.00	10.050
585.0	10.00	6.574
590.0	9.00	6.776
595.0	8.00	6.711
600.0	6.00	5.622
605.0	0.00	0.000

THE ADJUSTED STANDARD GIVES A RELATIVE AREA OF 0.4620E+05 AND THE UNKNOWN A QY OF 0.0384

```
$JOB
$ZERO
$FORTRAN
C   FOR WORK IN THE NEAR INFRARED ON THE BAIRD SF-1
C      SPECTRUM ADJUST PROGRAM FOR AN  IR  PHOTOTUBE WITH OPTION OF
C      CALCULATING QUANTUM YIELDS DIRECTLY,
C      THE CORRECTED INTENSITY IS PLOTTED TO GIVE A PLOT OF
C      ******WAVENUMBER VS. ADJ. INTENSITY ************
C      CALCULATING QUANTUM YIELDS DIRECTLY.  INPUT CONSISTS OF UNADUST-
C      ED SPECTRUM INTENSITIES EVERY 2.5 OR 5 NM. FROM 650 TO 1000 NM.
C
      COMMON WLA
      DIMENSION WLA(2,141),RUN(6),ADTA(141),ADJ(141),STAND(141),SDTA(141
     4)
    1 FORMAT(I3)
    2 FORMAT(16F5.2)
    3 FORMAT(6A5,5X,4I5,2F5.3)
    4 FORMAT(1H1,15HMEASUREMENT OF ,6A5/19HGAVE THE FOLLOWING-/)
    5 FORMAT(20X,10HWAVELENGTH,7X,8HRESPONSE,7X,13HADJ. RESPONSE/)
    6 FORMAT (21X,F6.1,9X,F8.2,11X,F7.3)
    7 FORMAT(1H0,37HTHE AREA UNDER THE ADJUSTED CURVE IS ,E11.4,15H RELA
     1TIVE UNITS)
    8 FORMAT(70HTHE QUANTUM YIELD CALCULATED FROM THIS RUN USING A QUANT
     2UM YIELD OF 0.,I2,1X,5HWITH ,6A5/14HAS A STANDARD./26X,28HTHE SPEC
     8TRUM OF THE STANDARD)
    9 FORMAT(47HTHE ADJUSTED STANDARD GIVES A RELATIVE AREA OF ,E11.4,1X
     3,24HAND THE UNKNOWN A QY OF ,F6.4)
   18 FORMAT(15H END OF PROGRAM)
      AI=0.
      DO 20 I=1,141
      WLA(1,I)=650.+AI
      AI=AI+2.5
   20 CONTINUE
      READ 2,(WLA(2,I),I=1,141)
      READ 1, NRUNS
      DO 10 IQ=1,NRUNS
      READ 3,(RUN(J),J=1,6),ISWL,N,INC,IND
      PRINT 4, (RUN(J),J=1,6)
      ISWL=(ISWL-6500)/25+1
      NI=ISWL+N
      READ 2,(ADTA(I),I=ISWL,NI,INC)
      CALL RSPEC(ADTA,ISWL,N,ADJ,INC,REL)
      PRINT 5
      PRINT6,(WLA(1,I),ADTA(I),ADJ(I),I=ISWL,NI,INC)
      UAREA=AREA(ADJ,ISWL,N,INC,REL)
      PRINT 7,UAREA
      CALL PAWN(ADJ,ISWL,NI,INC)
      IF(IND.EQ.0)GO TO 10
      READ 3,(STAND(I),I=1,6),IQY,IS,NPTS,INC,ODS,ODU
      QY=FLOAT(IQY)*0.01
      IS=(IS-6500)/25+1
      NNI=IS+NPTS
      READ 2,(SDTA(L),L=IS,NNI,INC)
      CALL RSPEC(SDTA,IS,NPTS,ADJ,INC,REL)
```

```
      PRINT 8,IQY,(STAND(I),I=1,6)
      PRINT 5
      PRINT 6,(WLA(1,I),SDTA(I),ADJ(I),I=IS,NNI,INC)
      SAREA=AREA(ADJ,IS,NPTS,INC,REL)
      UQY=UAREA*QY/SAREA
      IF(ODU.NE.0..AND.ODS.NE.0.)UQY=UQY*ODS/ODU
      PRINT 9, SAREA,UQY
      DO 30 I=1,141
   30 ADJ(I)=0.
   10 CONTINUE
      TYPE 18
      STOP
      END


$FORTRAN
      SUBROUTINE PAWN(ADJ,ISWL,NI,INC)
      COMMON WLA
      DIMENSION WN(2,218),WLA(2,141),PLOT(101),ADJ(141)
      REAL LOWER
      INTEGER PLOT,BLANK,POINT
      DATA WN/436*0./
      DATA PLOT,BLANK,POINT/102*1H ,1HX/
    1 FORMAT(1H1,41HRELATING THESE POINTS TO WAVENUMBER GIVES/20X,10HWAV
     1ENUMBER,7X,10HADJUSTED I/)
    2 FORMAT(22X,F6.0,10X,F6.2,30X,I5)
    3 FORMAT(8X,2H- ,101A1,2H -)
    4 FORMAT(2X,F6.0,2X,101A1,2H -)
    5 FORMAT(1H1)
C     CALCULATE WAVENUMBERS AND STORE IN WN
      DO 20 I=1,218
   20 WN(1,I)=15400.-25.*FLOAT(I)
C     FILL WN(2,N) WITH AVAILABLE VALUES OF ADJ
      PRINT 1
      DO 50 I=ISWL,NI,INC
      TEST=1.E07/WLA(1,I)
      DO 30 J=1,218
      IF(ABS(TEST-WN(1,J)).LE.12.5) GO TO 40
   30 CONTINUE
      GO TO 50
   40 WN(2,J)=ADJ(I)
      JSTOP=J
   50 CONTINUE
      TEST=1.E07/WLA(1,ISWL)
      DO 60 J=1,218
      IF(ABS(TEST-WN(1,J)).LE.12.5) GO TO 70
   60 CONTINUE
      J = 218
   70 JSAVE=J
C     PRINT WAVENUMBERS AND ADJUSTED INTENSITIES
      DO 80 J=JSAVE,JSTOP
      IF(WN(2,J).EQ.0.) GO TO 80
      PRINT 2, WN(1,J),WN(2,J)
   80 CONTINUE
```

```
      PRINT 5
C     PLOT WAVENUMBER AGAINST ADJUSTED INTENSITY
      J=1
      DO 101 I=JSAVE,JSTOP
      IF(WN(2,I).EQ.0.) GO TO 106
      UPPER=0.
      DO 102 J=1,101
      UPPER=UPPER+1.
      LOWER=UPPER-1.
      IF(WN(2,I).GE.LOWER.AND.WN(2,I).LT.UPPER) GO TO 103
  102 CONTINUE
      J=101
  103 PLOT(J)=POINT
  106 K=(I/5)*5
      IF(I.EQ.K) PRINT 4, WN(1,I),(PLOT(IQ),IQ=1,101)
      IF(I.NE.K) PRINT 3, (PLOT(IQ),IQ=1,101)
  105 PLOT(J)=BLANK
  101 CONTINUE
      RETURN
      END


$FORTRAN
      REAL FUNCTION AREA(T,ISWL,M,INC,REL)
      DIMENSION Z(141),T(141)
      NI=ISWL+M-1
      N=0
      DO 10 J=ISWL,NI,INC
      N=N+1
      Z(N)=T(J)
   10 CONTINUE
      H=INC
      S=0.
C
C    NEWTON-COTES QUADRATURE FORMULA,  CLOSED TYPE
C
      IF(N .LT. 5)  GO TO 840
C            FIVE POINT FORMULA
      DO 830  I=5,N,4
      S=S+7.*Z(I-4)+32.*Z(I-3)+12.*Z(I-2)+32.*Z(I-1)+7.*Z(I)
  830 CONTINUE
      S=S*2./45.
  840 J=N-((N/4)*4)+1
      GO TO (845,850,847,848),J
C            FOUR POINT FORMULA
  845 S=S+.375*(Z(N-3)+3.*Z(N-2)+3.*Z(N-1)+Z(N))
      GO TO 850
C            TWO POINT FORMULA
  847 S=S+(Z(N-1)+Z(N))/2.
      GO TO 850
C            THREE POINT FORMULA
  848 S=S+(Z(N-2)+4.*Z(N-1)+Z(N))/3.
  850 S=S*H
      AREA=S*REL
```

```
      RETURN
      END

$FORTRAN
      SUBROUTINE RSPEC(ADTA,ISWL,N,ADJ,INC,REL)
      COMMON WLA
      DIMENSION ADTA(141),WLA(2,141),ADJ(141)
      REL=0.
      NI=ISWL+N
      DO 200 I=ISWL,NI,INC
      ADJ(I)=ADTA(I)/WLA(2,I)
      TEST=ADJ(I)
      IF(TEST.GT.REL) REL=TEST
  200 CONTINUE
      DO 210 I=ISWL,NI,INC
      ADJ(I)=ADJ(I)*100./REL
  210 CONTINUE
      RETURN
      END

$LOAD
15.2 14.8 14.4 14.  13.6 13.2512.9512.6512.4 12.1 11.8511.6 11.3511.1 10.9 10.6
10.4510.2 10.  9.75 9.6  9.35 9.15 9.   8.88 8.8  8.75 8.7  8.74 8.8  8.84 8.8
8.78 8.7  8.53 8.2  7.85 7.4  7.   6.6  6.25 6.   5.8  5.6  5.4  5.2  5.05 4.85
4.7  4.55 4.4  4.25 4.1  4.   3.85 3.75 3.65 3.55 3.45 3.35 3.26 3.15 3.05 2.95
2.85 2.75 2.65 2.6  2.55 2.5  2.45 2.4  2.53 2.35 2.3  2.25 2.2  2.15 2.15 2.1
2.1  2.05 2.05 2.05 2.05 2.   2.   2.   2.   2.   2.   2.   2.   2.   2.   2.
1.95 1.95 1.95 1.95 1.9  1.9  1.9  1.85 1.85 1.85 1.8  1.8  1.8  1.75 1.75 1.75
1.7  1.7  1.65 1.65 1.65 1.6  1.6  1.55 1.55 1.53 1.50 1.5  1.45 1.45 1.4  1.4
1.35 1.35 1.3  1.3  1.25 1.25 1.25 1.2  1.2  1.15 1.15 1.1  1.1  1.05 1.05
  2
QUANTUM YLD CARBACETALD16-1C.2      6700  100    2    1
     2.9  5.8  8.3  12.1 22.1 20.7 18.1 18.  16.  14.9 14.9 15.  15.  14.9514.95
15.3 15.8 15.2 15.1 14.8 14.4 14.3 13.9 13.  12.4 12.  11.  10.2 9.1  8.2  7.1
6.3  5.9  5.1  4.7  4.1  3.7  3.2  3.   2.6  2.1  1.9  1.6  1.4  1.1  .9   .8
.6   .4   .1
QUININE SULFATE                        55 6700  100    2.114 .264
     2.   9.   22.  47.  91.  153. 239. 343. 449. 578. 675. 780. 870. 949. 994.
1017.1001.967. 922. 855. 794. 719. 659. 587. 527. 460. 390. 343. 297. 257. 225.
188. 153. 121. 100. 79.  67.  52.  41.  31.  28.  22.  19.  13.  11.  10.  5.

CARBAZOLYLACETALDEHYDE PHOS             7000   79    1
                         3.   32.  90.  107.267.  35.5 30.  41.9 47.8 48.5 64.
76.  71.  78.5 109. 121.294.  67.  51.7 54.  57.4 56.  52.9 58.  62.8 59.  51.5
49.5 51.5 50.9 41.  32.7 26.6 24.5 24.6 24.  23.4 20.  20.9 20.  20.5 17.7 15.2
14.  13.4 13.  11.1 9.   8.2  7.   6.6  6.4  5.9  5.5  5.   4.5  4.   3.5  3.3
3.   2.8  2.   2.   1.9  1.7  1.4  1.4  1.1  1.   .9   .9   .9   .8   .5
$EOJ
```

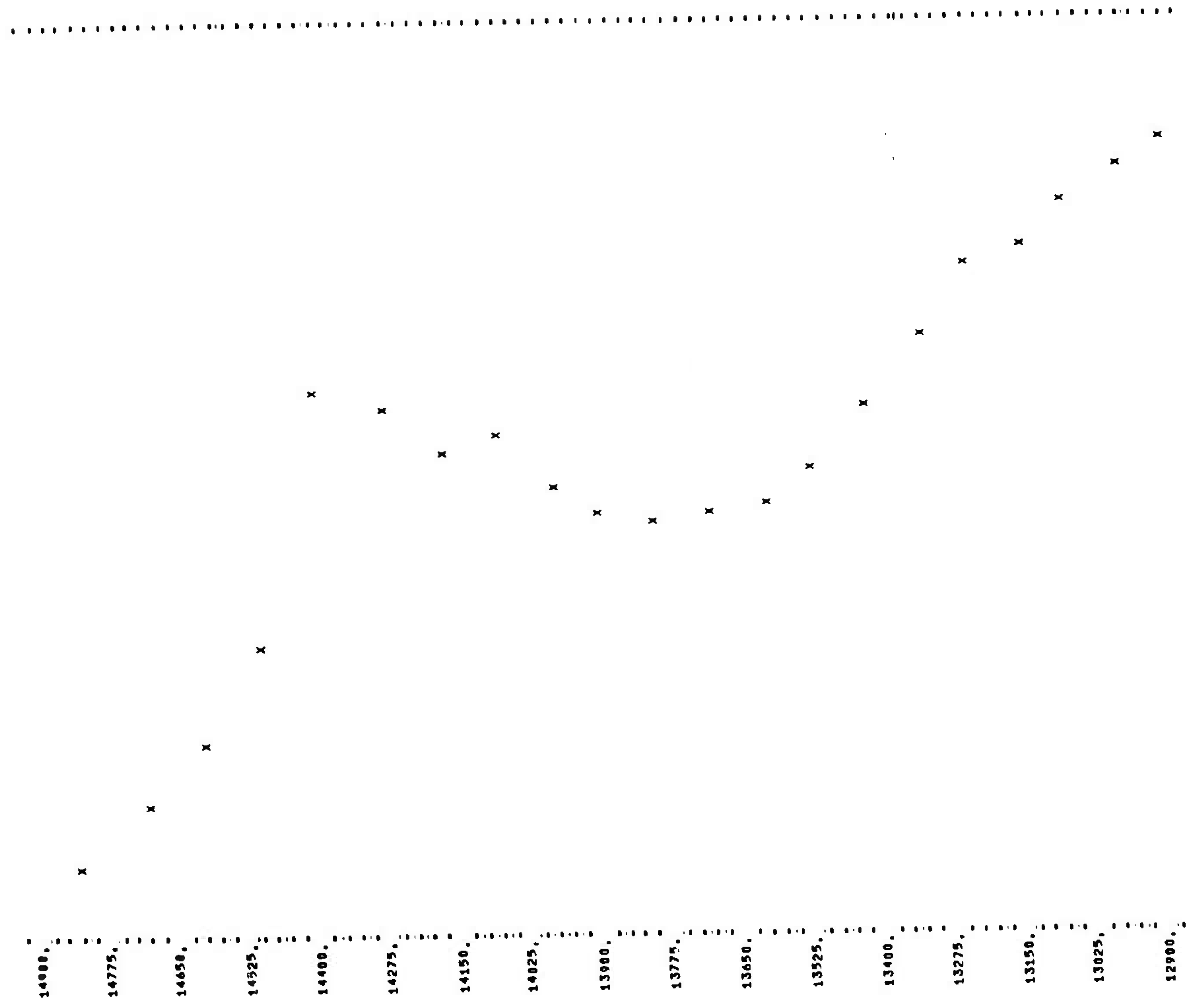
MEASUREMENT OF QUANTUM YLD CARBACETALD16-10.2
GAVE THE FOLLOWING-

WAVELENGTH	RESPONSE	ADJ. RESPONSE
670.0	0.00	0.000
675.0	2.90	6.648
680.0	5.80	13.883
685.0	8.30	20.687
690.0	12.10	31.456
695.0	22.10	60.038
700.0	20.70	58.578
705.0	18.10	53.740
710.0	18.00	55.068
715.0	16.00	49.676
720.0	14.90	46.314
725.0	14.90	45.790
730.0	15.00	46.412
735.0	15.00	47.773
740.0	14.95	51.738
745.0	14.95	58.020
750.0	15.30	66.504
755.0	15.80	74.006
760.0	15.20	76.469
765.0	15.10	81.231
770.0	14.80	85.546
775.0	14.40	88.909
780.0	14.30	94.752
785.0	13.90	98.082
790.0	13.00	96.758
795.0	12.40	97.643
800.0	12.00	100.000
805.0	11.00	97.978
810.0	10.20	97.228
815.0	9.10	93.289
820.0	8.20	87.359
825.0	7.10	78.728
830.0	6.30	67.648
835.0	5.90	69.688
840.0	5.10	62.977
845.0	4.70	59.388
850.0	4.10	53.040
855.0	3.70	49.033
860.0	3.20	42.407
865.0	3.00	40.750
870.0	2.60	35.317
875.0	2.10	28.525
880.0	1.90	25.808
885.0	1.60	21.733
890.0	1.40	19.504
895.0	1.10	15.325
900.0	0.90	12.868
905.0	0.80	11.439
910.0	0.60	8.811
915.0	0.40	6.037
920.0	0.10	1.509

THE AREA UNDER THE ADJUSTED CURVE IS 0.1983E+05 RELATIVE UNITS

RELATING THESE POINTS TO WAVENUMBER GIVES

WAVENUMBER	ADJUSTED I
14825.	6.65
14700.	13.88
14600.	20.69
14500.	31.46
14400.	60.04
14275.	58.58
14175.	53.74
14075.	55.07
13975.	49.68
13900.	46.31
13800.	45.79
13700.	46.41
13600.	47.77
13525.	51.74
13425.	58.02
13325.	66.50
13250.	74.01
13150.	76.47
13075.	81.23
12975.	85.55
12900.	88.91
12825.	94.75
12750.	98.08
12650.	96.76
12575.	97.64
12500.	100.00
12425.	97.98
12350.	97.23
12275.	93.29
12200.	87.36
12125.	78.73
12050.	67.65
11975.	69.69
11900.	62.98
11825.	59.39
11775.	53.04
11700.	49.03
11625.	42.41
11550.	40.75
11500.	35.32
11425.	28.53
11375.	25.81
11300.	21.73
11225.	19.50
11175.	15.32
11100.	12.87
11050.	11.44
11000.	8.81
10925.	6.04
10875.	1.51


14900.
14775.
14650.
14525.
14400.
14275.
14150.
14025.
13900.
13775.
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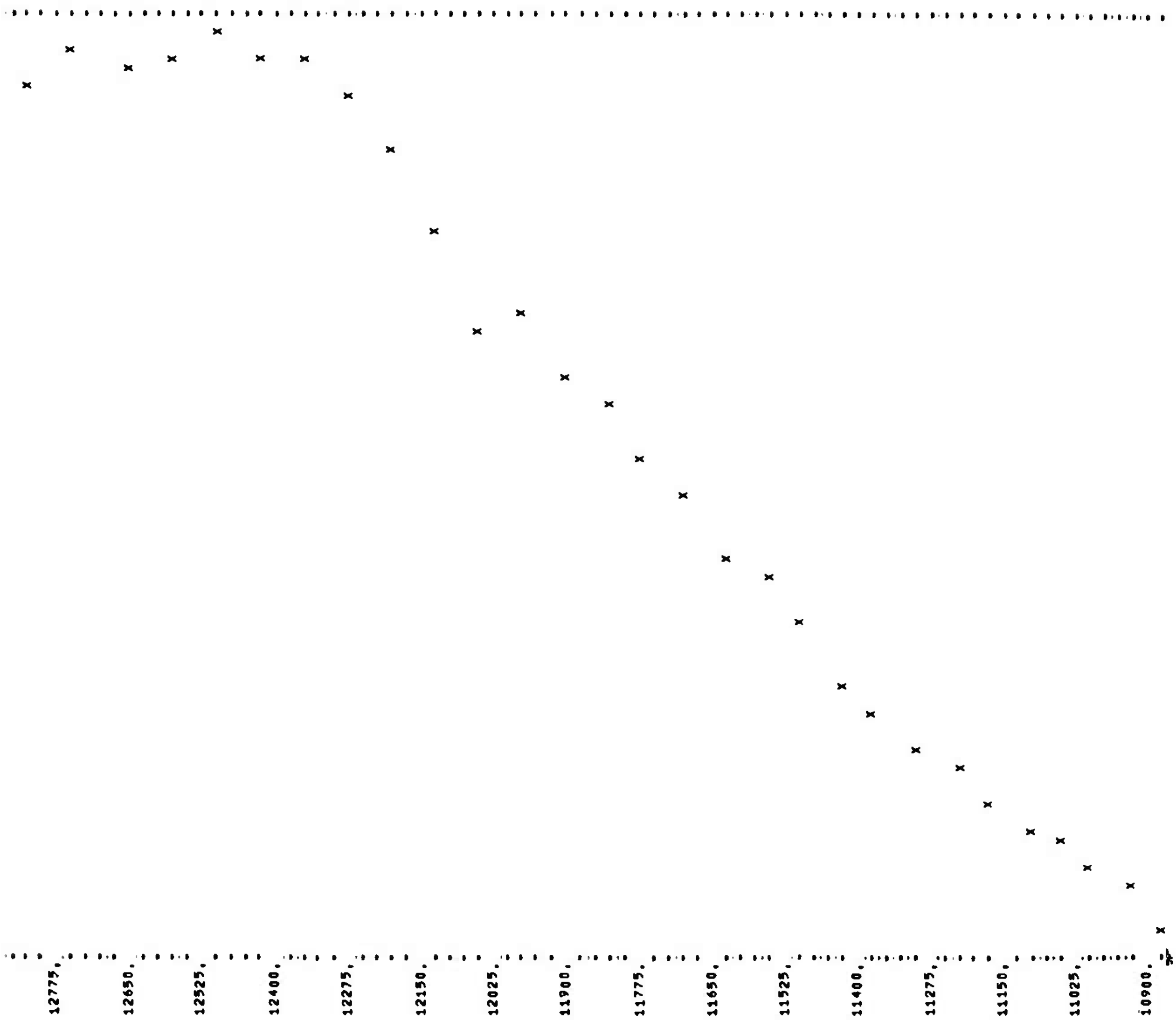
13525.
13400.
13275.
13150.
13025.
12900.


12775.
12650.
12525.
12400.
12275.
12150.
12025.
11900.
11775.
11650.
11525.
11400.
11275.
11150.
11025.
10900.

THE QUANTUM YIELD CALCULATED FROM THIS RUN USING A QUANTUM YIELD OF 0.55 WITH QUININE SULFATE AS A STANDARD.

THE SPECTRUM OF THE STANDARD

WAVELENGTH	RESPONSE	ADJ. RESPONSE
670.0	0.00	0.000
675.0	2.00	0.092
680.0	9.00	0.434
685.0	22.00	1.105
690.0	47.00	2.463
695.0	91.00	4.984
700.0	153.00	8.729
705.0	239.00	14.307
710.0	343.00	21.156
715.0	449.00	28.106
720.0	578.00	36.222
725.0	675.00	41.823
730.0	780.00	48.659
735.0	870.00	55.864
740.0	949.00	66.215
745.0	994.00	77.777
750.0	1017.00	89.125
755.0	1001.00	94.529
760.0	967.00	98.083
765.0	922.00	100.000
770.0	855.00	99.639
775.0	794.00	98.839
780.0	719.00	96.052
785.0	659.00	93.753
790.0	587.00	88.086
795.0	527.00	83.667
800.0	460.00	77.286
805.0	390.00	70.037
810.0	343.00	65.919
815.0	297.00	61.386
820.0	257.00	55.202
825.0	225.00	50.301
830.0	188.00	40.700
835.0	153.00	36.435
840.0	121.00	30.125
845.0	100.00	25.475
850.0	79.00	20.605
855.0	67.00	17.901
860.0	52.00	13.893
865.0	41.00	11.228
870.0	31.00	8.490
875.0	28.00	7.668
880.0	22.00	6.025
885.0	19.00	5.203
890.0	13.00	3.651
895.0	11.00	3.090
900.0	10.00	2.883
905.0	5.00	1.441
910.0	0.00	0.000
915.0	0.00	0.000
920.0	0.00	0.000

THE ADJUSTED STANDARD GIVES A RELATIVE AREA OF 0.7182E+06 AND THE UNKNOWN A QY OF 0.0066

MEASUREMENT OF CARBAZOLYLACETALDEHYDE PHOS
GAVE THE FOLLOWING•

WAVELENGTH	RESPONSE	ADJ, RESPONSE
700,0	0,00	0.000
702,5	0,00	0.000
705,0	0,00	0.000
707,5	0,00	0.000
710,0	0,00	0.000
712,5	3,00	1.758
715,0	32,00	18.859
717,5	90,00	53.346
720,0	107,20	63.250
722,5	67,00	39.262
725,0	35,50	20.709
727,5	30,00	17.580
730,0	41,90	24.609
732,5	47,80	28.333
735,0	48,50	29.320
737,5	64,00	40.248
740,0	76,00	49.925
742,5	71,00	49.477
745,0	78,50	57.829
747,5	109,00	85.165
750,0	121,20	100.000
752,5	94,00	80.789
755,0	67,00	59.570
757,5	51,70	47.608
760,0	54,00	51.568
762,5	57,40	56.923
765,0	56,00	57.184
767,5	52,90	56.246
770,0	58,00	63.637
772,5	62,80	71.175
775,0	59,00	69.148
777,5	51,50	62.488
780,0	49,50	62.259
782,5	51,50	66.393
785,0	50,90	68.176
787,5	41,00	56.381
790,0	32;70	46.199
792,5	26,60	38.639
795,0	24,50	36.621
797,5	24,60	37.868
800,0	24,00	37.964
802,5	23,40	38.307
805,0	20,00	33.815
807,5	20,90	36.534
810,0	20,00	36.188
812,5	20,50	38.441
815,0	17,70	34.443
817,5	15,20	30.147
820,0	14,00	28.312
822,5	13,40	27.640
825,0	13,00	27.362
827,5	11,10	23.850
830,0	9,00	18.344
832,5	8,20	17.994
835,0	7,00	15.595
837,5	6,60	15.127
840,0	6,40	15.002
842,5	5,90	14.151
845,0	5,50	13.192

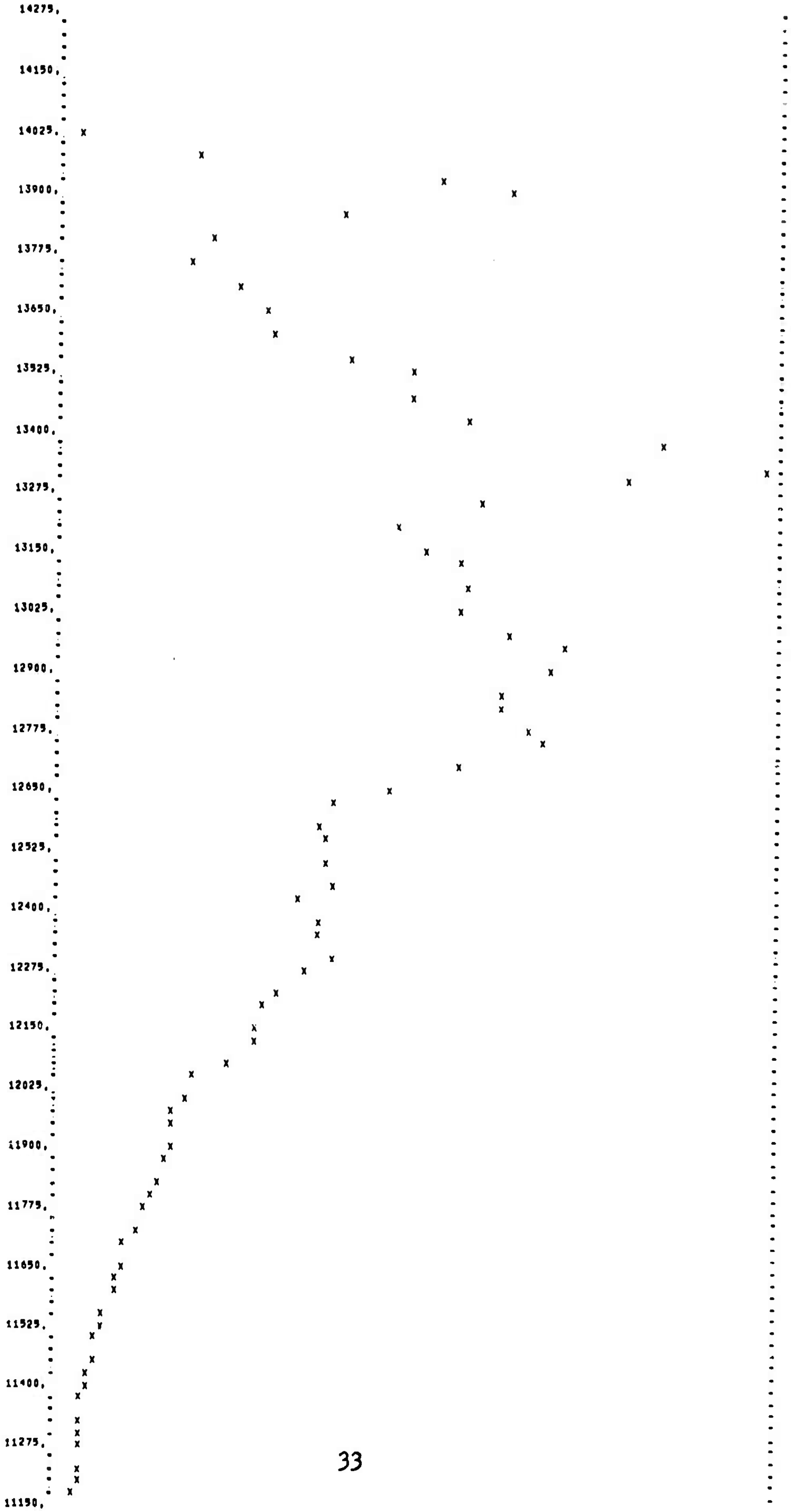
847,5	5,00	12.278
850,0	4,50	11.050
852,5	4,00	10.062
855,0	3,50	8.804
857,5	3,30	8.301
860,0	3,00	7.546
862,5	2,80	7.219
865,0	2,00	5.157
867,5	2,00	5.157
870,0	1,90	4.899
872,5	1,70	4.383
875,0	1,40	3.610
877,5	1,40	3.610
880,0	1,10	2.836
882,5	1,00	2.578
885,0	0,90	2.321
887,5	0,90	2.321
890,0	0,90	2.380
892,5	0,80	2.116
895,0	0,50	1.322
897,5	0,00	0.000

THE AREA UNDER THE ADJUSTED CURVE IS 0.4619E+05 RELATIVE UNITS

RELATING THESE POINTS TO WAVENUMBER GIVES

WAVENUMBER	ADJUSTED I
14025.	1.76
13975.	18.86
13925.	53.35
13900.	63.25
13850.	39.26
13800.	20.71
13750.	17.58
13700.	24.61
13650.	28.33
13600.	29.32
13550.	40.25
13525.	49.93
13475.	49.48
13425.	57.83
13375.	85.16
13325.	100.00
13300.	80.79
13250.	59.57
13200.	47.61
13150.	51.57
13125.	56.92
13075.	57.18
13025.	56.25
12975.	63.64
12950.	71.17
12900.	69.15
12850.	62.49
12825.	62.26
12775.	66.39
12750.	68.18
12700.	56.38
12650.	46.20
12625.	38.64
12575.	36.62
12550.	37.87
12500.	37.96
12450.	38.31
12425.	33.81
12375.	36.53
12350.	36.19
12300.	38.44
12275.	34.44
12225.	30.15
12200.	28.31
12150.	27.64
12125.	27.36
12075.	23.85
12050.	18.34
12010.	17.99
11975.	15.69
11950.	15.13
11900.	15.00
11875.	14.15
11825.	13.19
11800.	12.28
11775.	11.05
11725.	10.06
11700.	8.80
11650.	8.30
11625.	7.55
11600.	7.22

11550.	5.16
11525.	5.16
11500.	4.90
11450.	4.38
11425.	3.61
11400.	3.61
11375.	2.84
11325.	2.58
11300.	2.32
11275.	2.32
11225.	2.38
11200.	2.12
11175.	1.32


14275,
14150,
14025,
13900,
13775,
13650,
13525,
13400,
13275,
13150,
13025,
12900,
12775,
12650,
12525,
12400,
12275,
12150,
12025,
11900,
11775,
11650,
11525,
11400,
11275,
11150,

APPENDIX B

CALIBRATION CURVES

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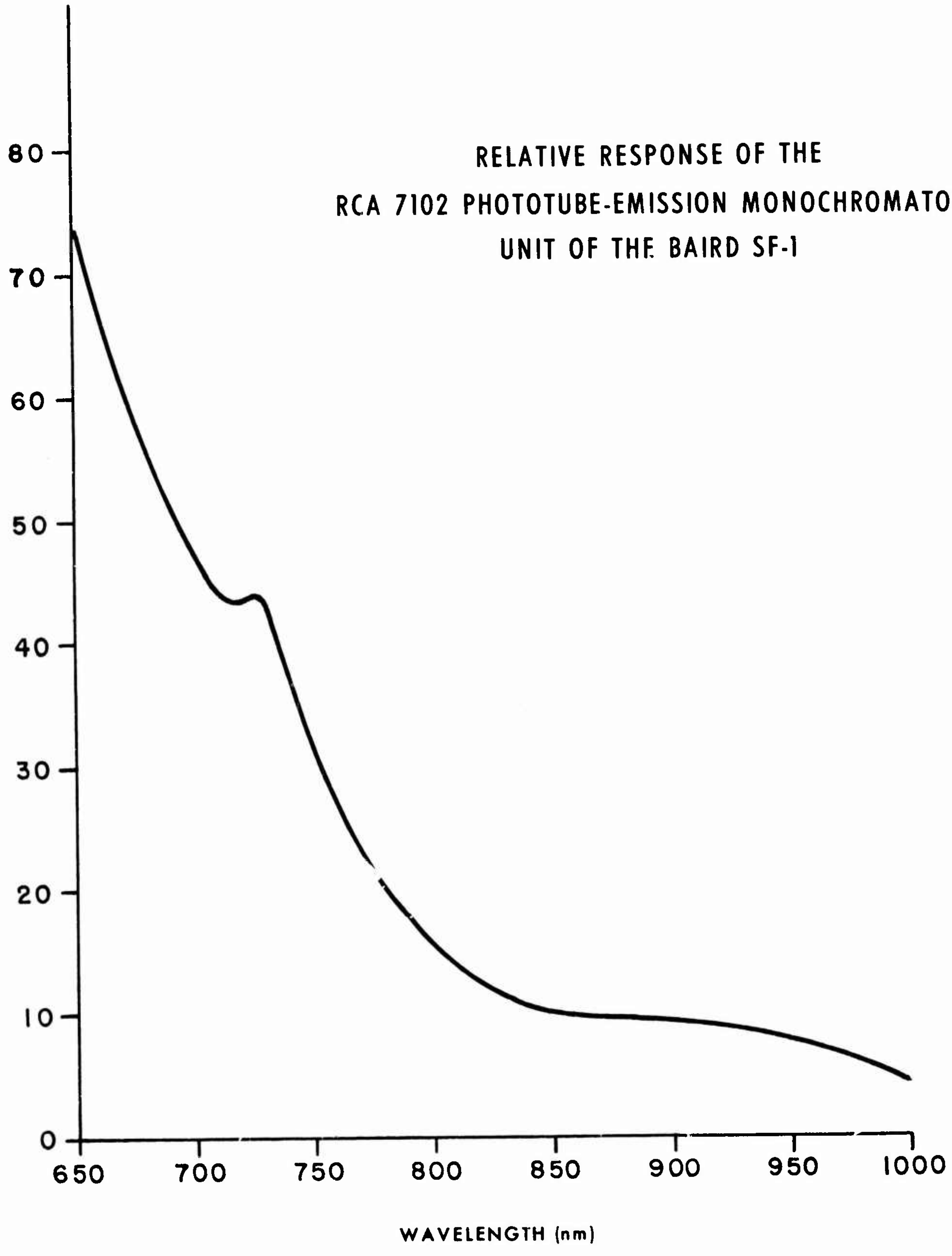
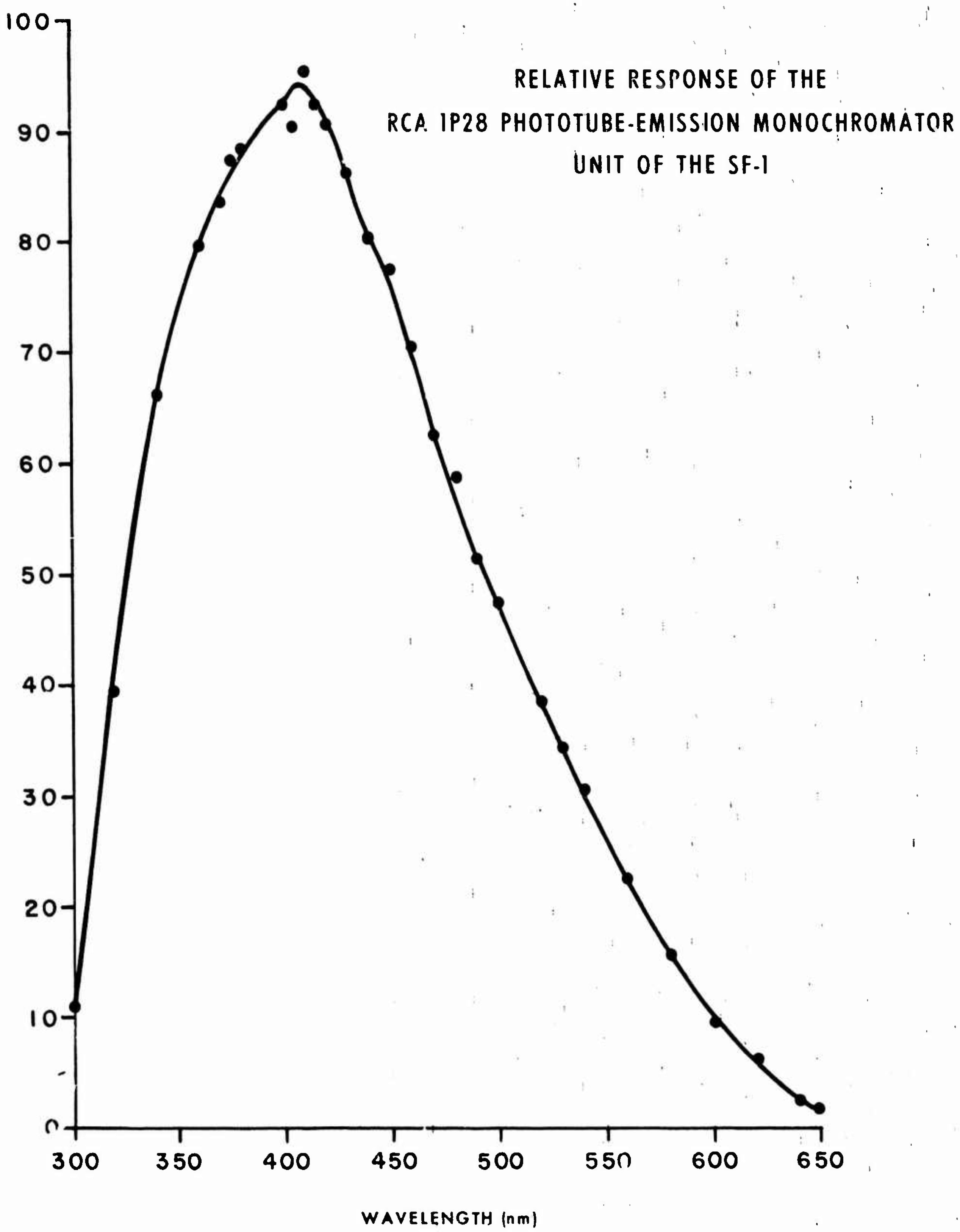

RELATIVE RESPONSE OF THE
RCA 7102 PHOTOTUBE-EMISSION MONOCHROMATOR
UNIT OF THE BAIRD SF-1
80
70
60
50
40
30
20
10
0
650
700
750
800
850
900
950
1000
WAVELENGTH (nm)


100
90
80
70
60
50
40
30
20
10
0
RELATIVE RESPONSE OF THE
RCA 1P28 PHOTOTUBE-EMISSION MONOCHROMATOR
UNIT OF THE SF-1
300
350
400
450
500
550
600
650
WAVELENGTH (nm)

APPENDIX C

ABBREVIATED MAIN PROGRAM