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by

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ALLCAL: AN INTERACTIVE BASIC PROGRAM FOR SPECTROCHEMICAL CALCULATIONS

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ABSTRACT

An interactive program, ALLCAL, has been developed at Los Alamos Scientific Laboratory (LASL) to calculate the results of spectrochemical measurements of impurities in production samples. The program generates a working curve from input data of standard samples to calculate the impurity concentrations.

ALLCAL permits use by individuals with minimal programming experience; it is truly interactive in providing periodic means to edit, modify, and change incorrect data that might have been introduced through various human error factors affecting any computer program, without the need to terminate and reinitialize after such editing. The program can be used as a research tool to manipulate data with minimum effort and eliminates repetitive input data from its operation. It also provides the spectroscopist a comparison mode to evaluate the effect of the use or nonuse of a given internal standard. ALLCAL accepts either optical density or percent transmittance data from photographic plates and films.

The program is written in BASIC language for a minicomputer with 28 000 octal words of core memory and has been shown to be adaptable to another computer system with slight modifications.

I. INTRODUCTION

Photographic methods are used for nearly all spectrochemical measurements at the Los Alamos Scientific Laboratory (LASL). Quantitative input data for the production samples is obtained with microphotometers as either percent transmittances or optical densities. Because many different spectrographs and photographic emulsions are used at LASL, the individual variations in their responses must be considered in the spectrochemical calculations. ALLCAL provides that capability.

II. THE ALLCAL PROGRAM

During past work on spectrochemical calculations at LASL, a preliminary program* was developed which performed satisfactorily but which had certain limitations. It could only receive numerical input and emulsion calibration values for a single photographic emulsion.

*LASL Identification No. LP-203. Described at the Rocky Mountain Spectroscopy Conference, Denver, CO, August 23, 1972, by the author and associates.

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The earlier program has been modified and expanded to accept alphanumeric input and to include reference tables of emulsion coefficients for all film and plate emulsions in the spectrographic laboratory. Designated ALLCAL (App. A), the improved program is written in the BASIC/RT-11 language¹ for use with a PDP-11 minicomputer,* also, it has been slightly modified and proven for use with KRONOS.**

ALLCAL uses the input data of the standards to generate a least squares working curve relating the logarithm of the intensity ratio to the logarithm of the concentration. With this curve, concentrations of the impurity elements in samples are then calculated. To enhance the program's operation, input data need be introduced only once; furthermore, to counteract the human factor of real people providing incomplete tabular data or data containing typographical errors, the program has an interactive feature which permits correction, deletion, or insertion of data as a part of the program run. This editing capability has probably contributed more than any other feature to the general acceptance of this program at LASL. It is a "Real Time—Real People" program.

III. ALLCAL HARDWARE

The minimum hardware configuration used at LASL for ALLCAL is the PDP-11 minicomputer, a Digital Equipment Corporation DECTape bulk storage device, and an ASR-33 TTY input-output terminal. The terminal is used for normal input and output of data during program execution and also provides access for the user to the several interactive EDIT subroutines incorporated in the program. As stated above, other computer systems such as KRONOS could be employed with slight modifications to the program.

IV. DATA INPUT

To give ALLCAL maximum possible flexibility, photometric data can be entered as optical densities or percent transmittances. A number of different emulsion calibration tables are included in the

*Manufactured by Digital Equipment Corporation (DEC), Maynard, MA.

**Produced by Control Data Corporation, Arden Hills, MN. One of the time-shared LASL computer systems.

program, any of which may be selected on the basis of the emulsion and spectrograph used. Also, the user may enter his own table of values. One has the option of using or ignoring the internal standard data and/or the background data as input. Standard base concentrations and sample numbers are entered at the beginning of the run, with identification numbers assigned. Gravimetric factors (including dilution factors) for different matrices are entered, as are element impurity levels. For example, with standard base concentrations of 1, 10, and 100 $\mu\text{g/g}$ for iron standards having an impurity level of 1 and for boron standards with an impurity level of 0.1, the nominal concentrations for iron standards are 1, 10, and 100 $\mu\text{g/g}$ and those for boron are 0.1, 1, and 10 $\mu\text{g/g}$.

Internal standard data (when needed), standard base data, and sample number data are always entered as input in their entirety. The program assigns "rack numbers" to the data as subscripts or data correlation numbers. Analytical line data for a given impurity element are then entered by identifying rack number to facilitate selection of the correct internal standard for a given impurity element intensity. Entering a zero for an impurity element optical density or percent transmittance omits that value from the calculating algorithm and the subsequent output.

V. EDIT SUBROUTINES

At selected points in the program, usually following the input of a long table, the program will ask the user "EDIT? YES=1, NO=0." If the user is confident that there are no input errors, he types "0" followed by a carriage return, and the program continues with execution of the input data to that point. If input data need to be corrected, the user types "1" followed by a carriage return, and a subroutine is called which interactively assists in the required corrections. The EDIT subroutines always terminate by repeating the question "EDIT? YES=1, NO=0." This permits corrections of more than one error in an input table or of errors generated while editing. This feature also allows changing impurity standard data without the need of reentering all impurity sample data.

Normal usage of the EDIT subroutines is shown in the first EDIT usage of a typical run (App. B), by the correction of the internal standard values in rack position 4 and by the correction of the gravimetric factor in sample number GRW-7007-A. Another example is shown on page 17, App. B, under

$$\text{Log } E = F + G \log R ,$$

where E is the calculated concentration, R is the intensity ratio, F is the least square intercept as calculated in the program run, and G is the calculated first-degree coefficient. Higher order fits have been tried but have generally been less satisfactory than the linear fit, particularly when analyzing samples of known composition.

The algorithm calculates the deviation of each standard from the computed curve and then calculates the average deviation of all standards from the curve in order to give one a feeling of how well the curve fits the data. The computed curve is then used to convert intensity ratios of samples into impurity concentrations. For replicate samples, averages and relative standard deviations are calculated and printed in the output.

VIII. SUMMARY AND CONCLUSIONS

This program has been used in our emission spectrographic laboratory for the past 14 months. Compared to hand-calculating, it offers the advantages of least square curve-smoothing and a time savings of 10-20 min per impurity element. The interactive

feature of the program provides the options of correcting, modifying, or deleting input data; omitting internal standard and/or background data from input; and comparing values calculated using an internal standard with those calculated using no internal standard. Each point in the program requiring input from the user explains at the terminal what type of input is expected before halting and waiting for the user's response. The simplicity of use, coupled with the program's versatility and on-the-spot editing capabilities on a periodic basis, have contributed greatly to its general acceptance at LASL.

REFERENCES

1. "BASIC/RT-11 Language Reference Manual," Digital Equipment Corporation Manual DEC-11-LBACA-B-D (1973).
2. J. R. Phillips, J. V. Pena, and C. T. Apel, Los Alamos Scientific Laboratory, unpublished data, 1969.
3. "Photographic Photometry in Spectrochemical Analysis," ASTM Method E 116, 1974 Annu. Book ASTM Stand., Part 42 (July 1974).

APPENDIX A

LASL Identification

PROGRAM LISTING - ALLCAL

No. LP-0549

THE FOLLOWING LISTING OF ALLCAL WAS MADE FROM A DEC PDP-11/20 COMPUTER WITH 28K OF MEMORY. REMARK (REM-) STATEMENTS ARE USED TO CONVEY PERTINENT INFORMATION AND TO DEFINE ALL VARIABLES. FOR THE MOST PART, PRINT STATEMENTS ARE SELF-EXPLANATORY.

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1 REM- PROGRAM NAME "ALLCAL" FEBRUARY 23, 1973 - THIS PROGRAM IS INTENDED
2 REM- TO RUN ON A 28K PDP-11/20 COMPUTER EQUIPPED WITH AN ASR-33 TTY
3 REM- FOR INPUT-OUTPUT AND A DISK OR DECTAPE FOR BULK STORAGE.
4 REM- SOFTWARE USED IS DIGITAL EQUIPMENT RT-11/BASIC. PROGRAM HAS
5 REM- NOT BEEN TESTED IN LESS THAN 28 K. DELETE ALL REMARK STATEMENTS
6 REM- BEFORE PROGRAM EXECUTION. PROGRAM USES CONVENTION FOR
7 REM- RESPONSES - YES = 1, NO = 0.
10 DIM X4(4,40),I4(4,40),K(20),H10(40),C1(40),X3(20),Y3(80),R(80)
20 DIM Z(80),F(80),B(2),D1(20),C0(5,8),C2(5,8),C1(5,8),M1(20)
30 DIM I(20),W3(5,8),W5(5,8),N1(8),S1(40),S3(40),X1(80),X2(80)
40 PRINT "PROGRAM - ALLCAL - HAS EVERYBODY'S COEFFICIENTS"
50 PRINT "APRIL 17, 1974 C. APEL"
70 W1=0
75 REM- W1 IS WAVELENGTH FLAG, USED TO TEST FOR THE
76 REM- EXISTENCE OF DATA IN THE SECOND HALF OF THE PROGRAM.
80 READ N2
85 REM- N2 IS THE NUMBER OF PHOTOGRAPHIC EMULSION DATA SETS USED.
90 FOR K=1 TO N2:READ E$(K):READ N1(K)
95 REM- E$(K) IS AN EMULSION DATA SET LABEL.
96 REM- N1(K) IS NUMBER OF WAVELENGTH REGIONS FOR A GIVEN EMULSION.
100 FOR L=1 TO N1(K)
110 READ W5(L,K),W3(L,K),C0(L,K),C1(L,K),C2(L,K):NEXT L
112 REM- W5(L,K) AND W3(L,K) ARE LOWER AND UPPER BOUNDARIES FOR
113 REM- EMULSION CALIBRATION WAVELENGTH REGIONS.
114 REM- C0(L,K) IS 0 DEGREE SEIDEL COEFFICIENT FOR REGION "L".
115 REM- C1(L,K) " 1ST " " " " " "
116 REM- C2(L,K) " 2ND " " " " " "
120 NEXT K
130 FOR K=1 TO N2
140 PRINT E$(K);"? YES=1 NO=0";\INPUT B1\IF B1=1GO TO 260
141 REM- B1 IS YES-NO SWITCH FOR EMULSION DATA SET CHOICE.
150 IF B1>1GO TO 140
160 NEXT K
170 LET K=N2+1
180 PRINT "TO ENTER YOUR OWN COEFFICIENTS. INPUT NUMBER OF REGIONS";
190 E$(K)="USER INPUT"
195 REM- NOT SATISFIED ? --- THEN INPUT YOUR OWN VALUES ! ! !
200 INPUT N1(K)
210 FOR L=1 TO N1(K)
220 PRINT "REGION WAVELENGTHS-LOW,HIGH";\INPUT W5(L,K),W3(L,K)
230 PRINT "0 DEGREE COEFFICIENT";\INPUT C0(L,K)
240 PRINT "1ST DEGREE COEFFICIENT";\INPUT C1(L,K)
250 PRINT "2ND DEGREE COEFFICIENT";\INPUT C2(L,K):NEXT L
260 G2=K:\PRINT "VERIFY COEFFICIENTS? YES=1, NO=0";\INPUT B2
265 REM- B2 IS YES-NO SWITCH FOR DATA VERIFICATION.
270 IF B2>1GO TO 260
280 IF B2=0GO TO 330
290 PRINT E$(G2):\PRINT N1(G2)
300 PRINT "LOW", "HIGH", "C0", "C1", "C2"
310 FOR L=1 TO N1(G2)
320 PRINT W5(L,G2),W3(L,G2),C0(L,G2),C1(L,G2),C2(L,G2):NEXT L
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330 RESTORE
340 PRINT "REDO CALIBRATION INPUT? YES=1 NO=0";\INPUT B3
345 REM- B3 IS YES-NO SWITCH FOR REPEATING EMULSION DATA SELECTION
350 IF B3=1 GO TO 80
360 IF B3>1 GO TO 350
370 DEF FNY(Z)=(LOG(Z))*434294
375 REM- FNY(Z) IS FUNCTION FOR CONVERTING NATURAL LOGS TO BASE 10.
380 PRINT "LOG SHEET NUMBER ";\INPUT N5
385 REM- N5 IS LOG SHEET OR OTHER RUN IDENTIFICATION NUMBER.
390 PRINT "DENSITIES(1) OR TRANSMITTANCES(2) ";\INPUT P1
395 REM- P1 IS SWITCH FOR DATA INPUT AS 1 (DENSITIES) OR 2 (TRANSMITTANCES).
400 IF P1<1 GO TO 390
410 IF P1>2 GO TO 390
420 PRINT "READ? (1)ALL, (2)NO I.S., (3)NO BKG., (4)LINE ONLY";
430 INPUT O
435 REM- O IS SWITCH DETERMINING IF INTERNAL STANDARDS OR BACKGROUNDS ARE USED.
440 IF O>4 GO TO 430
450 IF O<1 GO TO 430
460 PRINT "MAXIMUM NUMBER OF RACK POSITIONS";\INPUT J1
470 PRINT "MAXIMUM NUMBER OF STANDARDS";\INPUT J2
480 PRINT "MAXIMUM NUMBER OF SAMPLE NUMBERS";\INPUT J3
485 REM- J1,J2 & J3 ARE SELF-EXPLANATORY.
490 C6=0\VI=0
495 REM- C6 IS FLAG FOR ENTERING NEW INTERNAL STANDARD DATA.
497 REM- VI IS EDIT FLAG - EDIT MODE IS VI=1, NORMAL RUN IS VI=0.
500 U1=1\U2=J1
505 REM- U1 AND U2 ARE RACK NUMBER SUBSCRIPTS USED IN EDIT MODE.
510 FOR L=U1 TO U2\Y3(L)=1\NEXT L
515 REM- ALL Y(3)'S=1 KEEP US FROM ACCIDENTALLY DIVIDING BY ZERO LATER.
520 IF O=2 GO TO 710
530 IF O=4 GO TO 710
540 PRINT "I.S. ELEMENT NAME";\INPUT E2S
550 PRINT "I.S. WAVELENGTH";\INPUT W2\W4=W2\COSUB 2420
555 REM- WE NOW GO CHOOSE PROPER CALIBRATION COEFFICIENTS FOR
560 REM- THE WAVELENGTH REGION CONTAINING THE INTERNAL STANDARD LINE.
557 REM- W4 IS WAVELENGTH OVERLAY FOR ABOVE CALCULATION.
560 G=L\O2=G
565 REM- G IS SUBSCRIPT FOR COEFFICIENTS CALCULATED ABOVE.
566 REM- O2 IS SUBSCRIPT FOR INTERNAL STD. EMULSION CALB. COEFFICIENTS.
570 IF O=1 GO TO 590
580 PRINT "RACK#, I.S. "\IF O=3 GO TO 600
590 PRINT "RACK=, I.S., I.BKG."
600 FOR L=U1 TO U2\PRINT L;
605 REM- L=RACK NUMBER OR DATA LINE NUMBER
610 IF O=1 GO TO 630
620 INPUT A1\IF O=3 GO TO 640
625 REM- A1 = DENSITY OR TRANSMITTANCE VALUE OF LINE L.
630 INPUT A1,A2
635 REM- A2 = DENSITY OR TRANSMITTANCE BACKGROUND VALUE OF LINE L.
640 V=A1\Y1=1\Y2=0\COSUB 2680
645 REM- V = DENSITY OR TRANSMITTANCE OVERLAY FOR INTENSITY SUBROUTINE.
646 REM- SETTING Y1 = 1 AND Y2 = 0 ARE HOUSEKEEPING MANEUVERS.
550 Y1=X\IF O>2 GO TO 680
651 REM- X IS INTENSITY OVERLAY FROM INTENSITY SUBROUTINE.
660 V=A2\COSUB 2680
670 Y2=X
675 REM- Y1 AND Y2 ARE LINE AND BACKGROUND INTENSITIES.
680 Y3(L)=Y1-Y2\NEXT L
685 REM- Y3 = NET INTENSITY.
690 IF VI=0 GO TO 710
700 RETURN
710 PRINT "RACK#, CONC. STDS. "\U1=1\U2=J2
720 FOR L=U1 TO U2\PRINT L;\INPUT K(L)\NEXT L

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725 REM- K(L) = BASE CONCENTRATION OF STANDARD.
730 IF V1=0G0 TO 750
740 RETURN
750 U1=1\U2=J3
760 PRINT "SET*, SAMPLE*"
770 FOR K=U1 TO U2\PRINT K;\INPUT H1$(K)\NEXT K
775 REM- H1$(K) = SAMPLE NUMBER (ALPHANUMERIC TO 12 CHARACTERS).
780 PRINT "SAMPLE*, NO. OF REPLICATES, GRAV. FACTOR"
790 FOR K=U1 TO U2\PRINT H1$(K);\INPUT S1(K),G1(K)\NEXT K
795 REM- S1(K) = NO. OF REPLICATES, G1(K) = GRAVIMETRIC CONVERSION
796 REM- AND/OR DILUTION FACTOR.
800 IF V1=0G0 TO 820
810 RETURN
820 PRINT "EDIT? YES=1 NO=0";\INPUT V1
830 IF V1>1G0 TO 820
840 IF V1=0G0 TO 860
850 GOSUB 2480
860 IF V1=1G0 TO 820
870 IF W1=0G0 TO 920
880 G=01
885 REM- G=01 ASSURES PROPER EMULSION VALUE SUBSCRIPTS FOR RETURNING
886 REM- TO SECOND PORTION OF PROGRAM AFTER EDITING.
890 PRINT "SECOND HALF OF PROGRAM? YES=1 NO=0";\INPUT C7
895 REM- C7 = YES-NO SWITCH FOR RETURNING TO SECOND HALF OF PROGRAM
896 REM- IF DATA HAS ALREADY BEEN ENTERED THERE.
900 IF C7=1G0 TO 1580
910 IF C7>1G0 TO 890
920 I3=0
925 REM- I3 = FLAG CONTROLLING THE USE OR IGNORING OF INTERNAL STD.
930 PRINT "LOG SHEET * ";N5.DAT$
935 REM- DAT$ = CURRENT DATE (DD-MMM-YY) FROM RT-11 MONITOR.
940 PRINT "IMPURITY ELEMENT NAME";\INPUT E1$
950 PRINT "IMPURITY ELEMENT WAVELENGTH";\INPUT W1\W4=W1
960 GOSUB 2420
970 G=L\O1=G
975 REM- O1 IS SUBSCRIPT FOR ANALYTICAL LINE EMULSION CALIBRATION VALUES.
980 PRINT "IMPURITY FACTOR";\INPUT F3
985 REM- F3 IS IMPURITY FACTOR FOR CORRECTING STANDARDS TO PROPER LEVEL.
990 PRINT "USE I.S.? YES=1 NO=0";\INPUT I3
1000 IF I3>1G0 TO 990
1010 IF 0=1G0 TO 1040
1020 IF 0=3G0 TO 1040
1030 I3=0
1040 IF 0>2G0 TO 1060
1050 PRINT "RACK*, A.L., BKG." \IF 0<=2G0 TO 1070
1060 PRINT "RACK*, A.L."
1070 A1=0\A2=0\U1=1\U2=J2
1075 REM- MORE HOUSEKEEPING IN LINES 1070 & 1080 FOR A'S AND X'S.
1080 FOR L=U1 TO U2\M1(L)=0\X1=0\X2=0\PRINT L;
1085 REM- INITIALIZATION OF M1(L) WHICH IS CORRECTED STANDARD CONCENTRATION.
1090 IF 0>2G0 TO 1110
1100 \INPUT X1(L),X2(L)\IF 0<=2G0 TO 1120
1110 \INPUT X1(L)
1115 REM- X1(L) AND X2(L) ARE LINE AND BACKGROUND DENSITIES OR TRANSMITTANCES.
1120 NEXT L
1130 IF V1=0G0 TO 1150
1140 RETURN
1150 S2=J2\T1=1\PRINT "EDIT? YES=1 NO=0";\INPUT V1\V5=0
1151 REM- T1 IS "SKIP" BOOKKEEPING SUBSCRIPT.
1156 REM- V5 = EDIT FLAG FOR DISTINGUISHING SAMPLES FROM STANDARDS.
1160 IF V1>1G0 TO 1150
1170 IF V1=0G0 TO 1190
1180 GOSUB 2860

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1190 IF V1=1G0 TO 1150
1200 C9=0
1205 REM- C9 = COMPARE FLAG - KILLS DATA INPUT 'TIL COMPARISON DONE.
1210 FOR L=1 TO J2\A1=X1(L)\IF 0>2G0 TO 1230
1215 REM- A1 AND A2 ARE NOW LINE AND BACKGROUND DENSITY AND TRANSMITTANCE
1216 REM- OVERLAYS FOR STANDARDS AND SAMPLES.
1217 REM- INPUTTING 0 FOR X1(L) WILL CAUSE THAT SAMPLE OR STANDARD
1218 REM- TO BE SKIPPED.
1220 A2=X2(L)
1230 IF A1=0G0 TO 1300
1240 M1(T1)=F3*K(L)
1245 REM- M1(T1) = CORRECTED STANDARD CONCENTRATION ADJUSTED FOR
1246 REM- OMISSION OF DATA.
1250 I(T1)=L\X2=0\V=A1\GOSUB 2680
1251 REM- I(T1) = L IS FUNCTION TO AID IN SUBSCRIPT CHANGE.
1260 X1=X\IF 0>2G0 TO 1290
1270 V=A2\GOSUB 2680
1280 X2=X
1290 X3(T1)=X1-X2\T1=T1+1\G0 TO 1340
1295 REM- X3(T1) IS CORRECTED NET INTENSITY.
1296 REM- T1=T1+1 IS DEVICE FOR INCREMENTING T1.
1300 S2=S2-1
1305 REM- S2=S2-1 WE JUST LOST ONE SAMPLE OR STANDARD.
1310 X1=0\X3(L)=0
1320 IF 0>2G0 TO 1340
1330 X2=0
1340 NEXT L
1350 FOR L=1 TO S2\I2=I(L)
1355 REM- I2=I(L) IS SUBSCRIPT CORRECTION DEVICE.
1360 IF I3>=1G0 TO 1380
1370 R(L)=X3(L)\IF I3=0G0 TO 1390
1380 R(L)=X3(L)/Y3(I2)
1385 REM- R(L) IS INTENSITY RATIO OR RELATIVE INTENSITY
1390 GOSUB 2940
1400 F(L)=FNY(M1(L))
1405 REM- F(L) IS LOG BASE 10 OF ADJUSTED CONCENTRATION OF STANDARD L.
1410 NEXT L
1420 N=S2\GOSUB 2750
1430 PRINT \PRINT DAT\PRINT
1440 IF I3>=1G0 TO 1470
1450 GOSUB 2980
1460 IF I3=0G0 TO 1480
1470 GOSUB 2960
1480 PRINT "SLOPE=";B(2),"INTERCEPT=";B(1)
1485 REM- B(2) = 1ST DEGREE COEFFICIENT OF CALCULATED ANALYTICAL CURVE.
1486 REM- B(1) = 0
1490 PRINT "ADD.CONC.", "OBS.CONC.", "RATIO", "% DEV."
1500 E=0
1505 REM- E = SCRATCH VALJE FOR CALCULATING AVERAGE DEVIATION.
1510 FOR L=1 TO N
1520 D1(L)=((10^(Z(L)*B(2)+B(1))-M1(L))/M1(L))*100
1525 REM- D1(L) = DEVIATION BETWEEN OBSERVED INTENSITY OF POINT L AND
1526 REM- LEAST SQUARES CALCULATED FIT INTENSITY OF POINT L.
1527 REM- Z(L) = LOG BASE 10 OF RELATIVE INTENSITY OR INTENSITY RATIO.
1530 E=E+ABS(D1(L))
1540 PRINT M1(L),10^(Z(L)*B(2)+B(1)),R(L),D1(L)\NEXT L
1545 REM- LINE 1490 DEFINES EXPRESSIONS IN LINE 1540
1550 E1=E/N\PRINT "AVE. DEV. = ";E1
1555 REM- E1=AVERAGE DEVIATION OF STANDARDS.
1560 IF C9<>1G0 TO 1580
1570 C=01\S4=J2+1\G0 TO 1810
1575 REM- S4= LOWER LIMIT FOR NUMBER OF REPLICATES IN LOOP.
1580 PRINT "NEW ELEMENT(0),SAMPLES(1),END OF RUN(2),EDIT MODE(3),STOP(4)";

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1590 INPUT C3\IF C3>4 GO TO 1580
1591 IF C3=4 GOTO 2410
1595 REM- C3 = FLAG CONTROLLING CENTRAL SWITCHING POINT (LINE 1580) OF
1596 REM- PROGRAM. IF ONE HAS CHANGED DATA AFTER TYPING A 4 IN RESPONSE
1597 REM- TO LINE 1580, THE PROGRAM MAY BE RESTARTED BY TYPING "GO TO 1580".
1600 IF C3<3 GO TO 1660
1610 PRINT "EDIT-STDS(0),SAMPLES(1),FIRST PART OF PROGRAM(2)";
1620 G=01\INPUT C4\IF C4>2 GO TO 1610
1625 REM- C4 = FLAG CONTROLLING EDIT MODE SWITCHING POINT.
1630 IF C4=0 GO TO 1150
1640 IF C4=1 GO TO 1790
1650 IF C4=2 GO TO 820
1660 IF C3<1 GO TO 2820
1670 IF 0>2 GO TO 1700
1680 PRINT "RACK#, A.L., BKG."
1690 IF 0<2 GO TO 1710
1700 PRINT "RACK#, A.L."
1710 S4=J2+1
1720 U1=S4\U2=J1
1730 FOR L=U1 TO U2\PRINT L;\IF 0>2 GO TO 1750
1740 INPUT X1(L),X2(L)\IF 0<2 GO TO 1760
1750 INPUT X1(L)
1760 NEXT L
1770 IF V1=0 GO TO 1790
1780 RETURN
1790 S4=J2+1\PRINT "EDIT? YES=1 NO=0":\INPUT V1\V5=1
1800 IF V1<1 GO TO 1790
1810 IF V1=0 GO TO 1840
1820 GOSUB 2360
1830 GO TO 1790
1840 FOR K=1 TO J3
1850 T1=1\S2=S1(K)
1855 REM- S2 = NUMBER OF REPLICATES HANDLED IN LOOP.
1860 S5=S1(K)+S4-1
1865 REM- S5 = UPPER LIMIT FOR NUMBER OF REPLICATES IN LOOP.
1870 FOR L=S4 TO S5\X1=0\X2=0
1880 A1=X1(L)
1890 IF 0>2 GO TO 1910
1900 A2=X2(L)
1910 IF A1=0 GO TO 1970
1920 I4(T1,K)=L\V=A1\GOSUB 2680
1925 REM- I4(T1,K) = VARIABLE FOR SELECTION OF PROPER INTERNAL STANDARD
1926 REM- INTENSITY AND/OR SAMPLE NUMBER FOR RACK NUMBER SELECTED.
1930 X1=X1\IF 0>2 GO TO 1960
1940 V=A2\GOSUB 2680
1950 X2=X
1960 X4(T1,K)=X1-X2\T1=T1+1\GO TO 2000
1965 REM- X4(T1,K) = VARIABLE FOR SELECTION OF CORRECT INTENSITY RATIO
1966 REM- OR RELATIVE INTENSITY FOR RACK NUMBER CHOSEN.
1970 S2=S2+1
1980 IF 0>2 GO TO 2000
1990 X2=0
2000 NEXT L
2010 S4=S4+S1(K)
2020 S3(K)=S2
2025 REM- S3(K) = STORAGE FOR NUMBER OF REPLICATES IN LOOP K.
2030 NEXT K
2040 IF I3=1 GO TO 2070
2050 GOSUB 2980
2060 IF I3=0 GO TO 2080
2070 GOSUB 2960
2080 PRINT "SAMPLE#", "RATIO", "CONC-OXIDE", "CONC-OTHER"
2090 PRINT

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2100 FOR K=1 TO J3
2110 N=S3(K)\IF S3(K)=0GO TO 2310
2115 REM- N = NUMBER OF DATA POINTS IN LOOP N.
2120 Q=0\B=0
2125 REM- Q = SUBTOTAL OF CALCULATED SAMPLE CONCENTRATIONS IN LOOP.
2126 REM- B = SUBTOTAL OF DEVIATIONS FROM AVERAGE IN LOOP.
2130 FOR L=1 TO S3(K)\I2=14(L,K)
2140 IF I3=1GO TO 2160
2150 R(L)=X4(L,K)\IF I3=0GO TO 2170
2160 R(L)=X4(L,K)/Y3(I2)
2170 GOSUB 2940
2180 Q=Q+(10^(Z(L)*B(2)+B(1)))\NEXT L
2190 A=Q/N\H=Q/N\B=0
2200 FOR L=1 TO N\B=(10^(Z(L)*B(2)+B(1)))-A\B=D*D+P
2210 B=B+ABS(D)
2220 PRINT H1$(K),R(L),10^(Z(L)*B(2)+B(1));
2230 PRINT G1(K)*(10^(Z(L)*B(2)+B(1)))\NEXT L
2235 REM- LINE 2080 DEFINES EXPRESSIONS IN LINES 2220 AND 2230.
2240 IF S3(K)>1GO TO 2260
2250 PRINT
2260 IF S3(K)=1GO TO 2310
2270 C=P/(N-1)\M=C^.5\J=100*M/H
2275 REM- C = SUM OF SQUARES OF DEVIATIONS DIVIDED BY 1 LESS THAN
2276 REM- THE TOTAL NUMBER OF VALUES. M = STANDARD DEVIATION FOR ALL
2277 REM- DATA POINTS IN LOOP. J = STANDARD DEVIATION EXPRESSED AS
2278 REM- RELATIVE PERCENT.
2280 IF N<2GO TO 2310
2290 PRINT "AVE-OXIDE=";H;"AVE-OTHER=";G1(K)*H;"RSD=";J;"%"
2300 PRINT
2310 NEXT K
2320 C8=0\C9=0
2325 REM- C8 = COMPARE FLAG FOR USING OR IGNORING INTERNAL STANDARD.
2330 IF 0=2GO TO 1580
2340 IF 0=4GO TO 1580
2350 PRINT "COMPARE? YES=1 NO=0";\INPUT C8
2360 IF C8>1GO TO 2350
2370 IF C8=0GO TO 2390
2380 GOSUB 3000
2390 IF C9=1GO TO 1210
2400 GO TO 1580
2410 PRINT"RESTART AFTER CORRECTION BY TYPING GO TO 1580"\STOP
2420 FOR L=1 TO N1(G2)
2430 IF W4<=W3(L,G2)GO TO 2460
2440 NEXT L
2450 PRINT "WARNING-";CHR$(7);"CALIBRATION RANGE EXCEEDED";CHR$(7)
2460 RETURN
2470 STOP
2475 REM- LINES 2420 TO 2470 ARE CALIBRATION WAVELENGTH REGION SELECTION
2476 REM- SUBROUTINE.
2480 PRINT "EDIT I.S.(1),CONC.STDS.(2) OR SAMPLE'S(3)";\INPUT V2
2485 REM- V2 = EDIT FLAG FOR SWITCHING THROUGH EDIT MODE.
2490 PRINT "SEQUENCE OF RACK OR SET NUMBERS TO BE EDITED"
2500 PRINT "LOWEST? HIGHEST";\INPUT V3,V4\U1=V3\U2=V4
2505 REM- V3 AND V4 ARE LOWER AND UPPER RACK NUMBERS OF REGION TO BE EDITED.
2510 IF V2=1GO TO 2570
2520 IF V2=3GO TO 2550
2530 GOSUB 720
2540 IF V2=2GO TO 2560
2550 GOSUB 760
2560 IF V2>1GO TO 2660
2570 IF 0=2GO TO 2660
2580 IF 0=4GO TO 2660
2590 PRINT "NEW I.S.? YES=1 NO=0";\INPUT C6

```

```

2595 REM- C6 = INTERNAL STANDARD EDIT FLAG IN CASE WE CHANGE INTERNAL
2596 REM- STANDARD ELEMENTS.
2600 IF C6=1G0 TO 2590
2610 IF C6=0G0 TO 2630
2620 GOSUB 500
2630 IF C6=1G0 TO 2660
2640 G=02\IF V2=0G0 TO 2660
2650 GOSUB 600
2660 RETURN
2670 STOP
2675 REM- LINES 2480 TO 2670 ARE EDIT SUBROUTINE FOR FIRST PART OF PROGRAM.
2680 IF P1=2G0 TO 2710
2690 S=FNY((10^V)-1)
2700 IF P1=1G0 TO 2720
2710 S=FNY((100/V)-1)
2720 T=C0(G,G2)+C1(G,G2)*S+C2(G,G2)*S*S
2730 X=10^T\RETURN
2740 STOP
2745 REM- LINES 2680 TO 2740 ARE SUBROUTINE FOR CONVERTING DENSITIES OR
2746 REM- TRANSMITTANCES TO SEIDEL FUNCTIONS AND THEN TO INTENSITIES.
2750 E=N\F1=0\F0=0\Z1=0\Z2=0
2760 FOR L=1 TO N
2770 F1=F1+F(L)*Z(L)\LET F0=F0+F(L)\Z1=Z1+Z(L)
2780 Z2=Z2+Z(L)*Z(L)\NEXT L
2790 D=Z1*Z1-E*Z2\B(1)=(Z1*F1-F0*Z2)/D
2800 B(2)=(F0*Z1-E*F1)/D\RETURN
2810 STOP
2815 REM- LINES 2750 TO 2810 ARE SUBROUTINE USING LEAST SQUARES FIT
2816 REM- TO CALCULATE 0 AND 1ST DEGREE COEFFICIENTS OF ANALYTICAL
2817 REM- CURVE FOR STANDARDS.
2820 PRINT
2830 IF C3=2G0 TO 3260
2840 IF C3=0G0 TO 920
2850 STOP
2855 REM- LINES 2820 TO 2850 ARE SWITCHING POINT ROUTINE FROM LINE 1660
2856 REM- EITHER LOOPING THROUGH NEW ELEMENT OR TERMINATING RUN.
2860 PRINT "SEQUENCE OF RACK NUMBERS TO BE EDITED"
2870 PRINT "LOWEST? HIGHEST";\INPUT V3,V4\U1=V3\U2=V4\T1=1
2880 IF V5=1G0 TO 2910
2890 COSUB 1080
2900 IF V5=0G0 TO 2920
2910 GOSUB 1730
2920 RETURN
2930 STOP
2935 REM- LINES 2860 TO 2930 ARE EDIT SUBROUTINE FOR SECOND PART OF PROGRAM.
2940 Z(L)=FNY(R(L))\RETURN
2950 STOP
2955 REM- LINE 2940 IS SUBROUTINE FOR CALCULATING LOG BASE 10
2956 REM- OF INTENSITY RATIO.
2960 PRINT E1$;W1;" VS ";E2$;W2\RETURN
2970 STOP
2980 PRINT E1$;W1;" VS NO I.S."\RETURN
2990 STOP
3000 PRINT "RECALCULATE USING I.S.(1), IGNORING I.S.(0)";\INPUT I3
3010 IF I3=1G0 TO 3000
3020 IF I3=0G0 TO 3050
3030 PRINT "COMPARE MODE - USING I.S."
3040 IF I3=1G0 TO 3060
3050 PRINT "COMPARE MODE - IGNORING I.S."
3060 C9=1\S2=J2\T1=1\RETURN
3070 STOP
3075 REM- LINES 2960 TO 3070 ARE PRINT CONTROL SUBROUTINES.
3080 DATA 3

```

3090 DATA "MARTELL SA-1 PLATE JACO"
 3100 DATA 1
 3110 DATA 2483,3961,.6067,.3497,.0176
 3120 DATA "PENA SA-3 FILM L&N"
 3130 DATA 5
 3140 DATA 2415,2540,.115,.5591,.0539
 3150 DATA 2740,2870,-.0899,.6658,.0586
 3160 DATA 2978,3105,.0395,.6341,.0368
 3170 DATA 3218,3345,-.1747,.6434,.0958
 3180 DATA 4195,4325,.0395,.534,.0367
 3190 DATA "SIMI SA-1 PLATE L&N"
 3200 DATA 5
 3210 DATA 2500,2600,.6599,.422,.0193
 3220 DATA 2800,2900,.5893,.4181,.0451
 3230 DATA 2900,3100,.588,.4127,.6456
 3240 DATA 3350,3450,.5967,.3736,.0125
 3250 DATA 3920,3970,.4579,.2609,-5.80000E-03
 3255 REM- LINES 3080 TO 3250 ARE DATA LINES FOR EMULSION CALIBRATION
 3256 REM- COEFFICIENTS TO SATISFY READ STATEMENTS AT FIRST PART OF PROGRAM.
 3257 REM- DATA TABLES IDENTIFIED BY WORKER (ASSIGNED TO SPECTROGRAPH),
 3258 REM- FILM EMULSION DATA, AND DENSITOMETER.
 3260 END

APPENDIX B

TYPICAL RUN - ALLCAL

IN THE FOLLOWING TYPICAL RUN OF ALLCAL UNDER DEC BASIC/RT-11, THE RT-11 MONITOR IDENTIFIES ITSELF AND THE SYSTEM IS INITIALIZED AND DATED. BASIC IS CALLED AND ALL FUNCTIONS ARE USED. THE PROGRAM "ALLCAL" IS LOADED AND EXECUTED.

COMMENTS IN THE BOXES BOUNDED BY ASTERISKS IN THE RIGHT MARGIN ARE NOT PART OF A TYPICAL RUN BUT WERE ADDED LATER TO HELP IDENTIFY PORTIONS OF THE RUN WITH RESPECT TO THE MAIN BODY OF THE TEXT.

RT-11SJ Y02-10

.IN

.DAT 4-MAR-75

.R BASIC

BASIC V01-05

*A

READY

OLD"ALLCAL"

READY

RUN

ALLCAL 04-MAR-75 BASIC V01-05

PROGRAM - ALLCAL - HAS EVERYBODY'S COEFFICIENTS

APRIL 17, 1974 C. APEL

MARTELL SA-1 PLATE JACO? YES=1 NO=0?0

PENA SA-3 FILM L8N? YES=1 NO=0?1

VERIFY COEFFICIENTS? YES=1, NO=0?0

REDO CALIBRATION INPUT? YES=1 NO=0?0

LOG SHEET NUMBER ?23537

DENSITIES(1) OR TRANSMITTANCES(2) ?1

READ? (1)ALL, (2)NO I.S., (3)NO BKG., (4)LINE ONLY?1

MAXIMUM NUMBER OF RACK POSITIONS?18

MAXIMUM NUMBER OF STANDARDS?8

MAXIMUM NUMBER OF SAMPLE NUMBERS?5

I.S. ELEMENT NAME?COBALT

I.S. WAVELENGTH?2521

RACK#, I.S., I.BKG.

1 ?.79,.04
2 ?.83,.03
3 ?.89,.03
4 ?.96,.03
5 ?.96,.03
6 ?.92,.04
7 ?.96,.04
8 ?1.03,.04
9 ?1.1,.04
10 ?1.04,.04

*INTERNAL STANDARD OPTICAL *
*DENSITIES AND BACKGROUNDS *
*ARE ENTERED HERE. *

11 ?1.06,.05
 12 ?1.01,.05
 13 ?1.04,.04
 14 ?1.05,.05
 15 ?1.01,.04
 16 ?1...04
 17 ?1.03,.03
 18 ?1.03,.04

RACK#, CONC. STDS.

1 ?500
 2 ?200
 3 ?100
 4 ?50
 5 ?25
 6 ?10
 7 ?5
 8 ?1

SET#, SAMPLE#

1 ?NBL-95-2
 2 ?NBL-95-3
 3 ?NBL-95-4
 4 ?GRW-7007-B
 5 ?GRW-7007-A

SAMPLE#, NO. OF REPLICATES, GRAV. FACTOR

NBL-95-2?2,1.18

NBL-95-3?2,1.18

NBL-95-4?2,1.18

GRW-7007-B?2,1.18

GRW-7007-A?2,2.28

EDIT? YES=1 NO=0?1

EDIT I.S.(1), CONC.STDS.(2) OR SAMPLE#'S(3)?1

SEQUENCE OF RACK OR SET NUMBERS TO BE EDITED

LOWEST? HIGHEST?4,4

NEW I.S.? YES=1 NO=0?0

4 ?96...96,.03

EDIT? YES=1 NO=0?1

EDIT I.S.(1), CONC.STDS.(2) OR SAMPLE#'S(3)?1

SEQUENCE OF RACK OR SET NUMBERS TO BE EDITED

LOWEST? HIGHEST?4,4

NEW I.S.? YES=1 NO=0?0

4 ?1,.04

EDIT? YES=1 NO=0?1

EDIT I.S.(1), CONC.STDS.(2) OR SAMPLE#'S(3)?3

SEQUENCE OF RACK OR SET NUMBERS TO BE EDITED

LOWEST? HIGHEST?5,5

SET#, SAMPLE#

5 ?GRW-7007-A

SAMPLE#, NO. OF REPLICATES, GRAV. FACTOR

GRW-7007-A?2,1.18

EDIT? YES=1 NO=0?0

LOG SHEET # 23537

04-MAR-75

IMPURITY ELEMENT NAME?IRON

IMPURITY ELEMENT WAVELENGTH?2522

IMPURITY FACTOR?1

USE I.S.? YES=1 NO=0?1

RACK#, A.L., BKG.

1 ?1.13,.04
 2 ?.83,.03
 3 ?.57,.03
 4 ?.39,.04
 5 ?.25,.03
 6 ?.12,.04
 7 ?0,0

 STANDARD BASE CONCENTRATIONS
 *ARE ENTERED HERE. *

 *SAMPLE NUMBERS ARE ENTERED *
 *HERE. *

 *FIRST USAGE *
 *OF EDIT. *

 ANALYTICAL LINE OPTICAL
 *DENSITIES AND BACK- *
 *GROUNDS FOR STANDARDS *
 ARE ENTERED HERE. "0'S"
 *INDICATE OMITTED DATA. *

8 ?0,0
EDIT? YES=1 NO=0?0

04-MAR-75

IRON 2522 VS COBALT 2521

SLOPE= 1.21475 INTERCEPT= 2.34168

ADD. CONC.	OBS. CONC.	RATIO	% DEV.
500	475.23	1.88781	-4.95396
200	219.626	1	9.81298
100	100.118	.523775	.118332
50	43.6261	.264336	-12.7478
25	27.7121	.181936	10.8482
10	9.89423	.0779305	-1.05767

AVE. DEV. = 6.58984

NEW ELEMENT(0), SAMPLES(1), END OF RUN(2), EDIT MODE(3), STOP(4)?1

RACK#, A.L., BKG.

9 ?1.06,.04
10 ?1.03,.04
11 ?2.79,.05
12 ?2.73,.05
13 ?2.54,.04
14 ?2.50,.05
15 ?2.64,.04
16 ?2.66,.04
17 ?2.76,.03
18 ?2.77,.04

ANALYTICAL LINE OPTICAL
*DENSITIES AND BACK- *
*GROUNDS FOR SAMPLES *
*ARE ENTERED HERE. *

EDIT? YES=1 NO=0?0

IRON 2522 VS COBALT 2521

SAMPLE#	RATIO	CONC-OXIDE	CONC-OTHER
---------	-------	------------	------------

NBL-95-2	.930017	201.098	237.296
NBL-95-2	.981883	214.802	253.466
AVE-OXIDE=	207.95	AVE-OTHER=	245.381 RSD= 4.65984 %

NBL-95-3	.597702	117.535	138.691
NBL-95-3	.580048	113.332	133.731
AVE-OXIDE=	115.433	AVE-OTHER=	136.211 RSD= 2.57496 %

NBL-95-4	.36497	64.5556	76.1756
NBL-95-4	.318975	54.8113	64.6774
AVE-OXIDE=	59.6835	AVE-OTHER=	70.4265 RSD= 11.5446 %

GRW-7007-B	.483592	90.8665	107.222
GRW-7007-B	.514209	97.9015	115.524
AVE-OXIDE=	94.384	AVE-OTHER=	111.373 RSD= 5.27052 %

GRW-7007-A	.602365	118.65	140.007
GRW-7007-A	.610369	120.568	142.27
AVE-OXIDE=	119.609	AVE-OTHER=	141.139 RSD= 1.13378 %

COMPARE? YES=1 NO=0?1

RECALCULATE USING I.S.(1), IGNORING I.S.(0)?0

COMPARE MODE - IGNORING I.S.

04-MAR-75

IRON 2522 VS NO I.S.

SLOPE= 1.34121

ADD. CONC.	OBS. CONC.
500	434.765
200	210.086
100	102.763

INTERCEPT= 1.61369

RATIO	% DEV.
5.80646	-13.047
3.37605	5.04278
1.98088	2.7631

*IRON CALCULATIONS *
*REPEATED, IGNORING *
*INTERNAL STANDARD. *

30	53.1482	1.21159	6.29642
25	29.6175	.783468	18.4702
10	8.46006	.307813	-15.3994

AVE. DEV. = 10.1698

IRON 2522 VS NO I.S.

SAMPLE#	RATIO	CONC-OXIDE	CONC-OTHER
---------	-------	------------	------------

NBL-95-2	5.11557	366.83	432.859
NBL-95-2	4.84305	340.861	402.216
AVE-OXIDE= 353.846 AVE-OTHER= 417.538 RSD= 5.18953 %			

NBL-95-3	3.03057	181.767	214.485
NBL-95-3	2.68182	154.278	182.047
AVE-OXIDE= 168.022 AVE-OTHER= 198.266 RSD= 11.5685 %			

NBL-95-4	1.80018	90.3901	106.66
NBL-95-4	1.58787	76.3877	90.1374
AVE-OXIDE= 83.3889 AVE-OTHER= 98.3989 RSD= 11.8735 %			

GRW-7007-B	2.25772	122.471	144.516
GRW-7007-B	2.3569	129.741	153.094
AVE-OXIDE= 126.106 AVE-OTHER= 148.805 RSD= 4.07608 %			

GRW-7007-A	2.94723	175.095	206.612
GRW-7007-A	2.95605	175.797	207.441
AVE-OXIDE= 175.446 AVE-OTHER= 207.026 RSD= .28318 %			

COMPARE? YES=1 NO=0?0

NEW ELEMENT(0), SAMPLES(1), END OF RUN(2), EDIT MODE(3), STOP(4)?0

LOG SHEET # 23537 04-MAR-75

IMPURITY ELEMENT NAME? BORON

IMPURITY ELEMENT WAVELENGTH? 2497

IMPURITY FACTOR? .1

USE I.S.? YES=1 NO=0?0

RACK#, A.L., BKG.

1 ?1.76,.065

2 ?1.42,.05

3 ?1.1,.04

4 ?1.74,.03

5 ?1.52,.016

6 ?1.21,.02

7 ?1.124,.03

8 ?0.0

EDIT? YES=1 NO=0?0

04-MAR-75

BORON 2497 VS NO I.S.

SLOPE= 1.17765

INTERCEPT= .161119

ADD.CONC.	OBS.CONC.	RATIO	% DEV.
-----------	-----------	-------	--------

50	42.7367	17.7004	-14.5267
----	---------	---------	----------

20	21.0073	9.68465	5.03776
----	---------	---------	---------

10	10.7907	5.50051	7.90732
----	---------	---------	---------

5	4.93921	2.83274	-1.21586
---	---------	---------	----------

2.5	2.98802	1.84867	19.5209
-----	---------	---------	---------

1	.969163	.710614	-3.08369
---	---------	---------	----------

.5	.451034	.371155	-9.79325
----	---------	---------	----------

AVE. DEV. = 8.72649

NEW ELEMENT(0), SAMPLES(1), END OF RUN(2), EDIT MODE(3), STOP(4)?1

RACK#, A.L., BKG.

9 ?1.34,.026

10 ?1.34,.026

NORMAL CALCULATION OF BORON DATA

11 70.0
 12 70.0
 13 70.0
 14 70.0
 15 70.0
 16 70.0
 17 7.21,.03
 18 7.25,.04

EDIT? YES=1 NO=0?0

BORON 2497 VS NO I.S.

SAMPLE# RATIO CONC-OXIDE CONC-OTHER

NBL-95-2 1.10652 1.63263 1.9263
 NBL-95-2 1.10652 1.63263 1.9263
 AVE-OXIDE= 1.63263 AVE-OTHER= 1.9263 RSD= 0 %

GRW-7007-A .653503 .878105 1.03616
 GRW-7007-A .733747 1.00642 1.18758
 AVE-OXIDE= .942264 AVE-OTHER= 1.11187 RSD= 9.62944 %

COMPARE? YES=1 NO=0?0

NEW ELEMENT(0),SAMPLES(1),END OF RUN(2),EDIT MODE(3),STOP(4)?3

EDIT-STDS(0),SAMPLES(1),FIRST PART OF PROGRAM(2)?0

EDIT? YES=1 NO=0?1

SEQUENCE OF RACK NUMBERS TO BE EDITED

LOWEST? HIGHEST?1,1

1 70.0

EDIT? YES=1 NO=0?0

04-MAR-75

BORON 2497 VS NO I.S.

SLOPE= 1.13276

INTERCEPT= .163723

ADD. CONC.	OBS. CONC.	RATIO	% DEV.
20	19.0861	9.68465	-4.56943
10	10.0559	5.50051	.55893
5	4.74202	2.83274	-5.15963
2.5	2.92422	1.84867	16.9687
1	.990058	.710614	-.994206
.5	.474389	.371155	-5.12227

AVE. DEV. = 5.56219

NEW ELEMENT(0),SAMPLES(1),END OF RUN(2),EDIT MODE(3),STOP(4)?3

EDIT-STDS(0),SAMPLES(1),FIRST PART OF PROGRAM(2)?1

EDIT? YES=1 NO=0?0

BORON 2497 VS NO I.S.

SAMPLE# RATIO CONC-OXIDE CONC-OTHER

NBL-95-2 1.10652 1.635 1.9293
 NBL-95-2 1.10652 1.635 1.9293
 AVE-OXIDE= 1.635 AVE-OTHER= 1.9293 RSD= 0 %

GRW-7007-A .653503 .900417 1.06249
 GRW-7007-A .733747 1.02664 1.21144
 AVE-OXIDE= .96353 AVE-OTHER= 1.13697 RSD= 9.26348 %

COMPARE? YES=1 NO=0?0

NEW ELEMENT(0),SAMPLES(1),END OF RUN(2),EDIT MODE(3),STOP(4)?4

RESTART AFTER CORRECTION BY TYPING GO TO 1580

STOP AT LINE 2410

READY

 *EDITOR USED TO DROP 50 *
 *PPH STANDARD AND *
 *RECALCULATE BORON *
 *STANDARDS, PRODUCING *
 *NEW WORKING CURVE. *

 *EDITOR USED TO RE- *
 *CALCULATE SAMPLES *
 *FOR BORON FROM NEW *
 *WORKING CURVE WITH- *
 *OUT RE-ENTERING *
 *DATA, AS MENTIONED *
 *IN BODY OF TEXT. *

 *IMMEDIATE MODE USE *
 *AS MENTIONED IN *
 *BODY OF TEXT. *

LET W1=4000

LET E10="B"

GOTO 1580

NEW ELEMENT(0),SAMPLES(1),END OF RUN(2),EDIT MODE(3),STOP(4)?3

EDIT-STDS(0),SAMPLES(1),FIRST PART OF PROGRAM(2)?0

EDIT? YES=1 NO=0?0

04-MAR-75

B 4000 VS NO I.S.

SLOPE= 1.13276

INTERCEPT= .163723

ADD.CONC. OBS.CONC.

RATIO

% DEV.

20 19.0861 9.68465 -4.56943

10 10.0559 5.50051 .55893

5 4.74202 2.83274 -5.15963

2.5 2.92422 1.84867 16.9687

1 .990058 .710614 -.994206

.5 .474389 .371155 -5.12227

AVE. DEV. = 5.56219

NEW ELEMENT(0),SAMPLES(1),END OF RUN(2),EDIT MODE(3),STOP(4)?2

READY