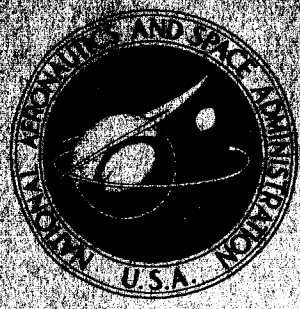


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by William A. Gordon and Anne K. Gallagher
Lewis Research Center
Cleveland, Ohio

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SUMMARY

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Calculations required to convert photographic densities of spectral lines to the concentration-related intensity parameter in spectrographic analysis have been programmed for digital computer processing.

The program produced an emulsion calibration curve for each data set and converted all percent transmission values to relative intensities. Further, the line intensity ratios of the analytical lines to the internal standard lines were printed out for each step and exposure. These calculations were made for a maximum of 50 elements, four internal standard lines, and 11 exposures made with a seven-step sector.

The program is written in Fortran IV (version 13) and is operational on the IBM 7094-2/7044 direct-coupled system of the Lewis Research Center.

INTRODUCTION

In emission spectrographic analysis the concentrations of the various elements in a sample are determined from the photographic density of selected spectral lines that are recorded on a photographic plate. The conversion of the data from photographic density to concentration requires lengthy calculations and graphical procedures that are adaptable to automatic processing. The description of the graphical construction of the emulsion calibration curve from step-sectored spectra follows a standard practice as described in reference 1. The processing of the most laborious steps in the calculations by an electronic computer is the subject of this report.

The program, described in appendix B determines the emulsion calibration curve for each photographic plate and converts all percent transmissions to the intensity parameters from which element concentrations are derived. Calculations were made for a maximum of 50 elements, in a maximum of 11 samples. In spectral analysis using photographic photometry it is customary to stepwise attenuate the intensity of the spectral lines along their length to calibrate the emulsion and also to extend the concentration range for each exposure. This program allows the recording of data in a maximum of seven steps of atten-

uation for each spectral line. Conventionally, the element line intensities are ratioed to an internal standard line intensity to compensate for some experimental errors in the procedure. In this program provisions were made for calculating these ratios using a maximum of four internal standard line intensities. This was done to facilitate selection of internal standard lines in the development of analytical methods. A typical set of calculations, requiring about 40 hours when performed manually, may be completed in about 1 minute of computer time. In addition, the automatic calculations are less subject to error than those performed manually.

PHOTOGRAPHIC DATA REDUCTION

The conversion of photographic density to element concentration can be arbitrarily divided into four basic operations. Two of the operations are performed manually and two by computer as indicated:

- (1) The conversion of photographic density into percent transmission using a densitometer (Manual)
- (2) Graphical determination of the relation between percent transmission and the spectral line intensity that produced the photographic density, referred to as the emulsion calibration curve (ECC) (Computer)
- (3) Calculation of the ratios of the analytical line intensities and the internal standard intensity, with appropriate background corrections (Computer)
- (4) Graphical conversion of the line intensity ratios to elemental concentrations by means of calibration curves prepared from standards for each element sought (Manual)

The automation of the second operation, which involves the plotting of experimental data followed by two separate curve-fitting procedures, provides the emulsion calibration curve ECC. Although the mathematical relation for an emulsion calibration curve can be approximated in general by a mathematical function, a more precise procedure is to determine experimentally the ECC for each photographic plate. It should also be noted that the ECC is a function of the wavelength of the exciting light and for highest precision should therefore be determined for selected wavelength intervals. In the present work, however, a single ECC is determined representing an average over the experimental wavelength region. Additions can be made to this program to take into account this wavelength dependency should this be desired.

In the first curve-fitting procedure in operation (2), the percent transmission readings of adjacent steps of each spectral line recorded on card 3 (appendix A, fig. 1(b)), are input on linear X-Y coordinates. These ordered pairs (X,Y) have a definite intensity relation, known as the "step factor," which is determined by the physical configuration of the step sector used in the procedure to stepwise attenuate the light. In this work the step factor is 2.0 (i.e., any two adjacent steps of a given line have an intensity relation of 2.0). Similarly, alternate steps for a given line have an intensity

ratio of 2^2 , and for steps separated by n step positions the intensity ratio of the darker step to the lighter step is 2^n . Thus, for the preliminary curve each ordered pair (X,Y) is derived from transmission readings for $n = 1$ (i.e., adjacent steps in the same line). It should be noted that these ordered pairs (X,Y) are derived from line, not background readings.

The program, as designed, orders a maximum of 250 pairs (X,Y) from the input data including two pairs fixed at $(0,0)$ and $(100,100)$, which are weighted to force the fit. Should the maximum number of ordered pairs exceed 250, it may be necessary to revise card 1 (appendix A, fig. 1(a)), so that the ordering of the elements will provide representative data with respect to wavelength region and to the range of densities in the first 250 ordered pairs. After calibration all of the input data are used in the ratio calculations.

The total number of points registered are curve fitted to a polynomial of the form

$$Y = A_1 + A_2X + A_3X^2 + A_4X^3$$

by a general least-squares method using the Crout reduction and a method developed at the Lewis Research Center by Bert Henry to invert the matrix. The resulting coefficients describe a curve known as a "preliminary emulsion calibration curve." This curve-fitting operation serves to effectively smooth all the plotted data.

The second curve-fitting operation results in the final emulsion calibration curve ECC, which relates percent transmission (ordinate) to the intensity parameter (abscissa). Values for plotting this curve are derived from the preliminary curve as follows: start at $X = 0.02$ (2 percent transmission) on the preliminary curve, and compute Y_1 ; now let $Y_1 = X_2$, and find Y_2 corresponding to this X_2 from the preliminary curve function. Then set $Y_2 = X_3$, and compute Y_3 , . . . , etc. In this way a series of X 's (maximum of 10) is generated, which represent the smoothed percent-transmission readings whose intensity relation are known from the step factor as explained previously. In the experiments presented herein this relation may be expressed as the percent transmission $T = 2^nZ$, where n is the difference in step number and Z is the intensity parameter that is related to element concentration in analytical work. The conversion of all percent-transmission data to this intensity parameter is done by a Lagrange four-point interpolation technique. The interpolation was easily performed on a large-scale computer and yielded greater accuracy than the method of least squares.

The programming of operation (3) requires the straightforward calculations of spectral line intensity ratios using the intensity parameters derived from the percent transmissions and the ECC, as described in operation (2). All intensity ratios were tabulated in both the background-corrected and the non-corrected forms; however, when background readings were not entered on card 3 (appendix A, fig. 1(b)), for either the internal standard or the analytical line, a zero was printed in the column reserved for the background-corrected ratio, as shown in the sample output for nickel (appendix C). In the calculation of line intensity ratios instructions are programmed so that maximum use

is made of the available data. For example, percent-transmission readings in a given exposure may not be recorded in the same step for the internal standard and the analytical lines. When this occurs, a calculation is made that automatically corrects for any step difference between the internal standard and the analytical lines. This calculation is performed by using 2^n as a multiplier, where 2 is the known step factor and n is the step difference. The intensity ratios obtained by this procedure may be subject to extrapolative errors; therefore, it is desirable to identify such values to warn of possible error by printing an asterisk to the right of the intensity ratios obtained by extrapolation. It should also be noted on the sample output (appendix C) that an average value is printed for each element and exposure. In the calculation of this average the extrapolated intensity ratios are given the same weight as the other intensity ratios. Although this may not be a statistically valid procedure, the error due to this simplification is not significant for most work at the Lewis Research Center.

Since a considerable amount of manual effort is still necessary to record the input data, errors in input can be expected to arise with about the same frequency as when calculations are made manually. The error-searching procedure is performed manually and is similar to the general procedure used by the spectrographer when making manual calculations. The preliminary curve is printed out, and wide deviations from the average are often recognized as erroneous data. The dubious value can then be traced back through the input, reread on the densitometer, and corrected if necessary. In addition, the percentage deviation of each of the data points from the preliminary curve fit is printed out in tabular form and serves as a useful means for revealing questionable data.

The line intensity ratios calculated by the program are then converted manually to element concentrations by means of calibration curves prepared from standards for each element sought. These calibrations cannot be conveniently programmed because the parameters under study at the Lewis Research Center affect the positions of the concentration curves. Once these calibrations are permanently established, the last operation, conversion of line intensity ratios to concentrations, can be included in the computer program by using curve fitting techniques similar to those described previously.

This program for spectrographic calculations forms a basis to which additional modifications can be made to make it more comprehensive. In its present state, the program serves the needs of a spectrographic laboratory engaged in both research and service analyses.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, November 23, 1965.

APPENDIX A

INPUT

This data reduction program is written in Fortran IV and is operational on the IBM 7094-2/7044 direct coupled system of the Lewis Research Center. The main program and its eight subroutines require 8000)₈ store in common data, 30000)₈ store for the program, and 25000)₈ additional store for Lewis monitor systems routines. For a smaller computer installation, overlay or some other store-sharing technique would be necessary.

Figure 1 contains a list of the input with samples of the forms used at Lewis. The input in card type 3 is sorted in columns 11 to 7 to provide for the proper pairing of data in the preliminary curve fit.

The sample data (fig. 1) and the sample output (appendix C) are abbreviated to show only the first two internal standards and the element nickel.

Instructions for preparing the input are given in table I.

TABLE I. - INSTRUCTIONS FOR PREPARING INPUT

[See listing for specific formats.]

Card type	Number	Columns	Description of variables	
1 (Element data)	1	1 to 5	NEL	number of elements present (maximum, 50)
	NEL	7 to 12	EL	6 letter code for element
		19 to 24	ELB	6 letter code for element background
2 (Constants for one case)	1	2 to 5	NMAX	number percent transmissions recorded (maximum, 3850)
		10 to 15	PLATE	plate number
		16 and 17	KSTOP	number standards to be used (maximum, 4)
	1	18 and 19	NEXP	number exposures (maximum, 11)
	1	1 to 72	(DATE (I), I=1,12)	any statement about the data
3 (Data for one case)	NMAX	7 and 8	I	element number (must match order of type 1, 1 to 4 standards)
		9 and 10	J	exposure number
		11	K	step number (maximum, 7)
		13 to 18	CLU	percent transmission
		19 to 24	BAK	percent transmission of background

Card types 1 and 3 may be repeated for a number of cases, but card type 2 must be the same for all cases in a given run. Forms used at Lewis for card types 1 and 3 are shown in figure 1.

SPECTROGRAPHIC PLATE READINGS		NAME William A. Gordon																
AUTOMATIC DATA PROCESSING WORKSHEET		DATE August 1, 1965																
(CARD TYPE 3)		PLATE NO. 705																
		SAMPLE W - Re																
		PAGE 1																
7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	
ELEMENT NO.	EXPOSURE NO.	STEP NO.	BLANK SPACE	ELEMENT	TRANS. MISSION	BACKGROUND	TRANS. MISSION	BACKGROUND	ELEMENT	TRANS. MISSION	BACKGROUND	TRANS. MISSION	BACKGROUND	ELEMENT	TRANS. MISSION	BACKGROUND	TRANS. MISSION	BACKGROUND
1	1	1	1	7	7	7	7	7	1	1	1	1	1	1	1	1	1	1
2	1	2	2	4	4	4	4	4	2	2	2	2	2	2	2	2	2	2
3	1	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
4	1	4	4	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2
5	1	5	5	0	0	0	0	0	3	3	3	3	3	3	3	3	3	3
6	1	6	6	0	0	0	0	0	4	4	4	4	4	4	4	4	4	4
7	1	7	7	0	0	0	0	0	4	4	4	4	4	4	4	4	4	4
8	1	8	8	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2
9	1	9	9	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2
10	1	10	10	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2
11	1	11	11	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2
12	1	12	12	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2
13	1	13	13	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2
14	1	14	14	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2
15	1	15	15	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2
16	1	16	16	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2
17	1	17	17	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2
18	1	18	18	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2
19	1	19	19	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2
20	1	20	20	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2
21	1	21	21	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2
22	1	22	22	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2
23	1	23	23	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2
24	1	24	24	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2
25	1	25	25	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2
26	1	26	26	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2

(b) Card type 3.

Element	Column																		
	7	8	9	10	11	12	19	20	21	22	23	24							
1	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
2	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
3	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
4	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
5	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
6	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
7	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
8	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
9	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
10	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
11	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
12	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
13	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
14	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
15	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
16	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
17	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
18	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
19	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
20	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
21	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
22	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
23	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
24	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
25	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A
26	A	W	A	G	L	R	C	U	E	F	M	N	I	S	I	B	K	G	A

(a) Card type 1. Background measurements: L is measured on low wavelength side of line; H is measured on high wavelength side of line; A is measured as average of both sides of line.

Figure 1. - Sample input.

APPENDIX B

FORTTRAN IV PROGRAM

A synopsis of the subroutines and their content listed in order of calling sequence is as follows:

BEGIN MAIN PROGRAM
 (1) Inputs data
 (2) Sets up X,Y-pairs for PC curve fit
 (3) Outputs relative intensities

GLSQ1 Performs a least-squares polynomial fit on X,Y-pairs

PLOTXY Plots preliminary curve; PLOTXY is Lewis Monitor Subroutine (see ref. 2)

FUNC Function Subprogram to generate independent variable function

BFUNC Function Subprogram to backtransform independent variable function

DINVER Subroutine using Crout reduction and a routine to invert matrix

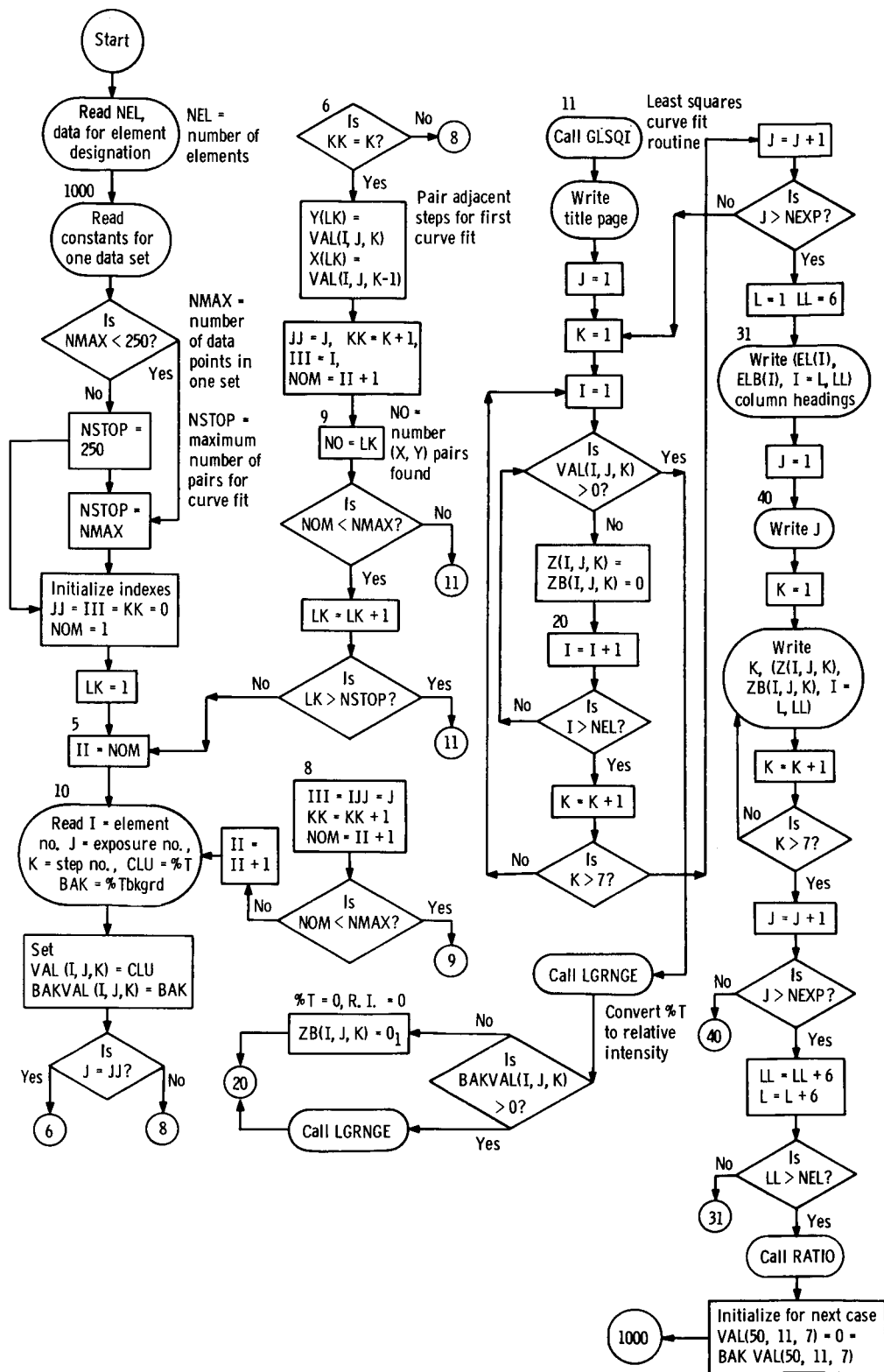
DMVMUL Subroutine to obtain solution vector from the inverse

CALC Subroutine to determine X,Y-pairs for the ECC from the fitted PC

LGRNGE Subroutine to perform four-point Lagrange interpolation; converts percent transmission to relative intensity

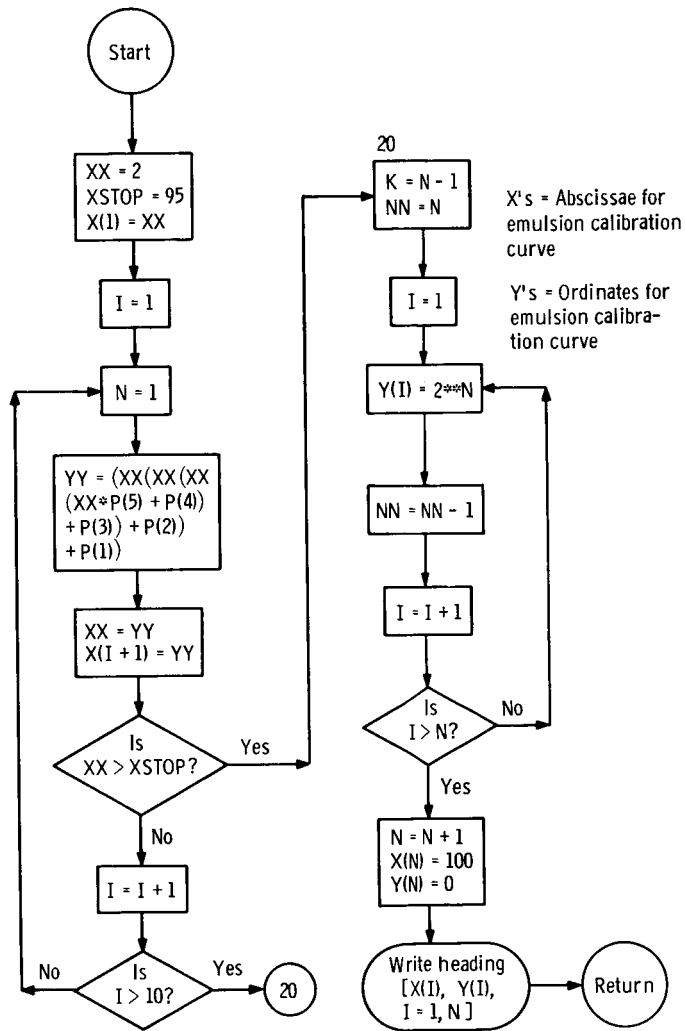
RATIO Subroutine which ratios relative intensity of an element to that of a standard and corrects for background if necessary (maximum number of standards, 4)

Flow charts of BEGIN, CALC, and RATIO are shown in figure 2. These three routines are pertinent to the spectrographic data analysis. The remaining subroutines are in general use at the Lewis Research Center. The main program and subroutines used for data reduction are presented after figure 2.



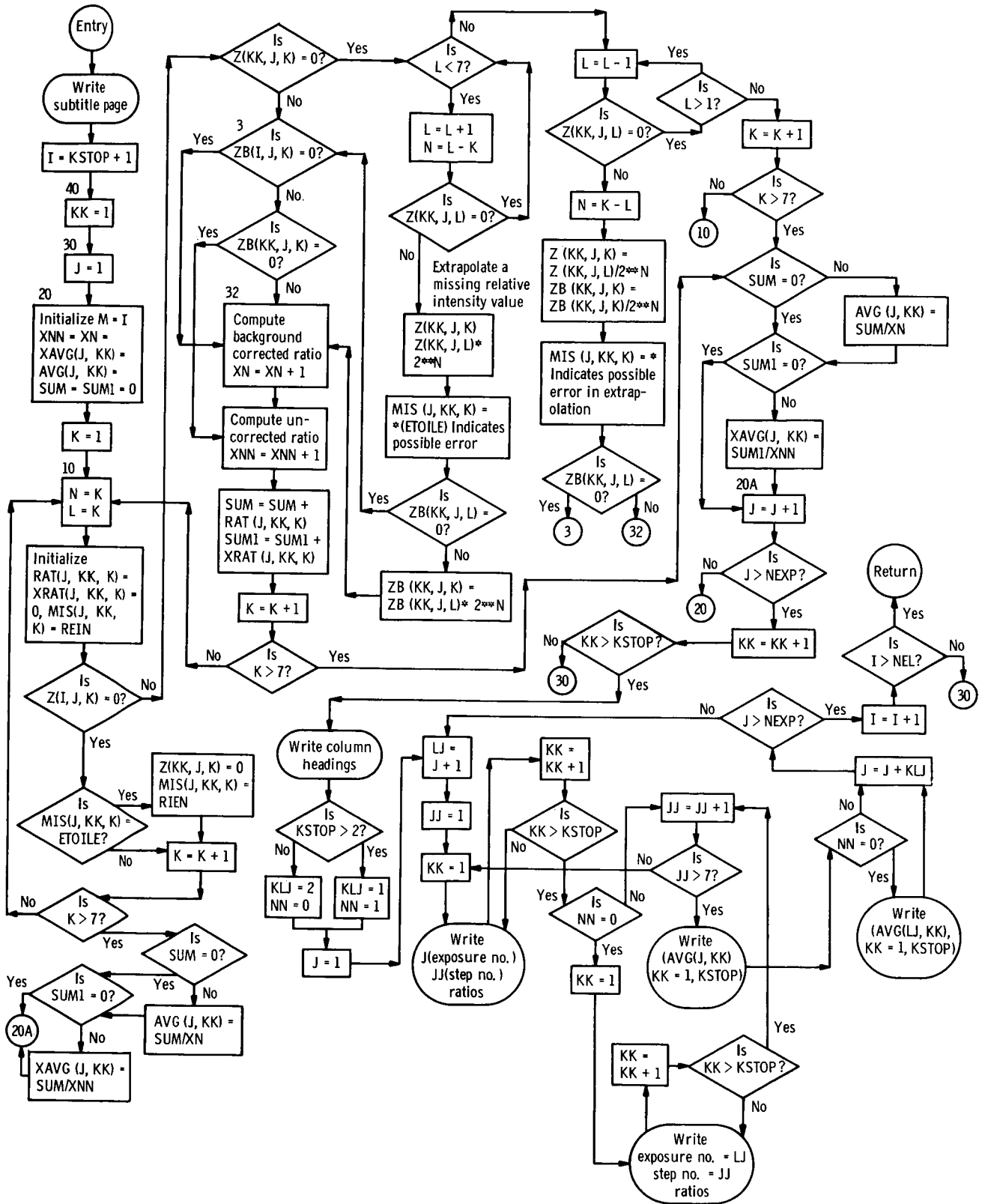
(a) Main program BEGIN.

Figure 2. - Flow charts.



(b) Subroutine CALC.

Figure 2. - Continued.



(c) Subroutine RATIO.

Figure 2. - Concluded.

\$IBFTC BEGIN LIST,DECK	BEG00000
C	BEG00010
C AUTOMATIC DATA PROCESSING FOR SPECTROGRAPHIC CALCULATIONS	BEG00020
COMMON IW,KSTOP,NEXP	BEG00030
COMMON Z(50,11,7),ZB(50,11,7)	BEG00040
COMMON EL(50),ELB(50)	BEG00050
DIMENSION VAL(50,11,7),BAKVAL(50,11,7),X(250),Y(500),P(35)	BEG00060
DIMENSION ZX(200),ZY(200)	BEG00070
DIMENSION DATE(12)	BEG00080
EQUIVALENCE (Z,VAL) , (ZB,BAKVAL)	BEG00090
READ(5,98) NEL	BEG00100
DO 1 I=1,NEL	BEG00110
1 READ(5,102)EL(I),ELB(I)	BEG00120
1000 WRITE(6,106)	BEG00130
READ(5,100) NMAX,PLATE,KSTOP,NEXP	BEG00140
READ(5,99) (DATE(I),I=1,12)	BEG00150
C	BEG00160
C	BEG00170
C NMAX= NUMBER READINGS ON THIS PLATE	BEG00180
C	BEG00190
C NEL= NUMBER OF ELEMENTS PRESENT IN THIS SAMPLE	BEG00200
C	BEG00210
C ELEMENTS INPUT FIRST (MAX=4) ARE TO BE USED AS INTERNAL STANDARDS.	BEG 220
C	BEG 230
C AG AND AGX = SILVER, A=ARGON, W = TUNGSTEN.	BEG 240
C	BEG00250
C	BEG00260
C EL AND ELB ALLOW A MAXIMUM 6 CHARACTER DESIGNATION FOR EACH	BEG00270
C ELEMENT AND ITS BACKGROUND TO BE USED AS COLUMN HEADINGS. READIN	BEG00280
C VALUE FOR - I - MUST MATCH ITS CODES IN EL(I), ETC)	BEG00290
C	BEG00300
IF (NMAX-250)3,3,2	BEG00310
2 NSTOP = 250	BEG00320
GO TO 4	BEG00330
3 NSTOP = NMAX	BEG00340
4 JJ=0	BEG00350
III = 0	BEG00360
KK = 0	BEG00370
NOM = 1	BEG00380
C BEGIN DETERMINATION OF POINTS TO BE USED IN FINDING THE PC	BEG00390
DO 5 LK=1,NSTOP	BEG00400
DO 10 II=NOM,NMAX	BEG00410
C	BEG00420
C I= ELEMENT NUMBER, XX , INTEGER VALUE FROM 1 TO 50	BEG00430
C J=EXPOSURE NUMBER, XX, INTEGER VALUE FROM 1 TO 11	BEG00440
C K= STEP NUMBER, X, INTEGER VALUE FROM 1 TO 7	BEG00450
C	BEG00460
C CLU = PERCENT T	BEG00470
C BAK = PERCENT T DUE TO BACKGROUND.	BEG00480
C	BEG00490
READ (5,101) I,J,K,CLU,BAK	BEG00500
VAL(I,J,K) = CLU	BEG00510
BAKVAL(I,J,K) = BAK	BEG00520
IF (JJ-J) 8,6,8	BEG00530
6 IF (KK-K) 8,7,8	BEG00540
7 Y(LK) = VAL(I,J,K)	BEG00550
X(LK)= VAL(I,J,K-1)	BEG00560
DEBUG LK,X(LK),Y(LK)	BEG00570
NOM = II+1	BEG00580
JJ = J	BEG00590
KK = K+1	BEG00600
III = I	BEG00610

GO TO 9	BEG00620
8 III=I	BEG00630
JJ = J	BEG00640
KK = K+1	BEG00650
NOM=II+1	BEG00660
IF(NOM-NMAX)10,10,9	BEG00670
10 CONTINUE	BEG00680
9 NO=LK	BEG00690
IF (NOM-NMAX) 5,11,11	BEG00700
5 CONTINUE	BEG00710
11 CONTINUE	BEG00720
C POINTS ARE AVAILABLE. CALL GLSQ1 TO DETERMINE PC	BEG00730
IW=1	BEG00740
CALL GLSQ1(X,Y,NO,P)	BEG00750
C PC HAS BEEN DETERMINED. ECC HAS BEEN DEFINED.	BEG00760
WRITE(6,106)	BEG00770
WRITE(6,104) PLATE	BEG00780
WRITE(6,105)	BEG00790
WRITE(6,107) (DATE(I),I=1,12)	BEG00800
KODE=1	BEG00810
C	BEG00820
C KODE = 1 INDICATES DERIVATIVE IS NOT TO BE CALCUALTED IN SUB. LGRNGE	BEG00830
C RENAME RESULTS OF SUB. CALC	BEG00840
DO 15 J=1,NO	BEG00850
ZX(J)=X(J)	BEG00860
15 ZY(J)=Y(J)	BEG00870
C TRANSFORM PERCENT TS TO RELATIVE INTENSITIES BY MEANS OF LAGRANGE	BEG00880
C INTERPOLATION.	BEG00890
DO 30 J=1,NEXP	BEG00900
DO 25 K=1,7	BEG00910
DO 20 I=1,NEL	BEG00920
IF (VAL(I,J,K)-1.)16,16,17	BEG00930
16 Z(I,J,K)=0.	BEG00940
ZB(I,J,K)=0.	BEG00950
GO TO 20	BEG00960
17 CALL LGRNGE(ZX,ZY,NO,VAL(I,J,K),Z(I,J,K),DER,KODE)	BEG00970
IF (BAKVAL(I,J,K)-1.)18,18,19	BEG00980
18 ZB(I,J,K)=0.	BEG00990
GO TO 20	BEG01000
19 CALL LGRNGE(ZX,ZY,NO,BAKVAL(I,J,K),ZB(I,J,K),DER,KODE)	BEG01010
20 CONTINUE	BEG01020
25 CONTINUE	BEG01030
30 CONTINUE	BEG01040
L=1	BEG01050
LL=6	BEG01060
C	BEG01070
C PRINT RELATIVE INTENSITIES	BEG01080
C	BEG01090
31 WRITE(6,108) (EL(I),ELB(I),I=L,LL)	BEG01100
DO 50 J=1,NEXP	BEG01110
WRITE(6,103) J	BEG01120
DO 40 K=1,7	BEG01130
WRITE(6,109) K,(Z(I,J,K),ZB(I,J,K),I=L,LL)	BEG01140
40 CONTINUE	BEG01150
50 CONTINUE	BEG01160
LL=LL+6	BEG01170
L=L+6	BEG01180
IF (LL-NEL)51,51,52	BEG01190
51 GO TO 31	BEG01200
C BEGIN FINDING RATIOS OF RELATIVE INTENSITIES.	BEG01210
52 CALL RATIO (NEL,Z,ZB)	BEG01220
WRITE(6,106)	BEG01230

DO 70 I=1,7	BEG01240
DO 65 J=1,11	BEG01250
DO 60 K=1,50	BEG01260
VAL(K,J,I)=0.	BEG01270
BAKVAL(K,J,I)=0.	BEG01280
60 CONTINUE	BEG01290
65 CONTINUE	BEG01300
70 CONTINUE	BEG01310
GO TO 1000	BEG01320
C	BEG01330
C	BEG01340
C	BEG01350
98 FORMAT (I5)	BEG01360
99 FORMAT (12A6)	BEG01370
100 FORMAT(X,I4,4X,A6,2I2)	BEG01380
101 FORMAT (6X,2I2,11,X,2F6.2)	BEG01390
102 FORMAT (6X,A6,6X,A6)	BEG01400
103 FORMAT(4H EXP,I2)	BEG01410
104 FORMAT(1H2,35X,45H SPECTROGRAPHIC CALCULATIONS FOR PLATE NO. ,	BEG01420
XA6)	BEG01430
105 FORMAT(1H0,30X,62H PER CENT TRANSMISSION READINGS CONVERTED TO R	BEG01440
XEL INTENSITY)	BEG01450
106 FORMAT(1H1)	BEG01460
107 FORMAT(1H0,29X,12A6)	BEG01470
108 FORMAT(1H1,6(A6,5X,A6,4X))	BEG01480
109 FORMAT(1H ,I2,(12G10.3))	BEG01490
STOP	BEG01500
END	BEG01510

```

$IBFTC GLSWR LIST,DECK,DEBUG                                GLS00000
      SUBROUTINE GLSQ1(X,Y,NSMALL,P)                          GLS00010
C                                                                 GLS00020
      COMMON IW                                               GLS00030
      DIMENSION X(250),Y(500),D(35),A(35,35),ASAVE(35,35)   GLS00040
      1,P(35),P1(35),YCALC(250),DELY(250),XP(250),YP(500),ERRATA(250) GLS00050
      2,ELM(2),TITLE(12),FMT(12),FMTO(12),W(250)            GLS00060
      DIMENSION AIN(35,35)                                    GLS00070
      DIMENSION FMTW(7),KMTW(7),PK(1),KPL(15),CC(35)        GLS00080
      EQUIVALENCE (FMTW(5),KMTW(5))                          GLS00090
      DATA (FMTW(I),I=1,7)/6H(22H0 ,6HTHE PA,6HRAMETE,6HRS (A0,6H-A I2,, GLS00100
      16H5H) AR,3HE )/,KMT51,KMT52/6H-A I1,,6H-A I2,/      GLS00110
      DATA(TITLE(I),I=1,12)/6HAUTOMA,6HTIC DA,6HTA PRD,6HCESSIN,6HG FOR GLS00120
      X,6HSPECTR,6HOGRAH,6HIC CAL,6HCULATI,6HONS ,6H ,6H / GLS00130
C                                                                 GLS00140
C MAIN PROGRAM FOR LEAST SQUARES ANALYSIS HAS BEEN ALTERED FOR THIS GLS00150
C SPECIFIC PROBLEM.                                         GLS00155
C                                                                 GLS00160
C ALL THE OPTIONS IN THE ORIGINAL PROGRAM HAVE BEEN REMOVED. GLS00170
      DOUBLE PRECISION A,D,CC,DXMAX,AIN                      GLS00180
      PK(1)=1.0                                               GLS00190
      KPL=64                                                  GLS00200
      KPL(2)=2                                                GLS00210
      POOL1=0.                                                 GLS00220
      POOL2=0.                                                 GLS00230
      NFMT0=NBIG*3 - 2                                        GLS00240
      NBIG=4                                                  GLS00250
      IPL=1                                                    GLS00260
      IY=0                                                     GLS00270
      NBIGSV=NBIG                                             GLS00280
C                                                                 GLS00290
C NSMALL=NO. OF DATA POINTS --- NBIG=NO. OF COEFFICIENTS DESIRED GLS00300
C THE ORIGINAL DATA IS PLOTTED                             GLS00310
C IF IT BECOMES DESIRABLE TO OMIT THE PLOT CHANGE IPL TO 0 GLS00320
      NNN=NBIG                                               GLS00330
      MAX =35                                                GLS00340
      DO 32 I=1,NSMALL                                       GLS00350
32  W(I)=1.                                                  GLS00360
      NSMALL=NSMALL+2                                        GLS00370
      NN=NSMALL                                             GLS00380
      X(NN-1)=0.                                             GLS00390
      Y(NN-1)=0.                                             GLS00400
      X(NN)=100.                                             GLS00410
      Y(NN)=100.                                             GLS00420
      W(NN)=50.                                             GLS00430
      W(NN-1)=50.                                           GLS00440
      KKK=1                                                 GLS00450
      SN=NSMALL                                             GLS00460
6000 DO 6010 I=1,NSMALL                                     GLS00470
      XP(I)=X(I)                                             GLS00480
6010 YP(I)=Y(I)                                             GLS00490
C                                                                 GLS00500
      NBIG=NBIGSV                                           GLS00510
      NSAME=NSAMSV                                           GLS00520
      SUMYP=0.                                               GLS00530
      XMAXX=0.                                               GLS00540
      DO 501 I=1,NSMALL                                       GLS00550
      IF (XMAXX-ABS(X(I))) 33,501,501                       GLS00560
33  XMAXX=ABS(X(I))                                         GLS00570
      DXMAX=XMAXX                                           GLS00580
501  CONTINUE                                               GLS00590

```


DO 20 I=1,NSMALL	GLS00600
X(I)=X(I)/XMAXX	GLS00610
XP(I)=X(I)	GLS00620
YP(I)=Y(I)	GLS00630
20 SUMYP=SUMYP+YP(I)	GLS00640
1903 SUMY=0.	GLS00650
CN=NBIG	GLS00660
KN=NBIG-1	GLS00670
DETNUM=0.	GLS00680
DETDEN=0.	GLS00690
YPMEAN=SUMYP/SN	GLS00700
YMEAN=YPMEAN	GLS00710
C	GLS00720
C	GLS00730
DO 23 I=1,NSMALL	GLS00740
IF(IY) 22,23,22	GLS00750
22 Y(I)=FUNC(IY,Y(I))	GLS00760
23 SUMY=SUMY+Y(I)	GLS00770
YMEAN=SUMY/SN	GLS00780
C	GLS00790
C	GLS00800
C	GLS00810
DO 2 I=1,NBIG	GLS00820
DO 2 J=1,NBIG	GLS00830
A(I,J)=0.	GLS00840
DO 2 K=1,NSMALL	GLS00850
FI=FUNC(I,X(K))	GLS00860
FJ=FUNC(J,X(K))	GLS00870
IF (IW) 35,36,35	GLS00880
35 A(I,J)=A(I,J)+FI*FJ*W(K)	GLS00890
GO TO 2	GLS00900
36 A(I,J)=A(I,J)+FI*FJ	GLS00910
2 CONTINUE	GLS00920
C	GLS00930
DO 14 I=1,NBIG	GLS00940
D(I)=0.	GLS00950
DO 14 K=1,NSMALL	GLS00960
FI=FUNC(I,X(K))	GLS00970
IF (IW) 37,38,37	GLS00980
37 D(I)=D(I)+Y(K)*FI*W(K)	GLS00990
GO TO 14	GLS01000
38 D(I)=D(I)+Y(K)*FI	GLS01010
14 CONTINUE	GLS01020
C	GLS01030
WRITE (6,397) TITLE	GLS01040
397 FORMAT(1H1,10X,12A6)	GLS01050
C	GLS01060
300 CALL DINVER (A,NNN,AIN,MAX,DET,ERR,D)	GLS01070
CALL DMVMUL(AIN,NNN,D,CC,MAX)	GLS01080
XXAXX=1./XMAXX	GLS01090
DO 301 J=1,NBIG	GLS01100
P(J)=CC(J)	GLS01110
301 P(J)=P(J)*FUNC(J,XXAXX)	GLS01120
C	GLS01130
C	GLS01140
C	GLS01150
130 CONTINUE	GLS01160
DEBUG (P(J),J=1,NBIG)	GLS01170
ERS=0.	GLS01180
DEV=0.	GLS01190
DO 8 I=1,NSMALL	GLS01200
X(I)=X(I)*XMAXX	GLS01210

K=NSMALL+I	GLS01220
Y(K)=0.	GLS01230
DO 9 J=1,NBIG	GLS01240
FJ=FUNC(J,X(I))	GLS01250
DEBUG FJ	GLS01260
9 Y(K)=Y(K)+P(J)*FJ	GLS01270
TEM=Y(I)-YMEAN	GLS01280
DETDEN=DETDEN+TEM*TEM	GLS01290
TEM=Y(K)-YMEAN	GLS01300
DETNUM=DETNUM+TEM*TEM	GLS01310
DELY(I)=Y(I)-Y(K)	GLS01320
ERRATA(I)=DELY(I)/Y(K)*100.	GLS01330
ERS=ERS+ERRATA(I)**2	GLS01340
8 DEV=DEV+DELY(I)*DELY(I)	GLS01350
POOL1=POOL1+DEV	GLS01360
ENDIV=SN-CN-1.	GLS01370
TVRDEN=TVRDEN+ENDIV	GLS01380
TVRNUM=POOL1	GLS01390
100 DEV=DEV/ENDIV	GLS01400
DVTN=SQRT(DEV)	GLS01410
ERS=ERS/SN	GLS01420
ERA=SQRT(ERS)	GLS01430
TOTVAR=TVRNUM/TVRDEN	GLS01440
TOTDEV=SQRT(TOTVAR)	GLS01450
DETRM=DETNUM/DETDEN	GLS01460
CORRL=SQRT(DETRM)	GLS01470
WRITE(6,401)	GLS01480
DO 10 I=1,NSMALL	GLS01490
K=NSMALL+I	GLS01500
10 WRITE(6,402) X(I),Y(I),Y (K),DELY(I),ERRATA(I)	GLS01510
WRITE(6,406)	GLS01520
406 FORMAT(41H0THE REGRESSION EQUATION FOR THE ABOVE IS /1H0,35H Y = A	GLS01530
X0 + A1*X + A2*X**2 + A3*X**3)	GLS01540
409 IF (KN-10) 407,405,405	GLS01550
405 KMTW(5)=KMT52	GLS01560
GO TO 408	GLS01570
407 KMTW(5)=KMT51	GLS01580
408 WRITE (6,FMTW) KN	GLS01590
WRITE (6,403) (P(I),I=1,NBIG)	GLS01600
WRITE (6,404) DEV,DVTN,DETRM,CORRL,TOTVAR,TOTDEV,ERS,ERA	GLS01610
WRITE (6,91) DET	GLS01620
91 FORMAT(13H0DETERMINANT= G14.6//)	GLS01630
IF(IW) 422,419,422	GLS01640
422 WRITE(6,430)	GLS01650
DO 420 I=1,NSMALL	GLS01660
IF (W(I)-1.) 421,420,421	GLS01670
421 WRITE(6,431)X(I),Y(I),W(I)	GLS01680
420 CONTINUE	GLS01690
419 CONTINUE	GLS01700
431 FORMAT(1H ,2X,2HX=G15.6,2X,2HY=G15.6,2X,12HWITH WEIGHT= F7.0)	GLS01710
430 FORMAT(44H0THE ABOVE DATA HAS BEEN WEIGHTED AS FOLLOWS)	GLS01720
401 FORMAT(1H0,2X,10H IND. VAR. ,8X,10H DEP.VAR. ,8X,12HCALC. FUNC.	GLS01730
X,6X,10H DEVIATION,8X,15H PER CENT ERROR)	GLS01740
402 FORMAT(1H ,(5(F12.4,6X)))	GLS01750
403 FORMAT(7G18.8)	GLS01760
404 FORMAT(1H0,2X,14H THE VARIANCE=G15.7,20H STANDARD DEVIATION=G15.7/GLS01770	GLS01770
13X,14H0DETERMINATION=G15.7,8X,12H0CORRELATION=G15.7/17H POOLED VARIAGLS01780	GLS01780
2NCE=G15.7,3X,17H0POOLED DEVIATION=G15.7/	GLS01790
3 1H0,2X,14H PCT VARIANCE=G15.7,20H STD. PCT DEVIATION=G15.7)GLS01800	GLS01800
GO TO (101,102),KKK	GLS01810
101 DO 24 I=1,NSMALL	GLS01820
K=NSMALL+I	GLS01830

IF (IY) 25,26,25	GLS01840
25 YP(K)=BFUNC(IY,Y(K))	GLS01850
GO TO 24	GLS01860
26 YP(K)=Y(K)	GLS01870
24 CONTINUE	GLS01880
IF (IPL-1) 29,803,801	GLS01890
803 KKK=2	GLS01900
801 CONTINUE	GLS01910
KPL(3)=NSMALL	GLS01920
K2N=NSMALL+NSMALL	GLS01930
102 WRITE(6,77)TITLE	GLS01940
77 FORMAT(2HPT,12A6/2HPT/2HPT,59X,7HNOTE---/2HPT/2HPT,59X,28HORIGINA	GLS01950
1 DATA PLOTTED WITH • /2HPT,59X,30HCALCULATED DATA PLOTTED WITH + /	GLS01960
X2HPT/2HPT,59X,14HPLOT OF PC)	GLS01970
CALL SCALE(NSMALL,X,KKLU)	GLS01980
CALL SCALE(K2N,Y ,KKLY)	GLS01990
CALL PLOTMY(X ,Y ,KPL,PK)	GLS02000
WRITE(6,78)	GLS02010
78 FORMAT(2HPL,59X,23HLIGHT STEP VS DARK STEP)	GLS02020
802 CONTINUE	GLS02030
GO TO (103,29),KKK	GLS02040
103 CONTINUE	GLS02050
27 DEV=0.	GLS02060
DETNUM=0.	GLS02070
DETDEN=0.	GLS02080
DO 28 I=1,NSMALL	GLS02090
K=NSMALL +I	GLS02100
X(I)=XP(I)	GLS02110
Y(I)=YP(I)	GLS02120
Y(K)=YP(K)	GLS02130
TEM=Y(I)-YPMEAN	GLS02140
DETDEN=DETDEN+TEM*TEM	GLS02150
TEM=Y(K)-YPMEAN	GLS02160
DETNUM=DETNUM+TEM*TEM	GLS02170
DELY(I)=Y(I)-Y(K)	GLS02180
ERRATA(I)=DELY(I)/YP(K)	GLS02190
28 DEV=DEV+DELY(I)*DELY(I)	GLS02200
POOL2=POOL2+DEV	GLS02210
TVRNUM=POOL2	GLS02220
KKK=2	GLS02230
GO TO 100	GLS02240
29 CALL CALC (XP,YP,NSMALL,NBIG,P)	GLS02250
DO 6 I=1,NSMALL	GLS02260
X(I)=XP(I)	GLS02270
Y(I)=YP(I)	GLS02280
6 CONTINUE	GLS02290
RETURN	GLS02300
END	GLS02310

\$IBFTC FLINFN LIST,DECK	FLI00000
C FUNCTION SUBROUTINE TO GENERATE INDEPENDENT VARIABLE FUNCTIONS	FLI00010
FUNCTION FUNC (I,X)	FLI00020
Z=X	FLI00030
K=I	FLI00040
C	FLI00050
C THE NUMBER OF THE STATEMENT IS IDENTICAL TO THE NUMBER OF THE TERM	FLI00060
C IN THE POLYNOMIAL TO BE FITTED.	FLI00070
C	FLI00080
IF (K-6) 100,6,7	FLI00090
7 WRITE (6,10) K	FLI00100
10 FORMAT(1H0,5X,72HTOO MANY COEFFICIENTS ASKED FOR - ONLY 6 ARE AV	FLI00110
1AAILABLE YOU CANNOT GET I3)	FLI00120
STOP	FLI00130
6 ANS=ALOG10(Z)	FLI00140
GO TO 99	FLI00150
100 IF (K-4) 101,4,5	FLI00160
5 ANS=Z*Z	FLI00170
ANS=ANS*ANS	FLI00180
GO TO 99	FLI00190
4 ANS=Z*Z*Z	FLI00200
GO TO 99	FLI00210
101 IF (K-2) 1,2,3	FLI00220
3 ANS=Z*Z	FLI00230
GO TO 99	FLI00240
2 ANS=Z	FLI00250
GO TO 99	FLI00260
1 ANS=1.	FLI00270
99 FUNC=ANS	FLI00280
RETURN	FLI00290
END	FLI00300

\$IBFTC BLINFN LIST,DECK	BLI00000
C SUBROUTINE TO BACK-TRANSFORM Y(I) ARRAY	BLI00010
FUNCTION BFUNC (I,X)	BLI00020
Z=X	BLI00030
K=I	BLI00040
C	BLI00050
C THE NUMBER OF THE STATEMENT IS THE NUMBER TO BE USED IN SPECIFYING	BLI00060
C THE TYPE OF CONVERSION.	BLI00070
C IT MUST AGREE WITH THE CONVERSION USED IN SUBROUTINE FUNC.	BLI00080
C	BLI00090
IF (K-6) 100,6,7	BLI00100
7 WRITE (6,10) K	BLI00110
10 FORMAT(1H0,5X,44HWRONG BACK-TRANSFORMATION OF Y REQUESTED, K= I)	BLI00120
STOP	BLI00130
6 ANS=10.**Z	BLI00140
GO TO 99	BLI00150
100 IF (K-4) 101,4,5	BLI00160
5 ANS=SQRT(Z)	BLI00170
ANS=SQRT(ANS)	BLI00180
GO TO 99	BLI00190
4 ANS=Z** .333333333	BLI00200
GO TO 99	BLI00210
101 IF (K-2) 1,2,3	BLI00220
3 ANS=SQRT(Z)	BLI00230
GO TO 99	BLI00240
2 ANS=Z	BLI00250
GO TO 99	BLI00260
1 ANS=1.	BLI00270
99 BFUNC=ANS	BLI00280
RETURN	BLI00290
END	BLI00300

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$IBFTC DINV LIST,DECK,DEBUG
C SUBR USING CROUT REDUCTION AND HENRY INVERSE ROUTINE
SUBROUTINE DINVER(B,NNN,A,MAX,DET,ERR,D)
DIMENSION A(MAX,MAX),B(MAX,MAX),D(MAX),AN(60)
DOUBLE PRECISION A,B,D,AN
KMI=NNN
MM1=KMI-1
MP1=KMI+1
DO 25 I=1,KMI
A(I,MP1)=D(I)
DO 25 J=1,KMI
25 A(I,J)=B(I,J)
DO 15 N=2,MP1
15 A(1,N)=A(1,N)/A(1,1)
DO 7 J=2,MP1
M=0
L=J-1
DO 7 I=2,KMI
M=M+1
IF(M-L) 10,10,9
9 M=L
10 DO 6 N=1,M
6 A(I,J)=A(I,J)-A(N,J)*A(I,N)
IF(I-J) 12,7,7
12 A(I,J)=A(I,J)/A(I,I)
7 CONTINUE
DO 11 II=1,KMI
DEBUG(A(II,II),II=1,MP1)
11 CONTINUE
DET=1.0
DO 2 I=1,KMI
B(I,MP1)=A(I,I)*A(I,MP1)**2
DET=DET*A(I,I)
2 A(I,I)=1./A(I,I)
DO 3J=1,MM1
N=J+1
DO 4I=N,KMI
KJ=J
MJ=I-N
A(I,J)=A(I,J)+A(I,KJ)*A(KJ,J)
IF(MJ) 4,4,5
5 DO 16 K=1,MJ
KJ=KJ+1
16 A(I,J)=A(I,J)+A(I,KJ)*A(KJ,J)
4 A(I,J)=-A(I,J)*A(I,I)
3 CONTINUE
DO 17 J=1,MM1
KJ=KMI-J
DO 8 I=1,KJ
DO 8 K=1,J
KK=MP1-K
8 A(KJ,I)=A(KJ,I)-A(KJ,KK)*A(KK,I)
17 CONTINUE
DO 19 J=1,MM1
KK=KMI-J
KJ=MP1-J
DO 110 I=KJ,KMI
110 A(MP1,I)=A(KK,I)
DO 111 K=KJ,KMI
A(KK,K)=0.
DO 111 L=KJ,KMI

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DIN00000
DIN00010
DIN00020
DIN00030
DIN00040
DIN00050
DIN00060
DIN00070
DIN00080
DIN00090
DIN00100
DIN00110
DIN00120
DIN00130
DIN00140
DIN00150
DIN00160
DIN00170
DIN00180
DIN00190
DIN00200
DIN00210
DIN00220
DIN00230
DIN00240
DIN00250
DIN00260
DIN00270
DIN00280
DIN00290
DIN00300
DIN00310
DIN00320
DIN00330
DIN00340
DIN00350
DIN00360
DIN00370
DIN00380
DIN00390
DIN00400
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DIN00470
DIN00480
DIN00490
DIN00500
DIN00510
DIN00520
DIN00530
DIN00540
DIN00550
DIN00560
DIN00570
DIN00580
DIN00590
DIN00600

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111 A(KK,K)=A(KK,K)-A(MP1,L)*A(L,K)	DIN00610
19 CONTINUE	DIN00620
DO 88 II=1,KM1	DIN00630
DEBUG(A(II,JJ),JJ=1,MP1)	DIN00640
88 CONTINUE	DIN00650
REWIND 7	DIN00660
WRITE (7) ((B(I,J),I=1,KM1),J=1,KM1)	DIN00670
DO 114 I=1,KM1	DIN00680
DO 112 J=1,KM1	DIN00690
AN(J)=0.	DIN00700
DO 112 K=1,KM1	DIN00710
112 AN(J)=AN(J)+B(I,K)*A(K,J)	DIN00720
DO 114 II=1,KM1	DIN00730
B(I,II)=(-AN(II))	DIN00740
IF (II-I) 114,113,114	DIN00750
113 B(I,II)=B(I,II)+1.	DIN00760
114 CONTINUE	DIN00770
DO 117 I=1,KM1	DIN00780
DO 115 J=1,KM1	DIN00790
AN(J)=0.	DIN00800
DO 115 K=1,KM1	DIN00810
115 AN(J)=AN(J)+A(I,K)*B(K,J)	DIN00820
DO 116 II=1,KM1	DIN00830
116 A(I,II)=A(I,II)+AN(II)	DIN00840
117 CONTINUE	DIN00850
DO 18 II=1,KM1	DIN00860
DEBUG(A(II,JJ),JJ=1,MP1)	DIN00870
DEBUG(B(II,JJ),JJ=1,MP1)	DIN00880
18 CONTINUE	DIN00890
REWIND 7	DIN00900
READ (7) ((B(I,J),I=1,KM1),J=1,KM1)	DIN00910
ERR=0.	DIN00920
DO 20 I=1,KM1	DIN00930
DO 20 K=1,KM1	DIN00940
ERR1=0.	DIN00950
DO 21 J=1,KM1	DIN00960
21 ERR1=B(I,J)*A(J,K)+ERR1	DIN00970
IF (I-K) 23,22,23	DIN00980
22 ERR1=1.-ERR1	DIN00990
23 ERR1=ABS(ERR1)	DIN01000
IF (ERR-ERR1) 24,20,20	DIN01010
24 ERR=ERR1	DIN01020
20 CONTINUE	DIN01030
RETURN	DIN01040
END	DIN01050

\$IBFTC DSLV	LIST,DECK,DEBUG	DSL00000
C	SUBROUTINE TO OBTAIN SOLUTION VECTOR FROM INVERSE B	DSL00010
C		DSL00020
C	SOLUTION VECTOR IS RETURNED IN THE AN ARRAY AND IN ((B(I,NP1),I=1,NNN)	DSL00030
C	WHICH IS THE AUGMENTED MATRIX INVERTED	DSL00040
C		DSL00050
	SUBROUTINE DMVMUL(B,NNN,D,AN,MAX)	DSL00060
	DIMENSION B(MAX,MAX),D(MAX),AN(MAX)	DSL00070
	DOUBLE PRECISION B,D,AN	DSL00080
	M=NNN	DSL00090
	NP1=NNN+1	DSL00100
	DO 100 I=1,M	DSL00110
	AN(I)=0.	DSL00120
	DO 100 J=1,M	DSL00130
100	AN(I)=B(I,J)*D(J)+AN(I)	DSL00140
	DO 11 II=1,M	DSL00150
	DEBUG(B(II,JJ),JJ=1,M)	DSL00160
11	CONTINUE	DSL00170
	DEBUG(AN(II),II=1,M)	DSL00180
	DO 4 I=1,NNN	DSL00190
4	B(I,NP1)=AN(I)	DSL00200
	WRITE (6,15)	DSL00210
	DO 14 J=1,M	DSL00220
	DO 13 I=1,M	DSL00230
13	B(MP1,I)=B(I,J)/SQRT(B(I,I)*B(J,J))	DSL00240
14	WRITE (6,16)(B(MP1,K),K=1,M)	DSL00250
15	FORMAT(20H0CORRELATION MATRIX=)	DSL00260
16	FORMAT(1H08G16.8)	DSL00270
	RETURN	DSL00280
	END	DSL00290

\$IBFTC CAL	LIST,DECK	CAL00000
	SUBROUTINE CALC(X,Y,N,K,P)	CAL00010
C		CAL00020
C	DETERMINE AN EMULSION CALIBRATION CURVE FOR INPUT TO LAGRANGE	CAL00030
C	INTERPOLATION ROUTINE.	CAL00040
	COMMON IW	CAL00050
	DIMENSION X(250),Y(500),P(35)	CAL00060
1	XX=2.	CAL00070
	XSTOP=95.	CAL00080
	X(1)=XX	CAL00090
	DO 10 I=1,10	CAL00100
	N=I	CAL00110
	YY=P(1)+P(2)*XX+P(3)*XX**2+P(4)*XX**3 +P(5)*XX**4	CAL00120
	XX=YY	CAL00130
	X(I+1)=YY	CAL00140
	IF (XX-XSTOP) 10,10,20	CAL00150
10	CONTINUE	CAL00160
20	K=N-1	CAL00170
	NN=N	CAL00180
4	DO 30 I=1,N	CAL00190
	Y(I)=2.**NN	CAL00200
	NN=NN-1	CAL00210
30	CONTINUE	CAL00220
	N=N+1	CAL00230
	X(N)=100.	CAL00240
	Y(N)=0.	CAL00250
	WRITE(6,99)	CAL00260
	WRITE(6,103) (X(I),Y(I),I=1,N)	CAL00270
99	FORMAT(1H0,100H X VS. Y (DEFINES EMULSION CALIBRATION	CAL00280
	XCURVE) FOR INPUT TO LAGRANGE ROUTINE.)	CAL00290
103	FORMAT(1H0,2F10.4)	CAL00300
	IW=0	CAL00310
101	RETURN	CAL00320
	END	CAL00330

\$IBFTC LGRN	LIST,DECK,DEBUG	LGR00000
	SUBROUTINE LGRNGE(X,Y,N,ARG,ANS,DER,KODE)	LGR00010
	DIMENSION X(200),Y(200),A(10),C(4)	LGR00020
	EQUIVALENCE (XX,A(1)),(X0,A(2)),(X1,A(3)),(X2,A(4)),(X3,A(5)),	LGR00040
	1(Y0,A(6)),(Y1,A(7)),(Y2,A(8)),(Y3,A(9)),(C1,C(1)),(C2,C(2)),(C3,C(LGR00050
	23)),(C4,C(4))	LGR00060
	IF(ARG-X(2))10,10,11	LGR00070
10	MX=1	LGR00080
	GO TO 51	LGR00090
11	IF(ARG-X(N-1)) 12,12,13	LGR00100
13	MX=N-3	LGR00110
	GO TO 51	LGR00120
12	K=N-1	LGR00130
	DO 14 JA=2,K	LGR00140
	IF(ARG-X(JA))15,15,14	LGR00150
15	MX=JA-2	LGR00160
	GO TO 51	LGR00170
14	CONTINUE	LGR00180
51	IF(KODE-1)1,2,1	LGR00190
1	CON=0.0	LGR00200
	GO TO 50	LGR00210
2	CON=1.	LGR00220
50	XX=ALOG(ARG+CON)	LGR00230
	DO 3 I=1,4	LGR00240
	MXI=MX+I-1	LGR00250
	A(I+1)=ALOG(X(MXI)+CON)	LGR00260
3	A(I+5)=ALOG(Y(MXI)+CON)	LGR00270
	DEBUG XX,X0,X1,X2,X3	LGR00280
	ANS=((XX-X1)*(XX-X2)*(XX-X3)/((X0-X1)*(X0-X2)*(X0-X3)))*Y0 +((XX-X0)	LGR00290
	1)*(XX-X2)*(XX-X3) *Y1/((X1-X0)*(X1-X2)*(X1-X3)) +(XX-X0)*(XX-X1)*	LGR00300
	2(XX-X3)*Y2/((X2-X0)*(X2-X1)*(X2-X3))+((XX-X0)*(XX-X1)*(XX-X2)*Y3/	LGR00310
	3((X3-X0)*(X3-X1)*(X3-X2))	LGR00320
	ANS=EXP(ANS)-CON	LGR00330
	DEBUG ANS	LGR00340
	GO TO (5,4),KODE	LGR00350
4	DO 7 I=2,5	LGR00360
7	C(I-1)=XX-A(I)	LGR00370
	CC0=Y0/(X0-X1)/(X0-X2)/(X0-X3)	LGR00380
	CC1=Y1/(X1-X0)/(X1-X2)/(X1-X3)	LGR00390
	CC2=Y2/(X2-X0)/(X2-X1)/(X2-X3)	LGR00400
	CC3=Y3/(X3-X0)/(X3-X1)/(X3-X2)	LGR00410
	DER=ANS/ARG*(CC0*(C2*C3+C2*C4+C3*C4)+CC1*(C1*C3+C1*C4+C3*C4)+CC2*(LGR00420
	1C1*C2+C1*C4+C2*C4)+CC3*(C1*C2+C1*C3+C2*C3))	LGR00430
5	RETURN	LGR00440
	END	LGR00450

\$IBFTC RAT	LIST,DECK	RAT00000
	SUBROUTINE FATID (NEL,Z,ZB)	RAT00010
C		RAT00020
C	COMPUTES RATIO OF RELATIVE INTENSITY OF AN ELEMENT TO RELATIVE	RAT00030
C	INTENSITY OF A STANDARD, MAXIMUM NUMBER OF STANDARDS IS FOUR,	RAT00040
C	MAXIMUM NUMBER OF ELEMENTS IS FIFTY.	RAT00050
C		RAT00060
	REAL MIS	RAT00070
	COMMON Iw,KSTOP,NEXP	RAT00080
	COMMON Z(50,11,7),ZB(50,11,7)	RAT00090
	COMMON EL(50)	RAT00100
	DIMENSION RAT (11,4,7),XRAT(11,4,7),AVG(11,4),XAVG(11,4)	RAT00110
	DATA RIEN,ETOILE/6H ,3H* /	RAT00120
	DIMENSION MIS(11,4,7)	RAT00130
	WRITE(6,98)	RAT00140
	WRITE(6,99)(FL(I),I=1,KSTOP)	RAT00150
	WRITE(6,101)	RAT00160
	WRITE(6,105)	RAT00170
	WRITE(6,106)	RAT00180
	KST=KSTOP+1	RAT00190
	DO 40 I=KST,NEL	RAT00200
	DO 30 KK=1,KSTOP	RAT00210
	DO 20 J=1,NEXP	RAT00220
	M=I	RAT00230
	XN=0.	RAT00240
	XNN=0.	RAT00250
	XAVG(J,KK)=0.	RAT00260
	AVG(J,KK)=C.	RAT00270
	SUM=0.	RAT00280
	SUM1=0.	RAT00290
	DO 10 K = 1,7	RAT00300
	N=K	RAT00310
	L=K	RAT00320
	RAT(J,KK,K)=0.	RAT00330
	XRAT(J,KK,K)=0.	RAT00340
	IF(I-KST)1,4,1	
	4 MIS(J,KK,K)=RIEN	RAT00360
C		RAT00370
C	ARRAY MIS SHOWS PROGRAM EXTRAPOLATED A REL INTENSITY IF THERE WAS	RAT00380
C	NO ORIGINAL DATA FOR THAT EXPOSURE AND STEP.	RAT00390
C		
	1 IF (Z(I,J,K))2,6,2	
	6 IF (MIS(J,KK,K)-ETOILE)10,7,10	
	7 Z(KK,J,K)=0.	
	MIS(J,KK,K)=RIEN	
	GO TO 10	
	2 IF (Z(KK,J,K)) 3,11,3	RAT00410
C	TEST FOR BACKGROUND	RAT00420
	3 IF (ZB(I,J,K)) 32,5,32	RAT00430
	5 IF (ZB(KK,J,K)) 32,31,32	RAT00440
C	IF IN STEP 7 GO TO 21 AND START SEARCHING LOWER STEPS.	RAT00450
C	IF NOT IN STEP 7 START SEARCHING HIGHER STEPS.	RAT00460
	11 IF (L-7) 12,21,21	RAT00470
	12 L = L+1	RAT00480
	N=L-K	RAT00490
	IF(Z(KK,J,L)) 13,11,13	RAT00500
C	CORRECT FOR STEP MOVEMENTS	RAT00510
	13 Z(KK,J,K) = Z(KK,J,L) * 2.**N	RAT00520
	MIS(J,KK,K)=ETOILE	RAT00530
	14 IF (ZB(KK,J,L)) 15,3,15	RAT00540
	15 ZB(KK,J,K) = ZB(KK,J,L) * 2.**N	RAT00550
	GO TO 32	RAT00560
C	START SEARCH OF LOWER STEPS	RAT00570

21 IF (L-7) 11,22,22	RAT00580
22 L = L-1	RAT00590
IF(Z(KK,J,L)) 23,27,23	RAT00600
23 N = K-L	RAT00610
C CORRECT FOR STEP MOVEMENT	RAT00620
Z(KK,J,K)=Z(KK,J,L)/2.**N	RAT00630
MIS(J,KK,K)=ETOILE	RAT00640
ZB(KK,J,K)=ZB(KK,J,L)/2.**N	RAT00650
IF(ZB(KK,J,L)) 32,3,32	RAT00660
27 IF (L-1) 10,10,22	RAT00670
C DETERMINE RATIO	RAT00680
32 RAT(J,KK,K) = (Z(I,J,K) - ZB(I,J,K))/(Z(KK,J,K) - ZB(KK,J,K))	RAT00690
XN=XN+1.	RAT00700
31 XRAT(J,KK,K) = Z(I,J,K) / Z(KK,J,K)	RAT00710
XNN=XNN+1.	RAT00720
33 SUM = SUM + RAT(J,KK,K)	RAT00730
SUM1=SUM1+XRAT(J,KK,K)	RAT00740
10 CONTINUE	RAT00750
IF(SUM)35,34,35	RAT00760
35 AVG(J,KK) = SUM/XN	RAT00770
34 IF(SUM1) 36,20,36	RAT00780
36 XAVG(J,KK) = SUM1/XNN	RAT00790
20 CONTINUE	RAT00800
30 CONTINUE	RAT00810
WRITE(6,102) (EL(I),EL(KK),KK=1,KSTOP)	RAT00820
IF(KSTUP-2)47,47,46	RAT00830
47 KLJ=2	RAT00840
NN=0	RAT00850
GO TO 45	RAT00860
46 KLJ=1	RAT00870
NN=1	RAT00880
45 DO 50 J=1,NEXP,KLJ	RAT00890
LJ=J+1	RAT00900
WRITE(6,104)	RAT00910
DO 51 JJ=1,7	RAT00920
WRITE(6,100) J,JJ,(RAT(J,KK,JJ),XRAT(J,KK,JJ),MIS(J,KK,JJ),KK=1,	RAT00930
XKSTOP)	RAT00940
IF(NN)51,53,51	RAT00950
51 WRITE(6,107) LJ,JJ,(RAT(LJ,KK,JJ),XRAT(LJ,KK,JJ),MIS(LJ,KK,JJ),KK	RAT00960
X=1,KSTOP)	RAT00970
51 CONTINUE	RAT00980
WRITE(6,103) (AVG(J,KK),XAVG(J,KK),KK=1,KSTOP)	RAT00990
IF(NN)50,48,50	RAT01000
48 WRITE(6,108) (AVG(LJ,KK),XAVG(LJ,KK),KK=1,KSTOP)	RAT01010
50 CONTINUE	RAT01020
40 CONTINUE	RAT01030
C	RAT01040
C	RAT01050
C	RAT01060
98 FORMAT(1H1)	RAT01070
99 FORMAT(1H2,57X,16HINTENSITY RATIOS //,37X,59H THE FOLLOWING-ELEMENRAT09300	
XNTS ARE CONSIDERED INTERNAL STANDARDS- //,46X,(4(A6,4X)))	RAT09350
100 FORMAT(1H ,214,4X,(4(2G11.4,A3)))	RAT09380
101 FORMAT(1H0,15X,105H COLUMNS 1,4,7,10 ARE BACKGROUND CORRECTED RATIO	RAT01110
XOS. COLS. 2,5,8,11 ARE THE UNCORRECTED RATIOS.)	RAT01120
102 FORMAT(1H1,12H EXP STEP ,X,4(A6,2H /,A6,11X))	RAT09500
103 FORMAT(1H ,5X,3HAVG,4X,(4(2G11.4,3X)))	RAT01140
104 FORMAT(1H0)	RAT01150
105 FORMAT(1H0,35X,60H * IN COL. 3,6,9,12 MEANS VALUE OF STD. IS EXTRARAT01160	
XPOLATED.)	RAT01170
106 FORMAT(1H0,32X,64H A BLANK IN THESE COLUMNS MEANS RATIO WAS CALCURAT01180	
XLATED DIRECTLY.)	RAT01190
107 FORMAT(1H+60X,214,(2(2G11.4,A3)))	RAT01200
108 FORMAT(1H+64X,3HAVG,2X,(2(2G11.4,3X)))	
RETURN	RAT01220
END	RAT01230

APPENDIX C

SAMPLE OUTPUT FROM SUBROUTINE RATIO

The following output is a typical example from the subroutine RATIO:

INTENSITY RATIOS

THE FOLLOWING ELEMENTS ARE CONSIDERED INTERNAL STANDARDS-

A 4044 W 4008 AG2929 AG3501

COLUMNS 1,4,7,10 ARE BACKGROUND CORRECTED RATIOS. COLS. 2,5,8,11 ARE THE UNCORRECTED RATIOS.

* IN COL. 3,6,9,12 MEANS VALUE OF STD. IS EXTRAPOLATED.

A BLANK IN THESE COLUMNS MEANS RATIO WAS CALCULATED DIRECTLY.

EXP	STEP	NI3566 /A 4044		NI3566 /W 4008		NI3566 /AG2929		NI3566 /AG3501		
1	1	C.1459	0.1743	* 32.655	5.0638	0.3581	0.4277	0.1020	0.1218	*
1	2	C	0	0	0	0	0	0	0	
1	3	0	0	0	0	0	0	0	0	
1	4	0	0	0	0	0	0	0	0	
1	5	C	0	0	0	0	0	0	0	
1	6	C	0	0	0	0	0	0	0	
1	7	C	0	0	0	0	0	0	0	
	AVG	0.1459	0.1743	32.655	5.0638	0.3581	0.4277	0.1020	0.1218	
2	1	C	0	0	0	0	0	0	0	
2	2	0	0.8380	* 0	0.8663E-01*	0	0.2285	* 0	0.1537	*
2	3	C	0.8498	0	0.8785E-01*	0	0.2317	* 0	0.1558	*
2	4	C	0.9295	0	0.8646E-01*	0	0.2281	* 0	0.1534	*
2	5	C	0	0	0	0	0	0	0	
2	6	0	0	0	0	0	0	0	0	
2	7	C	0	0	0	0	0	0	0	
	AVG	0	0.8724	0	0.8698E-01	0	0.2294	0	0.1543	
3	1	C	0	0	0	0	0	0	0	
3	2	0	0	0	0	0	0	0	0	
3	3	C	0	0	0	0	0	0	0	
3	4	0	2.9449	* 0	0.1648	* 0	0.8834	0	0.6593	
3	5	0	3.1737	* 0	0.1776	* 0	0.9145	0	0.7719	
3	6	0	0	0	0	0	0	0	0	
3	7	0	0	0	0	0	0	0	0	
	AVG	0	3.0553	0	0.1712	0	0.8990	0	0.7156	
4	1	C.2297	0.2774	* 0.3154E-01	0.3810E-01*	0.6918E-01	0.8356E-01*	0.5894E-01	0.7119E-01*	
4	2	0.2630	0.2818	0.3611E-01	0.3870E-01*	0.7920E-01	0.8488E-01*	0.6748E-01	0.7231E-01*	
4	3	C	0	0	0	0	0	0	0	
4	4	0	0	0	0	0	0	0	0	
4	5	0	0	0	0	0	0	0	0	
4	6	0	0	0	0	0	0	0	0	
4	7	C	0	0	0	0	0	0	0	
	AVG	0.2463	0.2796	0.3383E-01	0.3840E-01	0.7419E-01	0.8422E-01	0.6321E-01	0.7175E-01	

5	1	C.5671E-01	0.1359	*	0.7482E-02	0.1052E-01*	0.4045E-01	0.5685E-01*	0.3139E-01	0.4412E-01*
5	2	0.1244	0.1379		0.9628E-02	0.1067E-01*	0.5206E-01	0.5769E-01*	0.4040E-01	0.4477E-01*
5	3	C	0		0	0	0	0	0	0
5	4	0	0		0	0	0	0	0	0
5	5	0	0		0	0	0	0	0	0
5	6	0	0		0	0	0	0	0	0
5	7	0	0		0	0	0	0	0	0
	AVG	C.1106	0.1369		0.8555E-02	0.1059E-01	0.4625E-01	0.5727E-01	0.3590E-01	0.4445E-01
6	1	C	0		0	0	0	0	0	0
6	2	C	0		0	0	0	0	0	0
6	3	0	0		0	0	0	0	0	0
6	4	0	4.9703	*	0	0.7166	0	0.9195	0	0.6623
6	5	0	5.0939	*	0	0.7344	0	0.8736	0	0.7682
6	6	0	0		0	0	0	0	0	0
6	7	0	0		0	0	0	0	0	0
	AVG	C	5.0321		0	0.7255	0	0.8965	0	0.7153
7	1	0	0		0	0	0	0	0	0
7	2	0	0.8036		0	0.1225	*	0.2686	*	0.2009
7	3	C	1.0517		0	0.1363	*	0.2988	*	0.2235
7	4	0	0		0	0	0	0	0	0
7	5	0	0		0	0	0	0	0	0
7	6	0	0		0	0	0	0	0	0
7	7	0	0		0	0	0	0	0	0
	AVG	0	0.9276		0	0.1294	0	0.2837	0	0.2122
8	1	C	C.4080	*	0	0.9922E-01*	0	0.1167	*	0
8	2	C	0.4189	*	0	0.1019	*	0.1199	*	0
8	3	0	0		0	0	0	0	0	0
8	4	0	0		0	0	0	0	0	0
8	5	0	0		0	0	0	0	0	0
8	6	0	0		0	0	0	0	0	0
8	7	0	0		0	0	0	0	0	0
	AVG	0	0.4135		0	0.1005	0	0.1183	0	0.9329E-01

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