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User's Guide for the Computer Program REsponse FACtor

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USER'S GUIDE FOR THE COMPUTER PROGRAM REsponse FACtor

by

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SECTION 1

SCOPE AND CONTENT

Each analyte in the internal standard quantitative analysis by electron impact Gas Chromatography/Mass Spectroscopy has a constant associated with it called the response factor (RF). For comparable injected weights, the response factor of an analyte is simply a ratio of the ion current of analyte and internal standard at their respective quantitation m/z values. It has been shown in an interlaboratory study for extractable priority pollutants that Fused Silica Capillary Column Gas Chromatography/Mass Spectroscopy (FSCC GC/MS) can yield similar response factors (1) and that the RF values can be effectively instrument independent when adequate quality control is maintained (2). Thus, the acquisition and monitoring of RF data are important in determining the level of instrument/laboratory performance and the acceptability of GC/MS data in interlaboratory applications of this technology and ultimately for determining the amount of analyte present in a sample. A quality control (QC) protocol to standardize experimental FSCC GC/MS acquisition parameters, acquisition sequence and data reporting was written and has been subsequently updated to reflect programmatic and other changes in the U.S. Environmental Protection Agency's Contract Laboratory Program (3).

The Consensus Organic Protocol of the Contract Laboratory Program requires two processes to establish and subsequently monitor system performance using the response factor. The first process, INITIALIZATION, requires the analysis of the system performance standard, followed by data acquisition of five multilevel, multianalyte calibration standards. The ONGOING or monitoring process requires the running of the system performance standard and a single level, multianalyte calibration standard at the beginning of each day or at a minimum of every 8 hours of GC/MS data acquisition. In both the INITIALIZATION and the ONGOING process, the resulting response factors are compared to contract specified criteria. The computer program, REsponse FACtor (REFAC), simply facilitates the examination and reporting of the response factors.

REFAC is written in FORTRAN IV as implemented by the Data General Corporation. It reads response lists for any given set of analytes, calculates the statistics required for system monitoring as determined by the Quality Control Protocol for the Contract Laboratory Program referenced above, and also provides additional response factor statistics, including correlation coefficients of ion current ratio plots, standard errors for linear fit and average relative retention times. REFAC creates a disk file to store the initialization statistics for later use in the ONGOING process. REFAC not only eliminates time-consuming hand calculations and transcription errors, which can occur in multianalyte quantitative GC/MS, but also facilitates the identification of

potential problems. As currently written, REFAC is only compatable with the INCOS Disk Operating System and Finnigan MAT file structures.

The purpose of this manual is to describe REFAC to the user and to demonstrate how to run the program. A description of the INITIALIZATION and ONGOING process is given in Section 2 along with the formulas used to calculate relevant statistics. Section 3 describes the running of REFAC, provides a command list, and also gives examples of REFAC generated output for both ONGOING and INITIALIZATION processes. REFAC variables and data structures are presented along with the source listing in Section 4.

SECTION 2

HOW REFAC WORKS

Using Finnigan MAT system software, the analyst can reduce raw GC/MS data into a quantitation list. This list contains the compounds detected in the data file by the MSDS program SEARch, the ion current area at the quantitation m/z value determined by the MSDS program CHROmatogram, the calculated extract concentration consistent with the reference library, and other data. The MSDS program QUANtitate (QUAN) can be used to display results and to create (or append) a response list for each compound in the quantitation list. REFAC reads the response lists and computes the statistics stipulated by the user (see Section 3). An example of REFAC output from MSDS generated response lists is given below. It should be noted that REFAC calculates statistics using data read from the response lists, and the program assumes that the results passed to REFAC are accurate.

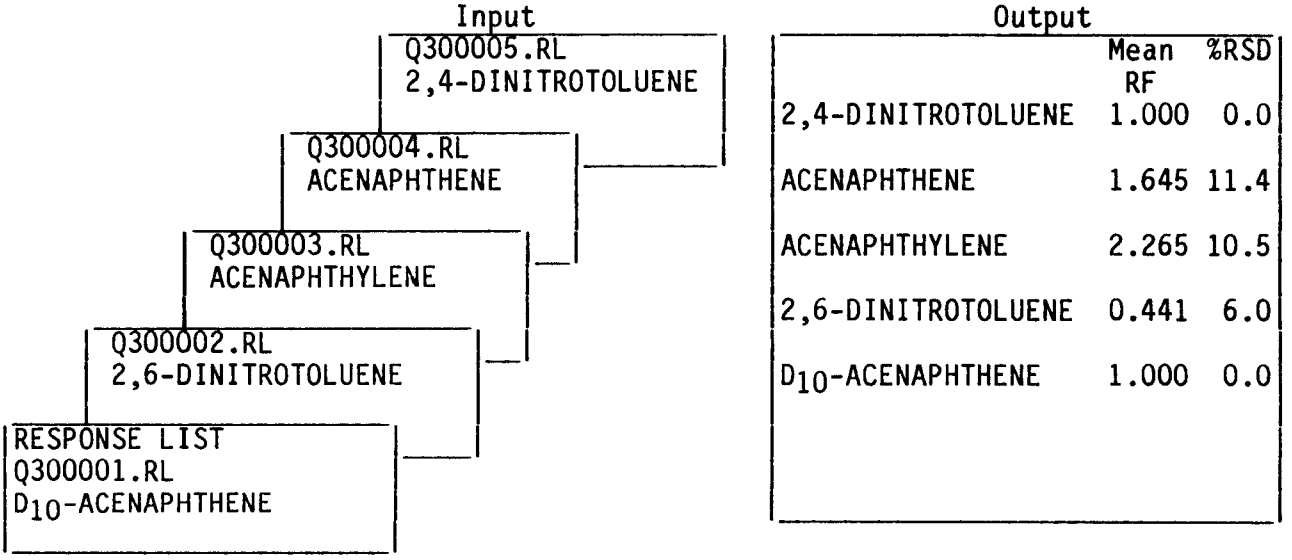

Figure 1. Statistics are performed and information is printed out on one sheet.

REFAC was written using the current QC protocol as a guideline (3), however, it can be easily updated to meet modified versions (see Section 4). The referenced QC protocol contains requirements that must be met in order for the data processed to be considered acceptable. These requirements can be classified into three groups:

1. QC requirements during the initialization process
2. QC requirements during sample analysis
3. QC requirements during the ongoing calibration

Only the INITIALIZATION and ONGOING processes have QC requirements involving response factor calculations, and consequently, only these processes will be considered below.

INITIALIZATION PROCESS

The INITIALIZATION process requires five calibration standards (concentrations of 20, 50, 80, 120, 160 µg/mL/analyte) to be run. Each of these standards contains the 61 semivolatile priority pollutants. For each of the compounds a response list is created by the user. Each response list should contain a response factor for each of the five runs. For specific analytes (Benzoic acid, 2,4,5-Trichlorophenol, 4-Nitroaniline, 3-Nitroaniline, 2-Nitroaniline, 4-Nitrophenol, Pentachlorophenol, and 4,6-Dinitro-2-Methylphenol) only 4 response factors may result because th 20 µg/mL concentration level approaches the detection limit for these compounds. In this case the output for REFAC in the 20 ng column is set to zero and is not averaged into the mean response factor calculations. For the remaining compounds, REFAC calculates the mean response factor and the relative standard deviation assuming that 5 entries are in each response list. See Figure 3 for an example of INITIALIZATION output for REFAC. As the statistics are calculated, the data are written to an LN.IN file, where LN is the first two letters of the response list name and IN is the extension given by REFAC. This file is subsequently used to do calculations in the ONGOING process for any response lists corresponding to the initialization response lists. Unless reinitialization is necessary this file is retained since ONGOING will access it.

REFAC users are cautioned that output will be only as valuable as the quality of the quantitation list from which response lists, and subsequent REFAC output is derived. Also, REFAC does not check to see if the results are within the QC requirements; this is left up to the user.

In initialization the average response factor is calculated using:

$$RF_{ave} = \left(\sum_{i=1}^{n} RF_i\right)/n$$

where RF_i is the corresponding response factor for the i^{th} entry, and n is set to 4 or 5. Relative standard deviation is calculated using:

$$\% \text{ RSD} = \frac{\sqrt{\left[\sum_{i=1}^{n} (RF_i - RF_{ave})^2\right]/n}}{RF_{ave}} \times 100$$

where RF_i, RF_{ave} and n are defined as above. The correlation coefficient is calculated using:

$$CC = \frac{\sum_{i=1}^{n} C_i \frac{AC_i}{AIS_i} - \left[\left(\sum_{i=1}^{n} C_i\right) \left(\sum_{i=1}^{n} \frac{AC_i}{AIS_i}\right)\right] /n}{\sqrt{\left[\sum_{i=1}^{n} C_i^2 - \left(\sum_{i=1}^{n} C_i\right)^2 /n\right] \sum_{i=1}^{n} \left(\frac{AC_i}{AIS_i}\right)^2 - \left(\sum_{i=1}^{n} \frac{AC_i}{AIS_i}\right)^2 /n}}$$

where n is defined as above, C_i is the concentration of the compound in the i^{th} run, AC_i is the area of the compound found in the ith run and AIS_i is the area of the internal standard found in the ith run. The formulas used for the standard error for linear fit are as follows:

$$S = \sqrt{\left[\sum_{i=1}^{n} \left(\frac{AC_i}{AIS_i} - \frac{AC_i}{AIS_i \text{ est}}\right)^2\right] /n}$$

with $\frac{AC_i}{AIS_i \text{ est}} = a + b\, C_i$. a and b are defined as follows:

$$b = \frac{n \sum_{i=1}^{n} C_i \frac{AC_i}{AIS_i} - \left(\sum_{i=1}^{n} C_i\right) \left(\sum_{i=1}^{n} \frac{AC_i}{AIS_i}\right)}{n \sum_{i=1}^{n} C_i^2 - \left(\sum_{i=1}^{n} C_i\right)^2}$$

$$a = \left(\sum_{i=1}^{n} \frac{AC_i}{AIS_i} /n\right) - b \left(\sum_{i=1}^{n} C_i\right) /n$$

This compares the area of the compound divided by the area of the internal standard to the amount of the compound.

ONGOING PROCESS

To monitor system performance, the QA/QC requirements contained in the Consensus Organic Protocol of the Contract Laboratory Program requires a single level multianalyte standard at a concentration of 50 µg/mL to be run at the beginning of each day or after every 8 hours of data acquisition. After the sample is run and the raw data are reduced to a quantitation list as described in the INITIALIZATION process, REFAC assumes that the response lists are appended, and consequently, the last entry in each response list will correspond to the run currently completed. REFAC reads the last response factor and performs ONGOING calculations. The referenced QC protocol only requires the calculation of the percentage difference but REFAC also calculates the standard error of the linear fit of all response factors in each list.

To calculate the percentage difference, data are needed for comparison from the INITILIZATION process. The INITIALIZATION data are read from the LN.IN file generated during the INITIALIZATION process. (If the .IN file is accidentally destroyed, re-initialize and only intialization points will be taken from the response list generating a new .IN file. The formula used to calculate the percentage difference is as follows:

$$\% D = \frac{RF_O - \overline{RF}_I}{\overline{RF}_I} \times 100$$

where RF_O is the response factor from the current run and $\overline{RF}_I$ is the average response factor from the initialization process. Standard error from the linear fit is calculated the same as in the initialization process, except that n is set to the number of entries read in from the response list. Normally this can be a maximum of 300; however, for this program the maximum is 50.

SECTION 3

RUNNING REFAC

In the implementation of REFAC, certain assumptions were required due to the nature of a computer and its limitations in handling exceptions while still being reasonably efficient. Before explaining how to run REFAC it will be helpful to know these basic assumptions. They are listed below:

1. REFAC assumes that there are 5 response factors contained in each list including the response lists for compounds that are not detected at 20 µg/mL. For these compounds, data should be recorded, but the data will not be considered accurate. As explained in INITIALIZATION, REFAC will disregard the 20 µg/mL run and only use the other four response factors present.

2. To print output data in a format acceptable for the Contractor Laboratory Program (in IFB format), compounds in the response list must be spelled exactly the same as in the file CMPND.DS (see Figure 6).

3. If REFAC receives as input a response list identifier that does not exist an error message will result. Be sure to check that each response list exists input by the user or read from the library list using the @ command.

To run REFAC, type onto the terminal: RUN REFAC

The program will respond by welcoming you to REFAC, and asking which process (initialization or ongoing) is wanted. Respond with I or O. Note: Within REFAC, the process (I or O) cannot be changed once selected. If you wish to change the process, then exit and restart the program.

REFAC will then ask the user if IFB format is wanted. Respond with Y or N. If the user responds N, then REFAC will skip IFB headings and ask about hardcopy. If IFB format is wanted REFAC will then select the proper heading depending on the process selected, and will print it to the terminal. For initialization it will look as follows:

INITIAL CALIBRATION DATA - SEMIVOLATILE HSL COMPOUNDS

CASE NO. 87654321 CONTRACT LAB: LEMSCO
CONTRACT NO. DA1202 INSTRUMENT IDENTIFIER: FINNIGAN 4010
CALIBRATION DATE: 3/22/84
MINIMUM MEAN RF FOR SPCC IS 0.05
MAXIMUM %RSD FOR CCC IS 30%

For Ongoing, the heading will look as follows:

CALIBRATION CHECK - SEMIVOLATILE HSL COMPOUNDS

```
CASE NO. 87654321                              CONTRACT LAB:  LEMSCO
CONTRACT NO. DA1202                INSTRUMENT IDENTIFIER:  FINNIGAN 4010
CALIBRATION DATE:  3/22/84
STANDARD FILE:  ABCDEFGHIJK
DATE:  3/1/84     TIME:  10:23
MAXIMUM % D FOR CCC IS 20
```

REFAC then asks if you want to make changes to the heading, type Y or N.

If the response is Y, REFAC will display a portion of the heading at a time. If a value different from the default value is desired, type in the new value and then carriage return. If no change is desired just type carriage return and the default value will be used.

When finished with changes to the heading, or if a typed N response was given when REFAC inquired "DO YOU WANT TO MAKE CHANGES," REFAC will enter command mode and prompt with "REFAC:"

REFAC COMMAND LIST

```
    N     ;  cancels hardcopy
    H     ;  resets hardcopy
    E     ;  exits the program
    ?     ;  lists REFAC commands
```

Variable Initialization Formats

```
    C     ;  outputs correlation coefficient to initialization output
    L     ;  outputs linear standard error to initialization output
    R     ;  outputs average relative retention time to initialization
             output
```

Variable Ongoing Format

```
    L     ;  adds linear standard error to ongoing output
```

To Perform Statistics

```
  $ LN, I, J ;  $ denotes consecutive entries from I to J in response lists LN
 #LN, I, J, K ;  # denotes separate entries I, J, K, etc. in response lists LN
          @ ;  uses library list
```

When in REFAC command mode, the user can cancel or reset hardcopy, choose the column heading format wanted and then perform statistics. If the user entered 'Y' to "IFB FORMAT (Y or N)" at the beginning of REFAC, then any format change commands are ignored. All the user needs to enter is one of the statistic commands.

REFAC will always default to output relative standard deviation in initialization and percent difference in ongoing unless one of the column heading change commands is entered before the first statistic command. A flowchart (Figure 1) and sample output (Figures 2 and 3) are provided on the following pages to clarify REFAC questions and commands. In Figures 2 and 3 the response factors are not necessarily indicative of values obtained following the current QC protocol and the operator should not use the response factor data as a determination for acceptable response factors.

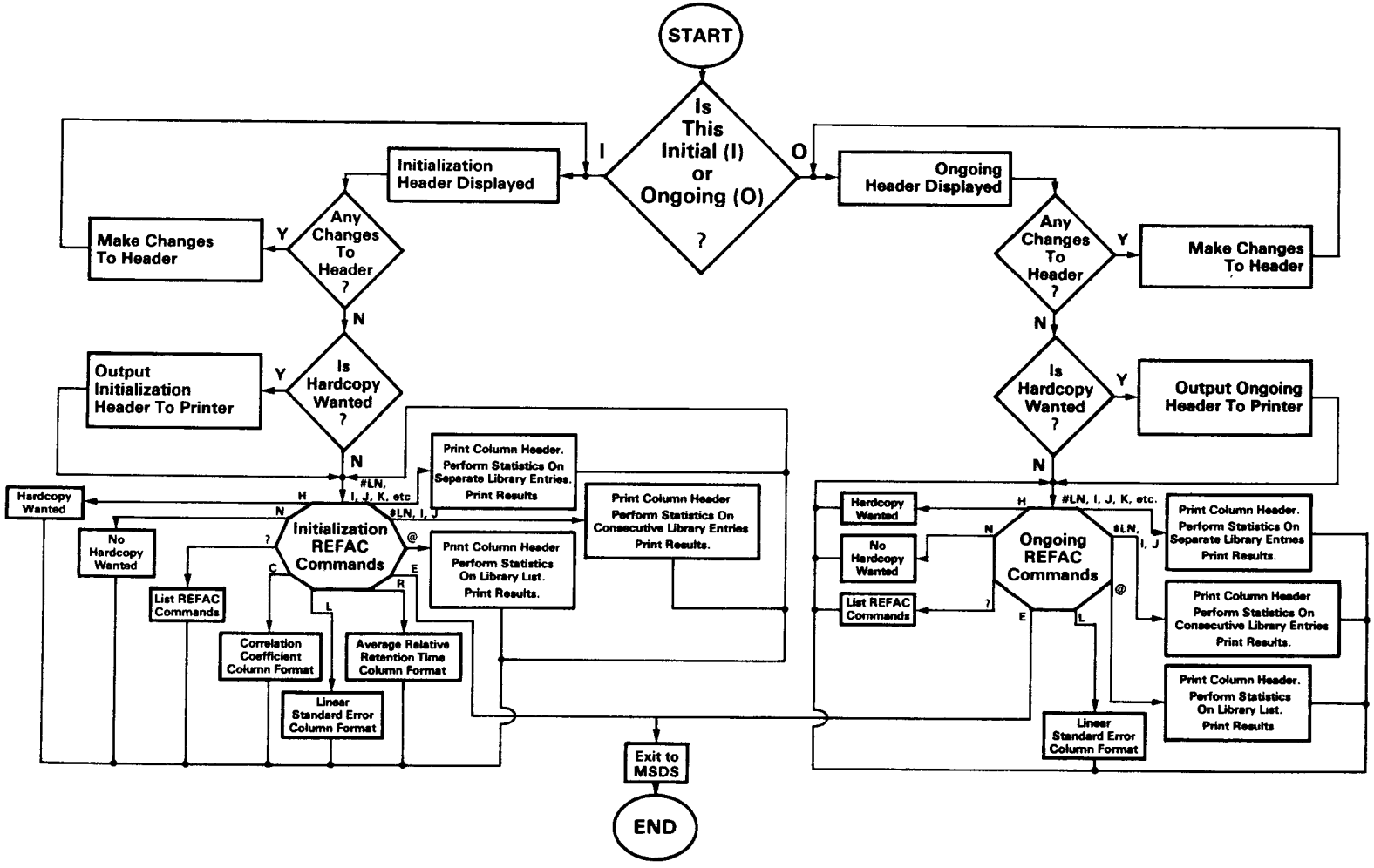

Figure 2. REFAC and user interaction flowchart.

COMPOUND	RF 20NG	RF 50NG	RF 80NG	RF 120NG	RF 160NG	MEAN RF	%RSD
D4-1,4 DICHLOROBENZENE	0.000	1.000	1.000	1.000	1.000	1.000	0.0
N-NITROSODIMETHYLAMINE	1 491	0.819	0.842	1.214	1.529	1.179	25.8
2-FLUOROPHENOL	1.959	1.230	1.287	1.328	1.442	1.449	18 2
2-FLUOROANILINE	1.912	1.607	1.641	1.735	1.843	1.747	6 6
PENTAFLUOROPHENOL	0.818	0.825	0.787	0.808	0.839	0.815	2 1
D5-PHENOL SURROGATE	1.613	1.534	1.533	1.561	1.607	1.570	2.2
PHENOL	2.316	2.219	2.310	2.102	2.186	2.227	3.5
ANILIN	2.503	2.434	2.547	2.646	2.696	2.565	3.6
BIS(2-CHLOROETHYL)ETHER	1.640	1.655	1.649	1.710	1.757	1.682	2.6
2-CHLOROPHENOL	1.477	1.475	1.490	1.626	1.694	1.553	5.8
1,3-DICHLOROBENZENE	1.524	1.690	1.694	1.814	1.800	1.704	6.1
1,4-DICHLOROBENZENE	1.587	1.754	1.734	1.811	1.845	1.746	5.0
BENZYL ALCOHOL	0.969	1.130	1.115	1.053	1.040	1.061	5.4
1,2-DICHLOROBENZENE	1.374	1.615	1.593	1.581	1.622	1.557	5.9
ORTHO CRESOL	1.360	1.567	1.497	1.423	1.474	1.464	4.7
BIS(2-CHLOROISOPROPYL)ETHER	2 847	3.637	3.708	2.938	2.917	3.210	11.8
PARA CRESOL	1.354	1.645	1.590	1.402	1.457	1.490	7.4
N-NITROSO-DI-N-PROPYLAMINE	0.000	0.979	1.023	0.924	0.708	0.909	13.3
HEXACHLOROETHANE	0.444	0.589	0.557	0.492	0.544	0.525	9.7
D8-NAPHTHALENE	1.000	1.000	1.000	1.000	1.000	1.000	0.0
D5-NITROBENZENE SURROGATE	0.165	0.176	0.175	0.180	0.192	0.178	4.8
NITROBENZENE	0.351	0.357	0.375	0.496	0.355	0.387	14.2
DECAFLUOROBIPHENYL	0.189	0.264	0.278	0.295	0.278	0.261	14.2
ISOPHORONE	0.614	0.659	0.681	0.772	0.589	0.663	9.5
2-NITROPHENOL	0.163	0.194	0.199	0.242	0.192	0.198	12.7
2,4-DIMETHYLPHENOL	0.318	0.322	0.335	0.382	0.307	0.333	7.8
BIS(2-CHLOROETHOXY)METHANE	0.454	0.506	0.499	0.563	0.482	0.501	7.1
BENZOIC ACID	0 000	0.156	0.140	0.164	0.191	0.163	11.2
2,4-DICHLOROPHENOL	0.315	0.337	0.339	0.390	0.358	0.348	7.1
1,2,4-TRICHOROBENZENE	0.317	0.359	0.356	0.396	0.369	0.359	7.0
NAPHTHALENE	1.059	1.190	1.187	1.354	1.217	1.201	7.8
4-CHLOROANILIN	0.401	0.423	0.451	0.481	0.474	0.446	6.8
HEXACHLOROBUTADIENE	0.166	0.180	0.178	0.185	0.187	0.179	4.1
4-CHORO-3-METHYLPHENOL	0.316	0.291	0.312	0.281	0.309	0.302	4.5
2-METHYLNAPHTHALENE	0.796	0.790	0.812	0.785	0.874	0.811	4.0
D10-ACENAPHTHENE	1.000	1.000	1.000	1.000	1.000	1.000	0.0
HEXACHLOROCYCLOPENTADIENE	0.000	0.538	0.475	0.529	0.565	0.527	6.2
2,4,6-TRICHLOROPHENOL	0.450	0.548	0.554	0.557	0.590	0.540	8.7
2,4,5-TRICHLOROPHENOL	0.502	0.578	0.531	0.637	0.614	0.572	8.7
2-FLUOROBIPHENYL	2.162	2.496	2.492	2.615	2.554	2.464	6.3
2-CHLORONAPHTHALENE	1.897	2.248	2.170	2.554	2.410	2.256	9.8
2-NITROANILINE	0.523	0.601	0.617	0.662	0.683	0.617	8.9
DIMETHYLPHTHALATE	1.740	1.882	1.842	2.183	2.025	1.934	7.9
ACENAPHTHYLENE	2.561	2.870	2.723	3.195	3.059	2.882	7.8
2,6-DINITROTOLUENE	0.381	0.434	0.425	0.468	0.468	0.435	7.4
3-NITROANILINE	0.416	0.438	0.454	0.508	0.534	0.470	9.3
ACENAPHTHENE	1.777	1.882	1.812	2.279	2.134	1.977	9.9
2,4-DINITROPHENOL	0.000	0.081	0.089	0.108	0.117	0.099	14.5
4-NITROPHENOL	0.000	0.261	0.308	0.281	0.315	0.292	7.4
DIBENZOFURAN	2.404	2.445	2.335	2.953	2.831	2.594	9.6
2,4-DINITROTOLUENE	0.421	0.435	0.429	0.479	0.461	0.445	4.8
DIETHYLPHTHALATE	1.725	1.594	1.599	2.107	1.895	1.784	10.9
FLUORENE	1.998	2.008	1.970	2.607	2.449	2.206	12.1
4-CHLOROPHENYL-PHENYL ETHER	1.098	1.139	1.123	1.535	1.379	1.255	13.7
4-NITROANILINE	0.377	0.374	0.323	0.411	0.434	0.384	9.8
D10-PHENANTHRENE	0.000	1.000	1.000	1.000	1.000	1.000	0.0
4,6-DINITRO-O-CRESOL	0.050	0.078	0.095	0.082	0.089	0.079	19.6
N-NITROSODIPHENYLAMINE	0.270	0.316	0.330	0.322	0.319	0 311	6.8
2,4,6-TRIBROMOPHENOL	0.088	0.110	0.125	0.130	0.139	0.119	15.1
4-BROMOPHENYL-PHENYL ETHER	0.237	0.285	0.297	0.302	0.298	0.284	8.4
ALPHA-BHC	0.142	0.150	0.152	0.156	0.157	0.151	3.4
HEXACHLOROBENZENE	0.240	0.273	0.296	0.274	0.277	0.272	6.6
BETA-BHC	0.113	0.123	0.121	0.121	0.125	0.120	3.4

Figure 3. Initialization sample output.

COMPOUND	MEAN RF(I)	RF(O)	% D
D4-1,4 DICHLOROBENZENE	1.000	1.000	0.000
N-NITROSODIMETHYLAMINE	1.179	0.909	-22.897
2-FLUOROPHENOL	1.449	1.442	-0.466
2-FLUOROANILINE	1.747	1.625	-7.035
PENTAFLUOROPHENOL	0.815	0.770	-5.513
D5-PHENOL SURROGATE	1.570	1.498	-4.579
PHENOL	2.227	2.271	1.975
ANILIN	2.565	2.550	-0.600
BIS(2-CHLOROETHYL)ETHER	1.682	1.593	-5.322
2-CHLOROPHENOL	1.553	1.469	-5.353
1,3-DICHLOROBENZENE	1.704	1.587	-6.868
1,4-DICHLOROBENZENE	1.746	1.611	-7.723
BENZYL ALCOHOL	1.061	1.082	1.994
1,2-DICHLOROBENZENE	1 557	1.465	-5.941
ORTHO CRESOL	1.464	1.483	1.322
BIS(2-CHLOROISOPROPYL)ETHER	3.210	1.758	-45.215
PARA CRESOL	1.490	1.455	-2.337
N-NITROSO-DI-N-PROPYLAMINE	0.909	0.873	-3.904
HEXACHLOROETHANE	0.525	0.523	-0.318
D8-NAPHTHALENE	1.000	1.000	0.000
D5-NITROBENZENE SURROGATE	0.178	0.185	4.038
NITROBENZENE	0.387	0.373	-3.698
DECAFLUOROBIPHENYL	0.261	0.239	-8.497
ISOPHORONE	0.663	0.679	2.458
2-NITROPHENOL	0.198	0.201	1.356
2,4-DIMETHYLPHENOL	0.333	0.336	1.026
BIS(2-CHLOROETHOXY)METHANE	1.682	0.505	-69.942
BENZOIC ACID	0.163	0.150	-7.711
2,4-DICHLOROPHENOL	0.348	0.340	-2.328
1,2,4-TRICHOROBENZENE	0.359	0.350	-2.693
NAPHTHALENE	1.201	1.203	0.131
4-CHLOROANILIN	0 446	0.439	-1.544
HEXACHLOROBUTADIENE	0.179	0.179	-0.161
4-CHORO-3-METHYLPHENOL	0.302	0.289	-4.381
2-METHYLNAPHTHALENE	0.811	0.786	-3.159
D10-ACENAPHTHENE	1.000	1.000	0.000
HEXACHLOROCYCLOPENTADIENE	0.527	0.524	-0.522
2,4,6-TRICHLOROPHENOL	0.540	0.554	2.666
2,4,5-TRICHLOROPHENOL	0.572	0.578	0.935
2-FLUOROBIPHENYL	2.464	2.472	0.341
2-CHLORONAPHTHALENE	2.256	2.311	2.452
2-NITROANILINE	0.617	0.650	5.275
DIMETHYLPHTHALATE	1.934	2.080	7.543
ACENAPHTHYLENE	2.882	2.884	0.068
2,6-DINITROTOLUENE	0.435	0.441	1.425
3-NITROANILINE	0.470	0.530	12.729
ACENAPHTHENE	1.977	1.984	0.368
2,4-DINITROPHENOL	0.099	0.127	28.901
4-NITROPHENOL	0.292	0.317	8.759
DIBENZOFURAN	2.594	2.599	0.220
2,4-DINITROTOLUENE	0.445	0.505	13.449
DIETHYLPHTHALATE	1.784	1.862	4.370
FLUORENE	2.206	2.188	-0.813
4-CHLOROPHENYL-PHENYL ETHER	1.255	1.330	6.023
4-NITROANILINE	0.384	0.456	18.806
D10-PHENANTHRENE	1.000	1.000	0.000
4,6-DINITRO-O-CRESOL	0.079	0.096	21.797
N-NITROSODIPHENYLAMINE	0.311	0.335	7.554
2,4,6-TRIBROMOPHENOL	0.119	0.103	-13.330
4-BROMOPHENYL-PHENYL ETHER	0.284	0.275	-3.098
ALPHA-BHC	0.151	0.152	0.461
HEXACHLOROBENZENE	0.272	0.237	-12.723
BETA-BHC	0.120	0.123	2.271

Figure 4. Ongoing sample output.

SECTION 4

REFAC DOCUMENTATION

This section assumes the reader has a knowledge of FORTRAN IV and the INCOS Disk Operating System (IDOS) as used by the Finnigan Corporation for GC/MS data systems. The purpose of this section is to clarify REFAC code to help the user easily modify REFAC to fit various needs in different laboratory situations and to easily update it to keep up with IFB Contract Laboratory procurement changes. This section should be used as a reference when reading through the code before making changes. It is divided into three parts: an explanation of major variables, an explanation of subroutines and functions, and an explanation of file formats.

MAJOR VARIABLES

AC - an array dimensioned to 50 that contains the area of the compound divided by the area of the reference compound.

C - an array dimensioned to 50 that contains the amount of the compound for each entry in the response list.

CC - contains the correlation coefficient.

FNUM - an array dimensioned to 30 that contains any real numbers input to the terminal in REFAC command mode.

IANS - hardcopy flag.

IC - a counter set up to count the number of response lists read.

ICL - an integer array dimensioned to 10 that contains the name of the contract lab for the main header.

ICOMI(0)- an integer array dimensioned to 14 that contains the name of the compound for initialization (ongoing).

ICQHD - an integer array that contains all variable information pertaining to the main header. It is equivalenced to the CQHD common block.

ICR - a counter set up to count the number of entries in a response list.

ICSN - an integer array dimensioned to 5 that contains the case number for the main header.

ICTN - an integer array dimensioned to 5 that contains the contract number for the main header.

ID - an integer array dimensioned to 10 that contains the instrument identifier for the main heading.

IDATE - an integer array dimensioned to 4 that contains the calibration date for the main header.

IDESC - contains the file descriptor for the response lists.

IFB - IFB format flag.

IHEAD - an integer array dimensioned to 84 that holds the response list header information. It is equivalenced to the CHEAD common block.

IIN - a two dimensional array that holds initialization information for each compound.

INCNT - a counter set up to count the number of initialization compounds read in from the .IN file for use in ongoing calculations.

IOK - flag used to determine if main header changes are wanted.

ION - a two dimensional array that holds ongoing information for each compound.

IPROC - initialization or ongoing flag.

IQ - a two dimensional containing response list entry information for each run.

ISD - contains standard file date for the main header.

ISF - contains name of the standard file for the main header.

IST - contains standard file time for the main header.

JIN - an array that contains initialization information for the current compound.

JON - an array that contains ongoing information for the current compound.

JQ - an array that contains response list entry information for the current run.

KDESC - file descriptor for the file containing main header information.

LDESC - file descriptor for the file containing the initialization information. Ongoing reads from it and initialization writes to it.

MAXQ - the maximum amount of entries allowed in a response list.

MAXD - the maximum number of response lists that can be referenced.

MAXIN - the number of initialization runs.

NFL - column flag to determine which output to use.

NUM - an array dimensioned to 30 that contains any integers inputted to the terminal in REFAC command mode.

RETM - contains the average relative retention time.

RDEV - contains the relative standard deviation of the response factors.

RF - an array containing the response factors for a compound as read in from the response list.

RFL - contains the last response factor read in.

RFMI(0) - contains the mean response factor.

RLINI(0)- contains the standard error for linear fit with area of compound divided by area of reference compound plotted against amount.

RSUM - contains the summation of all response factors.

ST - contains the standard deviation of the response factors.

SUBROUTINES

Call IFORM (IPROC, NFL, ION, IIN, IDEV, IC)

This routine prints ongoing or initialization data out in IFB format. It will print out all semivolatile compounds. For the compounds that have no data, only the name will be printed out. The arguments are defined under explanation of major variables.

Call IZERO (IDESC)

This routine initializes a response list file descriptor.

Call QUEST ("string", I1, ICHAR, I2)

This routine prints out a string constant, an associated character variable and waits for input to change the character variable. A carriage return does not change the character variable. The arguments are defined as follows:

"string" - a string literal to be printed out as written.

I1 - an integer containing the number of characters in "string." I1 must be greater than 10 even if "string" is shorter.

ICHAR - a character array containing data pertaining to the string. It must be less than or equal to 9.

I2 - an integer containing the length of ICHAR.

Call SORT (RARY1, RARY2, I1)

This routine sorts the first I1 elements of two real arrays from smallest to largest. It does this by comparing values in RARY2. I1 cannot be greater than 5. Also, if the smallest element of RARY2 is 35, it only sorts I1-1 elements and sets the first element of RARY1 to 0.

FUNCTIONS

RMEAN (R, IC)

This function divides the real argument (R) by the integer argument (IC).

RST (R1, R2)

This function divides R1 by R2 and multiplies by 100.

STDEV (RARY, AVE, IC)

This function finds the standard deviation of an array of real numbers (RARY) containing up to 250 elements. AVE is the mean of the array and IC is the number of elements.

FILE FORMATS

LNOOOOn.RF

This file is a response list created by QUAN where LN is a one or two character library name and n is a right justified integer no larger than 5 digits. It consists of an 84 word header containing variables defined in the common block CHEAD. The header is followed by 22 word entries. Each file can have a maximum of 300 entries. The variables contained in each 22 word block are defined by the common block CLIST.

LN.IN

This file is created by REFAC when initialization is chosen. LN will be any one or two character library name. It consists of 34 word entries. It can have any amount of entries. The variables contained in each 34 word block are defined by the common block CIN.

HEAD.IN

This file is one 52 word block containing main header information for IFB output. The variables are defined by the common block CQHD.

CMPND.DS

This is a FORTRAN readable file containing in IFB order the 69 semivolatile compounds. It is used to sort ongoing or initialization data.

NOTES

To change the number of initialization runs the user needs to change the parameter MAXIN from 5 to the number of initialization points desired. Format statements to print column headings (labels 1170-1186) and initialization output (label 1230) will also need to be changed to reflect data output. The necessary format changes should be clear. It is suggested that the user copy REFAC to a file named to reflect the number of initialization points REFAC will use. For example, if 3 points are used call the new program REFAC3.FR.

To change the order or spelling of compounds in IFB format the user need only edit the file CMPND.DS. If different compounds or additional compounds are desired just insert them into the file where desired. CMPND.DS cannot have more than 75 compounds.

INITIAL CALIBRATION DATA - SEMIVOLATILE HSL COMPOUNDS[a]

CASE NO. 87654321 CONTRACT LAB: LEMSCO
CONTRACT NO. DA1202 INSTRUMENT IDENTIFIER: FINNIGAN 4010
CALIBRATION DATE: 3/22/84
MINIMUM MEAN RF FOR SPCC IS 0.05
MAXIMUM %RSD FOR CCC IS 30%

COMPOUND	RF 20NG	RF 50NG	RF 80NG	RF 120NG	RF 160NG	MEAN RF	%RSD
NITROSODIMETHYLAMINE							
PHENOL							
ANILINE							
BIS(2-CHLOROETHYL)ETHER	1.640	1.655	1.649	1.710	1.757	1.682	2.643
2-CHLOROPHENOL	1.477	1.475	1.490	1.626	1.694	1.553	5.843
1,3-DICHLOROBENZENE	1.524	1.690	1.694	1.814	1.800	1.704	6.101
1,4-DICHLOROBENZENE	1.587	1.754	1.734	1.811	1.845	1.746	5.078
BENZYL ALCOHOL	0.969	1.130	1.115	1.053	1.040	1.061	5.456
1,2-DICHLOROBENZENE	1.374	1.615	1.593	1.581	1.622	1.557	5.942
2-METHYLPHENOL							
N-NITROSO-DI-N-PROPYLAMINE	0.000	0.979	1.023	0.924	0.708	0.909	13.322
HEXACHLOROETHANE	0.444	0.589	0.557	0.492	0.544	0.525	9.761
NITROBENZENE							
ISOPHORONE							
2-NITROPHENOL	0.163	0.194	0.199	0.242	0.192	0.198	12.775
2,4-DIMETHYLPHENOL	0.318	0.322	0.335	0.382	0.307	0.333	7.833
BENZOIC ACID							
BIS(2-CHLOROETHYL)ETHER	1.640	1.655	1.649	1.710	1.757	1.682	2.643
2,4-DICHLOROPHENOL	0.315	0.337	0.339	0.390	0.358	0.348	7.168
1,2,4-TRICHLOROBENZENE							
NAPHTHALENE							
4-CHLOROANILIN	0.401	0.423	0.451	0.481	0.474	0.446	6.802
HEXACHLOROBUTADIENE	0.166	0.180	0.178	0.185	0.187	0.179	4.158
4-CHLORO-3-METHYLPHENOL							
2-METHYLNAPHTALENE							
HEXACHLOROCYCLOPENTADIENE	0.000	0.538	0.475	0.529	0.565	0.527	6.227
2,4,6-TRICHLOROPHENOL	0.450	0.548	0.554	0.557	0.590	0.540	8.726
2,4,5-TRICHLOROPHENOL	0.502	0.578	0.531	0.637	0.614	0.572	8.794
2-CHLORONAPHTHALENE	1.897	2.248	2.170	2.554	2.410	2.256	9.892
4-NITROANILINE	0.377	0.374	0.323	0.411	0.434	0.384	9.808
DIMETHYLPHTHALATE	1.740	1.882	1.842	2.183	2.025	1.934	7.973
ACENAPHTHYLENE	2.561	2.870	2.723	3.195	3.059	2.882	7.875
3-NITROANILINE	0.416	0.438	0.454	0.508	0.534	0.470	9.382
ACENAPHTHENE							
2,4-DINITROPHENOL	0.000	0.081	0.089	0.108	0.117	0.099	14.552
4-NITROPHENOL	0.000	0.261	0.308	0.281	0.315	0.292	7.462
DIBENZOFURAN							
2,4-DINITROTOLUENE	0.421	0.435	0.429	0.479	0.461	0.445	4.837
2,6-DINITROTOLUENE	0.381	0.434	0.425	0.468	0.468	0.435	7.402
DIETHYLPHTHALATE	1.725	1.594	1.599	2.107	1.895	1.784	10.942
4-CHLOROPHENYL-PHENYL ETHER	1.098	1.139	1.123	1.535	1.379	1.255	13.769
FLUORENE							
2-NITROANILINE	0.523	0.601	0.617	0.662	0.683	0.617	8.996
4,6-DINITRO-O-CRESOL	0.050	0.078	0.095	0.082	0.089	0.079	19.614
N-NITROSODIPHENYLAMINE	0.270	0.316	0.330	0.322	0.319	0.311	6.810
AZOBENZENE							
4-BROMOPHENYL-PHENYL ETHER	0.237	0.285	0.297	0.302	0.298	0.284	8.446
HEXACHLOROBENZENE	0.240	0.273	0.296	0.274	0.277	0.272	6.670
PENTACHLOROPHENOL	0.089	0.116	0.143	0.128	0.131	0.122	14.960
PHENANTHRENE							
ANTHRACENE							
DI-N-BUTYLPHTHALATE	1.239	1.346	1.323	1.660	1.463	1.406	10.357
FLUORANTHENE							
BENZIDINE							
PYRENE							

Figure 5. IFB format sample output.

BUTYLBENZYLPHTHALATE	0.791	0.898	0.899	0.987	0.965	0.908	7.540
3,3'-DICHLOROBENZIDINE	0.391	0.396	0.379	0.460	0.468	0.419	8.930
BENZO(A)ANTHRACENE	1.320	1.469	1.526	1.466	1.432	1.442	4.735
BIS(2-ETHYLHEXYL)PHTHALATE	0.818	0.919	0.919	1.013	1.010	0.936	7.664
CHRYSENE							
DI-N-OCTYLPHTHALATE	1.727	1.901	1.971	2.319	2.463	2.076	13.132
BENZO(B)FLUORANTHENE							
BENZO(K)FLUORANTHENE							
INDENO(1,2,3-CD)PYRENE							
DIBENZ(A,H)ANTHRACENE							
BENZO(GHI)PERYLENE							

Figure 5. Continued

[a] Output for some compounds are blank as a result of different spellings in the response list and the file CMPND.DS or the response list identifier (as described in Section 3) in REFAC command mode was not given.

```
N-NITROSODIMETHYLAMINE              1  5
PHENOL                              2  5
ANILINE                             3  5
BIS(2-CHLOROETHYL)ETHER             4  5
2-CHLOROPHENOL                      5  5
1,3-DICHLOROBENZENE                 6  5
1,4-DICHLOROBENZENE                 7  5
BENZYL ALCOHOL                      8  5
1,2-DICHLOROBENZENE                 9  5
2-METHYLPHENOL                     10  5
BIS(2-CHLOROISOPROPYL)ETHER        11  5
4-METHYLPHENOL                     12  5
N-NITROSO-DI-N-PROPYLAMINE         13  5
HEXACHLOROETHANE                   14  5
NITROBENZENE                       15  5
ISOPHORONE                         16  5
2-NITROPHENOL                      17  5
2,4-DIMETHYLPHENOL                 18  5
BENZOIC ACID                       19  5
BIS(2-CHLOROETHOXY)METHANE         20  5
2,4-DICHLOROPHENOL                 21  5
1,2,4-TRICHLOROBENZENE             22  5
NAPHTHALENE                        23  5
4-CHLOROANILINE                    24  5
HEXACHLOROBUTADIENE                25  5
4-CHLORO-3-METHYLPHENOL            26  5
2-METHYLNAPHTALENE                 27  5
HEXACHLOROCYCLOPENTADIENE          28  5
2,4,6-TRICHLOROPHENOL              29  5
2,4,5-TRICHLOROPHENOL              30  5
2-CHLORONAPHTHALENE                31  5
2-NITROANILINE                     32  5
DIMETHYL PHTHALATE                 33  5
ACENAPHTHYLENE                     34  5
3-NITROANILINE                     35  5
ACENAPHTHENE                       36  5
2,4-DINITROPHENOL                  37  4
4-NITROPHENOL                      38  4
DIBENZOFURAN                       39  5
2,4-DINITROTOLUENE                 40  5
2,6-DINITROTOLUENE                 41  5
DIETHYLPHTHALATE                   42  5
4-CHLOROPHENYL-PHENYLETHER         43  5
FLUORENE                           44  5
4-NITROANILINE                     45  5
4,6-DINITRO-2-METHYLPHENOL         46  4
N-NITROSODIPHENYLAMINE             47  5
4-BROMOPHENYL-PHENYLETHER          48  5
HEXACHLOROBENZENE                  49  5
PENTACHLOROPHENOL                  50  4
PHENANTHRENE                       51  5
ANTHRACENE                         52  5
DI-N-BUTYLPHTHALATE                53  5
FLUORANTHENE                       53  5
BENZIDINE                          55  4
PYRENE                             56  5
BUTYLBENZYLPHTHALATE               57  5
3,3'-DICHLOROBENZIDINE             58  5
BENZO(A)ANTHRACENE                 59  5
BIS(2-ETHYLHEXYL)PHTHALATE         60  5
CHRYSENE                           61  5
DI-N-OCTYL PHTHALATE               62  5
BENZO(B)FLUORANTHENE               63  5
BENZO(K)FLUORANTHENE               64  5
BENZO(A)PYRENE                     65  5
INDENO(1,2,3-CD)PYRENE             66  5
DIBENZ(A,H)ANTHRACENE              67  5
BENZO(GHI)PERYLENE                 68  5
```

Figure 6. Listing of CMPND.DS.

```
C  RF
C  MARY BATES 7/5/84
C  GLINN HANSEN 12/13/83
C
      PARAMETER MAXG=50, LEN=22, LENH=84, LENI=34, LENO=22, MAXD=100, MAXIN=5
      PARAMETER LENG=52, MAXS=200, TTO=10, DSK=1, LPT=2
      PARAMETER IDLEN=11, NLEN=35, ILEN=14
      INTEGER IIN(LENI,10), JIN(LENI), ION(LENO,MAXD), JON(LENO)
      INTEGER DFSW, DFSW1, DFILE, SFILE, CFL
      INTEGER IG(LEN,MAXG), JG(LEN), IHEAD(LENH)
C
      COMMON/CGHD/ICSN(5), ICL(10), ICTN(5), ID(10), IDATE(4),
     +            ISF(10), ISD(4), IST(4)
C
      COMMON/CHEAD/NAME(NLEN), FMASS, SMASS, IU1, IU2, LNAMER, LNUMR,
     +            NAMER(NLEN), FMASSR, SMASSR, IU3, IU4
C
      COMMON/CLIST/IDAY, IRUN, RET, METH(2), AREA,
     +            HIT, AMNT, RETR, METHR(2), AREAR, HITR, AMNTR
C
      COMMON/CIN/ICOMI(ILEN), RFC(5), RFMI, RSD, RETM, CC, RLINI
C
      COMMON/CON/ICOMO(ILEN), RFMO, RFL, PD, RLINO
C
      COMMON/CMAIN/NPROG, DFSW, DFSW1, ITEMP(15),
     + DFILE(12,6), SFILE(IDLEN,4), INSTD(3), IREFTABLE(IDLEN),
     + JUNK(7), LIBRNAME, LIBRNUMB, IBUF, ISCN(45), IACG(100), IDAT(45)
C
      INTEGER IDESC(IDLEN), KDESC(IDLEN), LDESC(IDLEN), JFILE(IDLEN)
      REAL RF(MAXG), RT(MAXG), AC(MAXG), C(MAXG)
      DIMENSION NUM(MAXD), FNUM(30), ICGHD(LENG), IS(2,MAXS)
C
C  THE PURPOSE FOR THE USE OF AN EQUIVALENCE STATEMENT IS TO
C  FACILITATE FILE I/O.  SINCE FM ROUTINES ARE USED FOR I/O,
C  DATA MUST BE READ INTO ARRAYS DIMENSIONED TO THE NUMBER
C  OF WORDS THE PROGRAMMER NEEDS TO READ.  THE EQUIVALENCE
C  STATEMENT ALLOWS THE PROGRAMMER TO READ A RECORD OF DATA
C  TYPES INTO AN ARRAY AND THEN ACCESS EACH COMPONENT BY NAME
C  AS NEEDED.  FOR EXAMPLE IHEAD IS AN ARRAY DIMENSIONED TO THE
C  LENGTH OF ALL COMPONENTS IN THE COMMON BLOCK CHEAD.  DATA ARE
C  READ INTO IHEAD IN FMRD AND THEN TO ACCESS ANY COMPONENT OF
C  CHEAD THE VARIABLE NAME IS USED.
C
      EQUIVALENCE (IHEAD,NAME),
     1            (JG,IDAY),
     1            (JIN,ICOMI),
     1            (JON,ICOMO),
     1            (ICGHD,ICSN)
C
      WRITE(10,1130)
C
C  ASK USER IF THIS IS ONGOING OR INITIALIZATION
C
   20 WRITE(10,1010)
 1010 FORMAT(" ONGOING OR INITIALIZATION (O OR I)?: ",Z)
      READ(11,1020) IPROC
 1020 FORMAT(A2Z)
      IF(IPROC .NE. "O " .AND. IPROC .NE. "I ") GO TO 20
C
C  ASK USER IF IFB FORMAT IS WANTED
C
   25 WRITE(10,1025)
 1025 FORMAT(" IFB FORMAT(Y OR N)?: ",Z)
      READ(11,1026) IFB
 1026 FORMAT(A2Z)
      IF (IFB .NE. "Y " .AND. IFB .NE. "N ") GO TO 25
```

```
      DO 27 I=1,LENG
   27 ICGHD(I) = "  "
      DO 30  I=1,IDLEN
   30 KDESC(I) = 0
      KDESC(1) = "1<0>"
      KDESC(3) = 1
      KDESC(4) = "HE"
      KDESC(5) = "AD"
      KDESC(10) = "IN"
      CALL FMCHK(KDESC,$50)
C
C  READ IN HEADER VALUES SINCE HEAD.IN HAS BEEN PREVIOUSLY SET
C
      CALL FMOPR(KDESC,ICH1,$8600,IERR)
      CALL FMRD(ICGHD,ICH1,LENG,$8200,IERR)
      CALL FMCLS(ICH1,$8600)
C
C  PRINT OUT HEADER FOR INITIALIZATION OR ONGOING
C
   50 IDEV = 10
   60 WRITE(10,1130)
      IF(IPROC .EQ. "O ") GO TO 70
      WRITE(IDEV,1030)
 1030 FORMAT(10X,"INITIAL CALIBRATION DATA - SEMIVOLATILE HSL
     +  COMPOUNDS")
      WRITE(IDEV) "  "
      WRITE(IDEV,1040) ICSN,ICL
 1040 FORMAT(" CASE NO. ",5A2,23X,"CONTRACT LAB: ",10A2)
      WRITE(IDEV,1050) ICTN,ID
 1050 FORMAT(" CONTRACT NO. ",5A2,10X,"INSTRUMENT IDENTIFIER: ",
     +        10A2)
      WRITE(IDEV,1060) IDATE
 1060 FORMAT(" CALIBRATION DATE: ",4A2)
      WRITE(IDEV,1070)
 1070 FORMAT(" MINIMUM MEAN RF FOR SPCC IS 0.05")
      WRITE(IDEV,1071)
 1071 FORMAT(" MAXIMUM %RSD FOR CCC IS 30%")
      WRITE(IDEV) "  "
      GO TO 80
   70 WRITE(IDEV,1080)
 1080 FORMAT(10X,"CALIBRATION CHECK - SEMIVOLATILE HSL COMPOUNDS")
      WRITE(IDEV,1040) ICSN,ICL
      WRITE(IDEV,1050) ICTN,ID
      WRITE(IDEV,1060) IDATE
      WRITE(IDEV,1090) ISF
 1090 FORMAT(" STANDARD FILE: ",10A2)
      WRITE(IDEV,1100) IBD,IST
 1100 FORMAT(" DATE: ",4A2,5X,"TIME: ",4A2)
      WRITE(IDEV,1110)
 1110 FORMAT(" MAXIMUM % D FOR CCC IS 20")
      WRITE(IDEV) "  "
C
C  ASK IF HEADER IS OKAY - IF SO CONTINUE
C
   80 IF (IDEV .EQ. 2) GO TO 135
   90 WRITE(10,1120)
 1120 FORMAT(" DO YOU WANT TO MAKE CHANGES (Y OR N)?: "Z)
      READ(11,1020) IOK
      IF(IOK .NE. "Y " .AND. IOK .NE. "N ") GO TO 90
      IF(IOK .EQ. "N ") GO TO 100
C
C  CHANGES WANTED, SO CLEAR THE SCREEN AND ASK QUESTIONS
C
      WRITE(10,1130)
 1130 FORMAT("1")
      I1 = 10
```

```
      I2 = 5
      CALL QUEST("CASE NO. ", I1, ICSN, I2)
      I1 = 13
      I2 = 9
      CALL QUEST("CONTRACT LAB", I1, ICL, I2)
      I2 = 5
      CALL QUEST("CONTRACT NO. ", I1, ICTN, I2)
      I1 = 22
      I2 = 9
      CALL QUEST("INSTRUMENT IDENTIFIER", I1, ID, I2)
      I1 = 16
      I2 = 4
      CALL QUEST("CALIBRATION DATE", I1, IDATE, I2)
      IF(IPROC .EQ. "I ") GO TO 60
      I1 = 14
      I2 = 9
      CALL QUEST("STANDARD FILE", I1, ISF, I2)
      I1 = 5
      I2 = 4
      CALL QUEST("DATE", I1, ISD, I2)
      CALL QUEST("TIME", I1, IST, I2)
      GO TO 60
C
C  HEADER IS CORRECT SO LET'S CONTINUE
C
  100 CALL FMOPN(KDESC, ICH1, $8600, IERR)
      CALL FMPOS(0, 0, ICH1, $8600, IERR)
      CALL FMWRT(ICGHD, ICH1, LENG, $8600, IERR)
      CALL FMCLS(ICH1, $8600)
      WRITE(10, 1130)
  130 N = 1
      IDEV = 10
      DO 131 I=1, MAXD
  131 NUM(I) = 0
      NIIN = 0
      NIC = 0
      IC = 0
      CFL = 0
      CALL RESET
  135 WRITE(10, 1150)
 1150 FORMAT(" REFAC: ", Z)
  136 CALL IGET1(INPUT, IFL, IBIT, 30, NUM, FNUM, $130, $8100)
C
C  DETERMINE WHICH REFAC COMMAND IS WANTED
C
      IF (IFL .EQ. "$ " .OR. IFL .EQ. "# ") GO TO 220
      IF(IFL .EQ. "@ ") GO TO 215
      IF (INPUT .EQ. "E ") GO TO 9000
      IF (INPUT .EQ. "H ") GO TO 160
      IF (INPUT .EQ. "Z ") GO TO 9000
      IF (INPUT .EQ. "N ") GO TO 170
      IF (IFL .EQ. "? ") GO TO 180
      IF (INPUT .EQ. "L ") GO TO 190
      IF (IPROC .EQ. "O ") GO TO 150
      IF (INPUT .EQ. "C ") GO TO 200
      IF (INPUT .EQ. "R ") GO TO 210
  150 WRITE(10, 1150)
      GO TO 136
C
C  HARDCOPY COMMAND REQUESTED
C
  160 IDEV = 2
      WRITE(10, 1130)
      WRITE(10, 99)
   99 FORMAT (" HARDCOPY ENABLED")
      CALL OPLPT(IDEV, $8500)
```

```
      GO TO 60
C
C  NO HARDCOPY COMMAND REQUESTED
C
  170  IDEV = 10
       WRITE(10,1130)
       WRITE(10,98)
   98  FORMAT (" HARDCOPY DISABLED")
       GO TO 130
C
C  LIST REFAC COMMANDS REQUESTED
C
  180  CALL COPY(IDEV)
       GO TO 130
C
C  LINEAR STANDARD ERROR REQUESTED IN OUTPUT
C
  190  CFL = 1
       WRITE(10,1130)
       GO TO 135
C
C  CORRELATION COEFFICIENT REQUESTED IN OUTPUT
C
  200  CFL = 2
       WRITE(10,1130)
       GO TO 135
C
C  AVERAGE RELATIVE RETENTION TIME REQUESTED IN OUTPUT
C
  210  CFL = 3
       WRITE(10,1130)
       GO TO 135
C
C  READ FROM THE LIBRARY LIST TO OUTPUT IN IFB FORMAT
C
  215  DO 216 I=1,IDLEN
  216  JFILE(I) = DFILE(I,2)
       WRITE(10,1130)
       CALL FMOPS(JFILE,ICH2,$8920,IEE)
       CALL FMPOS(0,0,ICH2,$8910,IEE)
       CALL FMRD(IS,ICH2,MAXS+MAXS,$217,IEE)
  217  CALL FMCLS(ICH2,$8600)
       ICS = (MAXS+MAXS+IEE)/2
       LIBNM = JFILE(4)
       GO TO 230
C
C  PREPARE TO PERFORM STATISTICS ON LIBRARY ENTRIES
C
  220  LIBNM = INPUT
       WRITE(10,1130)

C
C  OPEN LIBNM.IN FILE
C
  230  DO 240 I=1,IDLEN
  240  LDESC(I) = 0
       LDESC(1) = "0<0>"
       LDESC(3) = 1
       LDESC(4) = LIBNM
       LDESC(10) = "IN"
C
C  CHECK TO SEE IF INITIALIZATION OR ONGOING
C
       IF (IPROC .EQ. "0 ") GO TO 250
C
C  PRINT OUT THE APPROPRIATE COLUMN HEADER FOR INITIALIZATION
```

```
C
      CALL FMOPN(LDESC, ICHIN, $8915, IERR)
      CALL FMPOS(0, 0, ICHIN, $8915, IERR)
      IF (CFL .EQ. 1) WRITE(IDEV, 1172)
      IF (CFL .EQ. 2) WRITE(IDEV, 1174)
      IF (CFL .EQ. 3) WRITE(IDEV, 1176)
      IF (CFL .EQ. 0) WRITE(IDEV, 1170)
 1170 FORMAT(" ", 9X, "COMPOUND", T26, 5(5X, "RF"), 4X, "MEAN", 4X, "%RSD")
 1172 FORMAT(" ", 9X, "COMPOUND", T26, 5(5X, "RF"), 4X, "MEAN", 3X, "%LSD")
 1174 FORMAT(" ", 9X, "COMPOUND", T26, 5(5X, "RF"), 4X, "MEAN", 4X, "CC")
 1176 FORMAT(" ", 9X, "COMPOUND", T26, 5(5X, "RF"), 4X, "MEAN", 3X, "RETM")
 1180 FORMAT(T30, "20NG", 3X, "50NG", 3X, "80NG", 3X, "120NG", 2X, "160NG", 3X, "RF")
      WRITE(IDEV, 1180)
      WRITE(IDEV) " "
      GO TO 290
C
C  ONGOING CHOSEN
C
  250 CALL FMCHK(LDESC, $8900)
      WRITE(IDEV, 1190)
 1190 FORMAT(" ", T32, "MEAN")
      IF (CFL .EQ. 0) WRITE(IDEV, 1192)
      IF (CFL .EQ. 1) WRITE(IDEV, 1194)
 1192 FORMAT(" ", 11X, "COMPOUND", T32, "RF(I)", 6X, "RF(0)", 7X, "% D")
 1194 FORMAT(" ", 11X, "COMPOUND", T32, "RF(I)", 6X, "RF(0)", 7X, "% D", 7X, "%LSD")
      WRITE(IDEV) " "
C
C  CREATE THE FILE DESCRIPTOR
C
  290 CALL IZERO (IDESC)
  300 IC = IC + 1
      NIIN = NIIN + 1
      IF (IFL .EQ. "# " .OR. IFL .EQ. "@ ") GO TO 320
C
C  CREATE FILE DESCRIPTOR FOR CONSECUTIVE ENTRIES
C  THIS IS DONE BY MASKING THE LIBRARY NAME WITH A WORD OF
C  ONE'S TO DETERMINE THE LENGTH (1 OR 2 CHARACTERS).  THEN THE
C  LEFT MOST CHARACTER OF THE NUMBER IS DETERMINED AND MASKED
C  ONTO THE DESCRIPTER ALONG WITH THE LIBRARY NAME.  THIS IS DONE
C  ONE CHARACTER (OF THE NUMBER) AT A TIME.  THE NUMBER CAN BE
C  AT MOST FIVE CHARACTERS LONG.
C
      N = N + 1
      IF(NUM(2) .GT. NUM(3)) GO TO 470
      NUMB = NUM(2)
      IDESC(4) = LIBNM
      IBYTE = (LIBNM .AND. 377K) .EQ. 0
      DO 310 I=1, 5
        IDIG = "<0>0" + MOD(NUMB, 10)
        IB = 14 + IBYTE - I
        IB1 = IB .AND. 1
        IWORD = (IB + 1)/2
        LWD = IDESC(IWORD)
        IF (IB1) IDESC(IWORD) = (LWD.AND.377K) + ISHFT(IDIG, 8)
        IF (IB1 .EQ. 0) IDESC(IWORD) = (LWD.AND.177400K) + IDIG
        NUMB = NUMB/10
  310 CONTINUE
      NUM(2) = NUM(2) + 1
      GO TO 340
C
C  CREATE FILE DESCRIPTOR FOR SEPARATE ENTRIES OR ENTRIES TAKEN
C  FROM LIBRARY LIST
C
  320 N = N + 1
      IF (IFL .EQ. "# ") GO TO 325
      LIBNM = IS(1, N-1)
```

```
      NUM(N) = IS(2,N-1)
      IF (N-1 .GT. ICS) GO TO 470
  325 IF (NUM(N) .EQ. 0) GO TO 470
      IDESC(4) = LIBNM
      IBYTE = (LIBNM .AND. 377K) .EQ. 0
      NUMB = NUM(N)
      DO 330 I=1,5
        IDIG = "<O>O" + MOD(NUMB,10)
        IB = 14 + IBYTE - I
        IB1 = IB .AND. 1
        IWORD = (IB + 1)/2
        LWD = IDESC(IWORD)
        IF (IB1) IDESC(IWORD) = (LWD .AND. 377K) + ISHFT(IDIG,8)
        IF (IB1 .EQ. 0) IDESC(IWORD) = (LWD.AND.177400K) + IDIG
        NUMB = NUMB/10
  330 CONTINUE
C
C  OPEN THE CURRENT RESPONSE LIST FOR READING ONLY
C
  340 ICH = -1
      CALL FMOPR(IDESC,ICH,$8100,IERR)
C
C  INITIALIZE THE HEADER VARIABLES TO ZERO AND READ IN THE HEADER.
C
      CALL HINIT(IU5,IU6)
      CALL FMRD(IHEAD,ICH,LENH,$8200,IERR)
      DO 350 I=1,14
         ICOMI(I) = NAME(I)
         ICOMO(I) = NAME(I)
  350 CONTINUE
C
C  READ IN FROM THE .RL FILE A MAXIMUM OR 250 ENTRIES.   ICOUNT WILL
C  COUNT THE NUMBER OF ENTRIES ACTUALLY READ.
C
      ICR = 0
      DO 370 I=1,MAXQ
        CALL FMRD(JQ,ICH,LEN,$380,IERR)
        DO 360 J=1,LEN
          IQ(J,I) = JQ(J)
  360   CONTINUE
      ICR = ICR + 1
  370 CONTINUE
C
C  CHECK TO SEE IF THE NUMBER OF WORDS READ IS EQUAL TO THE PROPER
C  AMOUNT    IF NOT GIVE AN ERROR MESSAGE.
C
  380 IF (IERR .NE. -LEN) GO TO 8300
      CALL FMCLS(ICH,$8400)
C
C  CALCULATE THE RESPONSE FACTOR FOR EACH ENTRY.   STORE THIS
C  RF IN A TEMPORARY ARRAY ALONG WITH RELATIVE RETENTION TIME
C  AND THE RATIO OF THE INTERNAL STANDARD AREA DIVIDED BY
C  THE COMPOUND AREA.   THE ARRAYS USED ARE RESPECTIVELY "RF",
C  "RT", AND "AC".
C
C
      IF(IPROC .EQ. "I ") ICR = MAXIN
      DO 400 I=1,ICR
        DO 390 J=1,LEN
          JQ(J) = IQ(J,I)
  390   CONTINUE
        A = AREA + .5
        AR = AREAR + .5
        C(I) = AMNT + .0005
        RF(I) = (AREA/AREAR) * (AMNTR/AMNT) + .0005
        RT(I) = RET/RETR + .0005
```

```
        AC(I) = AREA/AREAR + .5
  400   CONTINUE
        RFL = RF(ICR)
        DO 401 I=1,MAXIN
  401   RFC(I) = RF(I)
C
C   INITIALIZE VARIABLES USED IN LINEAR ERROR AND
C   CORRELATION COEFFICIENT CALCULATIONS.   IF
C   INITIALIZATION SORT RF'S ACCORDING TO CORRESPONDING
C   AMOUNT SO THAT WHEN PRINTED OUT THEY WILL BE IN
C   CORRECT ORDER.
C
        X1=0
        X2=0
        Y1=0
        Y2=0
        IF (IPROC .EQ. "I ")CALL SORT(RFC,C,MAXIN,AC)
        M = ICR
        I1 = 1
        IF (RFC(1) .EQ. 0) I1 = 2
        IF (I1 .NE. 1) M = ICR - I1 + 1
        IF (CFL .NE. 1) GO TO 420
C
C   LINEAR ERROR CALCULATION
C
        DO 410 I=I1,ICR
           X1 = X1 + C(I)
           X2 = X2 + AC(I)
           Y1 = Y1 + C(I)*AC(I)
           Y2 = Y2 + C(I)*C(I)
  410   CONTINUE
        B = (M*Y1 - X1*X2)/(M*Y2 - X1*X1)
        A = X2/M - B * X1/M
        S=0
        DO 415 I = I1,ICR
           EST = A + B*C(I)
           S = S + (AC(I) - EST)**2
  415   CONTINUE
        RLINI = SQRT(S/M)* 100
        RLINO = RLINI
        GO TO 429
  420   IF (CFL .NE. 2) GO TO 429
        IF (ICR .GT. MAXIN) ICR = MAXIN
C
C   CORRELATION COEFFICIENT CALCULATIONS
C
        W=0
        DO 425 I = I1,ICR
           X1 =X1 + C(I) * C(I)
           X2 = X2 + C(I)
           W = W + C(I) * AC(I)
           Y1 = Y1 + AC(I)
           Y2 = Y2 + AC(I) * AC(I)
  425   CONTINUE
        X = W - (X2 * Y1)/M
        Z1 = X1 - (X2 * X2)/M
        Z2 = Y2 - (Y1 * Y1)/M
        CC = X/SQRT(Z1 * Z2)
C
  429   ICRT = ICR
        RSUM = SUM(RF,ICRT)
        IF(IPROC .EQ. "I ") RSUM = SUM(RFC,ICRT)
        RFMI = RMEAN(RSUM,ICRT)
        ST = STDEV(RF,RFMI,ICR)
        IF(IPROC .EQ. "I ") ST = STDEV(RFC,RFMI,ICR)
        RDEV = RST(ST,RFMI)
```

```
      RETM = SUM(R1, ICR)
      RETM = RMEAN(RETM, ICR)
      RFMO = RFMI
C
C  BRANCH TO INITIALIZATION OR ONGOING TO STORE DATA
C
      IF (IPROC .EQ. "I ") GO TO 450
C
C  THE ONGOING PROCESS IS DESIGNATED SO SEARCH THE INITIALIZATION
C  OUTPUT CORRESPONDING TO THE CURRENT ONGOING DATA AND PERFORM
C  PERCENTAGE DIFFERENCE CALCULATION.
C
      CALL FMCHK(LDESC, $8900)
      CALL FMOPR(LDESC, ICHIN, LENI, $8915, IERR)
        CALL FMPOS(0, 0, ICHIN, $8910, IEE)
        DO 431 I=1, MAXD
          CALL FMRD(JIN, ICHIN, LENI, $4311, IERR)
          DO 432 J=1, 7
            IF(ICOMI(J) .NE. ICOMO(J)) GO TO 431
 432      CONTINUE
          GO TO 433
 431    CONTINUE
4311    PD = 0
      GO TO 434
C
C  CALCULATE PERCENTAGE DIFFERENCE
C
 433  PD = (RFL - RFMI)/RFMI * 100
      RFMO = RFMI
C
C  STORE THE ONGOING DATA INTO AN ARRAY CALLED "ION" AND GO BACK TO
C  GET MORE DATA
C
 434  DO 440 I=1, LENO
       ION (I, IC) = JON(I)
 440  CONTINUE
      CALL FMCLS(ICHIN, $8600)
      GO TO 300
C
C  INITIALIZATION PROCESS IS DESIGNATED SO STORE DATA IN THE
C  ARRAY "IIN".   "IIN" ONLY HOLDS TEN RECORDS SINCE THE
C  FORTRAN RUN TIME STACK WILL OVERFLOW IF TOO MANY DATA STRUCTURES
C  ARE CREATED.   AS A RESULT WHEN TEN ENTRIES ARE FINISHED THE DATA
C  ARE WRITTEN TO THE FILE ON THE DISK AND "IIN" CAN THEN BE
C  OVERWRITTEN.
C
 450  RSD = RDEV
      DO 460 I=1, LENI
        IIN(I, NIIN) = JIN(I)
 460  CONTINUE
      I2 = 10
      MIC = MOD(IC, 10)
      IF (MIC .EQ. 0) GO TO 510
      GO TO 300
C
C  ALL OF THE DATA ARE WRITTEN.   DETERMINE WHICH FORMAT DATA ARE TO
C  BE PRINTED OUT IN.
C
C
 470  IC = IC - 1
      IF (IPROC .EQ. "O ") GO TO 481
      I2 = MOD(IC, 10)
      IF (I2 .NE. 0) GO TO 510
 481  IF (IFB .EQ. "Y ") CALL IFORM(IPROC, CFL, ION, IIN, IDEV, IC, LDESC)
      IF (IFB .EQ. "Y ") GO TO 130
      IF (IPROC .EQ. "I ") GO TO 490
```

```
C
C  PRINT OUT ONGOING DATA
C
       DO 480 I=1,IC
         DO 475 J=1,LENO
           JON(J) = ION(J,I)
  475    CONTINUE
         IF(CFL.EQ.1) WRITE(IDEV,1220)(ICOMO(K),K=1,14),RFMO,RFL,PD,RLINO
         IF(CFL.EQ.0) WRITE(IDEV,1220) (ICOMO(K),K=1,14),RFMO,RFL,PD
 1220    FORMAT(" ",14A2,T32,F5.3,6X,F5.3,4X,F7.3,4X,F7.3)
  480  CONTINUE
       GO TO 130
C
C  PRINT OUT INITIALIZATION DATA
C
  490  CALL FMOPR(LDESC,ICHIN,$8915,IERR)
       CALL FMPOS(0,0,ICHIN,$8915,IEE)
         JN = IC
         DO 506 J=1,JN
           CALL FMRD(JIN,ICHIN,LENI,$507,IEE)
           IF(CFL.EQ.1)WRITE(IDEV,1230)(ICOMI(K),K=1,14),(RFC(L),L=1,5),
     +     RFMI,RLINI
           IF(CFL.EQ.2)WRITE(IDEV,1231)(ICOMI(K),K=1,14),(RFC(L),L=1,5),
     +     RFMI,CC
           IF(CFL.EQ.3)WRITE(IDEV,1230)(ICOMI(K),K=1,14),(RFC(L),L=1,5),
     +     RFMI,RETM
           IF(CFL.EQ.0)WRITE(IDEV,1230)(ICOMI(K),K=1,14),(RFC(L),L=1,5),
     +     RFMI,RSD
 1230      FORMAT(" ",14A2,T30,5(F5.3,2X),F5.3,2X,F5.1)
 1231      FORMAT(" ",14A2,T30,5(F5.3,2X),F5.3,2X,F6.4)
  506    CONTINUE
  507  CALL FMCLS(LDESC,$8600)
       GO TO 130
C
C  WRITE INITIALIZATION DATA TO FILE
C
  510  CALL FMWRT(IIN,ICHIN,I2*LENI,$8600,IERR)
       NIIN = 0
       NIC = NIC + 1
       IF(I2 .EQ. 10) GOTO 300
       CALL FMCLS(LDESC,$8600)
       GO TO 481
C
C  WRITE OUT ERROR MESSAGES
C  CLOSE FILES AND END PROGRAM
C
 8100  WRITE(10) "OPEN RL FILE ERROR"
       GO TO 9000
 8200  WRITE(10) "FILE READ ERROR FOR HEADER"
       GO TO 9000
 8300  WRITE(10) "FILE READ ERROR FOR ENTRIES"
       GO TO 9000
 8400  WRITE(10) "FILE CLOSE ERROR"
       GO TO 9000
 8500  WRITE(10) "OPEN PRINTER ERROR"
       GO TO 9000
 8600  WRITE(10) " WRITE ERROR "
       GO TO 9000
 8900  WRITE(10) " YOU NEED TO INITIALIZE - START AGAIN"
       GO TO 9000
 8910  WRITE(10) "FILE POSITION ERROR"
       GO TO 9000
 8915  WRITE(10) "OPEN LN.IN FILE ERROR",IERR
       GO TO 9000
 8920  WRITE(10) "OPEN LIBRARY LIST ERROR"
       GO TO 135
```

```
9000  CONTINUE
      CALL FMCLS(ICHIN)
      CALL CLOSE(IDEV)
      CALL CLOSE(ICHAN)
      CALL LOADIT("EXEC")
      STOP
      END
```

```
C
C   THIS SUBROUTINE FINDS THE STANDARD DEVIATION OF AN
C   ARRAY OF REAL NUMBERS GIVEN THE AVERAGE VALUE AND
C   THE NUMBER OF ELEMENTS IN THE ARRAY.
C     RARAY - ARRAY OF REAL NUMBERS
C     AVE - MEAN REAL NUMBER OF THE ARRAY DETERMINED IN FUNCTION
C     ICOUNT - NUMBER OF ELEMENTS IN THE ARRAY
C
        FUNCTION STDEV(RARAY, AVE, ICOUNT)
        DIMENSION RARAY(250)
        SUM = 0.0
        DO 10 J=1, ICOUNT
          DET = (RARAY(J) - AVE)**2
          IF (RARAY(J).EQ.0) DET = 0
          SUM = SUM + DET
   10   CONTINUE
        STDEV = SQRT(SUM/FLOAT(ICOUNT))
        RETURN
        END
C
C
C   THIS FUNCTION FINDS THE RELATIVE STANDARD DEVIATION
C   GIVEN THE STANDARD DEVIATION AND THE AVERAGE
C     ST - THE STANDARD DEVIATION OF A SET OF NUMBERS
C     AVE - THE AVERAGE OF THE SAME SET OF NUMBERS
C
        FUNCTION RST(ST, AVE)
        RST = ST/AVE *100
        RETURN
        END
C
C
C   THIS FUNCTION SUMS AN ARRAY OF REAL NUMBERS AND
C   CHANGES THE VALUE OF ICOUNT TO SKIP ANY NUMBERS OF THE
C   ARRAY THAT WERE ZERO.
C     RF - THE REAL ARRAY INPUTTED BY USER
C     IC - THE NUMBER OF ELEMENTS IN THE ARRAY
C
        FUNCTION SUM(RF, IC)
        DIMENSION RF(200)
        SUM = 0.0
        IN = IC
        DO 10 I=1, IN
          IF(RF(I).EQ.0) IC = IC - 1
          SUM = SUM + RF(I)
   10   CONTINUE
        RETURN
        END
C
C
C   THIS FUNCTION FINDS THE AVERAGE GIVEN THE SUM OF
C   AN ARRAY AND THE NUMBER OF NON-ZERO ELEMENTS
C     RSUM - THE SUM OF AN ARRAY OF NUMBERS
C     ICOUNT - THE NUMBER OF ELEMENTS IN THE ARRAY
C
        FUNCTION RMEAN(RSUM, ICOUNT)
        RMEAN = RSUM / ICOUNT
        RETURN
        END
C
C
C   THIS SUBROUTINE INITIALIZES A .RL FILE DESCRIPTOR
C     JDESC - THE ARRAY THAT WILL CONTAIN THE DESCRIPTOR
C
        SUBROUTINE IZERO(JDESC)
        DIMENSION JDESC(11)
```

```
      JDESC(1) ="D<0>"
      JDESC(2) = 0
      JDESC(3) = 1
      DO 10 I=4,9
         JDESC(I) = 0
10    CONTINUE
      JDESC(10) ="RL"
      JDESC(11) = 0
      RETURN
      END
C
C   THIS SUBROUTINE INITIALIZES A RESPONSE LIST HEADER.
C     IU5 - USER PARAMETER
C     IU6 - USER PARAMETER
C
      SUBROUTINE HINIT(IU5,IU6)
      COMMON/CHEAD/NAME(35),FMASS,SMASS,IU1,IU2,LNAMER,LNUMR,
     +       NAMER(35),FMASSR,SMASSR,IU3,IU4
      DO 10 I = 1,35
         NAME(I) = 0
         NAMER(I) = 0
10    CONTINUE
      IU1 = 0
      IU2 = 0
      IU3 = 0
      IU4 = 0
      IU5 = 0
      IU6 = 0
      FMASS = 0
      SMASS = 0
      FMASSR = 0
      SMASSR = 0
      RETURN
      END
C
C
C   THIS SUBROUTINE PRINTS OUT A STRING AND ITS
C   DEFAULT VALUE AND WAITS FOR CARRIAGE RETURN
C   OR INPUT TO CHANGE THE DEFAULT VALUE.
C     NAME - A STRING LITERAL TO BE PRINTED OUT AS WRITTEN
C     I1 - AN INTEGER CONTAINING THE NUMBER OF CHARACTERS IN NAME.
C          I1 MUST BE GREATER THAN 10 EVEN IF NAME IS SHORTER.
C     ICH - A CHARACTER ARRAY CONTAINING DATA PERTAINING TO THE
C           NAME.   IT MUST BE LESS THAN OR EQUAL TO 9.
C     I2 - AN INTEGER CONTAINING THE LENGTH OF ICH
C
      SUBROUTINE QUEST(NAME,I1,ICH,I2)
C
      INTEGER FMT(13),ICH(9),ICH2(9)
C
      FMT(1) = "('"
      FMT(2) = " '"
      FMT(3) = ",S"
      FMT(4) = ((I1/10) + 60K) * 256 + (MOD(I1,10) + 60K)
      FMT(5) = ",'"
      FMT(6) = "('"
      FMT(7) = ",  "
      FMT(8) = (I2+48) * 256 + 101K
      FMT(9) = "2,"
      FMT(10) = "')"
      FMT(11) = ":  "
      FMT(12) = "',"
      FMT(13) = "Z)"
      WRITE(10,FMT) NAME,(ICH(I),I=1,I2)
      READ(11,110) (ICH2(I),I=1,I2)
110   FORMAT(10A2)
```

```
      IF(ICH2(1) .EQ. "  ") RETURN
      DO 20 I=1,I2
        ICH(I) = ICH2(I)
   20 CONTINUE
      RETURN
      END
C
C  THIS SUBROUTINE READS IN "CMPND.DS" TO SORT DATA
C  INTO IFB FORMAT
C
      SUBROUTINE IFORM(IPROC,NFL,ION,IIN,IDEV,IC,LDESC)
C
      COMMON/CIN/ICOMI(14),RFC(5),RFMI,RSD,RETM,CC,RLINI
C
      COMMON/CON/ICOMO(14),RFMO,RFL,PD,RLINO
C
      INTEGER IIN(34,10),JIN(34),ION(22,75),JON(22),NAME(14)
      INTEGER LDESC(11)
C
      EQUIVALENCE (JIN,ICOMI),(JON,ICOMO)
C
      IF(IDEV.EQ.2) CALL OPLPT(IDEV,$999)
      LENI = 34
      ICH1 = 1
      CALL OPENR("1-CMPND.DS",ICH1,IERR,$8000)
      CALL FMOPR(LDESC,ICHIN,$999,IERR)
  100 READ(ICH1,1000,END=999) (NAME(I),I=1,14)
 1000 FORMAT(14A2)
      IF (IPROC .EQ. "O ") GO TO 60
C
C  INITIALIZATION DATA
C
      CALL FMPOS(0,0,ICHIN,$999,IERR)
      JN = IC + 1
        DO 20 J=1,JN
          CALL FMRD(JIN,ICHIN,LENI,$45,IERR)
          DO 30 K=1,7
            IF(ICOMI(K) .NE. NAME(K)) GO TO 20
   30     CONTINUE
          WRITE(IDEV,1010) (ICOMI(K),K=1,14),(RFC(L),L=1,5),RFMI,RSD
 1010     FORMAT(" ",14A2,T31,5(F5.3,1X),3X,F5.3,3X,F7.3)
          GO TO 100
   20   CONTINUE
   45 IF(IERR .NE. -LENI) GO TO 8010
      DO 50 J=1,34
   50 JIN(J) = 0
      WRITE(IDEV,1011) (NAME(J),J=1,14)
 1011 FORMAT(" ",14A2)
      GO TO 100
C
C  ONGOING DATA
C
   60 DO 90 I=1,IC
        DO 70 J=1,22
   70   JON(J) = ION(J,I)
        DO 80 J=1,5
          IF(ICOMO(J)  NE. NAME(J)) GO TO 90
   80   CONTINUE
        WRITE(IDEV,1020) (ICOMO(K),K=1,14),RFMO,RFL,PD
 1020   FORMAT(" ",14A2,T32,F5.3,6X,F5.3,4X,F7.3)
        GO TO 100
   90 CONTINUE
      DO 110 I=1,22
  110 JON(I) = 0
      WRITE(IDEV,1011) (NAME(K),K=1,14)
      GO TO 100
```

```
 8000  WRITE(10,1025) IERR
 1025  FORMAT(" IDOS ERROR",I5," OPEN CMPND.DS ERROR")
       GO TO 999
 8010  WRITE(10,1026) IERR
 1026  FORMAT(" IDOS ERROR",I5," READ .IN FILE ERROR")
  999  CALL CLOSE(DSK,IE)
       CALL RESET
       RETURN
       END
C
C  THIS SUBROUTINE SORTS AN ARRAY DIMENSIONED TO 5 - SMALLEST
C  TO LARGEST.   IF THE SMALLEST NUMBER IS  GREATER THAN
C  35 IT ASSUMES THE FIRST ELEMENT OF THE ARRAY SHOULD NOT BE FOUND
C  SO IT SETS IT TO ZERO
C
       SUBROUTINE SORT(RFC,C,MAXIN)
C
       DIMENSION C(5),RFC(5)
C
       IN = MAXIN - 1
       DO 20 I=1,IN
         JN = MAXIN - I
         DO 10 J= 1,JN
           IF (C(J) .LE. C(J+1)) GO TO 10
           TEMP = C(J)
           C(J) = C(J+1)
           C(J+1) = TEMP
           TEMP = RFC(J)
           RFC(J) = RFC(J+1)
           RFC(J+1) = TEMP
   10    CONTINUE
   20  CONTINUE
       IF (C(1) .LT. 35) RETURN
       TEMP1 = RFC(1)
       RFC(1) = 0
       DO 30 I=2,MAXIN
         TEMP2 = RFC(I)
         RFC(I) = TEMP1
         TEMP1 = TEMP2
   30  CONTINUE
       RETURN
       END
```

REFERENCES

1. Sauter, A. D.; Mills, P. E.; Fitch, W. L.; Dyer, R. High Resolution Chromatography and Chromatography Communication 1982, 5, pp. 27-30.

2. Sauter, A. D.; Betowski, L. D.; Ballard, J. M. Analytical Chemistry 1983, 55, pp. 116-119.

3. Consensus Organic Protocol, Attachment I: Statement of Work, Exhibit E, Contract Number WA-84-A266/267.