APPENDIX A

DEVELOPMENT OF COMPUTER PROGRAMS FOR PROCESSING AND INTERPRETING HIGH RESOLUTION MASS SPECTRAL DATA OBTAINED WITH SAMPLE INTRODUCTION BY PROBE MICRODISTILLATION

INTRODUCTION

Processing and interpretation of the voluminous quantity of high resolution mass spectral data acquired in typical probe microdistillation/mass spectral (PMD/MS) experiments can be very labor-intensive without the aid of extensive computer software. A series of modifications to and extensions of computer programs for processing and interpretation of PMD/MS data such as those obtained on the Fischer-Tropsch synthesis waxes in this project have been completed.

Probe microdistillation data are acquired from samples placed in a quartz direct-introduction probe having a temperature range from -150° to +600° C (1,2). The apparatus is used to introduce low-volatility samples into a high resolution mass spectrometer. A programmer controls probe temperature in two modes, either linearly or nonlinearly (1), and a maximum linear rate of 200° C/min can be achieved with existing equipment. Most experiments are performed with a programming rate of about 10° C/min, however, because of the limited capability of the mass spectrometer to produce high resolution spectra at scan rates faster than 10 sec/decade.

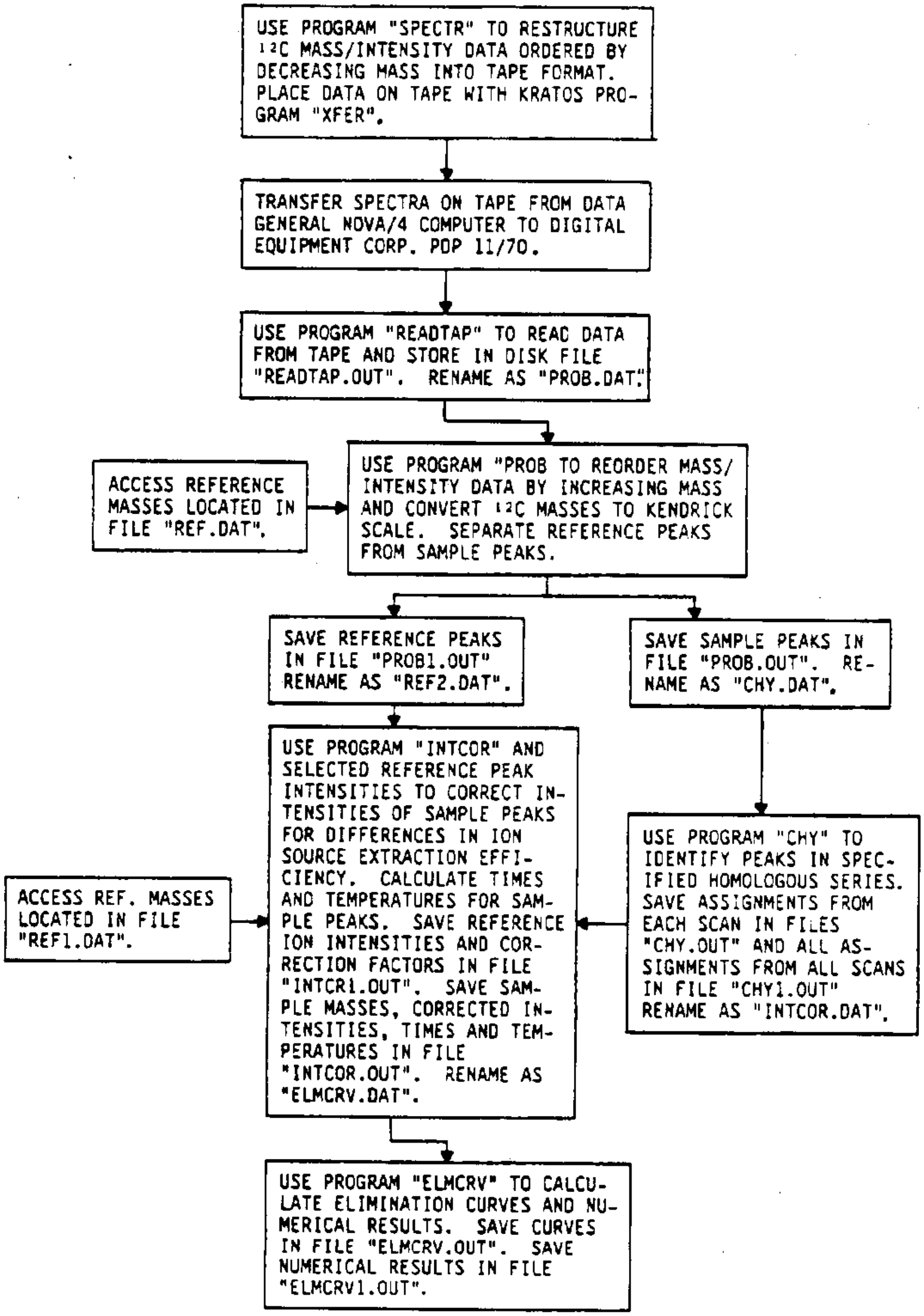
COMPUTER PROGRAM DESCRIPTIONS AND APPLICATIONS

Six FORTRAN programs, run sequentially, allow raw mass/intensity data from as many as 100 scans to be processed into qualitative and quantitative results with minimal manual intervention. These programs are named "SPECTR," "READTAP," "PROB," "CHY," "INTCOR," and "ELMCRV." Another program, "XFER," is required to place the mass/intensity data on magnetic tape for transfer to another computer. All programs except "SPECTR" and "XFER" run on Digital Equipment Corp. PDP 11/70 and MicroVAX II computers. "SPECTR" and "XFER" execute on a Data General NOVA/4 computer, which is a component part of the data acquisition system used with the Kratos MS-50 mass spectrometer on which the data were obtained. Program development was undertaken on the PDP 11/70 and MicroVAX II instead of the NOVA/4 because time on the latter computer is limited by demands for data acquisition from the mass spectrometer. With minor modifications, all programs should run on the NOVA/4 or any other computer having a FORTRAN compiler.

The relationship between programs and files is shown in Figure A-1. Working with a file containing high resolution mass/intensity data acquired by the data acquisition system, programs "SPECTR" and "XFER" restructure the data into a tape format compatible with the input requirements of the PDP 11/70. Transfer of data on tape to this computer is handled by program "READTAP," which places the data in file "READTAP.OUT." From this file, program "PROB" accepts the data, consisting of ^{12}C masses and intensities in order of decreasing mass, and converts the masses to the Kendrick scale, in which the mass of CH_2 is defined as exactly 14 amu (3-6). The data are reordered by increasing mass and processed to separate the reference peaks (originating from a calibration mixture run simultaneously with the sample) from the sample peaks. Each peak is matched against a set of reference masses contained in file "REF.DAT," and a peak is identified as a reference if its mass is within a specified parts-per-million (ppm) range of the mass of the reference ion. The maximum allowed error is usually set at 10 ppm or less, depending on the resolution at which the spectra were acquired and on other factors.

Two output files are generated by program "PROB": one, "PROB1.OUT," contains the identified reference peaks; and the other, "PROB.OUT", consists of all remaining peaks, which are assumed to arise from the sample. The latter file is renamed and used as input to program "CHY" which identifies ions belonging to specified homologous series; e.g., C_nH_{2n+z} or $C_nH_{2n+z}O$, where Z represents the degree of unsaturation. Separate output files, "CHY.OUT," are generated for each range of Z numbers, e.g., +2 through -53, corresponding to the specified elemental combination.

Program "CHY" assigns formulas to ions in a set of scans of a high resolution mass spectrum by fitting Kendrick experimental masses into an array having 14 columns and a variable number of rows, depending on the number of peaks in the spectrum (6). Theoretical Kendrick masses are calculated and compared to experimental masses, and an ion is placed at the proper location in the array only if the ppm error is within a specified range; e.g., 10 ppm. Masses having ppm errors outside this range are listed along with their intensities in nominal mass Z series at the end of the output file, "CHY.OUT" (4,7,8). Assigned masses and intensities from all scans are ordered according to decreasing Z number and increasing mass and placed in a separate output file, "CHY1.OUT."



USE PROGRAM "SPECTR" TO RESTRUCTURE ^{12}C MASS/INTENSITY DATA ORDERED BY DECREASING MASS INTO TAPE FORMAT. PLACE DATA ON TAPE WITH KRATOS PROGRAM "XFER".

TRANSFER SPECTRA ON TAPE FROM DATA GENERAL NOVA/4 COMPUTER TO DIGITAL EQUIPMENT CORP. PDP 11/70.

USE PROGRAM "READTAP" TO READ DATA FROM TAPE AND STORE IN DISK FILE "READTAP.OUT". RENAME AS "PROB.DAT".

ACCESS REFERENCE MASSES LOCATED IN FILE "REF.DAT".

USE PROGRAM "PROB TO REORDER MASS/INTENSITY DATA BY INCREASING MASS AND CONVERT ^{12}C MASSES TO KENDRICK SCALE. SEPARATE REFERENCE PEAKS FROM SAMPLE PEAKS.

SAVE REFERENCE PEAKS IN FILE "PROB1.OUT" RENAME AS "REF2.DAT".

SAVE SAMPLE PEAKS IN FILE "PROB.OUT". RENAME AS "CHY.DAT".

ACCESS REF. MASSES LOCATED IN FILE "REF1.DAT".

USE PROGRAM "INTCOR" AND SELECTED REFERENCE PEAK INTENSITIES TO CORRECT INTENSITIES OF SAMPLE PEAKS FOR DIFFERENCES IN ION SOURCE EXTRACTION EFFICIENCY. CALCULATE TIMES AND TEMPERATURES FOR SAMPLE PEAKS. SAVE REFERENCE ION INTENSITIES AND CORRECTION FACTORS IN FILE "INTCR1.OUT". SAVE SAMPLE MASSES, CORRECTED INTENSITIES, TIMES AND TEMPERATURES IN FILE "INTCOR.OUT". RENAME AS "ELMCRV.DAT".

USE PROGRAM "CHY" TO IDENTIFY PEAKS IN SPECIFIED HOMOLOGOUS SERIES. SAVE ASSIGNMENTS FROM EACH SCAN IN FILES "CHY.OUT" AND ALL ASSIGNMENTS FROM ALL SCANS IN FILE "CHY1.OUT" RENAME AS "INTCOR.DAT".

USE PROGRAM "ELMCRV" TO CALCULATE ELIMINATION CURVES AND NUMERICAL RESULTS. SAVE CURVES IN FILE "ELMCRV.OUT". SAVE NUMERICAL RESULTS IN FILE "ELMCRV1.OUT".

FIGURE A-1. - Flow chart showing relationship between programs and files.

Because probe microdistillation typically produces more than 30 scans with each containing several hundred peaks recorded at high resolution, the output files, "CHY.OUT," become quite voluminous. However, only those files from selected scans need to be printed, and all other output can be deleted from the disk. The usual procedure is to print the output from two or three scans, and upon examination, print output from additional scans for detailed interpretation. On the other hand, the "CHY1.OUT" file contains, for a particular elemental combination, such as $C_nH_{2n+z}O$, all of the assignments from all of the scans in a compressed format. This output can be examined quickly and used to help select additional "CHY.OUT" files to be printed, if necessary.

The high resolution data contained in file "CHY1.OUT," are renamed and used as input to program "INTCOR." This program also accepts a file renamed from "PROB1.OUT" containing all of the reference-ion peaks from all of the scans. Program "INTCOR" uses the intensities of the reference peaks to correct intensities of the sample peaks for variations in ion-source extraction efficiency caused by large changes in the total ion current encountered during a probe microdistillation experiment. The corrections are based on the assumption that the intensities of the reference ions should remain constant during the run. This is an approximation when the reference mixture is introduced through an expansion-volume inlet (the usual procedure) because the partial pressures of the components in the reference mixture are continuously decreasing while the data are being recorded.

Corrections to the intensities of the sample peaks are calculated from the intensities of selected reference ions by summing the reference intensities for each scan and taking the average of the sums over all scans. Correction factors are calculated by dividing this average by the reference intensity sum for each scan (1). Thus, if the extraction efficiency is low for a particular scan as compared to the average, the sum of the reference ion intensities will be low, causing the correction factor to be greater than one. On the other hand, if the extraction efficiency is higher than the average over all scans, the correction factor will be less than one. The factors therefore permit the sample-ion intensities to be corrected as if the extraction efficiency had not changed during the experiment.

In addition to correcting the sample-ion intensities, program "INTCOR" assigns times or probe temperatures or both to the sample ions. These two variables are calculated from the scan time and scan rate or the linear temperature programming rate and the initial probe temperature, which are entered from the terminal when the program is run. Output from program "INTCOR" is saved in two files. The first, "INTCR1.OUT," contains the reference-ion data, including intensity sum and correction factor for each scan. The second output file, "INTCOR.OUT," contains the Z number, mass, scan number, time, temperature, raw intensity, corrected intensity, and correction factor for all sample peaks in all of the scans.

File "INTCOR.OUT" provides the input to program "ELMCRV," which calculates elimination curves for the sample ions. By using nonlinear regression, the time/intensity or temperature/intensity data for each mass and Z number, describing each ion, are used to evaluate four parameters A, B, C, and D in the skewed Gaussian equation:

$$I = A \cdot e^{-\left[\frac{T - B}{C - D(T - B)}\right]^{2}} \qquad (1)$$

in which I is the intensity of a sample peak and T is time or the absolute temperature. After they are evaluated, the parameters are used to calculate the maximum intensity of the curve, IMAX, the time or temperature at which the maximum occurs, T(IMAX), and the area under the curve, AREA. Ninety percent confidence intervals are included.

Output, consisting of line-printer plots of the curves and other results, is saved in file "ELMCRV.OUT." Given with each curve are the name of the data set, the maximum ppm error, elemental combination, Z number, and mass. If the regression analysis is successful, the goodness of fit (R^2), number of the best iteration obtained by minimizing the sum of the squares, maximum number of iterations allowed, values of IMAX, T(IMAX), AREA, and the parameters with 90% confidence intervals are included.

Figure A-2 illustrates the type of output obtained when the ion current as a function of temperature is strong. It is evident that the curve is almost Gaussian with slight skewing on the right-hand side. Nearly symmetrical curves are typical for the distillation of abundant components from a complex mixture. On the other hand, distillation of an abundant component from a simple mixture produces a curve skewed to the left with an almost vertical drop of intensity to zero on the right-hand side. The difference in distillation behavior can be ascribed to variations in thermodynamic properties of components in simple versus complex mixtures, and a detailed explanation is outside the scope of the present discussion. The extent of skewing determines the value of D in equation (1), and it is seen that this parameter is near zero for the data shown in Figure A-2.

When an ion has less than a minimum allowed number of temperature/intensity values (usually set at ten), the data are ignored. However, because the input file to program "ELMCRV" contains all of the assignments from all of the scans, the data are not lost. This file, "ELMCRV.DAT," can be printed and saved for reference. If a curve cannot be calculated because low intensities cause excessive data scatter, only the points are plotted. In this case, the temperature centroid (moment) and area obtained by adding the areas of trapezoids are calculated and given along with the minimum allowed value of R^2, the maximum intensity, and the corresponding time or temperature. An example is shown in Figure A-3.

The ratio of the areas for the data plotted in Figures A-2 and A-3 is about 32:1. On the assumption of equimolar sensitivities, this ratio represents the relative abundances of components corresponding to the two molecular masses and elemental compositions. The data do not distinguish between isomers unless differences in volatility are sufficient to produce distinguishable curves. Usually, this is not the case, especially when complex mixtures are being distilled.

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SRCFRS. 11/26/86. SRC-II >325 DEG C STRONG ACIDS, FRACTION 5     SCANS:  50-120
MAXIMUM PPM ERROR =  4.0      ELEMENTAL COMPOSITION: C(N)H(2N+Z)O(2)
Z = -14   MASS =  186.   GOODNESS OF FIT (R**2) =  0.993   BEST ITERATION NO. = 20   NUMBER ALLOWED = 20
IMAX/10000 = 148.66 +-  8.78   T(IMAX) = 404.90 +-  0.29 K   AREA/10000 =  9213.25 +-  581.34
A/10000 = 148.66 +-  8.78   B = 404.90 +-  0.29 K   C =  34.55 +-  0.75 K   D =  -0.09 +-  0.02
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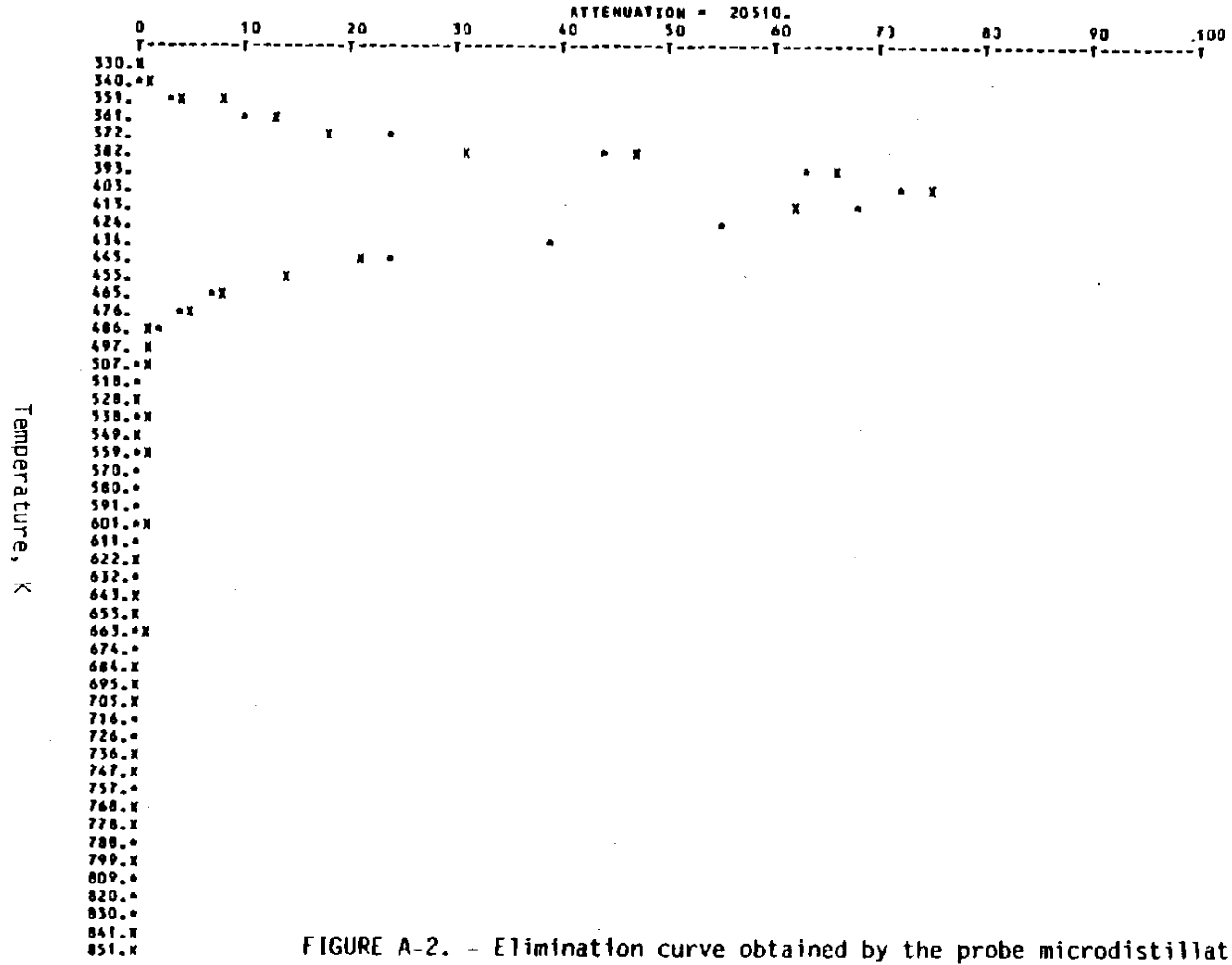
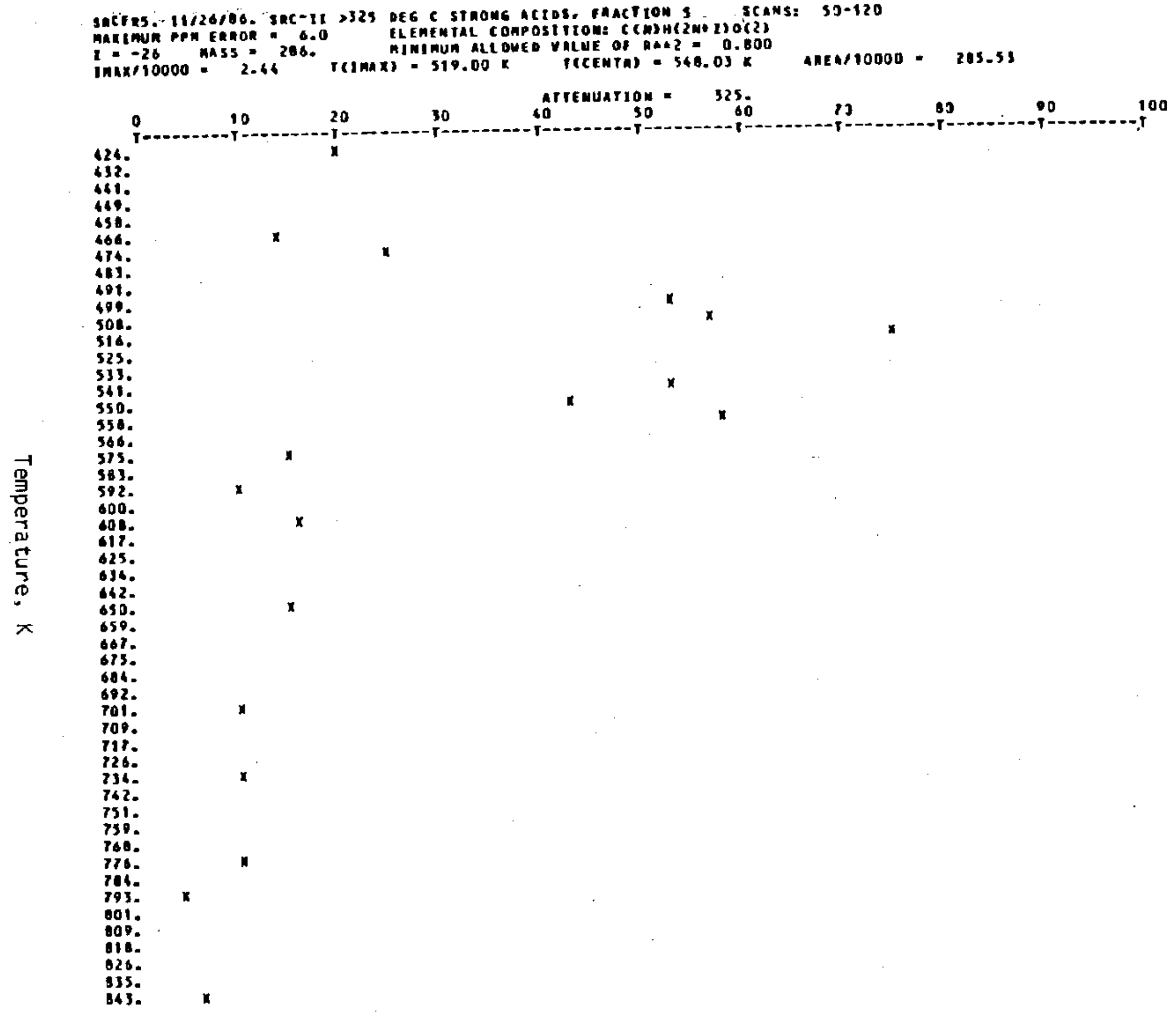


FIGURE A-2. – Elimination curve obtained by the probe microdistillation of $C_{12}H_{10}O_2$, M = 186, from acids subfraction No. 5 isolated from the >325° C distillate of an SRC-II coal liquid. Plot of ion current (arbitrary units) vs. temperature in Kelvin. Experimental points are denoted by "X" and calculated points by "*".



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SRCFR5. 11/26/86. SRC-II >325 DEG C STRONG ACIDS, FRACTION 5     SCANS:  50-120
MAXIMUM PPM ERROR =  6.0        ELEMENTAL COMPOSITION: C(N)H(2N+Z)O(2)
Z = -26    MASS =  286.         MINIMUM ALLOWED VALUE OF R**2 =  0.800
IMAX/10000 =    2.44      T(IMAX) = 519.00 K      T(CENTR) = 548.03 K      AREA/10000 =    285.53
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FIGURE A-3. - Data plotted for the probe microdistillation of $C_{20}H_{14}O_2$, M = 286, from acids subfraction No. 5 isolated from the 325° C distillate of an SRC-II coal liquid. Ion current in arbitrary units versus temperature in Kelvin. Experimental points are denoted by "X.".

Regression analysis on the data shown in Figure A-3 produced a goodness of fit, R^2, less than the minimum allowed value (0.8), which was entered from the terminal during execution of the program. When this occurs, the program plots the data points only and calculates nonstatistical parameters to represent the data set. The T(IMAX) value is simply the temperature corresponding to the maximum intensity, and the area is that obtained by adding the areas of trapezoids, as explained previously. The temperature centroid (moment) is calculated by adding the temperature-intensity products and dividing by the sum of the intensities. It is evident that T(IMAX) and T(CENTR) will converge when the distribution of data points becomes Gaussian; therefore, the difference between the two (29.03 K for the data shown in Figure A-3) is an indication of data skewing and, usually, of the amount of data scatter when the results of the regression analysis are omitted.

Program "ELMCRV" produces a separate output file, "ELMCRV1.OUT," in which a table is printed showing the T(IMAX), IMAX, AREA, and other information for each ion arranged in order of decreasing Z number and increasing mass. Ninety percent confidence intervals are included with the statistical output. As an example of this output, Table A-1 shows the results for molecular ions of elemental combination $C_nH_{2n+z}O_2$ originating from an acid subfraction of an SRC-II coal liquid. Compounds of this type were detected over a molecular-mass range from 172 to 366 and in corresponding Z series from -14 (O_2) to -30 (O_2). The output has been edited to remove fragment ions and a few extraneous ions believed to arise either from the reference mixture (i.e., ions not removed from the spectra by program "PROB") or from rearrangement mechanisms taking place in the molecular ions from the sample. Both this table and another, described below, are formatted for easy editing to remove any ions that do not belong in the homologous molecular-ion series. Comparison of the areas under the curves provides an estimate of the relative abundances of the components of the given elemental combination. By far, the most abundant compound type is $C_{13}H_{12}O_2$, whose Z number and molecular mass are -14 and 200 amu, respectively. This composition corresponds to isomers of methyldihydroxybiphenyl. The confidence interval on the area represents a relative error of 7.4%. Errors on the areas and other quantities increase dramatically as the abundances decrease toward zero, as seen from m/z 172, the first member detected in the $C_nH_{2n-14}O_2$ series. Because the first member of the

TABLE A-1. - Edited output from program "ELMCRV" showing statistical results for $C_nH_{2n+z}O_2$ assignments from 70 scans of the high resolution mass spectrum of an acids subfraction from an SRC-II coal liquid[1]

SRCFR5. 11/26/86. SRC-II >325 DEG C STRONG ACIDS, FRACTION 5 SCANS: 50-120

MAXIMUM PPM ERROR = 6.0 ELEMENTAL COMPOSITION: C(N)H(2N+Z)O(2)

STATISTICAL RESULTS ORDERED BY DECREASING Z NUMBER AND INCREASING MASS

Z	M/Z	T(IMAX), K	IMAX/10,000	AREA/10,000	NO. PTS.
-14	172.	399.94 ± 41.20	0.68 ± 0.70	36.22 ± 58.60	5
-14	186.	404.90 ± 0.29	148.66 ± 8.78	9213.25 ± 581.34	39
-14	200.	406.95 ± 2.11	682.18 ± 34.92	35480.75 ± 2607.88	44
-14	214.	416.79 ± 1.10	107.14 ± 3.00	6915.78 ± 275.03	49
-14	228.	422.69 ± 0.50	13.52 ± 0.78	950.53 ± 57.95	40
-16	226.	419.54 ± 3.98	22.34 ± 5.66	2174.52 ± 599.34	58
-18	210.	461.77 ± 4.26	3.16 ± 1.46	554.13 ± 263.52	27
-18	224.	486.70 ± 14.20	5.25 ± 1.99	508.84 ± 202.73	31
-18	238.	467.45 ± 0.74	13.37 ± 0.94	1071.96 ± 78.32	29
-18	252.	465.68 ± 2.07	22.63 ± 5.43	1677.27 ± 414.43	37
-18	266.	466.31 ± 0.60	12.95 ± 0.83	1034.15 ± 68.54	23
-18	280.	467.19 ± 1.78	5.04 ± 0.79	302.05 ± 85.66	20
-20	250.	461.71 ± 0.19	9.19 ± 0.89	878.94 ± 154.17	25
-20	264.	476.55 ± 5.70	7.38 ± 1.77	671.66 ± 361.56	22
-20	278.	458.05 ± 9.17	8.40 ± 1.61	818.32 ± 270.76	14
-20	292.	475.99 ± 4.99	3.78 ± 1.02	402.84 ± 119.23	18
-20	306.	476.36 ± 2.55	1.52 ± 0.17	177.23 ± 41.98	15
-22	262.	469.95 ± 5.87	9.00 ± 0.88	846.16 ± 113.88	23
-22	276.	470.20 ± 0.55	18.94 ± 2.43	1540.98 ± 213.80	24
-22	290.	474.44 ± 0.51	12.03 ± 2.91	1039.00 ± 259.46	31
-22	304.	478.70 ± 16.40	5.43 ± 1.79	536.45 ± 186.52	26
-22	318.	478.74 ± 1.37	2.33 ± 0.31	161.70 ± 54.96	6
-24	274.	479.81 ± 3.79	2.99 ± 0.25	480.71 ± 60.45	28
-24	288.	480.90 ± 4.52	4.25 ± 1.25	820.17 ± 267.68	22
-24	302.	493.33 ± 14.55	5.77 ± 1.93	691.32 ± 242.35	25
-24	316.	482.73 ± 6.46	4.53 ± 1.25	581.80 ± 172.36	20
-26	300.	516.84 ± 8.12	3.62 ± 1.84	417.76 ± 222.01	21
-26	314.	533.33 ± 6.10	3.67 ± 1.27	344.02 ± 123.86	18
-26	328.	514.26 ± 6.21	3.21 ± 0.30	343.07 ± 79.59	14
-26	342.	500.56 ± 3.25	2.34 ± 0.79	256.83 ± 95.48	15
-28	312.	537.55 ± 9.58	6.16 ± 2.70	337.46 ± 439.72	11
-28	326.	517.12 ± 16.47	6.92 ± 1.52	727.85 ± 173.53	24
-28	340.	526.96 ± 12.46	5.00 ± 2.04	513.51 ± 214.13	23
-28	354.	544.16 ± 2.34	2.41 ± 0.27	289.60 ± 34.51	13
-30	324.	529.30 ± 2.23	2.09 ± 0.20	298.55 ± 41.76	13
-30	352.	537.31 ± 3.47	2.47 ± 0.98	334.93 ± 138.57	26
-30	366.	534.13 ± 2.81	2.47 ± 1.11	289.64 ± 135.10	21

[1] Results for fragment ions and several extraneous ions have been excluded.

dihydroxybiphenyl homologs has a molecular mass of 186, the compound(s) of mass 172 in the -14 (O_2) Z series must belong to some other type. If equimolar sensitivities can be assumed, the abundance of this type is only 0.10% of the abundance of the methyldihydroxybiphenyls.

The T(IMAX) of a molecular ion in a homologous series is inversely proportional to its relative volatility; thus, T(IMAX) increases with increasing carbon number (1). This is evident for intense molecular ions having narrow confidence intervals around their T(IMAX) values, as seen for m/z 186, 200, and 214 in the -14 (O_2) Z series. An increase of about two to six degrees is typical for sequential members of a series. This small, but significant, difference is oftentimes sufficient to determine whether an ion does not belong in a series. However, the converse is not true; i.e., an ion may have a T(IMAX) that appears to fit with the other values for a series yet corresponds to a different compound type.

Nonstatistical results, i.e., temperature centroids, etc., are printed in a separate table at the end of the "ELMCRV1.OUT" file. For the $C_nH_{2n+z}O_2$ assignments from the acids subfraction, these results are shown in Table A-2. By comparison with the results in Table A-1, those in Table A-2 generally correspond to less abundant compounds. Consequently, scatter on the quantities given in the second table is greater. The results are significant, however, showing the presence of compound types having molecular masses from 184 to 442 in Z series from -14 (O_2) to -40 (O_2). Results in the two tables should be combined to obtain the overall distribution of compound types detected. For example, m/z 242 and 256 in the -14 (O_2) Z series in Table A-2 belong with the more abundant members listed in Table A-1. Thus, seven members in the -14 Z (O_2) series of elemental combination $C_nH_{2n+z}O_2$ were detected. Similarly, eight members were detected in the -16 (O_2) Z series and seven in the -30 (O_2) Z series of the same combination.

TABLE A-2. - Edited output from program "ELMCRV" showing nonstatistical results for $C_nH_{2n+z}O_2$ assignments from 70 scans of the high resolution mass spectrum of an acids subfraction from an SRC-II coal liquid[1]

SRCFR5. 11/26/86. SRC-II >325 DEG C STRONG ACIDS, FRACTION 5 SCANS: 50-120

MAXIMUM PPM ERROR = 6.0 ELEMENTAL COMPOSITION: C(N)H(2N+Z)O(2)

NONSTATISTICAL RESULTS ORDERED BY DECREASING Z NUMBER AND INCREASING MASS

Z	M/Z	T(CENTR), K	T(IMAX),	IMAX/10,000	AREA/10,000	NO. PTS.
-14	242.	530.74	432.00	3.00	400.08	25
-14	256.	514.54	416.00	0.88	117.81	16
-16	184.	524.70	393.00	0.97	194.16	16
-16	198.	548.57	456.00	8.47	1231.84	39
-16	212.	521.18	464.00	12.44	1824.61	39
-16	240.	548.63	432.00	8.74	1084.65	37
-16	254.	562.62	440.00	2.94	519.49	29
-16	268.	563.53	479.00	1.24	226.57	15
-16	282.	542.87	440.00	1.04	154.25	15
-18	196.	449.29	385.00	1.55	169.24	19
-18	294.	526.87	479.00	1.87	182.91	13
-20	236.	513.46	448.00	4.50	541.05	37
-20	320.	519.33	479.00	0.73	48.63	5
-22	234.	567.19	519.00	1.74	180.76	19
-22	248.	587.67	495.00	1.32	227.78	16
-22	332.	520.13	463.00	0.73	109.72	8
-24	246.	491.76	456.00	1.92	175.73	8
-24	260.	568.41	479.00	1.13	192.98	14
-24	330.	543.18	502.00	2.51	369.10	17
-24	344.	565.89	542.00	0.97	128.89	8
-26	272.	563.30	519.00	1.12	149.56	9
-26	286.	548.03	519.00	2.44	285.53	18
-26	356.	536.14	542.00	1.05	162.25	13
-26	370.	532.43	605.00	0.51	44.68	6
-28	284.	546.87	534.00	0.97	126.77	7
-28	298.	582.94	519.00	0.75	106.12	10
-28	368.	544.95	526.00	1.64	194.22	11
-28	382.	541.64	534.00	0.71	71.57	5

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[1] Results for fragment ions and several extraneous ions have been excluded.

TABLE A-2. - Edited output from program "ELMCRV" showing nonstatistical results for $C_nH_{2n+z}O_2$ assignments from 70 scans of the high resolution mass spectrum of an acids subfraction from an SRC-II coal liquid[1]--cont'd

SRCFR5. 11/26/86. SRC-II >325° C STRONG ACIDS, FRACTION 5 SCANS: 50-120

MAXIMUM PPM ERROR = 6.0 ELEMENTAL COMPOSITION: C(N)H(2N+Z)O(2)

NONSTATISTICAL RESULTS ORDERED BY DECREASING Z NUMBER AND INCREASING MASS

Z	M/Z	T(CENTR), K	T(IMAX), K	IMAX/10,000	AREA/10,000	NO. PTS.
-30	310.	560.44	558.00	2.24	266.14	15
-30	338.	590.22	558.00	2.97	352.73	23
-30	380.	571.88	542.00	1.34	155.24	9
-30	394.	551.09	526.00	0.65	100.20	5
-32	336.	604.83	597.00	0.62	98.05	6
-32	350.	602.26	518.00	0.83	150.73	14
-32	364.	580.73	550.00	1.70	216.97	9
-32	378.	592.48	558.00	1.36	164.21	13
-32	392.	552.40	550.00	0.99	143.79	7
-32	406.	575.41	542.00	0.88	93.90	5
-34	348.	587.90	526.00	0.50	76.12	6
-34	362.	585.27	573.00	1.43	190.95	8
-34	376.	575.37	565.00	2.18	208.03	13
-34	390.	601.03	557.00	1.92	191.18	11
-34	404.	558.24	605.00	1.42	237.42	9
-36	360.	582.96	518.00	0.48	79.11	7
-36	388.	635.11	621.00	1.16	117.46	8
-36	402.	610.82	573.00	1.26	135.53	10
-36	416.	581.05	565.00	1.74	129.15	9
-36	430.	589.59	557.00	0.65	90.86	6
-38	386.	610.10	597.00	0.64	86.18	6
-38	400.	644.08	549.00	0.56	112.32	6
-38	414.	638.14	684.00	1.08	125.93	11
-38	428.	611.62	613.00	0.92	90.60	5
-38	442.	590.17	581.00	0.75	82.33	6
-40	412.	659.94	660.00	0.73	40.92	5
-40	426.	663.02	660.00	0.43	79.67	5
-40	440.	614.32	597.00	1.05	121.02	6

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[1] Results for fragment ions and several extraneous ions have been excluded.

SUMMARY

Modifications to and extensions of a series of computer programs for processing and interpreting probe microdistillation/mass spectral data have been completed, as described in this Appendix. Application to the analysis of data obtained for an acid subfraction from an SRC-II coal liquid illustrates the utility of these programs. Application to PMD/MS data acquired on Fischer-Tropsch wax samples is similar in all respects and has been included in the final report to which this Appendix is attached. Use of these programs has resulted in significant savings in time and effort required to process and interpret the Fischer-Tropsch data.

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