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TOPICAL REPORT

PROCESSING OF HIGH RESOLUTION MASS SPECTRAL DATA BY USE OF KENDRICK MASSES IN A RECTANGULAR ARRAY

By
Ronald D. Grigsby

Work performed for the
U. S. Department of Energy
Under Cooperative Agreement
DE-FC22-83FE60149

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ABSTRACT

Computer programs based on the use of the Kendrick scale for calculating masses are described for rapidly assigning elemental formulas to ions in high resolution mass spectra. Output from the programs is displayed in the form of a rectangular array having fourteen columns and a variable number of rows, depending on the number of peaks in the spectrum. This type of layout permits formulas for the major ions to be identified almost as fast as the output is obtained from the printer. The array is especially useful for displaying the spectra of complex petroleum fractions, where molecular ions for 1000 or more components may be detectable.

The utility of the programs is illustrated with output from the mass spectrum of a fraction containing one-ring aromatic neutrals separated from the 200-425° C distillate of the Cerro Negro (Venezuela) heavy petroleum. The fraction was found to consist predominantly of C_nH_{2n+z} hydrocarbons with z numbers of -8 and -10. Virtually no oxygen- or nitrogen-containing compounds were detected, but sulfur compounds having formulas $C_nH_{2n+z}S$ with z numbers $\leq$ -4 were found. These types of compounds are in agreement with those anticipated from the HPLC method used in the fractionation of the distillate.

ACKNOWLEDGMENT

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PROCESSING OF HIGH RESOLUTION MASS SPECTRAL DATA BY USE OF KENDRICK MASSES IN A RECTANGULAR ARRAY

by

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INTRODUCTION

High resolution mass spectrometry (HRMS) is one of the most versatile methods available for analyzing petroleum and other sources of hydrocarbon fuels. Because it has the capability for measuring the masses of ions within a few parts per million, the technique can provide elemental compositions on molecules present in these complex mixtures.

Ordinarily, HRMS is not used to analyze crude petroleum, but it is employed instead after separation to analyze fractions produced from the original crude (1). Even when the petroleum is broken down according to compound type, the resultant fractions may still contain well over 1000 detectable components. Owing to this complexity, the identification of specific compounds is usually not attempted; instead, the method is used to identify compound types, e.g., alkylbenzenes. Because elemental compositions of the molecular ions are of greatest interest, the intensities of fragment ions are suppressed by using low-energy electrons or a high-intensity electric field for generating the ions.

Data produced by HRMS consist of masses accurate within a few parts per million (typically 10 ppm or 5 mmu at mass 500) and intensities falling within a dynamic range of 10,000 or more. When the spectrum of a single petroleum fraction (e.g., the aromatic neutrals) contains over 1000 molecular ions, the task of assigning elemental compositions to these ions becomes a formidable task that may consume so much time as to render the cost of the analysis prohibitive. Even when efficient computer programs are available to generate elemental compositions and theoretical masses for comparison with experimental masses, one or more criteria, besides the limit on experimental error, often times must be used to select a particular formula from those produced by the program. If the data are to be used in a quantitative analysis of the fraction, the intensities of the ions -- for which formulas have been assigned -- must be entered into another program (usually by hand) which then calculates the quantitative results. Thus, the slow step in processing high resolution

mass spectral data for a complex mixture is the assignment of the most probable formula to each significant ion, and any method that can reduce the time required for the assignments will result in a corresponding reduction in the cost of the analysis.

All manufacturers of high resolution mass spectrometers provide, as a part of their software packages, programs for assigning elemental formulas to ions in the spectra. These programs may or may not be adequate for processing the data, depending on the particular application. Any program used to process data from a single spectrum of a mixture containing 1000 or more components is inefficient in terms of time and cost if it produces a list of formulas which must be examined manually to select the best choice. This selection process may take days or even weeks, depending on the complexity of the spectrum and the amount of information that must be obtained from it. Clearly, any means by which the effort for this process can be reduced will be beneficial to the laboratory providing the analysis. For this reason, methods for automatic formula assignment have been investigated in our laboratory, leading to the development of computer programs that can partially assign formulas to the ions and produce an output easily edited to complete the assignments. These programs are described below along with output resulting from their execution on a typical data set obtained from the mass spectral analysis of a petroleum fraction.

The programs have been developed around the concept of a repeating unit that exists in compounds that can be classified into homologous series. For hydrocarbons and other compounds occurring in petroleum, this unit is CH_2 or methylene. Over two decades ago, Kendrick showed that the interpretation of high resolution mass spectra of hydrocarbon-derived mixtures could be simplified if the masses of the ions were based on CH_2 instead of carbon-12 (2). Ions are classified into homologous series whose members have masses differing by exactly 14 units, i.e, each member has exactly the same mass defect. Recently, the concept of the Kendrick mass scale has been generalized to include CF_2, CCl_2, and CBr_2, as additional repeating units, and programs for assigning elemental formulas based on these and the CH_2 unit are described in the literature (3,4).

DISCUSSION

The difference between the Kendrick and ordinary ^{12}C scales is seen from a comparison of masses defined by the two scales. In Figures 1 and 2, elemental compositions and masses are listed for C_nH_{2n} combinations. With the mass of carbon defined exactly as 12, the mass defects of the members increase with increasing elemental complexity (Figure 1). This causes the integer mass to be greater than the mass number (i.e., the sum of the numbers of protons and neutrons) when the mass defect exceeds 1.0000. (Note that the mass defect is defined as the difference between the mass of a species and its mass number [3].) Because the mass defect is not constant over a homologous series, combined with the fact that the integer mass is not always the same as the mass number, unnecessary complications in the interpretation of the spectrum arise. These can be avoided by replacing the ^{12}C mass scale with the Kendrick scale. Thus, in Figure 2, it is seen that the mass defect is the same over the series (0.0000 for C_nH_{2n}) and that the integer mass is identical to the mass number for all members of the series. For other series, the mass defects are not zero although they are constant over the range, and the integer masses are not necessarily equal to the mass numbers although the latter can be obtained by subtracting the Kendrick mass defects from the theoretical or calculated Kendrick masses. These concepts will be explained in detail below.

The Kendrick mass scale is readily incorporated into the processing of mass spectral data with output in the form of a rectangular array. This means of displaying a mass spectrum is consistent with the notion of nominal mass z series, and both concepts have been used for many years by researchers in the petroleum industry (3,5,6). The layout of mass numbers as an array for hydrocarbons is shown in Figure 3 in which the array has 14 columns and a variable number of rows, depending on the length of the spectrum. Adjacent elements in each column differ by 14 units, corresponding to CH_2. For high resolution spectra, this form of an array automatically classifies the ions into specific z series where z is defined by the formula C_nH_{2n+z}. Thus, the mass numbers for alkane molecular ions fall into the column for which z = +2 and those for alkylbenzenes in the z = -6 column. It is evident that major fragment ions fall into the column just to the left of that containing the molecular ions, i.e., z = +1 for alkane fragments and -7 for fragments from alkylbenzenes.

ORDINARY MASS SCALE

^{12}C MASS = 12.0000

ELEMENTAL COMPOSITION	MASS
CH_2	14.0156
C_2H_4	28.0313
C_3H_6	42.0470
....	....
$C_{40}H_{80}$	560.6260
....	....
$C_{100}H_{200}$	1401.5650
....	....

FIGURE 1. - Elemental combinations and masses for C_nH_{2n} combinations with mass defined by the ^{12}C scale.

KENDRICK MASS SCALE

CH_2 MASS = 14.0000

ELEMENTAL COMPOSITION	MASS
CH_2	14.0000
C_2H_4	28.0000
C_3H_6	42.0000
....	....
$C_{40}H_{80}$	560.0000
....	....
$C_{100}H_{200}$	1400.0000
....	....

FIGURE 2. - Elemental combinations and masses for C_nH_{2n} combinations with mass defined by the Kendrick scale.

Nominal mass z series numbers (NMZ) are identical to specific z series numbers (SPZ) -11 through +2 for hydrocarbon spectra. However, NMZ's are also useful for describing ions in the spectra of heteroatomic compounds even though the NMZ's and SPZ's do not necessarily coincide. Thus, in Figure 4 molecular ions for carboxylic acids fall into the column with NMZ = -10 although the SPZ = 0, i.e., the NMZ depends only on the mass number and not on the elemental composition. This leads to the definition of the nominal mass z series number as the remainder obtained when the mass number is divided by 14. According to conventional terminology used in petroleum mass spectrometry, the remainder is forced to fall between -11 and +2 (3,6). This is equivalent to the statement that 14 is to be subtracted from the mass number n times such that the remainder falls between -11 and +2, i.e., $-11 \leq NMZ \leq +2$.

The relationship between nominal mass z and specific z series is further exemplified in Figure 5 which shows the layout of mass numbers for heteroatomic compounds containing a single nitrogen. Molecular ions for amines fall in the column with NMZ = -11 and SPZ = +3. Pyridines, on the other hand produce molecular ions with the same SPZ and NMZ, i.e., -5.

Because each element of a column differs by exactly 14 from the adjacent elements, the Kendrick mass is automatically specified for any ion having a given mass number once the mass of any other ion in the series is identified. Furthermore, the mass of any ion of a given mass number in any row is also specified because masses corresponding to adjacent row elements differ exactly by the mass of the hydrogen atom. These statements can be clarified by considering the following arguments. Because the Kendrick mass scale is defined to make the mass of CH_2 = 14.0000, the relationship between Kendrick mass and ^{12}C mass is

$$M(CH_2) = 0.9988834 \times M(^{12}C) \qquad (1)$$

where the Kendrick mass factor, KMF = 0.9988834, is 14 divided by the mass of CH_2 as defined by the ^{12}C scale. Thus, any Kendrick mass can be calculated from the corresponding ^{12}C mass simply by multiplying the latter by 0.9988834. For example, the mass of the hydrogen atom on the Kendrick scale is 1.007825 x 0.9988834 = 1.006700. For hydrocarbons having a specific z

NAME: PSPCNM. 12-AUG-86. CN 200-425 DEG C 1-RING COMPDS. RUN 1, SCAN 1

MAXIMUM PPM ERROR = 0.1 TOTAL ION CURRENT = 0.3152E+07 ELEMENTAL COMPOSITION: C(N)H(2N+Z)

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.9263	0.9330	0.9397	0.9464	0.9531	0.9598	0.9665	0.9732	0.9799	0.9866	0.9933	1.0000	1.0067	1.0134

SPECIFIC Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	N	2N+2
MASS/INTENSITY/PPM ERROR															
3.0	4.0	5.0	6.0	7.0	8.0	9.0	10.0	11.0	12.0	13.0	14.0	15.0	16.0	1	4
17.0	18.0	19.0	20.0	21.0	22.0	23.0	24.0	25.0	26.0	27.0	28.0	29.0	30.0	2	6
31.0	32.0	33.0	34.0	35.0	36.0	37.0	38.0	39.0	40.0	41.0	42.0	43.0	44.0	3	8
45.0	46.0	47.0	48.0	49.0	50.0	51.0	52.0	53.0	54.0	55.0	56.0	57.0	58.0	4	10
59.0	60.0	61.0	62.0	63.0	64.0	65.0	66.0	67.0	68.0	69.0	70.0	71.0	72.0	5	12
73.0	74.0	75.0	76.0	77.0	78.0	79.0	80.0	81.0	82.0	83.0	84.0	85.0	86.0	6	14
87.0	88.0	89.0	90.0	91.0	92.0	93.0	94.0	95.0	96.0	97.0	98.0	99.0	100.0	7	16
101.0	102.0	103.0	104.0	105.0	106.0	107.0	108.0	109.0	110.0	111.0	112.0	113.0	114.0	8	18
115.0	116.0	117.0	118.0	119.0	120.0	121.0	122.0	123.0	124.0	125.0	126.0	127.0	128.0	9	20
129.0	130.0	131.0	132.0	133.0	134.0	135.0	136.0	137.0	138.0	139.0	140.0	141.0	142.0	10	22

FIGURE 3. - Partial layout of mass numbers for hydrocarbons with specific z numbers from -11 through +2.

NAME: RSPCNM. 12-AUG-86. CN 200-425 DEG C 1-RING COMPDS. RUN 1, SCAN 1

MAXIMUM PPM ERROR = 6.0 TOTAL ION CURRENT = 0.3152E+07 ELEMENTAL COMPOSITION: C(N)H(2N+Z)O(2)

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.9474	0.9541	0.9608	0.9675

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

-1	0	1	2	N	2N+2
45.0	46.0	47.0	48.0	1	4
59.0	60.0	61.0	62.0	2	6
73.0	74.0	75.0	76.0	3	8
87.0	88.0	89.0	90.0	4	10
101.0	102.0	103.0	104.0	5	12
115.0	116.0	117.0	118.0	6	14
129.0	130.0	131.0	132.0	7	16
143.0	144.0	145.0	146.0	8	18
157.0	158.0	159.0	160.0	9	20
171.0	172.0	173.0	174.0	10	22

FIGURE 4. - Partial layout of mass numbers for CHO_2 combinations with specific z numbers from -1 through +2.

NAME: RSPCNM. 12-AUG-86. CN 200-425 DEG C 1-RING COMPDS. RUN 1, SCAN 1

MAXIMUM PPM ERROR = 6.0 TOTAL ION CURRENT = 0.3152E+07 ELEMENTAL COMPOSITION: C(N)H(2N+Z)N

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

1.0075

SPECIFIC Z NUMBERS

3

MASS/INTENSITY/PPM ERROR

	N	2N+3
31.0	1	5
45.0	2	7
59.0	3	9
73.0	4	11
87.0	5	13
101.0	6	15
115.0	7	17
129.0	8	19
143.0	9	21
157.0	10	23

FIGURE 5. - Partial layout of mass numbers for CHN combinations with a specific z number of 3.

number of zero, e.g., olefins, the masses and mass numbers are identical, e.g., 14, 28, 42, ... Because the specific z number is defined by the formula C_nH_{2n+z}, the difference in mass numbers between elements in a given row of the array is the same as the difference in z numbers. Thus, the difference in mass numbers between benzene and hexene is 78 - 84 = -6, which is the same as the difference in the SPZ's. This value is also equal to the difference in the number of hydrogen atoms between the two species. Because the mass of hexene is exactly 84 on the Kendrick scale, the mass of benzene is 84 - 6 x 1.006700 = 77.9598 on the same scale. The Kendrick mass of any other member of the alkylbenzene series is also defined because the fractional mass, 0.9598, is the same for all members of the series. For example, propylbenzene has a mass of 119.9598 on the Kendrick scale. In the same way, the Kendrick mass of any ion having a mass number given in the array shown in Figure 3 is specified by adding to the mass of the olefin in the same row the product of the SPZ for the series and the mass of the hydrogen atom on the Kendrick scale.

Another way to specify the mass corresponding to any mass number in Figure 3 is to add the Kendrick mass defect (KMD) to the mass number. This follows from the definition of KMD as the difference between the Kendrick mass and the mass number. Thus, KMD is negative when the Kendrick mass is less than the mass number. For example, benzene has a KMD of 77.9598 - 78 = -0.040200, or conversely, the Kendrick mass of benzene is 78 - 0.040200 = 77.9598. As a corollary to the definition of the Kendrick mass defect, the fractional Kendrick mass (FKM) for a series is given by KMD + 1.0000. Between columns, the difference in FKM is constant and given by the fractional Kendrick mass of the hydrogen atom, i.e., 0.006700. Because the FKM is 1.0000 when z = 0 (e.g., for olefins), the FKM for any column is 1.0000 + z x 0.006700. Thus, for alkylbenzenes, FKM = 1.0000 -6 x 0.006700 = 0.9598. With these thoughts in mind, it becomes a simple matter to identify the mass of any ion whose mass number is given in the array by adding the FKM to one less than the mass number for the ion. The Kendrick mass of decane, for example, is 142 +1.0134 - 1.0000 = 142.0134.

By using 14 columns to lay out the array, the mass numbers in each row correspond to ions all having the same number of carbons, given by

$$N_C = (MN-z)/14 \qquad (2)$$

where MN is the mass number. To facilitate identification of the elemental composition corresponding to any mass number in the array, the carbon number for each row is given on the right-hand side. The number of hydrogens, N_h, for any member of a row is then specified by

$$N_h = 2N_c+z \qquad (3)$$

or N_h can be obtained by starting with the maximum number of hydrogens on the right ($2N_c+2$) and subtracting one for each member of the row when counting from right to left. (Note that combinations containing a negative number of hydrogens, i.e., those in the upper left of the array are not automatically excluded.)

If the compounds contain a heteroatom, X, the array can be laid out once the Kendrick mass defect of the heteroatom is calculated. Because KMD for CH_2 is 0.0000, KMD for CH_2X (and all homologs in the series for which SPZ = 0) is given simply by the KMD for X. Therefore, the fractional Kendrick mass of the column for which SPZ = 0 is the same as FKM for the heteroatom, i.e., FKM = KMD + 1. For example, the array for CHN combinations, shown in Figure 5, can be set up once the FKM is known for nitrogen. Thus, FKM = 14.003074 x KMF - 14 + 1 = 0.9874 where 14.003074 is the ^{12}C mass of nitrogen. The FKM of 0.9874 corresponds to the column for which SPZ = 0. Therefore, the FKM for all columns is automatically determined, as explained previously. The CHX array is not limited to any particular isotope of heteroatom X. As an example, an array for a minor isotope, ^{34}S, is shown in Figure 6.

For combinations containing ^{13}C, the setup is somewhat more complicated. When specifying the mass of the heteroatomic group, the mass of $^{13}CH_2$, i.e., 15.019005 on the ^{12}C scale, must be added to the ^{12}C mass of the heteroatomic group. Thus, for $CH^{13}CNO$ combinations, FKM = KMF(15.019005 + 29.997989) - 45 + 1 = 0.9667 when SPZ = 0. Also, when the number of C atoms is calculated for a row, an additional carbon must be added because ^{13}C has been removed from the CH part and included with the heteroatomic group. Combinations containing more than one ^{13}C would be handled in a similar manner. Figure 7 shows the array set up for $CH^{13}CNO$ combinations.

Once the array is laid out for a particular elemental combination, it is a relatively simple matter to match experimental masses against theoretical masses and thus specify the most probable formula for an ion. Although this task can be managed by various algorithms, the current programs select the

NAME: RSPCNM. 12-AUG-86. CN 200-425 DEG C 1-RING COMPDS. RUN 1, SCAN 1

MAXIMUM PPM ERROR = 6.0 TOTAL ION CURRENT = 0.3152E+07 ELEMENTAL COMPOSITION: C(N)H(2N+Z)34S

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.9098	0.9165	0.9232	0.9299	0.9366	0.9433

SPECIFIC Z NUMBERS

-3	-2	-1	0	1	2	N	2N+2
MASS/INTENSITY/PPM ERROR							
45.0	46.0	47.0	48.0	49.0	50.0	1	4
59.0	60.0	61.0	62.0	63.0	64.0	2	6
73.0	74.0	75.0	76.0	77.0	78.0	3	8
87.0	88.0	89.0	90.0	91.0	92.0	4	10
101.0	102.0	103.0	104.0	105.0	106.0	5	12
115.0	116.0	117.0	118.0	119.0	120.0	6	14
129.0	130.0	131.0	132.0	133.0	134.0	7	16
143.0	144.0	145.0	146.0	147.0	148.0	8	18
157.0	158.0	159.0	160.0	161.0	162.0	9	20
171.0	172.0	173.0	174.0	175.0	176.0	10	22

FIGURE 6. - Partial layout of mass numbers for $CH^{34}S$ combinations with specific z numbers from -3 through +2.

NAME: RSPCNM. 12-AUG-86. CN 200-425 DEG C 1-RING COMPDS. RUN 1, SCAN 1

MAXIMUM PPM ERROR = 6.0 TOTAL ION CURRENT = 0.3152E+07 ELEMENTAL COMPOSITION: C(N-1)H(2N+Z)13CNO

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.9667	0.9734	0.9801	0.9868

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

0	1	2	3	N	2N+3
59.0	60.0	61.0	62.0	2	7
73.0	74.0	75.0	76.0	3	9
87.0	88.0	89.0	90.0	4	11
101.0	102.0	103.0	104.0	5	13
115.0	116.0	117.0	118.0	6	15
129.0	130.0	131.0	132.0	7	17
143.0	144.0	145.0	146.0	8	19
157.0	158.0	159.0	160.0	9	21
171.0	172.0	173.0	174.0	10	23
185.0	186.0	187.0	188.0	11	25

FIGURE 7. - Partial layout of mass numbers for $CH^{13}CNO$ combinations with specific z numbers from 0 through +3.

best fit within a specified parts-per-million error, E_{ppm}, according to the following procedure. First, the theoretical Kendrick mass is calculated for the smallest mass number in the array. The smallest experimental mass is obtained, and the experimental ppm error is calculated from the difference between the theoretical and experimental masses. If this error is less than (i.e., more negative than) $-E_{ppm}$, the theoretical mass is replaced by the mass corresponding to the next mass number in the array. If the experimental ppm error is greater than $+E_{ppm}$, the experimental mass is rejected and the next experimental mass obtained. If the experimental ppm error is within the range of $-E_{ppm}$ and $+E_{ppm}$, any previously selected experimental mass giving an error within the range is replaced by the new experimental mass. In this way, the experimental mass having the smallest absolute ppm error within the specified range is selected. The associated intensity and ppm error are then placed in the array just below the corresponding mass number. The whole procedure is then repeated for the next mass number. All rejected mass/intensity values are saved for possible assignment in arrays having more negative z numbers, and any unassigned masses are sorted according to nominal mass z series and printed along with their intensities at the end of the output. In addition, the assigned mass/intensity values are duplicated in a separate output file for entry into separate programs used to produce a carbon-number distribution and other information for the sample. These programs and their output will be described in a future report.

The use of the array programs to process a high resolution mass spectrum is illustrated with data recorded for a petroleum fraction separated from the 200-425° C distillate of the Cerro Negro (Venezuela) heavy petroleum. This distillate has been fractionated into acid, base, and aromatic neutral fractions with subfractionation of each according to aromatic ring number (1). The subfraction considered here consists predominantly of 1-ring aromatics separated from the aromatic neutrals fraction. A Kratos MS-50 high resolution mass spectrometer (Kratos Analytical Instruments, Manchester, U.K.)* was used

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*Trade names are used for identification only and do not imply endorsement by the National Institute for Petroleum and Energy Research.

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to record the spectrum at a resolution of 40,000 (10 percent valley definition). The sample was introduced through an all-glass expansion volume inlet (R. J. Brunfeldt Co., Bartlesville, OK), at 350° C, and ionization was effected by electron impact at a nominal energy of 10 eV.

Output from the programs for CH, $CH^{13}C$, and CHS combinations is shown in Appendices I-III, respectively. The data were also processed through programs for CHO and CHN combinations, but no significant assignments were made; therefore, this output has been omitted. The programs are written in FORTRAN-77 and execute on a Digital Equipment Corp. PDP 11/70 computer operating under RSX-11M-PLUS. Data are entered from a tape created by a Data General Nova IV computer with RDOS operating system, which serves as the hardware for the Kratos DS-55 data acquisition system. File manipulation, data editing, and program execution on the PDP 11/70 are all handled from a remote DEC VT-100 terminal. The data, as entered into the PDP 11/70 from the tape, consist of the name of the spectrum and the mass/intensity data in order of decreasing mass. A short utility program, READATA5, is used to rearrange the data in order of increasing mass and convert the masses from the ^{12}C scale to the Kendrick scale. The program also counts the peaks and, as an option, removes any unwanted data, e.g., reference masses and intensities from the spectrum. A ppm error range must be entered for matching the unwanted masses against those specified in a reference file, REF.DAT, and the task is accomplished with the same algorithm described above for the array programs. The unwanted masses and intensities are placed in a separate output file, REF.OUT, which contains, among other information, the theoretical and experimental masses of the peaks, their intensities, and the ppm errors.

The REF.OUT file for the Cerro Negro fraction is contained in Appendix IV. These data are useful for interpreting the output from the array programs. For example, the ppm errors on the reference masses show the range of error expected for the sample masses in the same region of the spectrum. This information must be considered with caution, however, because the three-point interpolation used in the Kratos algorithm for calculating the experimental sample masses from the masses of the reference ions forces the errors on the latter to be zero. The fact that many errors are not zero in the REF.OUT file shown in Appendix IV is a consequence of small differences in the masses entered into the Kratos DS-55 software and the REF.DAT file used

with the READATA5 program. For example, the theoretical Kendrick mass 143.85341 corresponding to $C_7H_6F^{35}Cl$ in the REF.DAT file is not exactly equal to the mass entered into the DS-55 file (shown as experimental reference mass 143.85339). This difference results in a ppm error of 0.1. On the other hand, $C_7H_6F^{37}Cl$ is not used as a reference ion by DS-55 (theoretical mass shown as 145.84824) and the 1.3 ppm error calculated for the experimental reference mass, 145.84805, represents the true error calculated for the mass, i.e., DS-55 calculated this mass as if it were one of the sample masses. Therefore, errors associated with the sample ions in the region about m/z 146 are expected to be around 1.3 ppm. The actual error on a sample mass, e.g., $C_{11}H_{14}$ at m/z 146, may be different because of variations in intensities and other factors. The problem of not calculating true ppm errors for the reference masses can be avoided by using a different algorithm for calculating the masses. A program based on least squares has been written and tested, but its description and a discussion of the results obtained from it must be deferred as the subject of a later report.

The output containing the sample spectrum from READATA5 consists of the name of the data set, the number of peaks, and the Kendrick masses and associated intensities in order of increasing mass. This file is structured exactly the same as the input file required for the array programs, and only the name has to be changed, e.g., READATA5.OUT to CH.DAT, to allow the file to be used with any of the programs. During execution, the data file is automatically linked to the program, e.g., CH, and as the program executes, several entries are requested at the terminal. These include: (a) the most positive and most negative z numbers, e.g., +2 and -53,; (b) the maximum ppm error; and (c) the total ion current, TIC. If the latter is not entered, it is calculated by summing the intensities of the peaks in the spectrum. This sum is then normalized to 100,000. If the intensities have already been normalized (e.g., if the input is taken from the output of another program) then a TIC of 100,000 is entered.

Each array program typically executes in less than one minute on the PDP 11/70 and additional programs can be run by copying the data file from one program to another. In this way, output for selected elemental compositions is produced. For petroleum fractions, CH, CHO, CHN, and CHS are usually run first. Then, if additional combinations are suggested by the output, other

programs can be run. For example, strong CHO peaks may suggest the presence of CHO_2 and CHO_3 peaks, as well. At the present time, programs are available for running 18 elemental combinations, and only a few changes are required to set up a new program. These include the elemental composition and mass of the heteroatomic group and minor changes in the format of the output. Eventually, all programs will be combined into one with elemental combinations to be selected from a menu displayed on the terminal when the program is run.

A principal advantage of displaying the spectrum in the array format is that the major compound types can be immediately identified. For example, by looking at the CH output for the Cerro Negro fraction (Appendix I), it is evident from the assignments in the columns and from the intensity sums at the ends of the columns that the major CH compound types range from C_nH_{2n-6} through C_nH_{2n-16}. The most abundant types are C_nH_{2n-8} (tetralins and indans) and C_nH_{2n-10} (dinaphthenobenzenes) as shown by the column sums for molecular ions of 10578 and 10142 divisions per 100,000 divisions, respectively. These major compound types are in agreement with the 1-ring aromatics predicted by the separation scheme.

The capability of the programs for making proper assignments is seen by examining the CH output in detail. Assignments in the alkylbenzene series, C_nH_{2n-6}, are continuous from m/z 92 through m/z 400 with the exception of "holes" at m/z 106, 120, and 260. Whether an assignment is made depends on the specified maximum ppm error, which was set at 6 ppm for the output shown. Because the spectrum was not scanned below m/z 73, no peaks appear below this limit. Excluding the reference peaks, which appear in the printed output from READATA5 (Appendix IV), all peaks not assigned by the program will be found at the end of the array output ordered by nominal mass z series. Therefore, when a peak is missing from a series, it is a simple matter to search the unassigned list or the reference list for the peak, and if it is found it can be included with the series. For example, the first member of the alkylbenzene series is benzene, itself, having a Kendrick mass of 77.9598 (78 - 1 +0.9598). This peak is missing because it was used as a reference. It therefore appears in the REF.OUT file with a raw intensity of 16067 divisions (Appendix IV). Its approximate normalized intensity can be calculated by dividing 16067 by the TIC for the sample spectrum, 0.3152×10^7 and multiplying by 1.0×10^5 Thus $I_{78} = 509.7$. Similarly, m/z 105.9598, C_8H_{10},

is missing because it was removed from the sample spectrum by READATA5. Its raw intensity is 61630 divisions from which an approximate normalized intensity of 1955.3 is calculated. The peak at m/z 119.9598 is not part of the reference file, but instead it is found in the list of unassigned peaks at m/z 119.9610. Its normalized intensity is 1174.5. This peak was omitted from the series because the experimental error of -10.0 ppm is greater than the 6 ppm limit set when the program was run. (Note that a negative ppm error means the experimental mass is greater than the theoretical mass.) The only other peak missing from the series up to m/z 399.9598 is found at 259.9598. Because peaks above and below it in the series have significant intensities (430.2 and 291.7 for m/z 245.9598 and 273.9598, respectively, a peak at 259.9598 is expected. Examination of the unassigned list shows that the peak occurs at m/z 259.9634 with an intensity of 391.3. The experimental error is -13.8 ppm. All peaks in the alklybenzene series are thus accounted for up to m/z 399.9598. Whether the series extends beyond 399.9598, can be determined by looking for the higher mass homologues in the unassigned list. An examination shows that no additional members of the series are present.

Returning to the discussion of the missing peak at 259.9598, it is seen that all peaks are missing from m/z 254.9263 through 259.9598. These are found in the unassigned list with ppm errors slightly more than the 6 ppm limit. Examination of the reference peak output shows the absence of reference ions with mass numbers between 255 and 271. This fact may explain why the mass calibration is not quite as good in the range from m/z 255-260 as compared to that over the rest of the sectrum. An error of -4.0 ppm for mass 254.67793 [$C_9{}^{13}CH_7I$] in the REF.OUT file is greater than the average error for peaks in the file, showing that the mass calibration is not quite as good in this region of the spectrum.

Excluding the masses at m/z 77.9598 and 105.9598, which were used as references, the RMS error over the whole -6 z series through m/z 399.9598 and including the peaks at 119.9598 and 259.9598 is $\pm$ 4.6 ppm. This error is typical of that observed for the entire spectrum as long as unresolved multiplets are not encountered.

Output showing the ^{13}C isotope peaks of the hydrocarbons is shown in Appendix II. Although not nearly as intense as the ^{12}C peaks, the ^{13}C peaks are prominent in the -8 and -10 z series. At a resolution of 40,000 the ^{12}C

hydrocarbon fragment ions are resolved from the ^{13}C molecular ions to m/z 180. Comparison of the CH and $CH^{13}C$ output shows that the peaks are resolved -- at least partially -- to somewhat higher masses. For example, the 216.9531/216.9486 doublet [$C_{16}H_{25}/C_{15}{}^{13}CH_{24}$] is resolved with intensities of 153.6/136.0, as shown in the list of unresolved peaks at the end of the CH output. The expected intensity of the ^{13}C isotope peak is 166.7, which compares favorably with the observed intensity of 136.0.

CHS combinations for the Cerro Negro fraction given in Appendix III show the presence of fragment and molecular ions containing one sulfur atom at low masses. At a resolution of 40,000, these are expected to be resolved from the hydrocarbon ions to m/z 136. Comparison of the CH and CHS output indicates that the C_3-SH_4 doublet is resolved to somewhat higher mass. For example, starting at m/z 127 the C_nH_{2n-13} peak is resolved, at least partially, from the $C_nH_{2n-3}S$ peak up to m/z 197. Because the maximum positive z number for CHS compounds is +2 and because the difference in z numbers for overlapping CH/CHS combinations is -10, the CH output will not contain overlapping peaks for z numbers more positive than -8. Thus, the alkylbenzene series (z = -6) will be free of overlap from CHS peaks.

The most abundant molecular ions for CHS compounds are found in the z = -6 column (unedited sum = 2554.9). These peaks are relatively free from overlap with CH peaks in the z = -16 series because the separation scheme limits the abundant hydrocarbon types to those containing one aromatic ring. By the same reasoning, relatively few overlapping peaks are expected between CH and CHS combinations for z numbers corresponding to the latter compounds more negative than -6.

CONCLUSION

High resolution mass spectra of mixtures consisting of components that can be classified into homologous series are readily processed by using Kendrick masses in a rectangular array laid out according to nominal mass z series. This approach leads to partial assignment of elemental compositions to masses in a spectrum that is easily edited to complete the assignments. The use of the array for displaying the computer output is beneficial for interpreting the spectra of complex petroleum fractions, and only a cursory examination of the output is required to identify the major compound types.

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Appendix I

CH Output from the Mass Spectrum of One-Ring Aromatic Neutrals Separated from the 200-425° C Distillate of the Cerro Negro (Venezuela) Heavy Petroleum.

NATIONAL INSTITUTE FOR PETROLEUM AND ENERGY RESEARCH, P.O. BOX 2128, BARTLESVILLE, OK 74005

HIGH RESOLUTION MASS SPECTRUM

NAME: RSPCNM. 12-AUG-86. CN 200-425 DEG C 1-RING COMPDS. RUN 1, SCAN 1

ELEMENTAL COMPOSITION: C(N)H(2N+Z)

NAME: RSPCNM. 12-AUG-86. CN 200-425 DEG C 1-RING COMPDS. RUN 1, SCAN 1

MAXIMUM PPM ERROR = 6.0 TOTAL ION CURRENT = 0.3152E+07 ELEMENTAL COMPOSITION: C(N)H(2N+Z)

NOMINAL MASS Z NUMBERS	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
KENDRICK MASS DEFECT + 1.0000	0.9263	0.9330	0.9397	0.9464	0.9531	0.9598	0.9665	0.9732	0.9799	0.9866	0.9933	1.0000	1.0067	1.0134

SPECIFIC Z NUMBERS	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	N	2N+2
MASS/INTENSITY/PPM ERROR																
	3.0	4.0	5.0	6.0	7.0	8.0	9.0	10.0	11.0	12.0	13.0	14.0	15.0	16.0	1	4
	17.0	18.0	19.0	20.0	21.0	22.0	23.0	24.0	25.0	26.0	27.0	28.0	29.0	30.0	2	6
	31.0	32.0	33.0	34.0	35.0	36.0	37.0	38.0	39.0	40.0	41.0	42.0	43.0	44.0	3	8
	45.0	46.0	47.0	48.0	49.0	50.0	51.0	52.0	53.0	54.0	55.0	56.0	57.0	58.0	4	10
	59.0	60.0	61.0	62.0	63.0	64.0	65.0	66.0	67.0	68.0	69.0	70.0	71.0	72.0	5	12
	73.0	74.0	75.0	76.0	77.0	78.0	79.0	80.0	81.0 81.2 2.4	82.0	83.0 119.0 1.7	84.0	85.0	86.0	6	14
	87.0	88.0	89.0	90.0	91.0	92.0 111.0 1.1	93.0	94.0	95.0	96.0 23.6 -0.7	97.0	98.0	99.0 24.0 4.4	100.0	7	16
	101.0	102.0	103.0	104.0 63.9 -1.0	105.0 206.1 2.1	106.0	107.0	108.0 46.9 1.0	109.0 182.5 -0.2	110.0	111.0 211.9 5.8	112.0	113.0 29.2 -4.7	114.0	8	18
	115.0	116.0 62.0 4.5	117.0 96.5 -0.1	118.0 273.3 -5.1	119.0	120.0	121.0	122.0	123.0	124.0	125.0	126.0	127.0 29.0 0.1	128.0	9	20
	129.0 41.7 2.1	130.0 271.1 -3.5	131.0	132.0	133.0	134.0 1038.2 -5.2	135.0	136.0 45.2 -1.5	137.0 115.0 -3.2	138.0	139.0 54.1 -3.4	140.0	141.0	142.0	10	22
	143.0 149.8 -1.2	144.0 353.3 0.0	145.0 1221.7 1.2	146.0 450.2 0.8	147.0 623.7 3.5	148.0 482.2 1.5	149.0 64.7 0.3	150.0 39.1 1.3	151.0 56.0 1.9	152.0	153.0 33.9 -3.8	154.0	155.0	156.0	11	24

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.9263	0.9330	0.9397	0.9464	0.9531	0.9598	0.9665	0.9732	0.9799	0.9866	0.9933	1.0000	1.0067	1.0134

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	N	2N+2
157.0	158.0	159.0	160.0	161.0	162.0	163.0	164.0	165.0	166.0	167.0	168.0	169.0	170.0	12	26
649.6	497.5	1378.6	455.6	412.7	347.7	70.4		62.7							
-4.5	0.9	0.6	1.5	2.2	1.2	-3.0		1.1							
171.0	172.0	173.0	174.0	175.0	176.0	177.0	178.0	179.0	180.0	181.0	182.0	183.0	184.0	13	28
	355.4	1260.9	783.6	301.3	304.8	76.7		47.1							
	-5.6	-1.3	-1.0	-2.3	-1.6	1.2		2.9							
185.0	186.0	187.0	188.0	189.0	190.0	191.0	192.0	193.0	194.0	195.0	196.0	197.0	198.0	14	30
804.5	643.6	1014.9	1093.1	232.4	379.8	35.8		45.4							
-3.8	-1.9	1.9	2.8	0.6	-0.6	2.2		-2.8							
199.0	200.0	201.0	202.0	203.0	204.0	205.0	206.0	207.0	208.0	209.0	210.0	211.0	212.0	15	32
836.2	790.4	646.8	1403.2	186.3	471.2	19.9		18.3							
-2.4	0.8	0.2	2.4	0.5	2.0	6.0		4.2							
213.0	214.0	215.0	216.0	217.0	218.0	219.0	220.0	221.0	222.0	223.0	224.0	225.0	226.0	16	34
793.3	1032.6		946.7		462.2										
0.2	3.8		5.2		5.0										
227.0	228.0	229.0	230.0	231.0	232.0	233.0	234.0	235.0	236.0	237.0	238.0	239.0	240.0	17	36
		503.8	994.6		430.3										
		-5.0	-1.6		-0.5										
241.0	242.0	243.0	244.0	245.0	246.0	247.0	248.0	249.0	250.0	251.0	252.0	253.0	254.0	18	38
	1070.5	315.3		179.2	430.2										
	-4.5	-3.5		2.1	-5.6										
255.0	256.0	257.0	258.0	259.0	260.0	261.0	262.0	263.0	264.0	265.0	266.0	267.0	268.0	19	40
						55.8									
						3.3									
269.0	270.0	271.0	272.0	273.0	274.0	275.0	276.0	277.0	278.0	279.0	280.0	281.0	282.0	20	42
451.6	799.7		678.9	28.6	291.7										
0.1	0.9		1.2	-0.7	1.9										
283.0	284.0	285.0	286.0	287.0	288.0	289.0	290.0	291.0	292.0	293.0	294.0	295.0	296.0	21	44
162.3	638.5	153.1	695.7	7.3	246.8										
0.4	2.9	1.3	0.6	-4.4	-0.6										
297.0	298.0	299.0	300.0	301.0	302.0	303.0	304.0	305.0	306.0	307.0	308.0	309.0	310.0	22	46
365.4	711.9	220.0	570.8	16.2	179.1										
1.0	-1.6	5.3	0.2	-3.2	-0.2										
311.0	312.0	313.0	314.0	315.0	316.0	317.0	318.0	319.0	320.0	321.0	322.0	323.0	324.0	23	48
270.6	570.9	202.4	479.4		122.7										
1.7	-2.9	5.6	-4.4		-5.1										

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
KENDRICK MASS DEFECT + 1.0000													
0.9263	0.9330	0.9397	0.9464	0.9531	0.9598	0.9665	0.9732	0.9799	0.9866	0.9933	1.0000	1.0067	1.0134

SPECIFIC Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	N	2N+2
MASS/INTENSITY/PPM ERROR															
325.0	326.0	327.0	328.0	329.0	330.0	331.0	332.0	333.0	334.0	335.0	336.0	337.0	338.0	24	50
237.0	454.0		401.0	31.6	96.8										
5.0	0.3		1.3	3.1	1.4										
339.0	340.0	341.0	342.0	343.0	344.0	345.0	346.0	347.0	348.0	349.0	350.0	351.0	352.0	25	52
	489.8		475.4	24.4	99.0										
	3.0		1.2	2.7	2.5										
353.0	354.0	355.0	356.0	357.0	358.0	359.0	360.0	361.0	362.0	363.0	364.0	365.0	366.0	26	54
					43.6										
					-4.9										
367.0	368.0	369.0	370.0	371.0	372.0	373.0	374.0	375.0	376.0	377.0	378.0	379.0	380.0	27	56
268.9	477.0		214.0		63.5										
3.1	-0.8		-2.5		2.0										
381.0	382.0	383.0	384.0	385.0	386.0	387.0	388.0	389.0	390.0	391.0	392.0	393.0	394.0	28	58
77.8	302.9		182.0		66.5										
-2.3	0.9		0.7		-3.2										
395.0	396.0	397.0	398.0	399.0	400.0	401.0	402.0	403.0	404.0	405.0	406.0	407.0	408.0	29	60
20.3	202.6	19.3	154.4		45.7										
-5.5	-3.1	0.1	-1.8		0.1										
409.0	410.0	411.0	412.0	413.0	414.0	415.0	416.0	417.0	418.0	419.0	420.0	421.0	422.0	30	62
53.5	205.5		115.8	56.4		11.5									
-1.2	-4.2		-1.3	3.4		-2.1									
423.0	424.0	425.0	426.0	427.0	428.0	429.0	430.0	431.0	432.0	433.0	434.0	435.0	436.0	31	64
36.2			39.9	10.6											
-3.7			-3.2	1.4											
437.0	438.0	439.0	440.0	441.0	442.0	443.0	444.0	445.0	446.0	447.0	448.0	449.0	450.0	32	66
	98.1	13.6	46.0												
	-0.7	-0.3	-0.4												
451.0	452.0	453.0	454.0	455.0	456.0	457.0	458.0	459.0	460.0	461.0	462.0	463.0	464.0	33	68
	79.1		14.9												
	2.0		2.9												
465.0	466.0	467.0	468.0	469.0	470.0	471.0	472.0	473.0	474.0	475.0	476.0	477.0	478.0	34	70
	19.7		45.4												
	2.8		4.5												
479.0	480.0	481.0	482.0	483.0	484.0	485.0	486.0	487.0	488.0	489.0	490.0	491.0	492.0	35	72

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.9263	0.9330	0.9397	0.9464	0.9531	0.9598	0.9665	0.9732	0.9799	0.9866	0.9933	1.0000	1.0067	1.0134

SPECIFIC Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	N	2N+2
MASS/INTENSITY/PPM ERROR															
493.0	494.0 16.0 1.7	495.0	496.0	497.0	498.0	499.0	500.0	501.0	502.0	503.0	504.0	505.0	506.0	36	74
507.0	508.0	509.0	510.0	511.0	512.0	513.0	514.0	515.0	516.0	517.0	518.0	519.0	520.0	37	76
521.0	522.0	523.0	524.0	525.0	526.0	527.0	528.0	529.0	530.0	531.0	532.0	533.0	534.0	38	78
535.0	536.0	537.0	538.0	539.0	540.0	541.0	542.0	543.0	544.0	545.0	546.0	547.0	548.0	39	80
549.0	550.0	551.0	552.0	553.0	554.0	555.0	556.0	557.0	558.0	559.0	560.0	561.0	562.0	40	82
563.0	564.0	565.0	566.0	567.0	568.0	569.0	570.0	571.0	572.0	573.0	574.0	575.0	576.0	41	84
577.0	578.0	579.0	580.0	581.0	582.0	583.0	584.0	585.0	586.0	587.0	588.0	589.0	590.0	42	86
591.0	592.0	593.0	594.0	595.0	596.0	597.0	598.0	599.0	600.0	601.0	602.0	603.0	604.0	43	88
605.0	606.0	607.0	608.0	609.0	610.0	611.0	612.0	613.0	614.0	615.0	616.0	617.0	618.0	44	90
619.0	620.0	621.0	622.0	623.0	624.0	625.0	626.0	627.0	628.0	629.0	630.0	631.0	632.0	45	92
633.0	634.0	635.0	636.0	637.0	638.0	639.0	640.0	641.0	642.0	643.0	644.0	645.0	646.0	46	94
647.0	648.0	649.0	650.0	651.0	652.0	653.0	654.0	655.0	656.0	657.0	658.0	659.0	660.0	47	96

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.9263	0.9330	0.9397	0.9464	0.9531	0.9598	0.9665	0.9732	0.9799	0.9866	0.9933	1.0000	1.0067	1.0134

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2	N	2N+2
661.0	662.0	663.0	664.0	665.0	666.0	667.0	668.0	669.0	670.0	671.0	672.0	673.0	674.0	48	98
675.0	676.0	677.0	678.0	679.0	680.0	681.0	682.0	683.0	684.0	685.0	686.0	687.0	688.0	49	100
689.0	690.0	691.0	692.0	693.0	694.0	695.0	696.0	697.0	698.0	699.0	700.0	701.0	702.0	50	102
703.0	704.0	705.0	706.0	707.0	708.0	709.0	710.0	711.0	712.0	713.0	714.0	715.0	716.0	51	104
COLUMN SUMS:															
5218.4	10142.2	7046.8	10578.0	2316.8	5712.9	334.8	131.1	608.2	23.6	418.9	0.0	82.2	0.0		

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.8325	0.8392	0.8459	0.8526	0.8593	0.8660	0.8727	0.8794	0.8861	0.8928	0.8995	0.9062	0.9129	0.9196

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

-25	-24	-23	-22	-21	-20	-19	-18	-17	-16	-15	-14	-13	-12	N	2N-12
73.0	74.0	75.0	76.0	77.0	78.0	79.0	80.0	81.0	82.0	83.0	84.0	85.0	86.0	7	2
87.0	89.0	89.0	90.0	91.0	92.0	93.0	94.0	95.0	96.0	97.0	98.0	99.0	100.0	8	4
101.0	102.0	103.0	104.0	105.0	106.0	107.0	108.0	109.0	110.0	111.0	112.0	113.0	114.0	9	6
115.0	116.0	117.0	118.0	119.0	120.0	121.0	122.0	123.0	124.0	125.0	126.0	127.0 27.3 1.6	128.0 8.6 -2.0	10	8
129.0	130.0	131.0	132.0	133.0	134.0	135.0	136.0	137.0	138.0	139.0	140.0	141.0	142.0	11	10
143.0	144.0	145.0	146.0	147.0	148.0	149.0	150.0	151.0	152.0	153.0	154.0	155.0	156.0 10.5 -4.7	12	12
157.0	158.0	159.0	160.0	161.0	162.0	163.0	164.0	165.0	166.0	167.0	168.0	169.0 26.0 3.1	170.0	13	14
171.0	172.0	173.0	174.0	175.0	176.0	177.0	178.0	179.0	180.0	181.0	182.0	183.0	184.0 184.5 5.5	14	16
185.0	186.0	187.0	188.0	189.0	190.0	191.0	192.0	193.0	194.0	195.0	196.0 39.6 1.0	197.0 103.7 2.1	198.0 210.2 -0.8	15	18
199.0	200.0	201.0	202.0	203.0	204.0	205.0	206.0	207.0	208.0 10.5 2.8	209.0	210.0 118.8 -0.9	211.0	212.0 265.1 -0.1	16	20
213.0	214.0	215.0	216.0	217.0	218.0	219.0	220.0	221.0	222.0 7.2 4.6	223.0 55.0 0.8	224.0	225.0	226.0	17	22
227.0	228.0	229.0	230.0	231.0	232.0	233.0	234.0	235.0	236.0	237.0	238.0 202.7 -1.3	239.0 389.4 -5.9	240.0	18	24

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.8325	0.8392	0.8459	0.8526	0.8593	0.8660	0.8727	0.8794	0.8861	0.8928	0.8995	0.9062	0.9129	0.9196

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

-25	-24	-23	-22	-21	-20	-19	-18	-17	-16	-15	-14	-13	-12	N	2N-12
241.0	242.0	243.0	244.0	245.0	246.0	247.0	248.0	249.0	250.0	251.0	252.0 219.9 -1.8	253.0 761.8 -1.6	254.0 529.0 -0.9	19	26
255.0	256.0	257.0	258.0	259.0	260.0	261.0	262.0	263.0	264.0	265.0	266.0	267.0	268.0 697.9 -2.8	20	28
269.0	270.0	271.0	272.0	273.0	274.0 24.9 4.7	275.0 21.1 3.9	276.0	277.0 23.3 1.0	278.0 312.3 -2.1	279.0 118.0 -0.9	280.0 206.1 -2.0	281.0 303.8 3.5	282.0 627.9 1.8	21	30
283.0	284.0 14.7 -5.3	285.0	286.0 17.5 -3.7	287.0	288.0	289.0	290.0	291.0 87.2 -5.1	292.0	293.0 97.2 2.5	294.0 392.8 -3.3	295.0 238.7 -1.0	296.0 586.0 0.9	22	32
297.0	298.0	299.0	300.0	301.0	302.0	303.0 46.1 0.3	304.0	305.0 116.3 -5.7	306.0 295.5 -5.3	307.0 67.1 1.5	308.0 327.1 -3.9	309.0 148.7 -4.8	310.0 408.1 -2.2	23	34
311.0	312.0	313.0	314.0	315.0	316.0	317.0 41.5 3.5	318.0 26.5 1.9	319.0 169.3 -4.2	320.0 251.1 -4.6	321.0 160.6 0.2	322.0 331.7 -2.8	323.0	324.0 405.6 -2.6	24	36
325.0	326.0	327.0	328.0	329.0	330.0	331.0 66.1 -0.3	332.0 159.8 -5.7	333.0 56.8 2.3	334.0 228.8 0.5	335.0 55.5 -5.7	336.0 351.1 2.3	337.0	338.0 351.2 3.9	25	38
339.0	340.0	341.0 25.2 -5.4	342.0	343.0 36.4 -4.3	344.0	345.0	346.0	347.0 48.3 -0.5	348.0 254.5 -1.9	349.0 50.9 5.5	350.0	351.0	352.0	26	40
353.0	354.0 35.0 -4.2	355.0	356.0 105.7 -2.7	357.0 39.5 -2.7	358.0 164.8 -5.9	359.0 38.3 1.6	360.0 102.1 -5.0	361.0	362.0 204.2 -3.0	363.0 147.9 1.4	364.0 274.7 -5.0	365.0 261.7 -0.8	366.0 357.0 -2.1	27	42
367.0	368.0	369.0	370.0	371.0 17.2 0.2	372.0	373.0 45.2 -0.2	374.0 108.3 -2.0	375.0 42.3 2.5	376.0	377.0 93.2 -2.6	378.0 301.1 -5.3	379.0 94.3 3.4	380.0 315.1 -0.8	28	44
381.0	382.0	383.0	384.0	385.0	386.0	387.0 25.4 0.6	388.0	389.0	390.0 182.9 -4.1	391.0 44.6 -1.4	392.0 98.9 4.0	393.0 120.5 1.9	394.0 197.0 -0.7	29	46
395.0	396.0	397.0	398.0	399.0 22.6 0.7	400.0	401.0 31.2 5.6	402.0 110.4 -4.9	403.0 27.8 -3.9	404.0 133.1 -4.9	405.0 51.7 -2.6	406.0 150.8 -2.7	407.0 40.5 -1.8	408.0 252.1 -1.9	30	48

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
KENDRICK MASS DEFECT + 1.0000													
0.8325	0.8392	0.8459	0.8526	0.8593	0.8660	0.8727	0.8794	0.8861	0.8928	0.8995	0.9062	0.9129	0.9196

SPECIFIC Z NUMBERS

-25	-24	-23	-22	-21	-20	-19	-18	-17	-16	-15	-14	-13	-12	N	2N-12
MASS/INTENSITY/PPM ERROR															
409.0	410.0	411.0	412.0	413.0	414.0	415.0 16.4 0.4	416.0	417.0	418.0	419.0	420.0	421.0	422.0	31	50
423.0	424.0	425.0	426.0	427.0	428.0	429.0	430.0	431.0 33.8 -5.0	432.0 18.6 -1.3	433.0 29.6 -3.5	434.0 81.9 -3.2	435.0 18.4 5.8	436.0 88.1 -3.2	32	52
437.0	438.0	439.0	440.0 70.3 -5.1	441.0 13.7 -0.7	442.0 53.8 -3.5	443.0	444.0 16.0 -4.7	445.0	446.0 58.3 -5.7	447.0	448.0 65.3 -3.5	449.0	450.0 96.9 0.1	33	54
451.0	452.0	453.0	454.0	455.0	456.0 29.8 -4.7	457.0	458.0	459.0	460.0 84.5 -3.3	461.0 25.2 2.3	462.0 20.2 4.8	463.0	464.0 41.6 2.0	34	56
465.0	466.0	467.0	468.0	469.0	470.0 33.2 -3.8	471.0	472.0	473.0	474.0 34.7 -1.5	475.0	476.0 22.8 2.2	477.0	478.0 31.3 3.5	35	58
479.0	480.0	481.0	482.0	483.0	484.0	485.0	486.0	487.0	488.0 24.9 1.6	489.0	490.0	491.0	492.0	36	60
493.0	494.0 14.8 -5.2	495.0	496.0	497.0	498.0 8.2 -2.4	499.0	500.0	501.0	502.0 14.3 -4.8	503.0	504.0	505.0	506.0	37	62
507.0	508.0	509.0	510.0	511.0	512.0	513.0	514.0	515.0	516.0	517.0	518.0	519.0	520.0	38	64
521.0	522.0	523.0	524.0	525.0	526.0	527.0	528.0	529.0	530.0	531.0	532.0	533.0	534.0	39	66
535.0	536.0	537.0	538.0	539.0	540.0	541.0	542.0	543.0	544.0	545.0	546.0	547.0	548.0	40	68
549.0	550.0	551.0	552.0	553.0	554.0	555.0	556.0	557.0	558.0	559.0	560.0	561.0	562.0	41	70
563.0	564.0	565.0	566.0	567.0	568.0	569.0	570.0	571.0	572.0	573.0	574.0	575.0	576.0	42	72

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
KENDRICK MASS DEFECT + 1.0000													
0.8325	0.8392	0.8459	0.8526	0.8593	0.8660	0.8727	0.8794	0.8861	0.8928	0.8995	0.9062	0.9129	0.9196

SPECIFIC Z NUMBERS

-25	-24	-23	-22	-21	-20	-19	-18	-17	-16	-15	-14	-13	-12	N	2N-12
MASS/INTENSITY/PPM ERROR															
577.0	578.0	579.0	580.0	581.0	582.0	583.0	584.0	585.0	586.0	587.0	588.0	589.0	590.0	43	74
591.0	592.0	593.0	594.0	595.0	596.0	597.0	598.0	599.0	600.0	601.0	602.0	603.0	604.0	44	76
605.0	606.0	607.0	608.0	609.0	610.0	611.0	612.0	613.0	614.0	615.0	616.0	617.0	618.0	45	78
619.0	620.0	621.0	622.0	623.0	624.0	625.0	626.0	627.0	628.0	629.0	630.0	631.0	632.0	46	80
633.0	634.0	635.0	636.0	637.0	638.0	639.0	640.0	641.0	642.0	643.0	644.0	645.0	646.0	47	82
647.0	648.0	649.0	650.0	651.0	652.0	653.0	654.0	655.0	656.0	657.0	658.0	659.0	660.0	48	84
661.0	662.0	663.0	664.0	665.0	666.0	667.0	668.0	669.0	670.0	671.0	672.0	673.0	674.0	49	86
675.0	676.0	677.0	678.0	679.0	680.0	681.0	682.0	683.0	684.0	685.0	686.0	687.0	688.0	50	88
689.0	690.0	691.0	692.0	693.0	694.0	695.0	696.0	697.0	698.0	699.0	700.0	701.0	702.0	51	90
703.0	704.0	705.0	706.0	707.0	708.0	709.0	710.0	711.0	712.0	713.0	714.0	715.0	716.0	52	92
COLUMN SUMS:															
0.0	64.5	25.2	193.4	129.4	314.8	331.3	523.0	605.1	2115.3	996.5	3205.6	2535.0	5663.6		

NAME: RSPCNM. 12-AUG-86. CN 200-425 DEG C 1-RING COMPDS. RUN 1, SCAN 1

MAXIMUM PPM ERROR = 6.0 TOTAL ION CURRENT = 0.3152E+07 ELEMENTAL COMPOSITION: C(N)H(2N+Z)

ORIGINAL NO. OF MASSES = 671 NO. OF MASSES ASSIGNED = 256 PERCENT OF TOTAL ION CURRENT ASSIGNED = 59.3

UNASSIGNED MASSES AND INTENSITIES:

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
100.929	115.936	117.015	131.942	118.950	119.924	120.963	93.972	94.979	109.986	96.933	97.989	85.006	113.923
86.1	14.0	20.2	36.4	17.4	19.2	117.3	11.8	124.5	31.4	11.8	34.4	78.6	26.8
114.930	143.928	130.937	131.948	118.954	119.956	120.967	121.974	108.924	123.988	96.934	97.995	126.894	127.769
178.2	19.0	10.8	467.4	590.2	20.0	34.7	43.9	241.3	36.0	12.9	12.1	7.7	12.8
128.930	157.928	130.941	145.942	132.949	119.958	134.956	135.962	122.981	137.897	96.994	111.910	126.916	127.923
270.6	38.7	587.6	115.3	37.1	13.0	213.4	1384.2	226.1	24.2	255.6	58.4	37.4	37.1
142.930	171.928	144.935	159.941	132.954	119.961	134.962	135.975	150.889	151.896	124.904	125.910	140.916	141.924
226.0	58.5	18.0	187.2	988.4	1174.5	62.4	8.5	11.6	17.1	103.0	79.8	39.8	21.1
170.928	171.931	172.934	173.942	146.948	133.951	134.964	177.883	164.890	179.895	124.994	125.911	140.917	155.922
651.6	28.7	21.2	134.8	50.5	31.1	43.8	14.5	21.8	22.4	183.1	33.5	21.5	13.9
170.933	185.928	186.935	187.941	160.943	133.956	134.968	205.745	164.891	193.895	138.903	139.910	154.916	155.923
18.4	82.7	46.3	119.8	13.0	79.3	16.1	14.7	22.7	22.7	157.2	68.6	97.5	11.0
198.920	199.928	200.935	215.941	160.948	147.955	148.963	205.883	178.890	193.897	152.903	153.909	155.005	169.921
35.6	72.5	105.3	52.7	64.4	39.0	39.0	21.0	97.2	30.6	143.4	22.4	16.6	114.3
212.921	227.935	214.922	229.940	174.945	175.963	162.876	205.972	178.981	207.895	166.903	153.910	168.816	183.922
33.1	1093.7	14.7	29.7	8.8	14.0	18.5	18.0	11.5	47.4	180.0	16.1	15.1	31.1
226.923	241.924	214.938	243.948	174.948	203.715	176.962	219.693	192.889	207.897	180.903	167.911	168.916	211.914
20.0	7.1	665.0	822.1	47.1	17.1	20.7	45.2	59.4	22.5	159.7	25.1	248.4	19.4
226.930	255.935	228.934	257.944	188.947	203.868	190.876	219.881	206.889	221.890	194.904	181.727	182.725	225.914
529.0	926.7	48.6	54.8	26.8	20.3	48.5	35.1	27.7	13.3	161.1	24.6	16.9	11.4
240.924	297.520	228.937	257.949	188.949	203.870	190.962	233.883	220.889	221.896	208.902	181.909	182.912	225.917
98.0	7.1	122.1	781.0	114.5	11.3	39.3	37.0	55.2	124.1	201.1	37.7	84.1	24.6
240.928	311.843	242.936	271.855	202.863	203.955	204.961	247.884	234.888	235.896	222.903	195.909	182.915	225.922
409.5	41.7	121.1	33.8	32.1	38.3	48.5	87.7	101.0	248.8	145.9	58.7	349.9	303.5
240.933	325.843	256.852	299.856	202.949	231.869	218.870	261.886	234.891	249.895	236.902	223.908	196.916	239.916
28.3	28.8	14.2	107.3	168.2	14.0	16.9	110.0	72.5	240.5	258.9	171.8	200.3	36.3
254.923	353.419	256.936	299.941	216.861	245.870	218.875	261.969	248.889	249.899	250.901	223.912	210.915	239.921
56.8	25.2	24.9	54.8	46.5	54.1	34.3	9.7	155.1	20.8	248.0	29.9	350.5	439.9
254.928	353.930	256.938	313.857	216.864	245.966	218.878	275.882	248.893	263.896	250.906	237.910	224.916	253.915
313.8	436.9	84.4	67.7	23.0	9.6	12.9	74.5	7.8	419.4	22.8	48.8	314.3	94.8
268.910	367.842	256.942	327.857	216.947	259.874	218.961	289.882	262.890	291.890	264.903	265.903	238.908	309.915
10.1	30.2	207.0	98.4	136.0	23.6	78.2	113.8	148.7	47.1	239.6	7.1	19.3	27.4

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
282.835 14.6	381.844 22.6	270.849 7.3	327.910 20.2	216.952 153.6	259.963 391.3	232.962 60.2	303.883 99.1	276.889 41.1	291.895 230.8	278.894 25.6	265.910 295.3	252.670 38.7	351.911 33.4
282.921 80.4	409.843 19.9	270.937 337.6	341.855 91.1	230.863 78.9	273.869 115.6	232.965 8.2	317.883 117.1	304.882 11.7	333.494 91.6	292.903 55.6	293.887 16.8	266.915 666.4	351.917 320.5
282.930 19.9	423.845 23.3	284.935 86.2	355.413 7.7	230.950 243.0	287.869 171.8	246.877 16.0	331.499 79.2	332.882 14.3	333.898 16.7	306.903 43.9	307.900 19.1	280.906 38.4	393.829 20.2
324.919 49.0	423.936 171.3	298.849 12.0	355.944 294.4	244.864 42.5	287.953 19.3	246.964 87.6	345.450 118.5	332.888 31.9	375.896 234.3	334.896 58.5	349.903 215.7	308.485 11.3	393.912 7.7
338.923 243.1	437.499 28.5	312.943 20.8	369.856 99.0	258.865 85.7	301.870 150.7	260.879 27.9	345.883 141.3	360.889 41.7	403.877 7.7	348.894 42.5	363.900 7.2	322.910 145.9	421.923 180.9
352.922 192.6	479.936 15.5	326.936 154.5	383.856 71.2	258.951 119.1	315.870 196.0	260.882 17.5	373.888 12.9	374.890 31.8	417.898 78.1	348.902 19.0	391.909 85.2	322.917 32.0	449.926 13.8
380.921 76.1	507.939 23.3	340.937 141.2	397.860 27.0	258.957 77.7	329.471 40.6	274.876 10.8	387.882 115.2	388.882 29.5	431.899 47.6	418.897 16.1	419.910 110.2	336.910 226.0	477.922 14.2
394.922 91.7	535.947 12.5	354.934 183.8	411.857 25.9	272.863 37.0	329.869 136.1	274.961 21.6	401.365 6.2	402.884 16.4		418.904 32.0	461.177 140.7	350.909 249.0	505.926 23.5
436.923 19.3		368.937 156.3	411.953 20.3	272.948 131.9	329.951 11.0	288.875 21.5	415.885 121.0	458.315 19.1		503.064 34.4	461.910 15.4	378.906 36.9	
478.922 16.3		382.936 104.6	425.271 6.4	286.862 32.6	343.862 12.6	288.961 25.8	429.884 102.0	458.881 21.9		531.020 174.8	489.909 12.9	378.918 6.6	
549.024 8.4		396.936 40.6	425.858 55.2	286.949 121.4	343.870 177.1	302.964 17.8	500.072 17.8	626.842 12.0		545.017 15.5	545.923 19.0	406.908 38.1	
		410.937 90.9	439.182 18.7	300.949 90.5	357.958 53.0	316.963 14.7						406.921 13.1	
		424.935 22.3		314.863 29.6	371.869 152.9	330.961 28.5						420.910 22.5	
		438.936 5.4		314.950 116.3	385.870 125.8	344.962 43.5						420.916 39.6	
		495.073 5.2		328.857 13.7	399.869 146.0	386.601 13.1						448.917 22.2	
				328.948 61.5	413.871 66.6	386.876 25.5						533.016 40.0	
				342.949 80.5	427.873 61.3	414.876 19.1							
				356.857 17.4	441.176 15.8	442.504 36.3							
				356.947 55.8	441.503 295.5	456.314 68.6							

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
				370.951	455.228	456.877							
				49.6	5.4	9.3							
				384.863	455.872	624.843							
				23.6	14.2	23.7							
				384.950	469.180								
				28.2	7.9								
				398.950	469.873								
				25.0	16.5								
				454.317									
				15.6									
				580.984									
				50.6									
				706.740									
				26.0									

Appendix II

$CH^{13}C$ Output from the Mass Spectrum of One-Ring Aromatic Neutrals Separated from the 200-425° C Distillate of the Cerro Negro (Venezuela) Heavy Petroleum.

NATIONAL INSTITUTE FOR PETROLEUM AND ENERGY RESEARCH, P.O. BOX 2128, BARTLESVILLE, OK 74005

HIGH RESOLUTION MASS SPECTRUM

NAME: RSPCNM. 12-AUG-86. CN 200-425 DEG C 1-RING COMPDS. RUN 1, SCAN 1

ELEMENTAL COMPOSITION: C(N-1)H(2N+Z)13C

NAME: RSPCNM. 12-AUG-86. CN 200-425 DEG C 1-RING COMPDS. RUN 1, SCAN 1

MAXIMUM PPM ERROR = 6.0 TOTAL ION CURRENT = 0.3152E+07 ELEMENTAL COMPOSITION: C(N-1)H(2N+Z)13C

NOMINAL MASS Z NUMBERS

-11 -10 -9 -8 -7 -6 -5 -4 -3 -2 -1 0 1 2

KENDRICK MASS DEFECT + 1.0000

1.0156

SPECIFIC Z NUMBERS

2

MASS/INTENSITY/PPM ERROR

	N	2N+2
31.0	2	6
45.0	3	8
59.0	4	10
73.0	5	12
87.0	6	14
101.0	7	16
115.0	8	18
129.0	9	20
143.0	10	22
157.0	11	24
171.0	12	26

NOMINAL MASS Z NUMBERS

-11 -10 -9 -8 -7 -6 -5 -4 -3 -2 -1 0 1 2

KENDRICK MASS DEFECT + 1.0000

1.0156

SPECIFIC Z NUMBERS

2

MASS/INTENSITY/PPM ERROR

	N	2N+2
185.0	13	28
199.0	14	30
213.0	15	32
227.0	16	34
241.0	17	36
255.0	18	38
269.0	19	40
283.0	20	42
297.0	21	44
311.0	22	46
325.0	23	48
339.0	24	50

NOMINAL MASS Z NUMBERS

-11 -10 -9 -8 -7 -6 -5 -4 -3 -2 -1 0 1 2

KENDRICK MASS DEFECT + 1.0000

1.0156

SPECIFIC Z NUMBERS

2

MASS/INTENSITY/PPM ERROR

	N	2N+2
353.0	25	52
367.0	26	54
381.0	27	56
395.0	28	58
409.0	29	60
423.0	30	62
437.0	31	64
451.0	32	66
465.0	33	68
479.0	34	70
493.0	35	72
507.0	36	74

NOMINAL MASS Z NUMBERS

-11 -10 -9 -8 -7 -6 -5 -4 -3 -2 -1 0 1 2

KENDRICK MASS DEFECT + 1.0000

1.0156

SPECIFIC Z NUMBERS

2

MASS/INTENSITY/PPM ERROR

	N	2N+2
521.0	37	76
535.0	38	78
549.0	39	80
563.0	40	82
577.0	41	84
591.0	42	86
605.0	43	88
619.0	44	90
633.0	45	92
647.0	46	94
661.0	47	96
675.0	48	98

NOMINAL MASS Z NUMBERS

-11 -10 -9 -8 -7 -6 -5 -4 -3 -2 -1 0 1 2

KENDRICK MASS DEFECT + 1.0000

1.0156

SPECIFIC Z NUMBERS

2

MASS/INTENSITY/PPM ERROR

	N	2N+2
689.0	49	100
703.0	50	102
717.0	51	104

COLUMN SUMS:
0.0

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
0.9218	0.9285	0.9352	0.9419	0.9486	0.9553	0.9620	0.9687	0.9754	0.9821	0.9888	0.9955	1.0022	1.0089

KENDRICK MASS DEFECT + 1.0000

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	N	2N+1
353.0 192.6 -1.1	354.0 436.9 -5.3	355.0 183.8 3.3	356.0	357.0 55.8 4.2	358.0	359.0	360.0	361.0	362.0	363.0	364.0	365.0	366.0	26	53
367.0	368.0	369.0 156.3 -4.7	370.0	371.0 49.6 -5.0	372.0	373.0	374.0	375.0	376.0	377.0	378.0	379.0	380.0	27	55
381.0 76.1 1.8	382.0	383.0 104.6 -2.9	384.0	385.0 28.2 -3.3	386.0	387.0	388.0	389.0	390.0	391.0	392.0	393.0	394.0	28	57
395.0 91.7 -1.6	396.0	397.0 40.6 -1.0	398.0	399.0 25.0 -4.5	400.0	401.0	402.0	403.0	404.0	405.0	406.0	407.0	408.0	29	59
409.0	410.0	411.0 90.9 -3.7	412.0	413.0	414.0	415.0	416.0	417.0	418.0	419.0	420.0	421.0	422.0	30	61
423.0	424.0	425.0 22.3 -0.4	426.0	427.0	428.0	429.0	430.0	431.0	432.0	433.0	434.0	435.0	436.0	31	63
437.0 19.3 -2.2	438.0	439.0 5.4 -1.6	440.0	441.0	442.0	443.0	444.0	445.0	446.0	447.0	448.0	449.0	450.0	32	65
451.0	452.0	453.0	454.0	455.0	456.0	457.0	458.0	459.0	460.0	461.0	462.0	463.0	464.0	33	67
465.0	466.0	467.0	468.0 45.4 -5.1	469.0	470.0	471.0	472.0	473.0	474.0	475.0	476.0	477.0	478.0	34	69
479.0 16.3 0.1	480.0	481.0	482.0	483.0	484.0	485.0	486.0	487.0	488.0	489.0	490.0	491.0	492.0	35	71
493.0	494.0	495.0	496.0	497.0	498.0	499.0	500.0	501.0	502.0	503.0	504.0	505.0	506.0	36	73
507.0	508.0	509.0	510.0	511.0	512.0	513.0	514.0	515.0	516.0	517.0	518.0	519.0	520.0	37	75

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.9218	0.9285	0.9352	0.9419	0.9486	0.9553	0.9620	0.9687	0.9754	0.9821	0.9888	0.9955	1.0022	1.0089

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	N	2N+1
521.0	522.0	523.0	524.0	525.0	526.0	527.0	528.0	529.0	530.0	531.0	532.0	533.0	534.0	38	77
535.0	536.0	537.0	538.0	539.0	540.0	541.0	542.0	543.0	544.0	545.0	546.0	547.0	548.0	39	79
549.0	550.0	551.0	552.0	553.0	554.0	555.0	556.0	557.0	558.0	559.0	560.0	561.0	562.0	40	81
563.0	564.0	565.0	566.0	567.0	568.0	569.0	570.0	571.0	572.0	573.0	574.0	575.0	576.0	41	83
577.0	578.0	579.0	580.0	581.0	582.0	583.0	584.0	585.0	586.0	587.0	588.0	589.0	590.0	42	85
591.0	592.0	593.0	594.0	595.0	596.0	597.0	598.0	599.0	600.0	601.0	602.0	603.0	604.0	43	87
605.0	606.0	607.0	608.0	609.0	610.0	611.0	612.0	613.0	614.0	615.0	616.0	617.0	618.0	44	89
619.0	620.0	621.0	622.0	623.0	624.0	625.0	626.0	627.0	628.0	629.0	630.0	631.0	632.0	45	91
633.0	634.0	635.0	636.0	637.0	638.0	639.0	640.0	641.0	642.0	643.0	644.0	645.0	646.0	46	93
647.0	648.0	649.0	650.0	651.0	652.0	653.0	654.0	655.0	656.0	657.0	658.0	659.0	660.0	47	95
661.0	662.0	663.0	664.0	665.0	666.0	667.0	668.0	669.0	670.0	671.0	672.0	673.0	674.0	48	97
675.0	676.0	677.0	678.0	679.0	680.0	681.0	682.0	683.0	684.0	685.0	686.0	687.0	688.0	49	99

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.9218	0.9285	0.9352	0.9419	0.9486	0.9553	0.9620	0.9687	0.9754	0.9821	0.9888	0.9955	1.0022	1.0089

SPECIFIC Z NUMBERS

-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	N	2N+1
MASS/INTENSITY/PPM ERROR															
689.0	690.0	691.0	692.0	693.0	694.0	695.0	696.0	697.0	698.0	699.0	700.0	701.0	702.0	50	101
703.0	704.0	705.0	706.0	707.0	708.0	709.0	710.0	711.0	712.0	713.0	714.0	715.0	716.0	51	103
COLUMN SUMS: 829.4	708.2	1349.9	746.5	1570.8	156.6	404.2	9.7	0.0	0.0	0.0	0.0	0.0	0.0		

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.8280	0.8347	0.8414	0.8481	0.8548	0.8615	0.8682	0.8749	0.8816	0.8883	0.8950	0.9017	0.9084	0.9151

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

-26	-25	-24	-23	-22	-21	-20	-19	-18	-17	-16	-15	-14	-13	N	2N-13
87.0	88.0	89.0	90.0	91.0	92.0	93.0	94.0	95.0	96.0	97.0	98.0	99.0	100.0	8	3
101.0	102.0	103.0	104.0	105.0	106.0	107.0	108.0	109.0	110.0	111.0	112.0	113.0	114.0	9	5
115.0	116.0	117.0	118.0	119.0	120.0	121.0	122.0	123.0	124.0	125.0	126.0	127.0	128.0	10	7
129.0	130.0	131.0	132.0	133.0	134.0	135.0	136.0	137.0	138.0	139.0	140.0	141.0	142.0	11	9
143.0	144.0	145.0	146.0	147.0	148.0	149.0	150.0	151.0	152.0	153.0	154.0	155.0	156.0	12	11
157.0	158.0	159.0	160.0	161.0	162.0	163.0	164.0	165.0	166.0	167.0	168.0	169.0	170.0	13	13
171.0	172.0	173.0	174.0	175.0	176.0	177.0	178.0	179.0	180.0	181.0	182.0	183.0	184.0	14	15
185.0	186.0	187.0	188.0	189.0	190.0	191.0	192.0	193.0	194.0	195.0	196.0	197.0	198.0	15	17
199.0	200.0	201.0	202.0	203.0	204.0	205.0	206.0	207.0	208.0	209.0	210.0	211.0	212.0 19.4 5.9	16	19
213.0	214.0	215.0	216.0	217.0	218.0	219.0	220.0	221.0	222.0	223.0	224.0	225.0	226.0	17	21
227.0	228.0	229.0	230.0	231.0	232.0	233.0	234.0	235.0	236.0	237.0	238.0	239.0 19.3 1.1	240.0 36.3 -3.2	18	23
241.0	242.0	243.0	244.0	245.0	246.0	247.0	248.0	249.0	250.0	251.0	252.0	253.0	254.0 94.8 1.6	19	25

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
0.8280	0.8347	0.8414	0.8481	0.8548	0.8615	0.8682	0.8749	0.8816	0.8883	0.8950	0.9017	0.9084	0.9151

KENDRICK MASS DEFECT + 1.0000

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

-26	-25	-24	-23	-22	-21	-20	-19	-18	-17	-16	-15	-14	-13	N	2N-13
255.0	256.0	257.0	258.0	259.0	260.0	261.0	262.0	263.0	264.0	265.0	266.0 7.1 -4.1	267.0	268.0	20	27
269.0	270.0	271.0	272.0	273.0	274.0	275.0	276.0	277.0	278.0	279.0 25.6 5.3	280.0	281.0	282.0	21	29
283.0	284.0	285.0	286.0	287.0	288.0	289.0	290.0	291.0	292.0 47.1 -5.4	293.0	294.0	295.0	296.0	22	31
297.0	298.0	299.0	300.0	301.0	302.0	303.0	304.0	305.0 11.7 0.5	306.0	307.0	308.0 19.1 5.6	309.0	310.0 27.4 0.3	23	33
311.0	312.0	313.0	314.0	315.0	316.0	317.0	318.0	319.0	320.0	321.0	322.0	323.0 145.9 -5.0	324.0	24	35
325.0	326.0	327.0	328.0	329.0	330.0	331.0	332.0	333.0 14.3 -2.2	334.0	335.0 58.5 -3.6	336.0	337.0 226.0 -5.1	338.0	25	37
339.0	340.0	341.0	342.0	343.0	344.0 12.6 -2.0	345.0	346.0	347.0	348.0	349.0 42.5 3.1	350.0 215.7 -4.9	351.0 249.0 -2.9	352.0	26	39
353.0	354.0	355.0	356.0	357.0	358.0	359.0	360.0	361.0	362.0	363.0	364.0 7.2 5.6	365.0	366.0	27	41
367.0	368.0	369.0	370.0	371.0	372.0	373.0	374.0	375.0	376.0	377.0	378.0	379.0	380.0	28	43
381.0	382.0	383.0	384.0	385.0	386.0	387.0	388.0	389.0 29.5 -2.1	390.0	391.0	392.0	393.0	394.0	29	45
395.0	396.0	397.0	398.0	399.0	400.0	401.0 31.2 -5.5	402.0	403.0 16.4 -5.7	404.0	405.0	406.0	407.0 38.1 1.1	408.0	30	47
409.0	410.0	411.0	412.0	413.0	414.0	415.0	416.0	417.0	418.0	419.0 16.1 -3.8	420.0	421.0 22.5 -3.0	422.0	31	49

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
0.8280	0.8347	0.8414	0.8481	0.8548	0.8615	0.8682	0.8749	0.8816	0.8883	0.8950	0.9017	0.9084	0.9151

KENDRICK MASS DEFECT + 1.0000

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

-26	-25	-24	-23	-22	-21	-20	-19	-18	-17	-16	-15	-14	-13	N	2N-13
423.0	424.0	425.0	426.0	427.0	428.0	429.0	430.0	431.0	432.0	433.0	434.0	435.0 18.4 -4.4	436.0	32	51
437.0	438.0	439.0	440.0	441.0	442.0	443.0	444.0	445.0	446.0	447.0	448.0	449.0	450.0	33	53
451.0	452.0	453.0	454.0	455.0	456.0	457.0	458.0	459.0 21.9 2.0	460.0	461.0	462.0 20.2 -4.9	463.0	464.0	34	55
465.0	466.0	467.0	468.0	469.0	470.0	471.0	472.0	473.0	474.0	475.0	476.0	477.0	478.0 31.3 -5.9	35	57
479.0	480.0	481.0	482.0	483.0	484.0	485.0	486.0	487.0	488.0	489.0	490.0	491.0	492.0	36	59
493.0	494.0	495.0	496.0	497.0	498.0	499.0	500.0	501.0	502.0	503.0	504.0	505.0	506.0	37	61
507.0	508.0	509.0	510.0	511.0	512.0	513.0	514.0	515.0	516.0	517.0	518.0	519.0	520.0	38	63
521.0	522.0	523.0	524.0	525.0	526.0	527.0	528.0	529.0	530.0	531.0	532.0	533.0	534.0	39	65
535.0	536.0	537.0	538.0	539.0	540.0	541.0	542.0	543.0	544.0	545.0	546.0	547.0	548.0	40	67
549.0	550.0	551.0	552.0	553.0	554.0	555.0	556.0	557.0	558.0	559.0	560.0	561.0	562.0	41	69
563.0	564.0	565.0	566.0	567.0	568.0	569.0	570.0	571.0	572.0	573.0	574.0	575.0	576.0	42	71
577.0	578.0	579.0	580.0	581.0	582.0	583.0	584.0	585.0	586.0	587.0	588.0	589.0	590.0	43	73

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.8280	0.8347	0.8414	0.8481	0.8548	0.8615	0.8682	0.8749	0.8816	0.8883	0.8950	0.9017	0.9084	0.9151

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

-26	-25	-24	-23	-22	-21	-20	-19	-18	-17	-16	-15	-14	-13	N	2N-13
591.0	592.0	593.0	594.0	595.0	596.0	597.0	598.0	599.0	600.0	601.0	602.0	603.0	604.0	44	75
605.0	606.0	607.0	608.0	609.0	610.0	611.0	612.0	613.0	614.0	615.0	616.0	617.0	618.0	45	77
619.0	620.0	621.0	622.0	623.0	624.0	625.0	626.0	627.0	628.0	629.0	630.0	631.0	632.0	46	79
633.0	634.0	635.0	636.0	637.0	638.0	639.0	640.0	641.0	642.0	643.0	644.0	645.0	646.0	47	81
647.0	648.0	649.0	650.0	651.0	652.0	653.0	654.0	655.0	656.0	657.0	658.0	659.0	660.0	48	83
661.0	662.0	663.0	664.0	665.0	666.0	667.0	668.0	669.0	670.0	671.0	672.0	673.0	674.0	49	85
675.0	676.0	677.0	678.0	679.0	680.0	681.0	682.0	683.0	684.0	685.0	686.0	687.0	688.0	50	87
689.0	690.0	691.0	692.0	693.0	694.0	695.0	696.0	697.0	698.0	699.0	700.0	701.0	702.0	51	89
703.0	704.0	705.0	706.0	707.0	708.0	709.0	710.0	711.0	712.0	713.0	714.0	715.0	716.0	52	91
COLUMN SUMS: 0.0	0.0	0.0	0.0	0.0	12.6	31.2	0.0	93.9	47.1	142.7	269.4	719.2	209.4		

NAME: RSPCNM. 12-AUG-86. CN 200-425 DEG C 1-RING COMPDS. RUN 1, SCAN 1

MAXIMUM PPM ERROR = 6.0 TOTAL ION CURRENT = 0.3152E+07 ELEMENTAL COMPOSITION: C(N-1)H(2N+Z)13C

ORIGINAL NO. OF MASSES = 671 NO. OF MASSES ASSIGNED = 101 PERCENT OF TOTAL ION CURRENT ASSIGNED = 7.3

UNASSIGNED MASSES AND INTENSITIES:

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
100.929	115.932	116.940	103.947	104.953	91.960	120.963	93.972	80.980	95.987	82.993	97.989	85.006	113.923
86.1	62.0	96.5	63.9	206.1	111.0	117.3	11.8	81.2	23.6	119.0	34.4	78.6	26.8
114.930	115.936	117.015	117.947	118.950	119.924	120.967	107.973	94.979	109.986	96.933	97.995	99.006	127.769
178.2	14.0	20.2	273.3	17.4	19.2	34.7	46.9	124.5	31.4	11.8	12.1	24.0	12.8
128.926	129.933	130.937	131.948	118.954	119.956	134.956	121.974	108.924	123.988	96.934	111.910	113.007	127.920
41.7	271.1	10.8	467.4	590.2	20.0	213.4	43.9	241.3	36.0	12.9	58.4	29.2	8.6
128.930	143.933	130.941	145.946	132.954	119.958	134.964	135.962	108.980	137.897	96.994	125.910	126.894	127.923
270.6	353.3	587.6	450.2	988.4	13.0	43.8	1384.2	182.5	24.2	255.6	79.8	7.7	37.1
142.926	157.933	144.940	159.946	146.948	119.961	134.968	135.973	122.981	151.896	110.993	125.911	126.913	141.924
149.8	497.5	1221.7	455.6	50.5	1174.5	16.1	45.2	226.1	17.1	211.9	33.5	27.3	21.1
142.930	171.931	158.940	173.947	146.953	133.951	148.966	135.975	136.980	179.895	124.904	139.910	126.916	155.920
226.0	28.7	1378.6	783.6	623.7	31.1	64.7	8.5	115.0	22.4	103.0	68.6	37.4	10.5
156.927	171.934	172.934	187.946	160.943	133.961	162.876	149.973	150.889	193.895	124.994	153.909	127.007	155.922
649.6	355.4	21.2	1093.1	13.0	1038.2	18.5	39.1	11.6	22.7	183.1	22.4	29.0	13.9
170.928	185.933	172.940	201.946	160.953	147.960	162.967	177.883	150.980	193.897	138.903	153.910	140.916	155.923
651.6	643.6	1260.9	1403.2	412.7	482.2	70.4	14.5	56.0	30.6	157.2	16.1	39.8	11.0
170.933	199.933	186.939	215.945	174.945	161.960	176.966	205.745	164.890	207.892	138.994	167.911	140.917	169.921
18.4	790.4	1014.9	946.7	8.8	347.7	76.7	14.7	21.8	10.5	54.1	25.1	21.5	114.3
184.927	213.932	200.940	229.940	174.954	175.960	190.876	205.883	164.891	207.895	152.903	181.727	154.916	183.919
804.5	1032.6	646.8	29.7	301.3	304.8	48.5	21.0	22.7	47.4	143.4	24.6	97.5	184.5
198.920	227.935	214.922	229.947	188.947	175.963	190.966	205.972	164.980	207.897	152.994	181.909	155.005	183.922
35.6	1093.7	14.7	994.6	26.8	14.0	35.8	18.0	62.7	22.5	33.9	37.7	16.6	31.1
198.927	241.924	214.938	243.948	188.953	189.960	204.965	219.693	178.890	221.890	166.903	195.906	168.816	197.920
836.2	7.1	665.0	822.1	232.4	379.8	19.9	45.2	97.2	13.3	180.0	39.6	15.1	210.2
212.926	241.934	228.937	257.944	202.863	203.715	218.870	219.881	178.979	221.892	180.903	195.909	168.912	211.920
793.3	1070.5	122.1	54.8	32.1	17.1	16.9	35.1	47.1	7.2	159.7	58.7	26.0	265.1
226.930	255.935	228.941	257.949	202.953	203.868	218.875	233.883	178.981	221.896	194.904	209.906	168.916	225.914
529.0	926.7	503.8	781.0	186.3	20.3	34.3	37.0	11.5	124.1	161.1	118.8	248.4	11.4
240.924	269.933	242.941	271.855	216.861	203.870	218.878	247.884	192.889	235.896	208.902	223.908	182.725	225.917
98.0	799.7	315.3	33.8	46.5	11.3	12.9	87.7	59.4	248.8	201.1	171.8	16.9	24.6
240.928	283.941	256.852	271.946	216.864	203.959	218.961	261.886	192.980	249.895	222.899	223.912	182.912	225.922
409.5	14.7	14.2	678.9	23.0	471.2	78.2	110.0	45.4	240.5	55.0	29.9	84.1	303.5

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
240.933 28.3	283.932 638.5	256.938 84.4	285.854 17.5	216.952 153.6	217.959 462.2	232.965 8.2	275.882 74.5	206.889 27.7	249.899 20.8	222.903 145.9	237.907 202.7	182.915 349.9	239.921 439.9
254.928 313.8	297.520 7.1	256.942 207.0	285.946 695.7	230.863 78.9	231.869 14.0	246.877 16.0	289.882 113.8	206.979 18.3	263.896 419.4	236.902 258.9	237.910 48.8	196.912 103.7	253.920 529.0
268.910 10.1	297.934 711.9	270.849 7.3	299.856 107.3	244.864 42.5	231.960 430.3	246.964 87.6	303.883 99.1	220.889 55.2	277.893 312.3	250.901 248.0	251.907 219.9	196.916 200.3	267.920 697.9
268.926 451.6	311.843 41.7	270.937 337.6	299.946 570.8	244.953 179.2	245.870 54.1	260.879 27.9	317.879 26.5	234.888 101.0	291.895 230.8	250.906 22.8	265.910 295.3	210.915 350.5	281.919 627.9
282.835 14.6	311.934 570.9	284.939 153.1	313.857 67.7	258.865 85.7	245.961 430.2	260.882 17.5	317.883 117.1	234.891 72.5	305.894 295.5	264.903 239.6	279.907 206.1	224.916 314.3	295.919 586.0
282.926 162.3	325.843 28.8	298.849 12.0	313.948 479.4	258.951 119.1	245.966 9.6	260.966 55.8	331.499 79.2	248.889 155.1	319.894 251.1	278.900 118.0	293.887 16.8	238.914 389.4	309.920 408.1
292.930 19.9	325.933 454.0	298.938 220.0	327.857 98.4	258.957 77.7	259.874 23.6	274.872 21.1	331.881 159.8	248.893 7.8	333.494 91.6	292.899 97.2	293.907 392.8	252.670 38.7	323.920 405.6
296.926 365.4	339.932 489.8	312.938 202.4	327.910 20.2	272.863 37.0	259.963 391.3	274.876 10.8	345.450 118.5	262.890 148.7	333.893 228.8	292.903 55.6	307.907 327.1	252.913 761.8	337.918 351.2
310.926 270.6	353.419 25.2	312.943 20.8	327.946 401.0	272.953 28.6	273.865 24.9	288.875 21.5	345.883 141.3	276.886 23.3	333.898 16.7	306.899 67.1	321.907 331.7	266.915 666.4	351.911 33.4
324.919 49.0	353.841 35.0	340.848 25.2	341.855 91.1	286.862 32.6	273.869 115.6	302.873 46.1	359.881 102.1	276.889 41.1	347.893 254.5	306.903 43.9	335.905 351.1	280.906 38.4	351.917 320.5
324.925 237.0	367.842 30.2	396.940 19.3	341.946 475.4	286.954 7.3	273.959 291.7	302.964 17.8	373.880 108.3	290.888 87.2	361.894 204.2	320.899 160.6	363.908 274.7	280.912 303.8	365.920 357.0
366.925 268.9	367.933 477.0	438.940 13.6	355.413 7.7	300.954 16.2	287.869 171.8	316.872 41.5	373.888 12.9	304.888 116.3	375.896 234.3	334.901 55.5	377.908 301.1	294.913 238.7	379.920 315.1
380.927 77.8	381.844 22.6	495.073 5.2	355.854 105.7	314.863 29.6	287.953 19.3	330.873 66.1	387.882 115.2	318.887 169.3	389.894 182.9	348.898 50.9	391.905 98.9	308.485 11.3	393.829 20.2
394.928 20.3	381.933 302.9		355.944 294.4	328.857 13.7	287.960 246.8	358.872 38.3	401.365 6.2	332.885 56.8	403.877 7.7	348.902 19.0	391.909 85.2	308.914 148.7	393.912 7.7
408.927 53.5	395.934 202.6		369.856 99.0	328.952 31.6	301.870 150.7	372.873 45.2	401.881 110.4	332.888 31.9	403.895 133.1	362.899 147.9	405.907 150.8	322.917 32.0	393.920 197.0
422.928 36.2	409.843 19.9		369.947 214.0	342.861 36.4	301.960 179.1	386.601 13.1	415.885 121.0	346.886 48.3	417.898 78.1	376.900 93.2	419.910 110.2	364.913 261.7	407.920 252.1
549.024 8.4	409.935 205.5		383.856 71.2	342.952 24.4	315.870 196.0	386.872 25.4	429.884 102.0	360.889 41.7	431.893 18.6	390.900 44.6	433.908 81.9	378.906 36.9	421.923 180.9
	423.845 23.3		383.946 182.0	356.857 17.4	315.961 122.7	386.876 25.5	443.882 16.0	374.885 42.3	431.899 47.6	404.901 51.7	447.908 65.3	378.912 94.3	435.921 88.1
	423.936 171.3		397.860 27.0	356.860 39.5	329.471 40.6	414.873 16.4	500.072 17.8	374.890 31.8	445.895 58.3	418.904 32.0	461.177 140.7	378.918 6.6	449.920 96.9

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
	437.499 28.5		397.947 154.4	370.859 17.2	329.869 136.1	414.876 19.1		402.888 27.8	459.894 84.5	432.901 29.6	461.910 15.4	392.912 120.5	449.926 13.8
	437.933 98.1		411.857 25.9	384.863 23.6	329.951 11.0	414.967 11.5		430.888 33.8	473.894 34.7	460.898 25.2	475.905 22.8	406.914 40.5	463.919 41.6
	451.932 79.1		411.947 115.8	398.859 22.6	329.959 96.8	442.504 36.3		458.315 19.1	487.892 24.9	503.064 34.4	489.909 12.9	406.921 13.1	477.922 14.2
	465.932 19.7		411.953 20.3	412.952 56.4	343.870 177.1	456.314 68.6		626.842 12.0	501.895 14.3	531.020 174.8	545.923 19.0	420.916 39.6	505.926 23.5
	479.936 15.5		425.271 6.4	426.952 10.6	343.959 99.0	456.877 9.3				545.017 15.5		448.917 22.2	
	493.842 14.8		425.858 55.2	440.860 13.7	357.868 164.8	624.843 23.7						533.016 40.0	
	493.932 16.0		425.948 39.9	454.317 15.6	357.958 53.0								
	507.939 23.3		439.182 18.7	580.984 50.6	357.962 43.6								
	535.947 12.5		439.855 70.3	706.740 26.0	371.869 152.9								
			439.947 46.0		371.959 63.5								
			453.945 14.9		385.870 125.8								
					385.961 66.5								
					399.869 146.0								
					399.960 45.7								
					413.871 66.6								
					427.873 61.3								
					441.176 15.8								
					441.503 295.5								
					441.868 53.8								

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
					455.228 5.4								
					455.868 29.8								
					455.872 14.2								
					469.180 7.9								
					469.868 33.2								
					469.873 16.5								
					497.867 8.2								

Appendix III

CHS Output from the Mass Spectrum of One-Ring Aromatic Neutrals Separated from the 200-425° C Distillate of the Cerro Negro (Venezuela) Heavy Petroleum.

NATIONAL INSTITUTE FOR PETROLEUM AND ENERGY RESEARCH, P.O. BOX 2128, BARTLESVILLE, OK 74005

HIGH RESOLUTION MASS SPECTRUM

NAME: RSPCNM. 12-AUG-86. CN 200-425 DEG C 1-RING COMPDS. RUN 1, SCAN 1

ELEMENTAL COMPOSITION: C(N)H(2N+Z)S

NAME: RSPCNM. 12-AUG-86. CN 200-425 DEG C 1-RING COMPDS. RUN 1, SCAN 1

MAXIMUM PPM ERROR = 6.0 TOTAL ION CURRENT = 0.3152E+07 ELEMENTAL COMPOSITION: C(N)H(2N+Z)S

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.9297	0.9364	0.9431	0.9498

SPECIFIC Z NUMBERS

-1	0	1	2	N	2N+2
MASS/INTENSITY/PPM ERROR					
45.0	46.0	47.0	48.0	1	4
59.0	60.0	61.0	62.0	2	6
73.0	74.0	75.0	76.0	3	8
87.0	88.0	89.0	90.0	4	10
101.0 86.1 3.3	102.0	103.0	104.0	5	12
115.0 178.2 -1.5	116.0 14.0 5.5	117.0	118.0	6	14
129.0 270.6 -2.6	130.0	131.0	132.0	7	16
143.0 226.0 -1.8	144.0	145.0	146.0	8	18
157.0	158.0	159.0	160.0	9	20
171.0	172.0	173.0	174.0	10	22
185.0	186.0	187.0	188.0	11	24

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
0.9297	0.9364	0.9431	0.9498										

KENDRICK MASS DEFECT + 1.0000

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

-1	0	1	2	N	2N+2
199.0	200.0	201.0	202.0	12	26
213.0	214.0	215.0	216.0	13	28
227.0 529.0 -0.3	228.0	229.0	230.0	14	30
241.0	242.0	243.0	244.0	15	32
255.0	256.0 926.7 4.1	257.0 207.0 4.8	258.0 781.0 1.8	16	34
269.0	270.0	271.0	272.0	17	36
283.0 19.9 -1.7	284.0	285.0	286.0	18	38
297.0	298.0	299.0	300.0	19	40
311.0	312.0	313.0 20.8 -0.9	314.0	20	42
325.0	326.0	327.0	328.0	21	44
339.0	340.0	341.0	342.0	22	46
353.0	354.0	355.0	356.0	23	48

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.9297	0.9364	0.9431	0.9498

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

-1	0	1	2	N	2N+2
367.0	368.0	369.0	370.0	24	50
381.0	382.0	383.0	384.0	25	52
395.0 20.3 3.1	396.0 202.6 5.4	397.0	398.0	26	54
409.0	410.0 205.5 4.0	411.0	412.0	27	56
423.0 36.2 4.3	424.0 171.3 1.1	425.0	426.0 39.9 4.7	28	58
437.0	438.0	439.0	440.0	29	60
451.0	452.0	453.0	454.0	30	62
465.0	466.0	467.0	468.0	31	64
479.0	480.0 15.5 0.9	481.0	482.0	32	66
493.0	494.0	495.0	496.0	33	68
507.0	508.0 23.3 -5.0	509.0	510.0	34	70
521.0	522.0	523.0	524.0	35	72

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.9297	0.9364	0.9431	0.9498

SPECIFIC Z NUMBERS

-1	0	1	2	N	2N+2
MASS/INTENSITY/PPM ERROR					
535.0	536.0	537.0	538.0	36	74
549.0	550.0	551.0	552.0	37	76
563.0	564.0	565.0	566.0	38	78
577.0	578.0	579.0	580.0	39	80
591.0	592.0	593.0	594.0	40	82
605.0	606.0	607.0	608.0	41	84
619.0	620.0	621.0	622.0	42	86
633.0	634.0	635.0	636.0	43	88
647.0	648.0	649.0	650.0	44	90
661.0	662.0	663.0	664.0	45	92
675.0	676.0	677.0	678.0	46	94
689.0	690.0	691.0	692.0	47	96

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.9297	0.9364	0.9431	0.9498

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

-1	0	1	2	N	2N+2
703.0	704.0	705.0	706.0	48	98
717.0	718.0	719.0	720.0	49	100
COLUMN SUMS:					
1366.2	1558.8	227.9	821.0		

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.8359	0.8426	0.8493	0.8560	0.8627	0.8694	0.8761	0.8828	0.8895	0.8962	0.9029	0.9096	0.9163	0.9230

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

-15	-14	-13	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	N	2N -2
45.0	46.0	47.0	48.0	49.0	50.0	51.0	52.0	53.0	54.0	55.0	56.0	57.0	58.0	2	2
59.0	60.0	61.0	62.0	63.0	64.0	65.0	66.0	67.0	68.0	69.0	70.0	71.0	72.0	3	4
73.0	74.0	75.0	76.0	77.0	78.0	79.0	80.0	81.0	82.0	83.0	84.0	85.0	86.0	4	6
87.0	88.0	89.0	90.0	91.0	92.0	93.0	94.0	95.0	96.0	97.0	98.0	99.0	100.0	5	8
101.0	102.0	103.0	104.0	105.0	106.0	107.0	108.0	109.0	110.0	111.0	112.0 58.4 0.1	113.0	114.0 26.8 -4.0	6	10
115.0	116.0	117.0	118.0	119.0	120.0	121.0	122.0	123.0	124.0	125.0	126.0 79.8 0.2	127.0 37.4 -1.4	128.0 37.1 3.4	7	12
129.0	130.0	131.0	132.0	133.0	134.0	135.0	136.0	137.0	138.0 24.2 -3.4	139.0 157.2 -1.8	140.0 68.6 -2.1	141.0 39.8 3.2	142.0 21.1 -4.9	8	14
143.0	144.0	145.0	146.0	147.0	148.0	149.0	150.0	151.0 11.6 2.8	152.0 17.1 -1.8	153.0 143.4 1.6	154.0 22.4 3.3	155.0 97.5 3.5	156.0 11.0 -2.9	9	16
157.0	158.0	159.0	160.0	161.0	162.0	163.0 18.5 0.7	164.0	165.0 21.8 -0.5	166.0	167.0 180.0 -0.5	168.0	169.0 248.4 -1.3	170.0	10	18
171.0	172.0	173.0	174.0	175.0	176.0	177.0	178.0 14.5 -3.3	179.0 97.2 -0.2	180.0	181.0 159.7 1.4	182.0 37.7 3.4	183.0 349.9 4.4	184.0 31.1 4.1	11	20
185.0	186.0	187.0	188.0	189.0	190.0	191.0 48.5 2.4	192.0	193.0 59.4 0.7	194.0 22.7 3.9	195.0 161.1 -3.9	196.0 58.7 1.1	197.0 200.3 -0.2	198.0	12	22
199.0	200.0	201.0	202.0	203.0 32.1 0.4	204.0 11.3 -3.4	205.0	206.0 21.0 -1.3	207.0 27.7 2.7	208.0 47.4 4.0	209.0 201.1 2.0	210.0	211.0	212.0	13	24

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
0.8359	0.8426	0.8493	0.8560	0.8627	0.8694	0.8761	0.8828	0.8895	0.8962	0.9029	0.9096	0.9163	0.9230

KENDRICK MASS DEFECT + 1.0000

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

-15	-14	-13	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	N	2N -2
213.0	214.0	215.0	216.0	217.0	218.0	219.0 34.3 4.1	220.0	221.0 55.2 3.3	222.0 124.1 1.4	223.0 145.9 -1.2	224.0	225.0 314.3 1.8	226.0 303.5 5.1	14	26
227.0	228.0	229.0	230.0	231.0 78.9 -1.9	232.0 14.0 2.1	233.0	234.0 37.0 1.1	235.0	236.0 248.8 -0.3	237.0 258.9 5.0	238.0 48.8 -3.2	239.0	240.0	15	28
241.0	242.0	243.0	244.0	245.0	246.0 54.1 -1.6	247.0 16.0 -2.0	248.0 87.7 -3.4	249.0 155.1 3.9	250.0 240.5 5.7	251.0	252.0	253.0	254.0	16	30
255.0	256.0	257.0	258.0	259.0	260.0	261.0	262.0	263.0 148.7 -0.9	264.0 419.4 -0.7	265.0 239.6 -1.3	266.0 295.3 0.0	267.0 666.4 4.2	268.0	17	32
269.0	270.0	271.0 7.3 2.3	272.0 33.8 2.2	273.0 37.0 0.1	274.0 115.6 1.2	275.0 10.8 1.8	276.0 74.5 3.9	277.0 41.1 2.6	278.0	279.0	280.0	281.0	282.0	18	34
283.0 14.6 2.8	284.0	285.0	286.0	287.0 32.6 1.4	288.0 171.8 0.4	289.0 21.5 2.7	290.0 113.8 4.1	291.0	292.0 230.8 5.1	293.0 55.6 -0.4	294.0	295.0	296.0	19	36
297.0	298.0	299.0 12.0 -0.3	300.0 107.3 -1.3	301.0	302.0 150.7 -3.0	303.0	304.0 99.1 0.9	305.0 116.3 5.3	306.0 295.5 5.8	307.0 43.9 -1.6	308.0	309.0	310.0	20	38
311.0	312.0 41.7 0.1	313.0	314.0 67.7 -3.2	315.0 29.6 0.4	316.0 196.0 -1.2	317.0	318.0 117.1 -1.2	319.0	320.0	321.0	322.0	323.0 32.0 -2.4	324.0	21	40
325.0	326.0 28.8 -1.5	327.0	328.0 98.4 -3.2	329.0	330.0 136.1 1.1	331.0	332.0 159.8 4.5	333.0 31.9 5.1	334.0 16.7 -5.8	335.0 55.5 4.3	336.0	337.0	338.0	22	42
339.0	340.0	341.0 25.2 4.5	342.0 91.1 2.3	343.0 36.4 5.5	344.0 177.1 -1.0	345.0	346.0 141.3 -1.1	347.0	348.0	349.0 19.0 2.5	350.0	351.0	352.0	23	44
353.0	354.0 35.0 5.3	355.0	356.0	357.0	358.0 164.8 3.6	359.0	360.0 102.1 4.4	361.0 41.7 1.1	362.0	363.0	364.0 274.7 4.2	365.0	366.0	24	46
367.0	368.0 30.2 2.2	369.0	370.0 99.0 -1.2	371.0	372.0 152.9 0.3	373.0	374.0	375.0 31.8 -0.6	376.0 234.3 1.2	377.0	378.0 301.1 3.6	379.0 6.6 -3.9	380.0	25	48

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
0.8359	0.8426	0.8493	0.8560	0.8627	0.8694	0.8761	0.8828	0.8895	0.8962	0.9029	0.9096	0.9163	0.9230

KENDRICK MASS DEFECT + 1.0000

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

-15	-14	-13	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	N	2N -2
381.0	382.0 22.6 -4.4	383.0	384.0 71.2 -1.2	385.0 23.6 -1.7	386.0 125.8 -0.3	387.0 25.5 0.1	388.0 115.2 2.5	389.0	390.0 182.9 4.6	391.0	392.0 85.2 0.8	393.0	394.0	26	50
395.0	396.0	397.0	398.0	399.0	400.0 146.0 1.2	401.0	402.0 110.4 3.6	403.0 27.8 4.5	404.0 133.1 3.5	405.0 51.7 5.7	406.0 150.8 5.6	407.0	408.0	27	52
409.0	410.0 19.9 -1.3	411.0	412.0 25.9 -2.4	413.0	414.0 66.6 -5.1	415.0 19.1 1.3	416.0	417.0	418.0 78.1 -4.2	419.0 32.0 -1.5	420.0 110.2 -0.1	421.0 39.6 1.4	422.0 180.9 -0.7	28	54
423.0	424.0 23.3 -5.6	425.0	426.0 55.2 -4.4	427.0	428.0	429.0	430.0 102.0 -2.9	431.0 33.8 2.8	432.0 47.6 -5.9	433.0 29.6 4.2	434.0 81.9 4.6	435.0	436.0 88.1 4.5	29	56
437.0	438.0	439.0	440.0 70.3 2.6	441.0	442.0 53.8 4.2	443.0	444.0 16.0 2.9	445.0	446.0 58.3 1.8	447.0	448.0 65.3 4.0	449.0 22.2 -2.6	450.0	30	58
451.0	452.0	453.0	454.0	455.0	456.0 29.8 2.7	457.0 9.3 -1.0	458.0	459.0	460.0 84.5 4.0	461.0	462.0 15.4 -1.4	463.0	464.0	31	60
465.0	466.0	467.0	468.0	469.0	470.0 33.2 3.4	471.0	472.0	473.0	474.0 34.7 5.6	475.0	476.0	477.0	478.0 14.2 1.8	32	62
479.0	480.0	481.0	482.0	483.0	484.0	485.0	486.0	487.0	488.0	489.0	490.0 12.9 0.6	491.0	492.0	33	64
493.0	494.0 14.8 1.7	495.0	496.0	497.0	498.0 8.2 4.4	499.0	500.0	501.0	502.0 14.3 1.9	503.0	504.0	505.0	506.0	34	66
507.0	508.0	509.0	510.0	511.0	512.0	513.0	514.0	515.0	516.0	517.0	518.0	519.0	520.0	35	68
521.0	522.0	523.0	524.0	525.0	526.0	527.0	528.0	529.0	530.0	531.0	532.0	533.0	534.0	36	70
535.0	536.0	537.0	538.0	539.0	540.0	541.0	542.0	543.0	544.0	545.0	546.0	547.0	548.0	37	72

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.8359	0.8426	0.8493	0.8560	0.8627	0.8694	0.8761	0.8828	0.8895	0.8962	0.9029	0.9096	0.9163	0.9230

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

-15	-14	-13	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	N	2N -2
549.0	550.0	551.0	552.0	553.0	554.0	555.0	556.0	557.0	558.0	559.0	560.0	561.0	562.0	38	74
563.0	564.0	565.0	566.0	567.0	568.0	569.0	570.0	571.0	572.0	573.0	574.0	575.0	576.0	39	76
577.0	578.0	579.0	580.0	581.0	582.0	583.0	584.0	585.0	586.0	587.0	588.0	589.0	590.0	40	78
591.0	592.0	593.0	594.0	595.0	596.0	597.0	598.0	599.0	600.0	601.0	602.0	603.0	604.0	41	80
605.0	606.0	607.0	608.0	609.0	610.0	611.0	612.0	613.0	614.0	615.0	616.0	617.0	618.0	42	82
619.0	620.0	621.0	622.0	623.0	624.0	625.0	626.0	627.0	628.0	629.0	630.0	631.0	632.0	43	84
633.0	634.0	635.0	636.0	637.0	638.0	639.0	640.0	641.0	642.0	643.0	644.0	645.0	646.0	44	86
647.0	648.0	649.0	650.0	651.0	652.0	653.0	654.0	655.0	656.0	657.0	658.0	659.0	660.0	45	88
661.0	662.0	663.0	664.0	665.0	666.0	667.0	668.0	669.0	670.0	671.0	672.0	673.0	674.0	46	90
675.0	676.0	677.0	678.0	679.0	680.0	681.0	682.0	683.0	684.0	685.0	686.0	687.0	688.0	47	92
689.0	690.0	691.0	692.0	693.0	694.0	695.0	696.0	697.0	698.0	699.0	700.0	701.0	702.0	48	94
703.0	704.0	705.0	706.0	707.0	708.0	709.0	710.0	711.0	712.0	713.0	714.0	715.0	716.0	49	96

COLUMN SUMS:

14.6	216.3	44.4	719.9	270.0	1807.9	203.3	1311.5	901.1	2554.9	1934.1	1767.2	2054.5	713.8

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.7421	0.7488	0.7555	0.7622	0.7689	0.7756	0.7823	0.7890	0.7957	0.8024	0.8091	0.8158	0.8225	0.8292

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

-29	-28	-27	-26	-25	-24	-23	-22	-21	-20	-19	-18	-17	-16	N	2N-16
129.0	130.0	131.0	132.0	133.0	134.0	135.0	136.0	137.0	138.0	139.0	140.0	141.0	142.0	9	2
143.0	144.0	145.0	146.0	147.0	148.0	149.0	150.0	151.0	152.0	153.0	154.0	155.0	156.0	10	4
157.0	158.0	159.0	160.0	161.0	162.0	163.0	164.0	165.0	166.0	167.0	168.0	169.0	170.0	11	6
171.0	172.0	173.0	174.0	175.0	176.0	177.0	178.0	179.0	180.0	181.0	182.0	183.0	184.0	12	8
185.0	186.0	187.0	188.0	189.0	190.0	191.0	192.0	193.0	194.0	195.0	196.0	197.0	198.0	13	10
199.0	200.0	201.0	202.0	203.0	204.0	205.0	206.0	207.0	208.0	209.0	210.0	211.0	212.0	14	12
213.0	214.0	215.0	216.0	217.0	218.0	219.0	220.0	221.0	222.0	223.0	224.0	225.0	226.0	15	14
227.0	228.0	229.0	230.0	231.0	232.0	233.0	234.0	235.0	236.0	237.0	238.0	239.0	240.0	16	16
241.0	242.0	243.0	244.0	245.0	246.0	247.0	248.0	249.0	250.0	251.0	252.0	253.0	254.0	17	18
255.0	256.0	257.0	258.0	259.0	260.0	261.0	262.0	263.0	264.0	265.0	266.0	267.0	268.0	18	20
269.0	270.0	271.0	272.0	273.0	274.0	275.0	276.0	277.0	278.0	279.0	280.0	281.0	282.0	19	22
283.0	284.0	285.0	286.0	287.0	288.0	289.0	290.0	291.0	292.0	293.0	294.0	295.0	296.0	20	24

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
0.7421	0.7488	0.7555	0.7622	0.7689	0.7756	0.7823	0.7890	0.7957	0.8024	0.8091	0.8158	0.8225	0.8292

KENDRICK MASS DEFECT + 1.0000

SPECIFIC Z NUMBERS

-29	-28	-27	-26	-25	-24	-23	-22	-21	-20	-19	-18	-17	-16	N	2N-16
MASS/INTENSITY/PPM ERROR															
297.0	298.0	299.0	300.0	301.0	302.0	303.0	304.0	305.0	306.0	307.0	308.0	309.0	310.0	21	26
311.0	312.0	313.0	314.0	315.0	316.0	317.0	318.0	319.0	320.0	321.0	322.0	323.0	324.0	22	28
325.0	326.0	327.0	328.0	329.0	330.0	331.0	332.0	333.0	334.0	335.0	336.0	337.0	338.0	23	30
339.0	340.0	341.0	342.0	343.0	344.0	345.0	346.0	347.0	348.0	349.0	350.0	351.0	352.0	24	32
353.0	354.0	355.0	356.0	357.0	358.0	359.0	360.0	361.0	362.0	363.0	364.0	365.0	366.0	25	34
367.0	368.0	369.0	370.0	371.0	372.0	373.0	374.0	375.0	376.0	377.0	378.0	379.0	380.0	26	36
381.0	382.0	383.0	384.0	385.0	386.0	387.0	388.0	389.0	390.0	391.0	392.0	393.0	394.0 20.2 0.7	27	38
395.0	396.0	397.0	398.0	399.0	400.0	401.0	402.0	403.0	404.0	405.0	406.0	407.0	408.0	28	40
409.0	410.0	411.0	412.0	413.0	414.0	415.0	416.0	417.0	418.0	419.0	420.0	421.0	422.0	29	42
423.0	424.0	425.0	426.0	427.0	428.0	429.0	430.0	431.0	432.0	433.0	434.0	435.0	436.0	30	44
437.0	438.0	439.0	440.0	441.0	442.0	443.0	444.0	445.0	446.0	447.0	448.0	449.0	450.0	31	46
451.0	452.0	453.0	454.0	455.0	456.0	457.0	458.0	459.0	460.0	461.0	462.0	463.0	464.0	32	48

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.7421	0.7488	0.7555	0.7622	0.7689	0.7756	0.7823	0.7890	0.7957	0.8024	0.8091	0.8158	0.8225	0.8292

SPECIFIC Z NUMBERS

-29	-28	-27	-26	-25	-24	-23	-22	-21	-20	-19	-18	-17	-16	N	2N-16
MASS/INTENSITY/PPM ERROR															
465.0	466.0	467.0	468.0	469.0	470.0	471.0	472.0	473.0	474.0	475.0	476.0	477.0	478.0	33	50
479.0	480.0	481.0	482.0	483.0	484.0	485.0	486.0	487.0	488.0	489.0	490.0	491.0	492.0	34	52
493.0	494.0	495.0	496.0	497.0	498.0	499.0	500.0	501.0	502.0	503.0	504.0	505.0	506.0	35	54
507.0	508.0	509.0	510.0	511.0	512.0	513.0	514.0	515.0	516.0	517.0	518.0	519.0	520.0	36	56
521.0	522.0	523.0	524.0	525.0	526.0	527.0	528.0	529.0	530.0	531.0	532.0	533.0	534.0	37	58
535.0	536.0	537.0	538.0	539.0	540.0	541.0	542.0	543.0	544.0	545.0	546.0	547.0	548.0	38	60
549.0	550.0	551.0	552.0	553.0	554.0	555.0	556.0	557.0	558.0	559.0	560.0	561.0	562.0	39	62
563.0	564.0	565.0	566.0	567.0	568.0	569.0	570.0	571.0	572.0	573.0	574.0	575.0	576.0	40	64
577.0	578.0	579.0	580.0	581.0	582.0	583.0	584.0	585.0	586.0	587.0	588.0	589.0	590.0	41	66
591.0	592.0	593.0	594.0	595.0	596.0	597.0	598.0	599.0	600.0	601.0	602.0	603.0	604.0	42	68
605.0	606.0	607.0	608.0	609.0	610.0	611.0	612.0	613.0	614.0	615.0	616.0	617.0	618.0	43	70
619.0	620.0	621.0	622.0	623.0	624.0	625.0	626.0	627.0	628.0	629.0	630.0	631.0	632.0	44	72

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2

KENDRICK MASS DEFECT + 1.0000

0.7421	0.7488	0.7555	0.7622	0.7689	0.7756	0.7823	0.7890	0.7957	0.8024	0.8091	0.8158	0.8225	0.8292

SPECIFIC Z NUMBERS

MASS/INTENSITY/PPM ERROR

-29	-28	-27	-26	-25	-24	-23	-22	-21	-20	-19	-18	-17	-16	N	2N-16
633.0	634.0	635.0	636.0	637.0	638.0	639.0	640.0	641.0	642.0	643.0	644.0	645.0	646.0	45	74
647.0	648.0	649.0	650.0	651.0	652.0	653.0	654.0	655.0	656.0	657.0	658.0	659.0	660.0	46	76
661.0	662.0	663.0	664.0	665.0	666.0	667.0	668.0	669.0	670.0	671.0	672.0	673.0	674.0	47	78
675.0	676.0	677.0	678.0	679.0	680.0	681.0	682.0	683.0	684.0	685.0	686.0	687.0	688.0	48	80
689.0	690.0	691.0	692.0	693.0	694.0	695.0	696.0	697.0	698.0	699.0	700.0	701.0	702.0	49	82
703.0	704.0	705.0	706.0	707.0	708.0	709.0	710.0	711.0	712.0	713.0	714.0	715.0	716.0	50	84
COLUMN SUMS: 0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	20.2		

NAME: RSPCNM. 12-AUG-86. CN 200-425 DEG C 1-RING COMPDS. RUN 1, SCAN 1

MAXIMUM PPM ERROR = 6.0 TOTAL ION CURRENT = 0.3152E+07 ELEMENTAL COMPOSITION: C(N)H(2N+Z)S

ORIGINAL NO. OF MASSES = 671 NO. OF MASSES ASSIGNED = 180 PERCENT OF TOTAL ION CURRENT ASSIGNED = 18.5

UNASSIGNED MASSES AND INTENSITIES:

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
128.926	115.932	116.940	103.947	104.953	91.960	120.963	93.972	80.980	95.987	82.993	97.989	85.006	127.769
41.7	62.0	96.5	63.9	206.1	111.0	117.3	11.8	81.2	23.6	119.0	34.4	78.6	12.8
142.926	129.933	117.015	117.947	118.950	119.924	120.967	107.973	94.979	109.986	96.933	97.995	99.006	127.920
149.8	271.1	20.2	273.3	17.4	19.2	34.7	46.9	124.5	31.4	11.8	12.1	24.0	8.6
156.927	143.928	130.937	131.942	118.954	119.956	134.956	121.974	108.924	123.988	96.934	125.911	113.007	155.920
649.6	19.0	10.8	36.4	590.2	20.0	213.4	43.9	241.3	36.0	12.9	33.5	29.2	10.5
170.928	143.933	130.941	131.948	132.949	119.958	134.962	135.962	108.980	179.895	96.994	153.910	126.894	155.922
651.6	353.3	587.6	467.4	37.1	13.0	62.4	1384.2	182.5	22.4	255.6	16.1	7.7	13.9
170.933	157.928	144.935	145.942	132.954	119.961	134.964	135.973	122.981	193.897	110.993	167.911	126.913	169.921
18.4	38.7	18.0	115.3	988.4	1174.5	43.8	45.2	226.1	30.6	211.9	25.1	27.3	114.3
184.927	157.933	144.940	145.946	146.948	133.951	134.968	135.975	136.980	207.892	124.904	181.727	127.007	183.919
804.5	497.5	1221.7	450.2	50.5	31.1	16.1	8.5	115.0	10.5	103.0	24.6	29.0	184.5
198.920	171.928	158.940	159.941	146.953	133.956	148.963	149.973	150.980	207.897	124.994	195.906	140.917	197.920
35.6	58.5	1378.6	187.2	623.7	79.3	39.0	39.1	56.0	22.5	183.1	39.6	21.5	210.2
198.927	171.931	172.934	159.946	160.943	133.961	148.966	205.745	164.891	221.890	138.994	209.906	155.005	211.914
636.2	28.7	21.2	455.6	13.0	1038.2	64.7	14.7	22.7	13.3	54.1	118.8	16.6	19.4
212.921	171.934	172.940	173.942	160.948	147.955	162.967	205.972	164.980	221.892	152.994	223.908	168.816	211.920
33.1	355.4	1260.9	134.8	64.4	39.0	70.4	18.0	62.7	7.2	33.9	171.8	15.1	265.1
212.926	185.928	186.935	173.947	160.953	147.960	176.962	219.693	178.979	249.899	222.899	223.912	168.912	225.914
793.3	82.7	46.3	783.6	412.7	482.2	20.7	45.2	47.1	20.8	55.0	29.9	26.0	11.4
226.923	185.933	186.939	187.941	174.945	161.960	176.966	219.881	178.981	277.893	250.901	237.907	182.725	225.917
20.0	643.6	1014.9	119.8	8.8	347.7	76.7	35.1	11.5	312.3	248.0	202.7	16.9	24.6
240.924	199.928	200.935	187.946	174.948	175.960	190.962	261.886	192.980	291.890	250.906	251.907	182.912	239.916
98.0	72.5	105.3	1093.1	47.1	304.8	39.3	110.0	45.4	47.1	22.8	219.9	84.1	36.3
240.928	199.933	200.940	201.946	174.954	175.963	190.966	261.969	206.979	319.894	278.894	265.903	196.912	239.921
409.5	790.4	646.8	1403.2	301.3	14.0	35.8	9.7	18.3	251.1	25.6	7.1	103.7	439.9
240.933	213.932	214.922	215.941	188.947	189.960	204.961	317.879	234.888	333.494	278.900	279.907	210.915	253.915
23.3	1032.6	14.7	52.7	26.8	379.8	48.5	26.5	101.0	91.6	118.0	206.1	350.5	94.8
254.923	227.935	214.938	215.945	188.949	203.715	204.965	331.499	234.891	333.893	292.899	293.887	238.908	253.920
56.8	1093.7	665.0	946.7	114.5	17.1	19.9	79.2	72.5	228.8	97.2	16.8	19.3	529.0
254.928	241.924	228.934	229.940	188.953	203.868	218.870	345.450	248.893	347.893	306.899	293.907	238.914	267.920
313.8	7.1	48.6	29.7	232.4	20.3	16.9	118.5	7.8	254.5	67.1	392.8	389.4	697.9

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
268.910 10.1	241.934 1070.5	228.937 122.1	229.947 994.6	202.949 168.2	203.955 38.3	218.878 12.9	373.880 108.3	276.886 23.3	361.894 204.2	320.899 160.6	307.900 19.1	252.670 38.7	281.919 627.9
268.926 451.6	269.933 799.7	228.941 503.8	243.948 822.1	202.953 186.3	203.959 471.2	218.961 78.2	373.888 12.9	290.888 37.2	403.877 7.7	334.896 58.5	307.907 327.1	252.913 761.8	295.919 586.0
282.921 80.4	283.841 514.7	242.936 121.1	257.944 54.8	216.861 46.5	217.959 462.2	232.962 60.2	401.365 6.2	304.882 11.7	431.893 18.6	348.894 42.5	321.907 331.7	280.906 38.4	309.915 27.4
282.926 162.3	283.932 638.5	242.941 315.3	271.946 678.9	216.864 23.0	231.960 430.3	232.965 8.2	415.885 121.0	318.887 169.3	487.892 24.9	348.898 50.9	335.905 351.1	280.912 303.8	309.920 408.1
296.926 365.4	297.520 7.1	256.852 14.2	285.854 17.5	216.947 136.0	245.961 430.2	246.964 87.6	500.072 17.8	332.882 14.3		362.899 147.9	349.903 215.7	294.913 238.7	323.920 405.6
310.926 270.6	297.934 711.9	256.936 24.9	285.946 695.7	216.952 153.6	245.966 9.6	260.879 27.9		332.885 56.8		376.900 93.2	363.900 7.2	308.485 11.3	337.918 351.2
324.919 49.0	311.934 570.9	256.938 84.4	299.941 54.8	230.950 243.0	259.874 23.6	260.882 17.5		346.886 48.3		390.900 44.6	391.905 98.9	308.914 148.7	351.911 33.4
324.925 237.0	325.933 454.0	270.937 337.6	299.946 570.8	244.864 42.5	259.963 391.3	260.966 55.8		374.885 42.3		418.897 16.1	461.177 140.7	322.910 145.9	351.917 320.5
338.923 243.1	339.932 489.8	284.935 86.2	313.948 479.4	244.953 179.2	273.865 24.9	274.872 21.1		388.882 29.5		460.898 25.2	461.904 20.2	336.910 226.0	365.920 357.0
352.922 192.6	353.419 25.2	284.939 153.1	327.910 20.2	258.865 85.7	273.959 291.7	274.961 21.6		402.884 16.4		503.064 34.4	475.905 22.8	350.909 249.0	379.920 315.1
366.925 268.9	353.930 436.9	298.938 220.0	327.946 401.0	258.951 119.1	287.953 19.3	288.961 25.8		458.315 19.1		531.020 174.8	545.923 19.0	364.913 261.7	393.912 7.7
380.921 76.1	367.933 477.0	312.938 202.4	341.946 475.4	258.957 77.7	287.960 246.8	302.873 46.1		458.881 21.9		545.017 15.5		378.906 36.9	393.920 197.0
380.927 77.8	381.933 302.9	326.936 154.5	355.413 7.7	272.948 131.9	301.960 179.1	302.964 17.8		626.842 12.0				378.912 94.3	407.920 252.1
394.922 91.7	437.499 28.5	340.937 141.2	355.854 105.7	272.953 28.6	315.961 122.7	316.872 41.5						392.912 120.5	449.920 96.9
408.927 53.5	437.933 98.1	354.934 183.8	355.944 294.4	286.949 121.4	329.471 40.6	316.963 14.7						406.908 38.1	449.926 13.8
436.923 19.3	451.932 79.1	368.937 156.3	369.947 214.0	286.954 7.3	329.951 11.0	330.873 66.1						406.914 40.5	463.919 41.6
478.922 16.3	465.932 19.7	382.936 104.6	383.946 182.0	300.949 90.5	329.959 96.8	330.961 28.5						406.921 13.1	477.918 31.3
549.024 8.4	493.932 16.0	396.936 40.6	397.860 27.0	300.954 16.2	343.862 12.6	344.962 43.5						420.910 22.5	505.926 23.5
	535.947 12.5	396.940 19.3	397.947 154.4	314.950 116.3	343.959 99.0	358.872 38.3						434.910 18.4	

NOMINAL MASS Z NUMBERS

-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
		410.937	411.947	328.857	357.958	372.873						533.016	
		90.9	115.8	13.7	53.0	45.2						40.0	
		424.935	411.953	328.948	357.962	386.601							
		22.3	20.3	61.5	43.6	13.1							
		438.936	425.271	328.952	371.959	386.872							
		5.4	6.4	31.6	63.5	25.4							
		438.940	439.182	342.949	385.961	400.870							
		13.6	18.7	80.5	66.5	31.2							
		495.073	439.947	342.952	399.960	414.873							
		5.2	46.0	24.4	45.7	16.4							
			453.945	356.857	427.873	414.967							
			14.9	17.4	61.3	11.5							
			467.944	356.860	441.176	442.504							
			45.4	39.5	15.8	36.3							
				356.947	441.503	456.314							
				55.8	295.5	68.6							
				370.859	455.228	624.843							
				17.2	5.4	23.7							
				370.951	455.872								
				49.6	14.2								
				384.950	469.180								
				28.2	7.9								
				398.859	469.873								
				22.6	16.5								
				398.950									
				25.0									
				412.952									
				56.4									
				426.952									
				10.6									
				440.860									
				13.7									
				454.317									
				15.6									
				580.934									
				50.6									
				706.740									
				26.0									

Appendix IV

READATA5 Output from the Mass Spectrum of One-Ring Aromatic Neutrals Separated from the 200-425° C Distillate of the Cerro Negro (Venezuela) Heavy Petroleum.

RSPCNM. 12-AUG-86. CN 200-425 DEG C 1-RING COMPDS. RUN 1, SCAN 1

TH. REF. MASS	EXP. REF. MASS	INTENSITY	PPM ERROR
42.97036			
57.97705			
72.97119	72.97118	10871.	0.1
77.95980	77.95981	16067.	-0.1
78.96204			
90.95310	90.95313	3978.	-0.3
91.95534			
95.93029	95.93029	14185.	0.0
96.93253			
105.95981	105.95980	61630.	0.1
106.96204	106.96205	6612.	-0.1
107.96427			
115.00618	115.00606	1256.	1.1
116.01134	116.01133	27328.	0.1
117.01357	117.01358	856.	-0.1
127.90078	127.90077	21505.	0.1
128.90302	128.90366	936.	-5.0
136.96307	136.96333	4785.	-1.9
137.96530			
143.85341	143.85339	13367.	0.1
144.85564	144.85518	437.	3.2
144.86011			
145.84824	145.84805	4289.	1.3
146.85045			
155.78333	155.78333	8370.	0.0
156.77171			
156.78555	156.78540	533.	1.0
157.77904	157.77881	9768.	1.5
158.78128			
167.81226	167.81226	20058.	0.0
168.81448			
179.72913	179.72911	14309.	0.1
180.73135			
181.72394	181.72340	12878.	2.9
182.72618			
183.71877	183.71834	5144.	2.3
184.72099			
185.71358			
185.78275			
186.71582			
186.78497			
187.75381			
188.75604			
189.74953	189.74869	809.	4.4
190.75175			
194.76923	194.76929	3057.	-0.3
197.78934	197.78929	19292.	0.2
198.79153			
205.74312	205.74280	1246.	1.6
207.73885	207.73883	1758.	0.1
221.68637	221.68636	29700.	0.1
222.68860	222.68925	1897.	-2.9
235.68637	235.68636	98260.	0.1
235.72375	235.72371	20781.	0.2
236.68860	236.68890	8820.	-1.3
236.72595	236.72568	1141.	1.2
253.67569	253.67567	34958.	0.1

271.68356	271.68353	10059.	0.1
272.68576	272.68631	885.	-2.0
281.53940	281.53900	5866.	1.4
283.53513	283.53510	7122.	0.1
293.56836	293.56833	33742.	0.1
294.57059	294.57019	1844.	1.3
305.48880	305.48907	8435.	-0.9
306.49103			
307.48450	307.48456	17448.	-0.2
308.48676	308.48770	689.	-3.1
309.48026	309.48120	9251.	-3.1
310.48248			
333.61111	333.60989	29943.	3.7
334.61334	334.61243	3214.	2.7
353.42136			
355.41708	355.41602	393.	3.0
361.57480	361.57474	18063.	0.2
362.57700	362.57751	2272.	-1.4
379.43176	379.43173	80744.	0.1
380.43399	380.43408	7715.	-0.2
389.25385	389.25348	1023.	0.9
391.24960	391.25003	2620.	-1.1
393.24530	393.24530	5351.	0.0
395.24103	395.24139	2628.	-0.9
397.23676			
401.35394	401.35391	33670.	0.1
402.35614	402.35675	1120.	-1.5
423.27252			
425.26825			
442.50562	442.50656	739.	-2.1
441.50339			
453.31714	453.31763	10878.	-1.1
455.31287	455.31287	17923.	0.0
457.30859	457.30838	9001.	0.5
471.20508	471.20511	22270.	-0.1
472.20731	472.20700	1714.	0.6
481.07739			
483.07309			
485.06832	485.06882	1886.	0.0
487.06454	487.06424	2346.	0.6
489.06027	489.05853	1531.	3.6
491.05600			
495.07739			
497.07309	497.07242	1043.	1.4
499.06882	499.06882	3886.	0.0
501.06454	501.06686	2753.	-4.6
503.06027			
505.05600			
543.00995			
543.02380	543.02356	206.	0.4
545.00568			
545.01953	545.02185	1309.	-4.3
547.00140			
547.01526	547.01654	2564.	-2.3
548.99713			
549.01093	549.00891	688.	3.7
550.99286			
551.00665			
553.00238			
586.93390	586.93390	16462.	0.0
587.93610	587.93439	326.	2.9

589.94965			
590.95190			
591.94537			
592.94757			
593.94110			
594.94330			
595.93683			
596.93903			
597.93256			
598.93475			
610.87506			
612.87079			
614.86652			
620.84729			
621.84955			
622.84302			
623.84528			
624.83875			
625.84100			
626.83447	626.83447	586.	0.0
627.83667			
628.83020	628.83264	479.	-3.9
629.83240			
630.82593	630.82538	354.	0.9
631.82812			
632.82166			
633.82385			
637.88220			
638.88892			
639.87793			
640.88464			
641.87366			
642.88037			
643.86938			
644.87610			
658.80762	658.80762	239.	0.0
660.80334			
668.77985			
670.77557			
672.77130	672.77161	341.	-0.5
674.76703			
676.76257			
678.75848			
688.69855			
690.69427			
692.69000			
694.68573			
698.67084			
700.66656			
702.66223			
704.65796			
706.65369			
708.64941			

NO. OF REFERENCE MASSES IN "REF.DAT" FILE = 201

NO. OF REFERENCE MASSES FOUND = 81

SUM OF REFERENCE ION INTENSITIES = 0.8696E+06

MAXIMUM PPM ERROR = 6.0