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# COMPUTER PROGRAMS IN BASIC LANGUAGE FOR ATOMIC ABSORPTION FLAME SPECTROSCOPY

## Part 1. Operating Instructions

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January 25, 1978

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MS. date: September 30, 1977

**NOTICE**

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## **FOREWORD**

This report covers work performed by the Lawrence Livermore Laboratory for the United States Environmental Protection Agency under Interagency Agreement EPA-1AG-D7-0321.

Part 2, "Documentation," of this UCRL report describes in detail the various aspects of each of the programs discussed here (Part 1) and contains flow charts, listings, definitions of variables, and symbol tables for these programs.

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# COMPUTER PROGRAMS IN BASIC LANGUAGE FOR ATOMIC ABSORPTION FLAME SPECTROSCOPY

## Part 1. Operating Instructions

### ABSTRACT

These instructions describe how to use three BASIC language programs to process data from atomic absorption spectrophotometers operated in the flame mode. These programs will also control an automatic sampler if desired. The instructions cover loading the programs, responding to computer prompts, choosing among various options for processing the data, operating the automatic sampler, and producing reports. How the programs differ is also explained. Examples of computer/operator dialogue are presented for typical cases.

### INTRODUCTION

These instructions are intended for the operator who is to run the BASIC\* programs that are used with atomic absorption (AA) flame spectrophotometers. More complete descriptions of these programs are found in the Computer Documentation Manual.

There are three programs available: a program called "Semiautomatic," which requires operator interaction to tell the computer what to do next; a program called "Random," which requires only minimal operator interaction and allows sampling of standards and unknowns in a random or sequential mode; and a program called "Bracket," which automatically tries to find standards that bracket each unknown. These programs may run with or without a computer-controlled automatic sampling device.

The generic names Semiautomatic, Random, and

Bracket, which will be used in this document, are not necessarily the names that are used to call the programs into the computer. The first two of these programs chain or call up other programs to do certain tasks. These other programs referred to as subprograms will be called "Least Squares," "Interim Report," and "Final Report." Bracket is a self-contained program and does not chain to other programs.

The names of these programs can be conveniently changed by the operator. Furthermore, the names of the files used in each program can also be changed, because the names are contained in string variables. Some examples of program names, the associated instruments, and file names are given in Appendix A. Columns are provided in Appendix A for recording the channel numbers and program names used in your particular installation.

### RUNNING THE PROGRAM

Illustrations are provided for your assistance in understanding the instructions. They are taken from demonstration runs of the programs.† You may

find it helpful to follow them along with the descriptions.

\*The BASIC interactive programming language used in this document is Data General's extended BASIC, operating under their Real Time Disk Operating System (RDOS).

† The illustrations are reproductions of the output of a Texas Instruments "Silent 700" terminal.

## PROGRAM SELECTION

The computer will request an identification code after the operator presses the ESC key. If the proper code letters are typed followed by a carriage return, the computer will display on the terminal some message indicating that the BASIC system is up.

The operator may then load the appropriate program by typing LOAD XXXX where XXXX is the program name. To start the program he types RUN. Alternatively, he may type RUN XXXX, which loads and starts the program (see Fig. 1).

## COMMON RESPONSES

All three programs have certain common beginning responses (see Fig. 2). The computer will ask OPERATOR'S NAME AND INSTRUMENT? to which the operator responds appropriately. Responses should use dashes as separators because commas will stop the program with an error message. This information is contained in one string and may really be any alphanumeric information the operator wishes. All responses must be followed by a carriage return.

Next, the computer asks ELEMENT AND SAMPLE SOURCE? The operator should respond with a title that names the element and describes the samples.

In response to MAX I.D. LENGTH, NO. OF SAMPLES? the operator should enter a number that represents the largest number of characters expected in the sample identification code, and then enter the number of samples. The maximum number of samples is 50. The computer then responds with the number 1 and a question mark, to which the operator replies with the appropriate sample identification code for unknown number 1. Then number 2, etc. with replies are entered until all samples have been identified and referenced to a sequential number.

The sample identifiers also must include any quality control samples that are to be run. These samples include check standards, duplicate unknowns, and spiked unknowns. Quality control samples are identified by means of the beginning letters CS (Check Standard), DU (DUPLICATE), or SP (SPiKE). For example, CS3 means standard number 3 is a check standard, DU6 means unknown number 6 is duplicated here, and SP17 means that spike number 1 (whose concentration will be entered later) is in unknown number 7. The concentrations of these quality control samples are returned just as though they were ordinary samples. In addition, the Percent Recovery is returned in the Interim and Final Reports. A maximum of nine spikes may be entered. A reagent blank may also be entered and must be identified by the letter R in the last allowed space for sample I.D.

Next, there is a routine for making corrections on the sample identification code. The computer asks CORRECTIONS Y/N? If the operator responds with a Y (yes), the computer asks NO. OF I.D. CORRECTIONS? The operator replies with the number of sample identifiers that need to be corrected. The computer prompts for each one by asking NO. AND I.D. OF SAMPLE? There is also an error recovery routine for too many characters; this routine will return the program to the user after an appropriate warning.

LATS READY

ACCOUNT-ID:

09/22/77 16:17 SIGN ON: 04

◆RUN "SMASH1.LL

OPERATOR'S NAME AND INSTRUMENT  
?

STOP AT 0960

◆

LOAD "SMASH1.LL

◆RUN

OPERATOR'S NAME AND INSTRUMENT  
?

STOP AT 0960

◆

BYE

09/22/77 16:18 SIGN OFF: 04

09/22/77 16:18 CPU USED: 5

09/22/77 16:18 I/O USED: 0

LATS READY

Fig. 1. Loading and starting the program.

LATS READY

ACCOUNT-ID:

09/21/77 14:41 SIGN ON: 04

◆LOAD "SMASH1.LL

◆RUN

OPERATOR'S NAME AND INSTRUMENT

? WALTER BOYLE--JA-82-536

ELEMENT AND SAMPLE SOURCE

? CALCIUM--SIMULATED DTA\_LATA

MAX ID LENGTH, NO. OF SAMPLES ? 9 ? 13

SAMPLE I. D. CODE

1 ? SIM1

2 ? SOM2\_\_\_IM2

3 ? SIM4

4 ? CS3

5 ? SP17

6 ? SIM4

7 ? SIM5

8 ? DU6

9 ? SP210

10 ? SIM6

11 ? CS2

12 ? DU10

13 ? SP310

CORRECTIONS Y/N ? Y

NO. OF I.D. CORRECTIONS ? 2

NO. AND I.D. OF SAMPLE ? 2 ? SIM2

NO. AND I.D. OF SAMPLE ? 3 ? SIM3

INSTRUMENT CONDITIONS OR LAMP 250V

BASELINE LIMIT

? 14000

UNITS

? PPM

INTEG. TIME IN SECONDS

? 5

37 POINTS

PAUSE TIME IN SECONDS

? 1

NO. OF STDS 5

CONC:

1 ? 250

2 ? 500

3 ? 750

4 ? 1000

5 ? 1250

NO. OF SPIKES 3

SPIKE NO. 1 VALUE 250

SPIKE NO. 2 VALUE 500

SPIKE NO. 3 VALUE 750

COVER SLIT; HIT RETURN WHEN READY

?

TAKE A READING

DARK CURRENT= 457.729

Fig. 2. Preliminary input.

The next prompts are INSTRUMENT CONDITIONS? to be answered with the appropriate alphanumeric message, BASELINE LIMIT? (to guard against excessive drift), UNITS? which can be any alphanumeric response, such as PPM or PPB, the INTEG. TIME IN SECONDS? which returns the number of points read, and the PAUSE TIME IN SECONDS? which is the elapsed time between the time the sample has been selected and the time the integration of the signal begins. The computer then asks for the NO. OF STDS? After this question is answered, the word CONC is given by the computer.

The number "1" is displayed, to which the operator replies with the concentration of the first and least concentrated standard; the number "2" is then displayed, and so on until all the standards have been entered in increasing order of concentration. A maximum of 10 standards is allowed. The computer then asks NO. OF SPIKES? The operator enters the number of spiked unknowns to be run. The computer prints SPIKE NO. X, and the operator enters the concentration of each spike as the computer numbers the values.

There is an extra input required for single-beam instruments. The computer will prompt by displaying COVER SLIT: RETURN WHEN READY. The light input slit of the instrument should be covered, and after the instrument response has

become stable a carriage return is entered. The computer reads this signal and stores it as "dark current" to be used in subsequent absorbance calculations. This operation is done only once during the course of an entire set of analyses, because the dark current is a relatively stable reading (see Fig. 2).

On the double-beam instruments for the two programs Semiautomatic and Random, the sample and reference beam values are displayed after each beginning baseline. The difference between these beams is also displayed, and this difference is used as a correction to the raw data. This correction helps to make the computer-calculated absorbances agree with the displayed instrumental absorbances (on certain instruments), especially if instrumental features such as the auto-zero button are frequently used.

The Bracket Program generally asks for similar responses although the prompts are in a slightly different order. There are no quality control options for this special purpose program. The Bracket Program also asks for an upper limit for a percent standard deviation by prompting RELATIVE STANDARD DEVIATION? The operator must enter the relative standard deviation that he expects will not be exceeded during the course of the Bracket analysis.

## SEMIAUTOMATIC PROGRAM

The prompt READ A BASELINE is given (see Fig. 3) and the computer automatically begins to read a baseline after a double pause. After that the operator must signal the computer what to do in response to a question mark. He tells the computer to read a baseline by typing B. By typing S1, S2, S3, etc., he tells the computer which standard to read. By typing U1, U2, U3, etc., he tells the computer to read an unknown. He signals the computer to take an average baseline by typing a !B after the sample or unknown designation; e.g., S3!B or U2!B. This designation will automatically direct the computer to read a second baseline and average the two. The computer always prints (1) the position it is expecting, (2) the words TAKE A READING, which means integration has commenced, (3) the optical absorbance, and (4) the value of the last baseline that has been read and that is used in subsequent calculations.

If the baseline is out of range an audible signal will be emitted and the words BASELINE OUT OF RANGE returned, but the program will continue.

The operator signals the computer to calculate by typing CI for interpolation, CA for the method of additions, or C1, C2, or C3 for least squares fitting of 1st, 2nd or 3rd degree (see Fig. 4). C1, C2, C3, or CA cause the program to chain to the Least Squares Subprogram, which does the appropriate fit and returns the coefficients of the fitted equation, the coefficient of determination and differences between the standards as entered, and the standards as calculated from the fitted equation. When CA is indicated (method of additions), it is assumed that the first standard entered is really an unspiked unknown, so that subsequently the same unknown would be used as standards with various values of spikes entered as the concentration; i.e., the first standard would be the unknown of interest with a concentration of zero. Also, the first sample should be this same unknown. If more samples are to be run using the same calibration curve, the curve is shifted to zero, and therefore the samples read off this curve should have a very similar matrix.

```

SET-UP FOR BASELINE AND HIT RETURN
?
READ A BASELINE
POSITION 0
TAKE A READING
12351.4

12351.4

* ? S1
POSITION 1
TAKE A READING
ABS= 4.64709E-02
12351.4

* ? U1
POSITION 6
TAKE A READING
ABS= 4.65554E-02
12351.4

* ? U6
POSITION 11
TAKE A READING
ABS= 4.64253E-02
12351.4

* ? U81B
POSITION 13
TAKE A READING
SET-UP FOR BASELINE AND HIT RETURN
?
READ A BASELINE
POSITION 0
TAKE A READING
ABS= 4.74586E-02
12397.5

* ? S2
POSITION 2
TAKE A READING
ABS= .100015
12397.5

* ? U2
POSITION 7
TAKE A READING
ABS= 9.99559E-02
12397.5

* ? U101B
POSITION 15
TAKE A READING
SET-UP FOR BASELINE AND HIT RETURN
?
READ A BASELINE
POSITION 0
TAKE A READING
ABS= .0990115
12350.3

```

Fig. 3. Responses for instructing computer.

When interpolation is signified (CI), nothing is really calculated at this point. Calculations are done entirely in the Interim Report Subprogram.

The Interim Program Subprogram is called by typing *R* in response to the question mark. This report then gives the results of the run and asks the following questions: HARD COPY (Y/N)? which will print out the Interim Report on the line printer, RECALCULATE (Y/N)? which will chain back to the main program and allow a new mode of calculation or another standard or sample to be rerun, ACCEPT OR REJECT (A/R)? which allows the results to be accepted or erased, and ANOTHER RUN? (Y/N)? which will cause another run to be started by the main program (positive responses assumed) (see Fig. 5).

If the response to ANOTHER RUN is N, the program asks for NO. OF DILUTIONS? and a routine to enter dilution factors ensues if the response is other than zero. This routine is self-explanatory and allows for corrections (see Fig. 6).

The Interim Report Subprogram then chains to the Final Report Subprogram, which is independent and writes a report by reading two files. One file contains standardization and initialization data, and the other contains the sample information. These files are named in the individual programs. For storage purposes the names must be changed, or the next time the program is run the old data will be overwritten, and the opportunity to change these names is afforded as well as the option to write reports with other renamed files.

The first query NUMBER OF PLACES AFTER DECIMAL POINT? determines the number of places after the decimal point in the final answers for average concentration and standard deviation. Next, the computer prompts STANDARD VARIABLE FILE NAMES? Y/N. If Y (yes) is answered, the computer lists the program names and asks PROGRAM NAME? From the answer to this question the program will use the proper established file names. If N (no) is answered, the program asks for the file names you desire to be used in writing the reports by FILE NAME FOR STORAGE OF VARIABLES AND FILE NAME FOR SAMPLE ID. These are usually used for extra copies of reports whose records have been saved on the disk by changing the file names, as explained further on.

If there is a reagent blank, it will be found and displayed, and the message SUBTRACT REAGENT BLANK? Y/N will be asked. If Y is the reply, the reagent blank will be subtracted from all unknowns and QC samples that are appropriate in the Final Report.

```

♦ ? C1
LEAST SQUARES
COEFFICIENTS Y0,Y1,Y2,Y3 ARE 9.95337 4937.05 0 0

COEFFICIENT OF DETERMINATION= .999744

CONC= 9.95337 + 4937.05 ♦ABS 0 ♦ABS^2 0 ♦ABS^3
1 DIFF 250 - 254.409 = -4.40877
2 DIFF 500 - 495.394 = 4.60596
3 DIFF 750 - 752.1 = -2.10034
4 DIFF 1000 - 992.487 = 7.51343
5 DIFF 1250 - 1255.6 = -5.59521

♦ ? C2
LEAST SQUARES
COEFFICIENTS Y0,Y1,Y2,Y3 ARE -3.81641 5173.12 -782 0

COEFFICIENT OF DETERMINATION= 1.0004

CONC= -3.81641 + 5173.12 ♦ABS -782 ♦ABS^2 0 ♦ABS^3
1 DIFF 250 - 250.411 = -.410904
2 DIFF 500 - 497.276 = 2.72363
3 DIFF 750 - 756.148 = -6.14771
4 DIFF 1000 - 994.727 = 5.27271
5 DIFF 1250 - 1251.61 = -1.60864

```

Fig. 4. Output from least squares calculation.

The Final Report Subprogram will produce two different Final Reports: one is for the operator and the other is for the customer. Hence, the Final Report Subprogram prompts with FINAL REPORT: OPERATOR OR CUSTOMER; OP/CU/NO? If the operator responds with OP or CU the computer produces the appropriate report. The operator may continue to produce reports until a NO is entered.

When the operator is finished producing reports, he types NO to the above question of the Final Report Subprogram. The program then asks CHANGE FILE NAMES? (Y/N). If the operator wishes to save the disk file records, he changes both names and keeps a record of these names; otherwise, he types N and the program ends (see Fig. 6); also, see Appendix E for examples of the Final Report.

## THE RANDOM PROGRAM

The following prompts must be answered after the initialization prompts common to both programs have been completed. The computer asks, BASELINE AVERAGE? Y/N. The operator decides whether to take a baseline after every reading and average it. If not (N), the computer asks, FREQUENCY OF BASELINE? to which the operator responds with a number designating the number of samples and standards run before a new baseline is taken. Finally, the operator designates the mode of operating in replying R or S to the prompt, RANDOM OR SEQUENTIAL?

The computer then takes over the operation of the program. If an automatic sampler is not used

the operator must allow enough time to select and to aspirate the designated sample or standard. An alternative method would be to modify the program to halt after the computer has made its selection, so that the operator can gain control until the solution has been aspirated. The program could be restarted with a carriage return.

During the course of a run the computer will print (1) the position the sampler is going to sample next, (2) the words TAKE A READING, which means integration has commenced, (3) the optical absorbance, and (4) the value of the last baseline that has been read (used in subsequent calculations).

		RUN NO. 2 (PPM)			
	SAMPLE NO.	VALUE	AVERAGE	SD	RCF
NO. 1	SIM1.....	245.936	248.575	3.731	1.501
NO. 2	SIM2.....	508.753	505.661	4.373	.865
NO. 3	SIM3.....	753.127	753.672	.771	.102
NO. 4	CS3.....	744.022	753.871	13.929	1.848
RECOVERY OF STANDARD	3	750 PPM IS	99.203 PERCENT		
NO. 5	SP17.....	1013.15	1010.58	3.635	.36
RECOVERY OF SPIKE	1	250 PPM IS	107.682 PERCENT		
NO. 6	SIM4.....	245.301	252.32	9.926	3.934
NO. 7	SIM5.....	743.94	753.503	13.524	1.795
NO. 8	DU6.....	250.37	243.305	9.991	4.107
RECOVERY OF UNKNOWN	6	IS 102.067	PERCENT		
NO. 9	SP210....	1013.35	999.633	19.399	1.941
RECOVERY OF SPIKE	2	500 PPM IS	101.851 PERCENT		
NO. 10	SIM6.....	504.094	499.185	6.942	1.391
NO. 11	CS2.....	499.448	502.833	4.786	.952
RECOVERY OF STANDARD	2	500 PPM IS	99.89 PERCENT		
NO. 12	DU10.....	500.327	497.878	3.464	.696
RECOVERY OF UNKNOWN	10	IS 99.253	PERCENT		
NO. 13	SP310....	1255.46	1248.16	10.323	.827
RECOVERY OF SPIKE	3	750 PPM IS	100.183 PERCENT		

HARD COPY (Y/N) ? N  
 RECALCULATE Y/N ? N  
 ACCEPT OR REJECT (A/R) ? A  
 ANOTHER RUN ? (Y/N)  
 ? N

Fig. 5. Example of Interim Report.

The BASELINE OUT OF RANGE message will still be given when required, but the program will continue running; it is up to the operator to decide whether to halt the program.

After the first run the message CALCULATE, CI, CA, C1, C2, or C3 will be displayed. This deter-

mines the mode of calculation, and after the results of the first run\* have been accepted this mode of calculation will continue for the rest of the program; i.e., until a Final Report has been requested.

The accepting or rejecting of results, the request for hard copies of Interim Reports, and the prompt for ANOTHER RUN are the same as before. This program uses the same Interim Report, Least Squares, and Final Report Subprogram as the Semiautomatic Program.

\*A run is defined as a complete set of data obtained from standards and samples and used to calculate unknown concentrations.

```

HARD COPY (Y/N) ? N
RECALCULATE Y/N ? N
ACCEPT OR REJECT (A/R) ? A
ANOTHER RUN ? (Y/N)
? N
NO. OF DILUTIONS 2
SAMPLE NUMBER, VOL 1, (DILUTED TO) VOL 2 ? 1 ? 1 ? 10
SAMPLE NUMBER, VOL 1, (DILUTED TO) VOL 2 ? 2 ? 1 ? 10
CORRECTIONS Y/N ? N
NUMBER OF PLACES AFTER DECIMAL POINT ? 2
STANDARD VARIABLE FILE NAMES ? Y/N Y
SMASH1.LL,RSASH1.LL,SM305.LL,RS305.LL
PROGRAM NAME ? SMASH1.LL
FINAL REPORT; OPERATOR OR CUSTOMER; OP/CU/NO ? OP
FINAL REPORT; OPERATOR OR CUSTOMER; OP/CU/NO ? CU
FINAL REPORT; OPERATOR OR CUSTOMER; OP/CU/NO ? NO
CHANGE FILE NAMES (Y/N) N
ALL DONE

END AT 0535
♦

```

Fig. 6. Responses at end of run.

## THE BRACKET PROGRAM

The baseline average and frequency of baseline prompts for the Bracket Program are the same as for the Random Program. Again the computer takes control, and the remarks about the automatic sampler and operator control apply here also.

There are no calculation options. Calculation is done by interpolation; only. Each bracketed sample is run three times, and a relative standard deviation (RSD) is calculated and checked against the RSD entered earlier. If the sample RSD falls below the entered RSD, the program continues with the next

sample. Otherwise, two more attempts are made before continuing.

There is an Interim Report hard copy option. A continuous output is simultaneously displayed on the terminal and written onto a disk file in ASCII mode. At the end of the analysis when all of the samples have been attempted, this Interim Report, which is a history of the bracketing results, may be obtained as a hard copy. Then the Final Report is automatically produced.

## NOTES ON AUTOMATIC SAMPLER

The automatic sampler is a device that moves an arm up and down or swings it in a 360-deg circle. The arm must be precisely positioned over the containers in the sample holder, which contains 40 locations. The positioning is done by raising the arm and putting the sampler in manual switch setting.

The first position contains solvent or blank solution and can be a flow-through cell to avoid frequent refilling. The sampler is then loaded in a

clockwise manner with the standards as entered in the computer (increasing concentration) and the unknowns in the order in which they were entered in the computer. The first position (blank) is number 0, and subsequent positions are numbered 1 to 39.

The sampler is initialized to a zero position when the program is started. Thus the sampler position at startup time is defined as zero and should be centered over the blank (or solvent) solution.

## CHAINING

As mentioned previously the two programs Semiautomatic and Random chain to other programs. This is to insure that the program resident in core is not too large for efficient use of the operating system. Both programs use the same subprograms. One of the programs chained to is the Least Squares Subprogram already described in the section on the Semiautomatic Program.

Another program mentioned earlier is the Interim Report Subprogram. This program gives the results of the last run and the average of that run with all accepted previous runs. It also reports the standard deviation, relative standard deviation, and quality control results. It run, or in case an unknown was omitted. The addition of extra unknowns is not reported. Up to a maximum of 10 runs may be made on any set of standards and unknowns. After the Interim Report has been displayed or printed on

the terminal and the options answered, the program either returns to the main program or chains to the subprogram called Final Report.

The Final Report Subprogram gives the final average results of the runs along with quality control results and certain additional information, depending on whether the report is for the operator or customer.

The Final Report Subprogram is independent and may be called separately to furnish a report of a previous run, providing the data have been saved by changing the file names as explained earlier. See Appendixes B and C for explanations of the file structure.

The program ends in the Final Report Subprogram section, and the main program must be recalled to initiate a new run for a new element and/or a new set of samples.

## HELPFUL HINTS

Familiarity with running these programs may be obtained by simply typing in data that would correspond to the sample beam reading were it averaging the signal from a real solution. To do this hand entry of data the three programs must be modified to circumvent the real data acquisition section and instead ask for typed data. This information is presented in Appendix D.

Most errors or mistakes can be fixed and the program continued from the line on which it stopped by entering RUN XXXX where XXXX is the line number. Values can be set by equals sign; i.e., X=2. Files can be closed by the command CLOSE. The computer can also be used in a calculator mode; i.e., PRINT (X+Y)/Z will print

the answer directly on the terminal.

Finally, a word of warning. Because many of the programs chain back and forth, it is important for the operator to know what program he actually has in core before doing a SAVE. A SAVE stores the program on the disk and will overwrite another program of the same name. Thus, if the operator performs a SAVE thinking that one of the main programs is in core and that program is not in core, the program that is in core will overwrite it and the main program will be lost. He can recover it by reading it back from a magnetic tape record. Because disk records are volatile, magnetic tape records should always be kept as a backup.

## APPENDIX A

### Examples of Names of Programs and Files

<u>Instrument</u>	<u>Program</u>	<u>Files</u>	<u>A/D channel number</u>	<u>Local file name</u>	
PE 503	Semiautomatic	SM503.EM			
	Random	RS503.EM			
	Bracket	BR503.EM			
Varian AA5	Semiautomatic	SMAA5.EM			
	Random	RSAA5.EM			
	Bracket	BRAA5.EM			
			V503.SM		
			ID503.SM		
			V503.RS		
		ID503.RS			
		IN503.BR			
		FN503.BR			
		VAA5.SM			
		IDAA5.SM			
		VAA5.RS			
		IDAA5.RS			
		INAA5.BR			
		FNAAS.BR			
	<u>Subprogram</u>	<u>Function</u>			
	LSQ.AA	Least Squares calculations			
	INT.EM	Interim Report and calculations			
	RPT.EM	Final Report			

## APPENDIX B

### File Structure for Semiautomatic and Random Programs\*

Record No.	Information
<b>A. File: Standardization and Initialization Data.</b>	
1 <sup>b</sup>	Concentration of standard, last absorbance of standard
2	Concentration of standard, last absorbance of standard
3	Concentration of standard, last absorbance of standard
4	Concentration of standard, last absorbance of standard
5	Concentration of standard, last absorbance of standard
6	Concentration of standard, last absorbance of standard
7	Concentration of standard, last absorbance of standard
8	Concentration of standard, last absorbance of standard
9	Concentration of standard, last absorbance of standard
10	Concentration of standard, last absorbance of standard
11	Concentration of spike
12	Concentration of spike
13	Concentration of spike
14	Concentration of spike
15	Concentration of spike
16	Concentration of spike
17	Concentration of spike
18	Concentration of spike
19	Concentration of spike
20	Number of standards, unknowns, spikes, alphanumerics, baseline limit, integration time, pause time
21	Number of runs, mode of calculations, baseline frequency
22	Least squares coefficients, coefficient of determination
23	Program name, sample file name, standard file name, random or sequential
<b>B. File: Sample I.D. and Results.</b>	
1 through 50	Sample name, last absorbance, average concentration, variance, interpolation flag, dilution factor

<sup>a</sup>Files opened in random mode.

<sup>b</sup>Records 1 through 19 are compressed upwards.

## **APPENDIX C**

### **File Structure for Bracket Program**

ASCII records are written into two files, one for the Interim Report and one for the Final Report. Each file has a separate name and may be printed by a short routine.

## APPENDIX D

### Entering Values Directly for Familiarization

For all three programs, at line 8018 replace GOTO 8025 with REM GOTO 8025. This replacement will skip the on-line call, set the reference beam to 10,000, and prompt SAMPLE for the value to be entered. Dark current should be entered as zero.

Some suggested values are listed below.

#### Standards

<u>Concentration (ppb)</u>	<u>Signal to be entered</u>	<u>Absorbance*</u>
1. 250	8910	0.05012
2. 500	7940	0.10018
3. 750	7080	0.14997
4. 1000	6310	0.19997
5. 1250	5620	0.25026

#### Unknowns

<u>I.D.</u>	<u>Signal to be entered</u>	<u>Absorbance*</u>
1. First	8910	0.05012
2. Second	7940	0.10018
3. Third	7080	0.14997
4. CS3	7080	0.14997
5. SP17	6310	0.19997
6. Fourth	8910	0.05012
7. Fifth	7080	0.14997
8. DU6	8910	0.05012
9. SP210	6310	0.19997
10. Sixth	7940	0.10018
11. CS2	7940	0.10018
12. DU10	7940	0.10018
13. SP310	5620	0.25026

#### Spikes (ppb equivalent)

1. (SP1) 250
2. (SP2) 500
3. (SP3) 750

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\*Baseline values should be entered as 10,000 for above values to be valid.

**APPENDIX E**  
**Examples of Final Report**

Table E1. Atomic absorption report—operator.

DATE: 4 / 22 / 1977      WALTER BOYLE--JA-82-536

ELEMENT AND SAMPLE SOURCE: CALCIUM--SIMULATED DATA

SAMPLE NO. AND DESCRIPTION	AVERAGE CONC.(PPM) OF 2 RUNS	STANDARD DEVIATION	% RELATIVE STANDARD DEVIATION	AVERAGE % RECOVERY SPIKE, STD, OR UNK.
NO. 1 SIM1.....	1242.87	3.73	1.50	-----
NO. 2 SIM2.....	2528.5	4.57	0.86	-----
NO. 3 SIM5.....	753.67	.77	0.10	-----
NO. 4 CS3.....	753.87	15.93	1.85	100.52
NO. 5 SP17.....	1010.58	3.63	0.36	102.83
NO. 6 SIM4.....	252.52	4.93	3.93	-----
NO. 7 SIM5.....	753.5	13.52	1.74	-----
NO. 8 DU6.....	243.31	9.99	4.11	96.43
NO. 9 SP210.....	999.63	19.4	1.94	100.09
NO. 10 SIM6.....	499.19	6.98	1.39	-----
NO. 11 CS2.....	502.83	4.79	0.95	100.57
NO. 12 DU10.....	897.88	3.46	0.69	99.74
NO. 13 SP310.....	1248.16	10.32	0.82	99.86

STANDARDS PPM  
 250  
 500  
 750  
 1000  
 1250

FREQUENCY OF BASELINE HEAVY VARIES

STANDARD CURVE DEGREE OF FIT 2

COEFFICIENT OF DETERMINATION: .999295

MODE OF ANALYSIS AND ORDER OF SAMPLING SEMIAUTO

INSTRUMENT CONDITIONS  
 CA LAMP 250V

Table E2. Atomic absorption analysis report.

DATE: 9 / 22 / 1977

ELEMENT AND SAMPLE SOURCE: CALCIUM--SIMULATED DATA

SAMPLE NO. AND DESCRIPTION	AVERAGE CONC. (PPM) OF 2 RUNS	STANDARD DEVIATION	% RELATIVE STANDARD DEVIATION	AVERAGE % RECOVERY SPIKE, STD, UNK.
NO. 1 SIM1.....	1242.87	5.73	1.50	-----
NO. 2 SIM2.....	2528.3	4.37	0.86	-----
NO. 3 SIM3.....	753.67	.77	0.10	-----
NO. 4 CS3.....	753.67	13.93	1.85	100.52
NO. 5 SP17.....	1010.58	3.63	0.36	102.83
NO. 6 SIM4.....	252.32	9.93	3.93	-----
NO. 7 SIM5.....	753.5	13.52	1.79	-----
NO. 8 DU6.....	243.31	9.99	4.11	96.43
NO. 9 SP210....	999.63	19.4	1.94	100.09
NO. 10 SIM6.....	499.19	6.94	1.39	-----
NO. 11 CS2.....	502.83	4.79	0.95	100.57
NO. 12 DU10.....	497.88	3.46	0.69	99.74
NO. 13 SP310....	1248.16	10.32	0.82	99.86