Designation: D 6729 – 01

An American National Standard

Standard Test Method for
Determination of Individual Components in Spark Ignition Engine Fuels by 100 Meter Capillary High Resolution Gas Chromatography[1]

This standard is issued under the fixed designation D 6729; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This test method covers the determination of individual hydrocarbon components of spark-ignition engine fuels and their mixtures containing oxygenate blends (MTBE, ETBE, ethanol, and so forth) with boiling ranges up to 225°C. Other light liquid hydrocarbon mixtures typically encountered in petroleum refining operations, such as blending stocks (naphthas, reformates, alkylates, and so forth) may also be analyzed; however, statistical data was obtained only with blended spark-ignition engine fuels.

1.2 Based on the cooperative study results, individual component concentrations and precision are determined in the range of 0.01 to approximately 30 mass %. The procedure may be applicable to higher and lower concentrations for the individual components; however, the user must verify the accuracy if the procedure is used for components with concentrations outside the specified ranges.

1.3 The test method also determines methanol, ethanol, t-butanol, methyl t-butyl ether (MTBE), ethyl t-butyl ether (ETBE), t-amyl methyl ether (TAME) in spark ignition engine fuels in the concentration range of 1 to 30 mass %. However, the cooperative study data provided sufficient statistical data for MTBE only.

1.4 Although a majority of the individual hydrocarbons present are determined, some co-elution of compounds is encountered. If this test method is utilized to estimate bulk hydrocarbon group-type composition (PONA) the user of such data should be cautioned that some error will be encountered due to co-elution and a lack of identification of all components present. Samples containing significant amounts of olefinic or naphthenic (for example, virgin naphthas), or both, constituents above *n*-octane may reflect significant errors in PONA type groupings. Based on the gasoline samples in the interlaboratory cooperative study, this procedure is applicable to samples containing less than 25 mass % of olefins. However, some interfering coelution with the olefins above C_7 is possible, particularly if blending components or their higher boiling cuts such as those derived from fluid catalytic cracking (FCC) are analyzed, and the total olefin content may not be accurate.

1.4.1 Total olefins in the samples may be obtained or confirmed, or both, if necessary, by Test Method D 1319 (volume %) or other test methods, such as those based on multidimensional PONA type of instruments.

1.5 If water is or is suspected of being present, its concentration may be determined, if desired, by the use of Test Method D 1744, or equivalent. Other compounds containing oxygen, sulfur, nitrogen, and so forth, may also be present, and may co-elute with the hydrocarbons. If determination of these specific compounds is required, it is recommended that test methods for these specific materials be used, such as Test Methods D 4815 and D 5599 for oxygenates, and D 5623 for sulfur compounds, or equivalent.

1.6 Annex A1 of this test method compares results of the test procedure with other test methods for selected components, including olefins, and several group types for several interlaboratory cooperative study samples. Although benzene, toluene, and several oxygenates are determined, when doubtful as to the analytical results of these components, confirmatory analyses can be obtained by using specific test methods.

1.7 The values stated in SI units are to be regarded as the standard. The values given in parentheses are provided for information purposes only.

1.8 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.*

2. Referenced Documents

2.1 *ASTM Standards:*

D 1319 Test Method for Hydrocarbon Types in Liquid Petroleum Products by Fluorescent Indicator Adsorption[2]

D 1744 Test Method for Determination of Water in Liquid Petroleum Products by Karl Fisher Reagent[3]

D 4815 Test Method for Determination of MTBE, ETBE,

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[1] This test method is under the jurisdiction of ASTM Committee D02 on Petroleum Products and Lubricantsand is the direct responsibility of Subcommittee D02.04 on Hydrocarbon Analysis.

Current edition approved Nov. 10, 2001. Published January 2002.

[2] *Annual Book of ASTM Standards*, Vol 05.01.

[3] Discontinued; see *1999 Annual Book of ASTM Standards*, Vol 05.01.

TAME, DIPE, *t*-Amyl Alcohol and C_1 to C_4 Alcohols in Gasoline by Gas Chromatography[4]

D 5599 Test Method for Determination of Oxygenates in Gasoline by Gas Chromatography and Oxygen Selective Flame Ionization Detection[4]

D 5623 Test Method for Sulfur Compounds in Light Petroleum Liquids by Gas Chromatography and Sulfur Selective Detection[4]

E 355 Practice for Gas Chromatography Terms and Relationships[5]

3. Terminology

3.1 *Definitions*—This test method makes reference to many common gas chromatographic procedures, terms, and relationships. Detailed definitions can be found in Practice E 355.

4. Summary of Test Method

4.1 Representative samples of the petroleum liquid are introduced into a gas chromatograph equipped with an open tubular (capillary) column coated with the specified stationary phase. Helium carrier gas transports the vaporized sample through the column, in which it is partitioned into individual components which are sensed with a flame ionization detector as they elute from the end of the column. The detector signal is recorded digitally by way of an integrator or integrating computer. Each eluting component is identified by comparing its retention time to that established by analyzing reference standards or samples under identical conditions. The concentration of each component in mass % is determined by normalization of the peak areas after correction of selected components with detector response factors. The unknown components are reported individually and as a summary total.

5. Significance and Use

5.1 Knowledge of the specified individual component composition (speciation) of gasoline fuels and blending stocks is useful for refinery quality control and product specification. Process control and product specification compliance for many individual hydrocarbons may be determined through the use of this test method.

6. Apparatus

6.1 *Gas Chromatograph*, a gas chromatograph equipped with cryogenic column oven cooling and capable of producing repeatable oven ramps from 0° to at least 300°C is required. The following features are useful during the sample analysis phase: electronic flow readout, electronic sample split-ratio readout, and electronic pneumatic control of flow. Though their use is not required, careful review of this test method will demonstrate the usefulness of a gas chromatograph equipped with these features. These features will replace the need to carry out the manual calculations that must be performed as listed in 8.1 and 8.2.

6.2 *Inlet*—a capillary split/splitless inlet system operated in the split mode is recommended. It must be operated in its linear range. Refer to 8.4 to determine the proper split ratio.

6.2.1 *Carrier Gas Pneumatic Control*—Constant carrier gas pressure control was used by all cooperative study participants. This may be either direct pressure to the inlet (injector) or by using a total flow/back pressure system.

6.2.2 *Pneumatic Operation of the Chromatograph*—The use of constant pressure was the mode of operating the gas chromatography used by the participants in the interlaboratory cooperative study. Other carrier gas control methods such as constant flow (pressure programming) may be used, but this may change the chromatography elution pattern unless the temperature programming profile is also adjusted to compensate for the flow differences.

6.2.3 *Temperature Control*—The injector operated in the split mode shall be heated by a separate heating zone and heated to temperatures of 200 to 275°C.

6.3 *Column*, a fused silica capillary column, 100 m in length by 0.25 mm inside diameter, coated with a 0.5 mm film of bonded dimethylpolysiloxane. The column must meet the resolution requirements expressed in 8.3. Columns from two different commercial sources were used in the interlaboratory cooperative study.

6.4 *Data System*, a computer based chromatography data system capable of accurately and repeatedly measuring the retention time and areas of eluting peaks. The system shall be able to acquire data at a rate of at least 10 Hz. Although it is not mandatory, a data system which calculates column resolution (R) is extremely useful as it will replace the need to carry out the manual calculations which must be performed as listed in 8.3.

6.4.1 *Electronic Integrators*, shall be capable of storing up to 400 components in the peak table and shall be able to acquire the data at 10 Hz or faster speeds. They shall be capable of integrating peaks having peak widths at half height which are 1.0s wide. The integrator must be capable of displaying the integration mode of partially resolved peaks. In addition, these integrators should be able to download a commonly readable format of data (that is, ASCII) to a computer in order to facilitate data processing.

6.5 *Sample Introduction*—Sample introduction by way of a valve, automatic injection device, robotic arm or other automatic means is highly recommended. An automatic sample introduction device is essential to the reproducibility of the analysis. Manual injections are not recommended. All of the reproducibility data reported by this test method for the samples analyzed were gathered using automatic injection devices.

6.6 *Flame Ionization Detector (FID)*—The gas chromatograph should possess a FID having a sensitivity of 0.005 coulombs/g for *n*-butane. The linear dynamic range of the detector should be 10^6 or better. The detector is heated to 300°C.

7. Reagents and Materials

7.1 *Calibrating Standard Mixture*—A spark ignition engine fuel standard of known composition and concentration by mass can be used. In order to corroborate the identification of the sample, a typical chromatogram (Fig. 1) was obtained from

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[4] *Annual Book of ASTM Standards*, Vol 05.03.

[5] *Annual Book of ASTM Standards*, Vol 14.02.

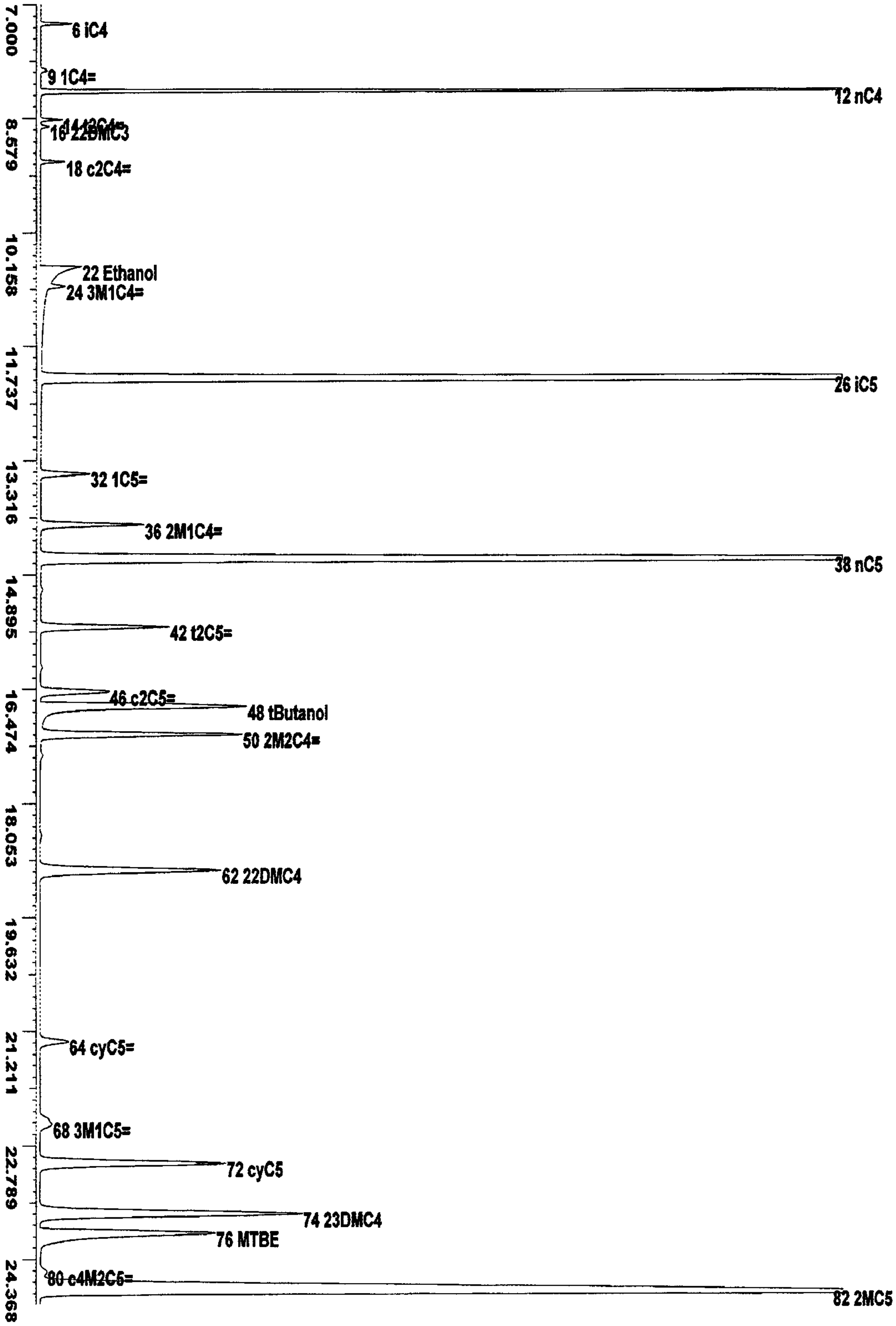

FIG. 1 Chromatogram for Reference Spiked Gasoline

reference sample ARC96OX.[6]

7.2 *Gas Chromatograph Gases*—All of the following gases shall have a purity of 99.999 % (V/V) or greater.

NOTE 1—**Warning:** Gases are compressed. Some are flammable and all gases are under high pressure.

7.2.1 *Helium*—The test data was developed with helium as the carrier gas. It is possible that other carrier gases may be used for this test method. At this time, no data is available from this test method with other carrier gases.

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[6] Reference spark ignition sample No. ARC 960X obtained from the Alberta Research Council, Edmonton, Alberta, Canada. Other samples are available from suppliers.

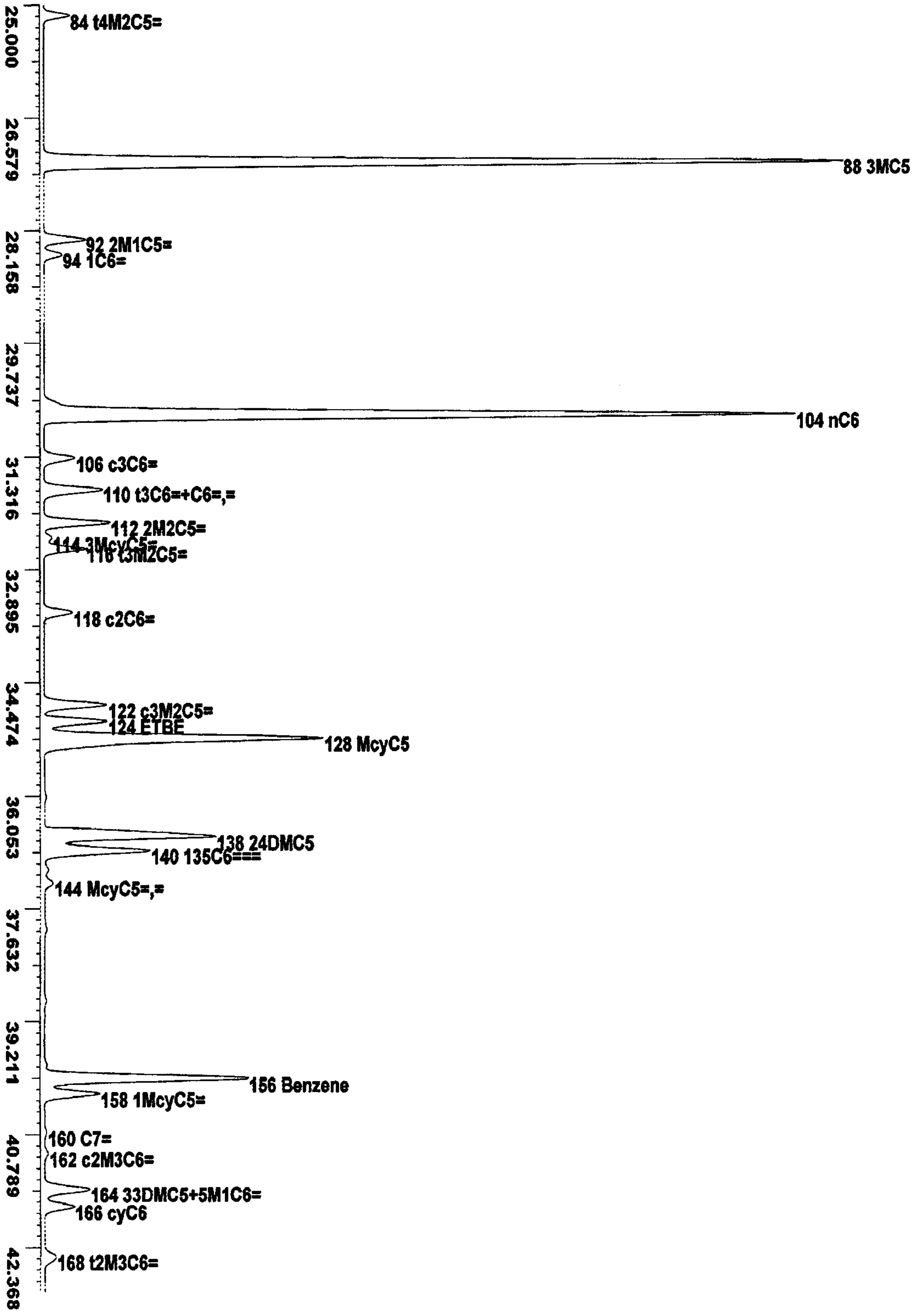

FIG. 1 Chromatogram for Reference Spiked Gasoline *(continued)*

7.2.2 *Air, Hydrogen and Make-up Gas (Helium or Nitrogen),* shall have a purity of 99.999 % (V/V) or greater.

8. Instrument Check Out Prior to Analysis

8.1 *Setting*:

8.1.1 *Linear Gas Velocity*—If the gas chromatograph is equipped with an electronic flow readout device, set the flow to 1.8 mL/min. This is achieved by setting the carrier gas flow rate by injection of methane or natural gas at 35°C. Ensure that the retention time is 7.00 ± 0.05 min. This corresponds to a linear velocity of 25 to 26 cm/s. This is equivalent to retention times of methane at 0°C ranging from 6.5 to 6.8 min.

8.1.2 If the gas chromatograph is not equipped with an

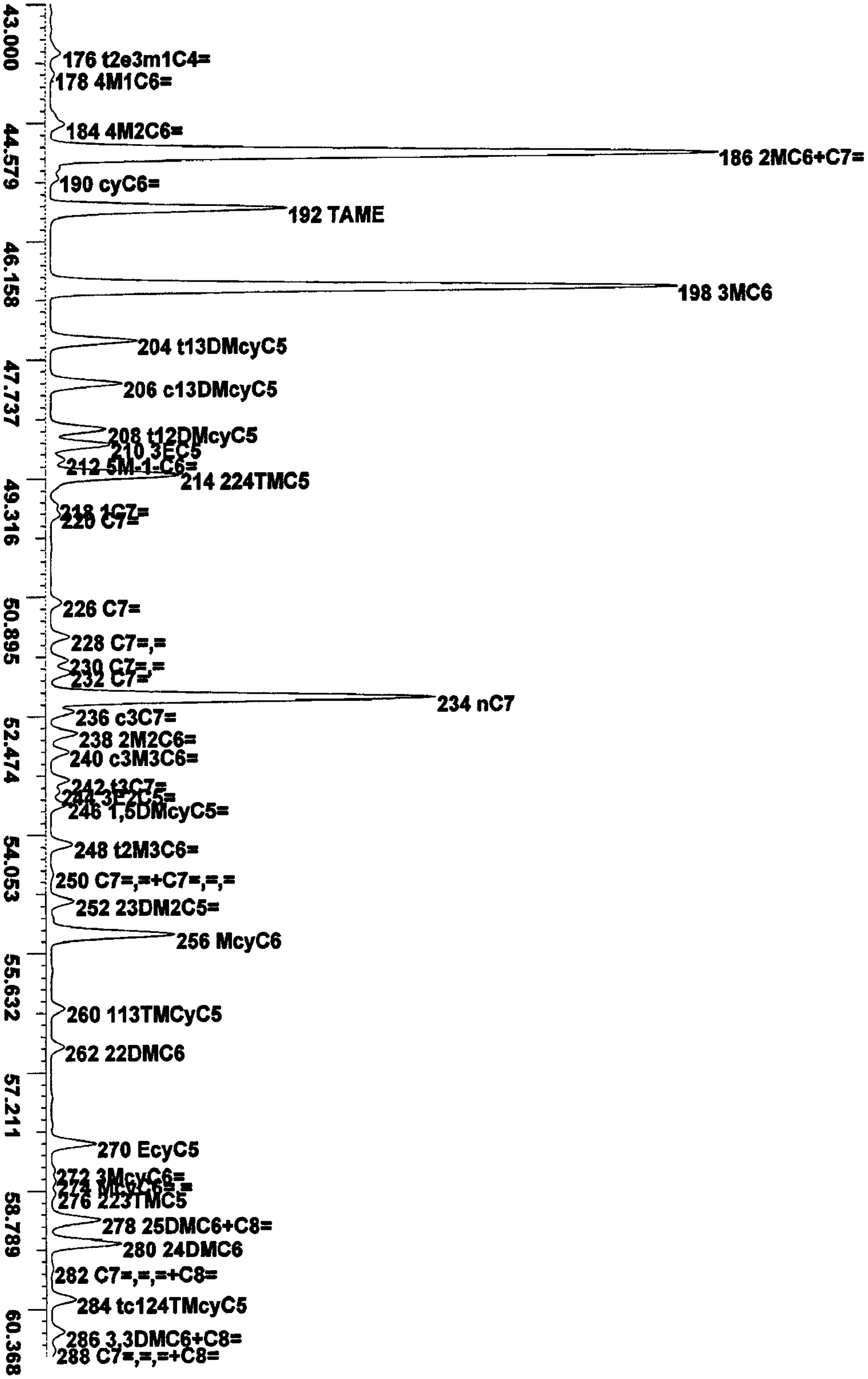

FIG. 1 Chromatogram for Reference Spiked Gasoline *(continued)*

electronic flow readout device, calculate the linear gas velocity in cm/s using Eq 1.

$$\text{linear gas velocity} = V = \frac{\text{column length (cm)}}{\text{retention time of methane(s)}} \tag{1}$$

8.1.3 The typical retention times for methane and linear gas velocity for helium are 6.5 to 6.8 and 24 to 26 cm/s, respectively.

8.2 *Setting the Split Ratio*—If the gas chromatograph is equipped with an electronic split-ratio readout device, set the split ratio to a sample split of 200:1. If the gas chromatograph

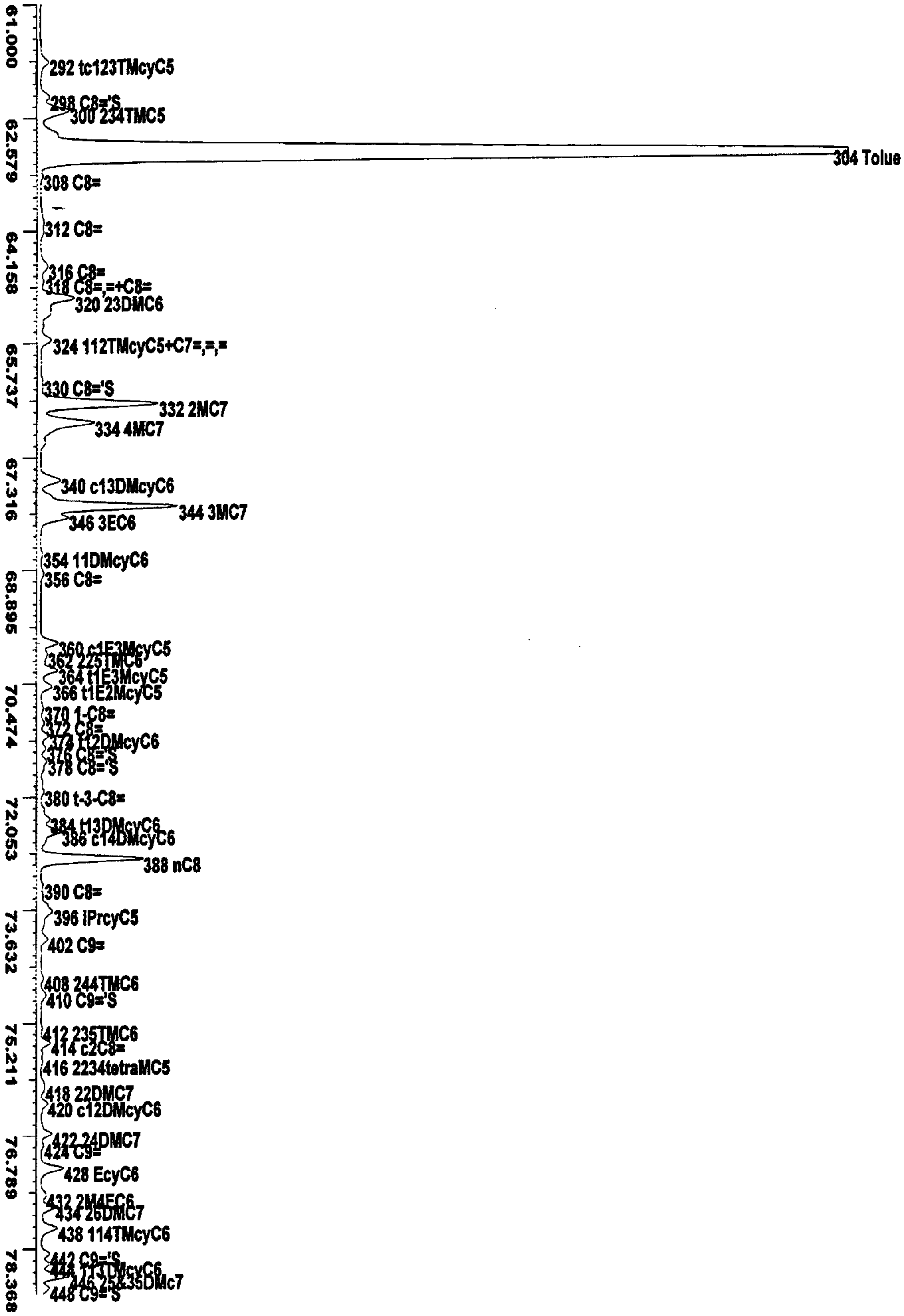

FIG. 1 Chromatogram for Reference Spiked Gasoline *(continued)*

is not equipped with an electronic split-ratio readout device, one must first calculate column flow rate and then proceed to calculating split ratio using Eq 2 and 3.

$$\text{column flow rate} = F = \frac{(60\,\pi\,r^2)\,L(T_{ref})\,2(P_i - P_o)}{(T)3(P_{ref})(P_i^2 - P_o^2)\mu} \qquad (2)$$

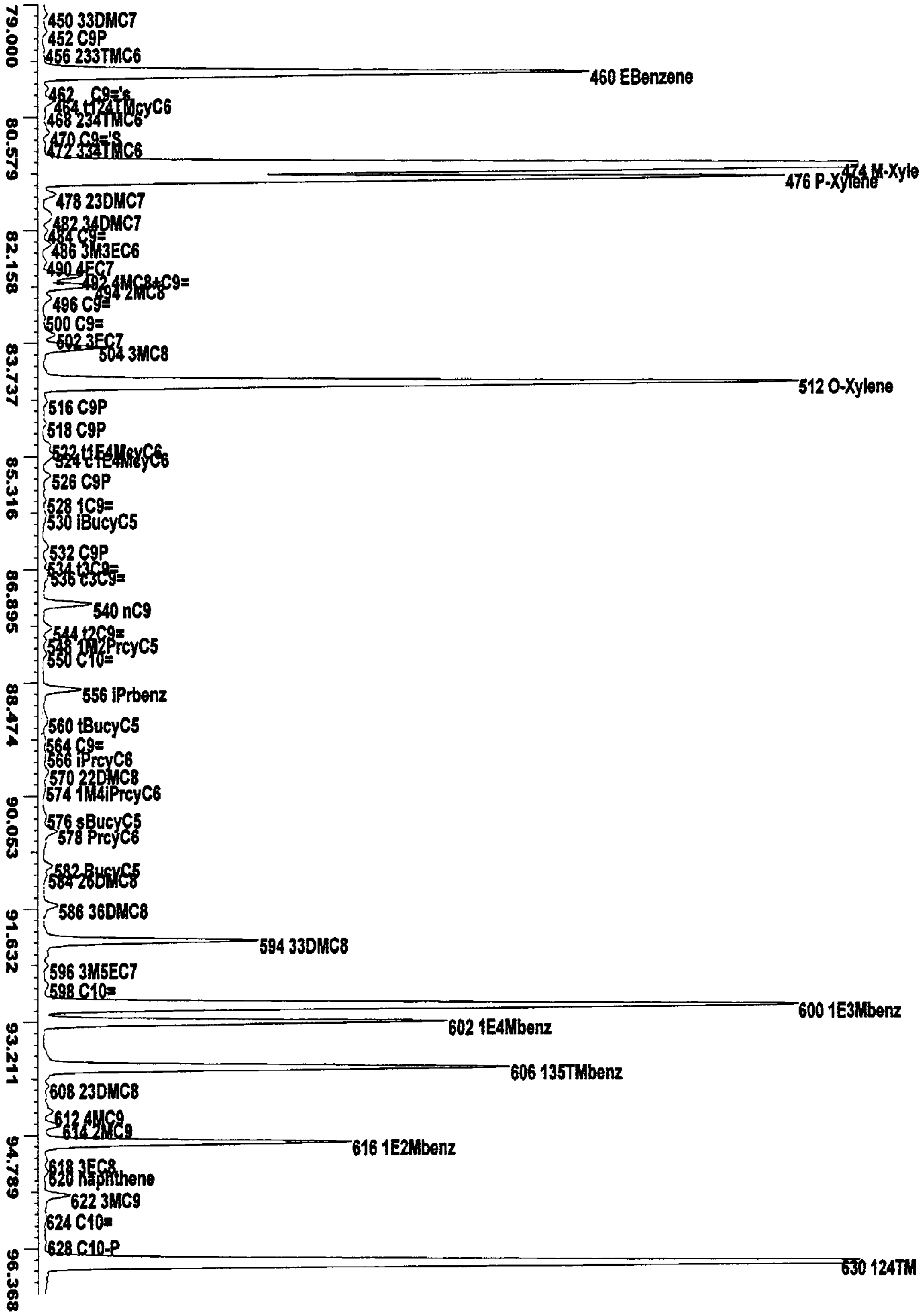

FIG. 1 Chromatogram for Reference Spiked Gasoline *(continued)*

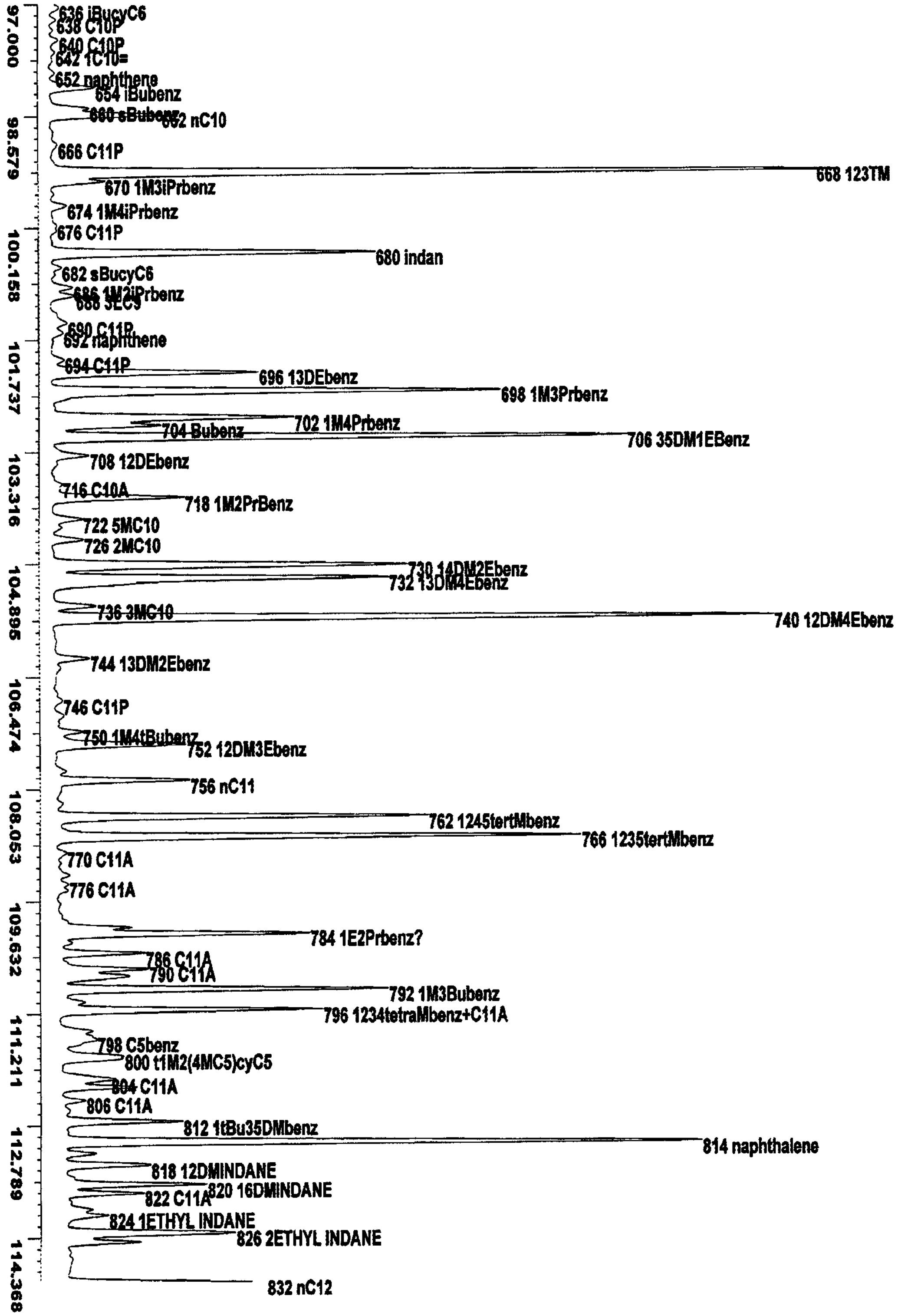

FIG. 1 Chromatogram for Reference Spiked Gasoline *(continued)*

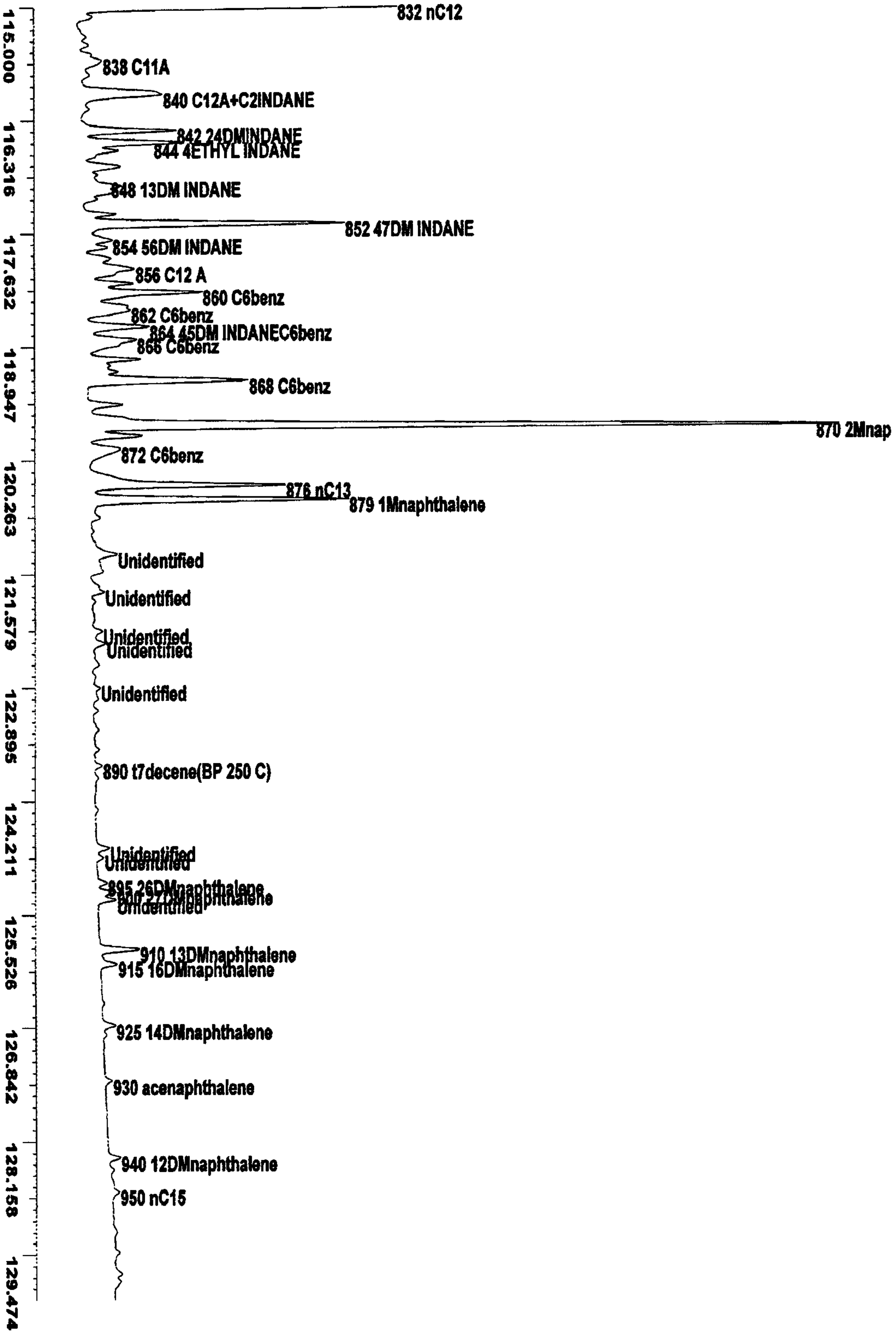

FIG. 1 Chromatogram for Reference Spiked Gasoline *(continued)*

where:

F = flow rate as calculated by using the equation,
r = column radius, cm,
L = column length, cm,
P_i = inlet pressure,
P_o = outlet pressure,
P_{ref} = reference pressure, 1 atm,
T = temperature of the column oven,
T_{ref} = temperature at the column outlet, and
μ = linear velocity, cm/s.

$$\text{split ratio} = S = \frac{\text{split vent flow} + F}{F} \tag{3}$$

8.2.1 The column flow rate is calculated by the use of Eq 2. Use the results obtained from Eq 3 to adjust the split flow until a split flow of approximately 200:1 is achieved.

8.3 *Evaluation of Column Performance*:

8.3.1 Prior to using the column described in Table 1, measure the resolution of the column under the conditions of Table 2. Check that the resolution for the following pairs of components is obtained using Eq 4 to calculate the resolution of a pair of components:

$$R = \frac{(t_{R2} - t_{R1})^2}{1.699\,(W_{h1} + W_{h2})} \tag{4}$$

where:

R = resolution,
t_{R2} = retention time of the first member of the pair,
t_{R1} = retention time of the second member of the pair,
W_{h1} = peak width at half height of the first member of the pair, and
W_{h2} = peak width at half height of the second member of the pair.

8.3.1.1 Column resolution should be checked frequently by examining the resolution of these compounds.

8.3.2 *Evaluation of the Baseline*—Carry out a blank baseline run utilizing no solvent injection, by setting the GC in accordance with the conditions of Table 1.

8.3.3 Subtract the baseline from a sample chromatogram and verify that the residual signal at the beginning of the chromatogram does not differ from the end of the chromatogram by more than 2 %.

TABLE 2 Resolution Performance Requirements

Component Pair	Minimum Resolution	Concentration of Each Component, W/W
Benzene 1-Methyl-cyclopentene	1.0	0.5 %–0.5 %
m-Xylene p-Xylene	0.4	2.0 %–2.0 %
n-Tridecane 1-Methylnaphthalene	1.0	0.5 %–0.5 %

8.4 *Evaluation of Splitter Linearity*—Using the reference gasoline sample, inject this sample according to the schedule listed in Table 3.

8.4.1 Select from the chromatogram about 10 to 15 components, which have concentrations in the range of .01 to 30 weight %. Tabulate for each split ratio the concentrations of the 10 to 15 components. Verify that for each component selected, its concentration does not vary by more than 3 %.

9. Procedure

9.1 Set the operating conditions of the gas chromatograph as shown in Table 1. These conditions will elute all components up to and including pentadecane (nC_{15}).

9.2 All of the parameters in Table 1 can be marginally changed to optimize for sample types and optimize for characteristics of each gas chromatographic system. The final

TABLE 1 Chromatographic Operating Conditions, Column Requirements and Data Acquisition Requirements

Chromatographic Conditions	Requirements
Injector settings	
Injector temperature, °C	250
Split ratio	175:1 - 275:1
Liner	deactivated glass
Injection volume, µL	0.2–0.5
Detector settings	
FID detector temperature, °C[A]	300–350
Gas flows	
Hydrogen, mL/min[B]	30–40
Air, mL/min	300–450
Nitrogen make up, mL/min	30
Column oven settings	
Initial temperature, °C	0
Initial time, min	15
1st ramp rate, °C/min	1
Final temperature, °C	50
Final time, min	0
2nd ramp rate, °C/min	2
Final temperature, °C	130
Final time, min	0
3rd ramp rate, °C/min	4
Final temperature, °C	270
Final time, min[C]	0
Column Requirements	
Length, m	100
Inside diameter, mm	0.25
Liquid phase	100 % dimethylpolysiloxane
Film thickness, µ	0.5
Pressure, psig	40–50
Flow, mL/min	1.7–2.0
Linear gas velocity, cm/s	24.5
Data acquisition, Hz	10–20
Total analysis time, min	140–150

[A] Set to 25–50°C above the highest column temperature.
[B] Values to be set as recommended by instrument manufacturer.
[C] Final temperature or time may be adjusted to ensure complete elution of the sample components.

TABLE 3 Injection Schedule

Split Ratio	Injection Volume, µL	Injection Temperature, °C
100:1	0.1	250
200:1	0.5	250
300:1	1.0	250

boiling point of samples should not exceed nC_{15} and the column resolution (R) performance requirements listed in Table 2 should not be compromised.

9.3 Obtain a representative sample following the guidelines of Practice D 4057 and any other applicable guidelines. Take precautions to minimize the loss of light ends from volatile samples. The sample container may be cooled prior to transfer of sample into it. Cool the sample to less than 4°C, maintain at that approximate temperature until the autosampler is loaded and analysis begins.

9.4 *Preparation/Storage*:

9.4.1 *Samples Stored in Vials*—Cool the original sample to less than 4°C prior to taking a sample aliquot or prior to filling the sample vials. The sample aliquot container, or the vial, or both, can also be cooled prior to the transfer of the original sample. Syringes may also be cooled along with the sample for manual injections.

9.4.2 *Samples Stored in Pressurized Containers*—It is recommended that they be kept away from direct heat or light. No other sample preparations are necessary for samples stored in pressurized containers. Avoid storage at temperatures greater than 25°C. Store pressure containers in accordance with the manufacturer's instructions.

9.5 It is recommended that a quality assurance (QA) sample similar to the reference material gasoline sample be run at regular intervals (see Fig. 1). An interval of once per week or after every 15 samples is recommended. The quantitation results use statistical quality control charts can track benzene. Other components of interest in the reference sample can be tracked in a similar manner. By monitoring these components over an extended period of time, the performance of the column and the chromatographic system can be determined.

10. Data Analysis

10.1 *Compound Identification*—Prepare a table listing all of the retention times of the components in the sample. Compare the retention time of each peak with that of the reference gasoline. Pay particular attention to the fact that columns can be overloaded, and peaks can shift in retention time. Observe the peak pattern so that proper identification is made by comparison with the reference material.

10.2 Consistency in peak identification can be achieved by using software (data handling software, spreadsheet software, and so forth). Alternatively, a retention index system can be used.

$$(R1)_i = 100n + 100\left[\frac{log\ (T_i) - log\ (T_n)}{log\ (TN) - log\ (T_n)}\right] \quad (5)$$

where:

$(R1)_i$ = retention index of component I bracketed by the *N*-paraffin, n in its lower boundary and *N*-paraffin N in its upper boundary,

T_i = adjusted retention time of component *i* (retention time of component *i* minus the retention time of methane),

T_n = adjusted retention time of *N*-paraffin n, and

TN = retention time of *N*-paraffin N.

10.3 Determine the hydrocarbon response factors by using the following equation.[7]

$$RRF_{CH4} = \frac{MW_i}{N_c} \times \frac{1}{MW_{CH4}} \quad (6)$$

where:

RRF_{CH4} = relative response factor of each component with respect to methane (RRF_{CH4}=1.000),

MW_i = molecular weight of the component, *i*,

N_c = number of carbon atoms in the molecule, and

MW_{CH4} = molecular weight of methane (16.04276).

10.4 Convert the acquired areas to corrected areas by multiplying each area by its corresponding relative response factor as indicated in the following equation.

$$A_{c_i} = (A)_I\ (RRF)_I \quad (7)$$

where:

$(A_c)_i$ = corrected area,

A_i = acquired area for an individual component, and

RRF = relative response factor (weight basis).

10.4.1 The percent weight (% W) is calculated as follows:

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[7] Sevcik, J., *Detectors in Gas Chromatography*, Elsevier, NY, 1976, p 94.

TABLE 4 Predominant Compounds and Identified Coeluting Compounds[A]

NOTE—The response factor of the predominant compound will be used for the analyte and this analyte will be used for the calculations.

Peak Number (from Annex A1)	Predominant Compound	Coeluting Compound(s)
164	3,3-dimethylpentane	5-methyl-1-hexene
186	2-methylhexane	C_7-olefin
278	2,5-dimethylhexane	C_8-olefin
286	3,3-dimethylhexane	C_8-olefin
304	toluene	2,3,3-trimethylpentane[B]
324	1,1,2-trimethylcyclopentane	C_7-triolefin
326	C_8-diolefin	C_8-paraffin
492	4-methyloctane	C_9-olefin
796	1,2,3,4-tetramethylbenzene	C_{11}-aromatic

[A] This is not an exhaustive list. Due to the possibility of coeluting peaks in other areas, the user is cautioned in the interpretation of the data.

[B] In most alkylated gasolines, a split may occur between toluene and 233 TMC5.

TABLE 5 Response Factors of Oxygenated Compounds

Analytes	Relative Response Factors	
	RRF C_7= 1.000	RRF CH_4= 1.000
Methanol	2.996	2.672
Ethanol	2.087	1.862
t-Butanol (TBA)	1.302	1.161
Methyl-t-butyl ether (MTBE)	1.577	1.407
Ethyl-t-butyl ether (ETBE)	1.407	1.255
t-Amyl methyl ether (TAME)	1.356	1.210

$$\% W_i = \frac{(A_C)_i}{\sum_{i=1}^{i=n} A_{c_i}} \times 100 \tag{8}$$

where:

$\% W$ = percent weight of the component i in the mixture, and

$\sum_{i=1}^{i=n} A_{c_i}$ = summation of all the corrected areas for the components analyzed.

10.4.1.1 The subscript i indicates that the operations are carried out for each individual component in the matrix.

10.5 In the case of unidentified components, utilize a relative response factor of 0.800 (relative to methane).

11. Oxygenates

11.1 A cooperative study for linearity was performed for methanol, ethanol, t-butanol, methyl-t-butyl ether (MTBE), ethyl-t-butyl ether (ETBE), and t-amyl methyl ether (TAME) in concentration ranges from 1.0 mass % up to 30 mass % (Annex A2). The average relative response factors for the oxygenates were calculated from the study and are listed in Table A2.1. They have been incorporated into the IHA Method. The percent standard deviation of these relative response values was as high as 7 %. MTBE was the only oxygenate that was present in sufficient number of samples to meet the ASTM requirements for round robin testing in accordance with RR: D02-1007. Therefore the statistical data for MTBE should be taken from Table A1.2.

12. Expression of Results

12.1 Report the concentration of each components as mass % (m/m) to the nearest 0.001 %.

12.2 The data for individual components may by grouped by summing the concentration of compounds in each particular group type such as paraffin, isoparaffin, olefin, aromatic, naphthene, oxygenates, and unknowns. Commercially available software may be used to provide this function, as well as the calculation of other properties of petroleum liquids.

13. Precision and Bias [8]

13.1 The repeatability and reproducibility precision estimates are quoted in Annex A1.

13.2 *Precision Statement Outline*—(> Analyte Qualification Process):

13.2.1 For each analyte to qualify for a precision statement, it must be present in at least six samples, and detected by at least six laboratories, at least once, in accordance with RR: D02-1007 requirements.

13.2.2 The (repeatability standard deviation)/mean value for each analyte/sample combination must be less than or equal to 0.1, in accordance with LOQ requirements which, while not a standard, is what CS94 is recommending.

13.3 A brief explanation of headers in Table A1.2 follows:

13.3.1 ID: self explanatory,

13.3.2 r_{min}: lower 95 % confidence limit of r_{est},

13.3.3 r_{est}: repeatability estimate in percentage of concentration,

13.3.4 r_{max}: upper 95 % confidence limit of r_{est},

13.3.5 R_{min}, R_{est}, R_{max}: same as above except for reproducibility,

13.3.6 C_{min}: lower concentration limit that rest, R_{est} is applicable, and

13.3.7 C_{max}: upper concentration limit that rest, R_{est} is applicable.

13.4 The summaries for the paraffins, isoparaffins, C_2 benzene, and oxygenates follow the same procedure that was used for the analytes and are listed in Table A1.3.

13.5 *Bias*—The bias of this test method cannot be determined since an appropriate standard reference material is not available.

14. Keywords

14.1 gas chromatograph; gasoline; individual hydrocarbon analysis; oxygenated fuels; spark-ignition engine fuels

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[8] Supporting data describing the interlaboratory cooperative study to determine precision and bias has been filed at ASTM International Headquarters and may be obtained by requesting RR: D02-1519.

ANNEXES

(Mandatory Information)

A1. HYDROCARBON DATA

A1.1 Table A1.1 presents the component retention times and properties.

A1.2 Table A1.2 represents the repeatability and reproducibility precision estimates prepared by statisticians of CS94 in accordance with RR: D02-1007. The analyte qualification process for precision statements is outlined as follows:

A1.2.1 For each analyte to qualify for a precision statement, it must be present in at least six samples, and detected by at least six laboratories, at least once, in accordance with RR: D02-1007 requirements.

A1.2.2 The (repeatability standard deviation)/mean value for each analyte/sample combination must be less than or equal to 0.1, in accordance with LOQ requirements which, while not a standard, is what CS94 is recommending.

A1.3 *Summary for Oxygenates:* **Warning—**The statistical data could be done on the oxygenates but there was not an equal number of all oxygenates in the round robin. MTBE was the largest contributor to the statistical results. The number of samples that contained each oxygenate is as follows:

Oxygenate Type	No. of Samples	Approximate Concentration Range
Ethanol	2	1 %, and 12 %
t-butanol	2	.20 %, and 1.0 %
MTBE	6	1, 2, 4, 4, 8 and 16 %
ETBE	1	0.50 %
TAME	1	15.00 %

A1.4 The precision statement for the olefins and cycloparaffins is determined by taking the square root of the value determined in the summary; multiply by the coefficient (r_{coef}) for repeatability and the coefficient (R_{coef}) for the reproducibility.

Name	r_{min}	r_{coef}	r_{max}	R_{min}	R_{coef}	R_{max}	C_{min}	C_{max}
Cycloparaffins	0.0726	0.08	0.098	0.286	0.384	0.586	2	10
Olefins	0.1555	0.18	0.21	0.382	0.555	1.012	2	25

A1.5 The precision for the aromatics does not depend on level and is stated below in weight %.

Name	r_{min}	r %	r_{max}	R_{min}	R %	R_{max}	C_{min}	C_{max}
Aromatics	0.8549	0.98	1.155	2.151	2.706	3.651	15	50

A1.6 The summaries for the paraffins, isoparaffins, C_2benzene and oxygenates follow the same procedure that was used for the analytes. The statistics for the grouping are shown in Table A1.3 as an indication of reproducibility and repeatability of reporting the results as a group summary. However, there is a possibility that significant error could occur due to co-elution of peaks, the presence of significant amounts of olefinic or naphthenic constituents, or both, above octane and the percent unknown in the sample. If more accurate summary results are needed that are not covered by the above precision statement, for some or all of the above families of components, please consider another ASTM test method.

TABLE A1.1 Component Retention Times and Properties

NOTE 1—The names used are from several other tables and changes have been made where the GCMS did not agree with the peak name or its retention time.

NOTE 2—n-propanol will coelute with 3M-1-C5=.

NOTE 3—MTBE will coelute with 23DN-1C4=.

NOTE 4—MSBE will coelute with 1-hexene.

NOTE 5—ETBE will coelute with 23DM-13C4= =.

NOTE 6—isobutanol will coelute with 44DM-1-c5=.

NOTE 7—233TM pentane will coelute with toluene when the ratio with toluene is greater than 5.0:1.

NOTE 8—The coeluting olefins in Notes 2-6 will usually be below 1000 ppm.

NOTE 9—In some instances the chemical group is known, but the chemical structure is not known (for example, C_6-olefin; the position of the double bond is not known).

NOTE 10—Relative response factors for six of the major oxygenated compounds have been determined by using the average results from seven laboratories analyzing six samples in duplicate. These same samples were used to determine linearity of methanol, ethanol, t-butanol, MTBE, ETBE and TAME from a concentration level ranging from 1 mass % up to 30 mass %.

Peak No.	New Name	Retention Time	Molecular Mass, MWt	Theoretical Mass, Rf, (C1)
1	Methane	6.74	16.04	1.000
2	Ethene	7.10	28.05	0.874
3	Ethane	7.21	30.07	0.937
4	Propene	7.41	42.05	0.874
5	Propane	7.87	44.11	0.916
6	Isobutane	8.26	58.12	0.906
7	Methanol	8.64	32.03	2.672
8	Isobutene	8.95	56.11	0.874
9	1-butene	8.99	56.11	0.874
10	1,3-butadiene	9.17	54.09	0.843
12	*N*-butane	9.28	58.12	0.906
14	Trans-2-butene	9.70	56.11	0.874

TABLE A1.1 *Continued*

Peak No.	New Name	Retention Time	Molecular Mass, MWt	Theoretical Mass, Rf, (C1)
16	2,2-dimethylpropane	9.82	72.15	0.899
18	Cis-2-butene	10.33	56.11	0.874
20	1,2-butadiene	10.88	54.09	0.843
22	Ethanol	11.39	46.07	1.862
24	3-methyl-1-butene	12.21	70.13	0.874
26	Isopentane	13.57	72.15	0.899
28	1,4-pentadiene	14.25	68.12	0.849
30	2-Butyne (dimethylacetylene)	14.57	54.09	0.843
32	1-pentene	15.03	70.13	0.874
34	Isopropanol	15.28	60.11	1.950
36	2-methyl-1-butene	15.76	70.13	0.874
38	*N*-pentane	16.24	72.15	0.899
40	2-methyl-1,3-butadiene	16.73	68.12	0.849
42	Trans-2-pentene	17.23	70.13	0.874
44	3,3-dimethyl-1-butene	17.86	84.16	0.874
46	Cis-2-pentene	18.17	70.13	0.874
48	Tert-butanol (TBA)	18.51	74.12	1.161
50	2-methyl-2-butene	18.76	70.13	0.874
52	Trans-1,3-pentadiene	19.12	68.12	0.849
54	3-methyl-1,2-butadiene	19.48	68.12	0.849
56	Cyclopentadiene	19.76	67.10	0.824
58	Cis-1,3-pentadiene	20.25	68.12	0.849
60	1,2-pentadiene	20.51	68.12	0.849
62	2,2-dimethylbutane	20.69	86.18	0.895
64	Cyclopentene	23.16	68.12	0.849
66	4-methyl-1-pentene	24.30	84.16	0.874
68	3-methyl-1-pentene	24.38	84.16	0.874
70	*n*-propanol	24.68	60.11	1.770
72	Cyclopentane	24.86	70.13	0.874
74	2,3-dimethylbutane	25.57	86.18	0.895
76	2,3-dimethyl-1-butene	25.99	84.16	0.874
78	Methyl tert-butyl ether (MTBE)	26.18	88.09	1.407
80	Cis-4-methyl-2-pentene	26.48	84.16	0.874
82	2-methylpentane	26.66	86.18	0.895
84	Trans-4-methyl-2-pentene	72.09	84.16	0.874
86	Methyl ethyl ketone (MEK)	28.00	72.06	1.570
88	3-methylpentane	29.15	86.18	0.895
90	C_6-olefin	29.61	84.16	0.874
92	2-methyl-1-pentene	30.29	84.16	0.874
94	1-hexene	30.52	84.16	0.874
96	Methyl sec-butyl ether (MSBE)	30.66	88.09	1.550
98	C_6-olefin	30.94	84.16	0.874
100	2-butanol	31.56	74.12	1.600
102	2ethyl-1-butene	32.47	84.16	0.874
104	*N*-hexane	32.75	86.18	0.895
106	Cis-3-hexene	33.41	84.16	0.874
108	Di-isopropyl ether (DIPE)	33.58	102.00	1.600
110	Trans-3-hexene+hexadiene	33.86	84.16	0.874
112	2-methyl-2-pentene	34.33	84.16	0.874
114	3-methylcyclopentene	34.57	82.10	0.853
116	Trans-3-methyl-2-pentene	34.71	84.16	0.874
118	Cis-2-hexene	35.62	84.16	0.874
120	3,3-dimethyl-1-pentene	36.04	98.19	0.874
122	Cis-3-methyl-2-pentene	36.92	84.16	0.874
124	Ethyl tert-butyl ether (ETBE)	37.07	102.18	1.255
126	2,3-dimethyl-1,3-butadiene	37.19	82.10	0.853
128	Methylcyclopentane	37.40	84.16	0.874
130	2,2-dimethylpentane	37.60	100.21	0.892
132	4,4-dimethyl-1-pentene	37.91	98.19	0.874
134	Isobutanol	38.06	74.12	1.500
136	2,3-dimethyl-2-butene	38.30	84.16	0.874
138	2,4-dimethylpentane	38.99	100.21	0.892
140	1,3,5-hexatriene	39.31	80.06	0.832
142	2,2,3-trimethylbutane	39.48	100.21	0.892
144	Methylcyclopentadiene	40.17	80.06	0.832
146	C_7-olefin	40.30	98.19	0.874
148	C_7-olefin	40.68	98.19	0.874
150	C_7-diolefin	41.20	96.18	0.856
152	4-methylcyclopentene	41.44	82.10	0.853
154	Methylenecyclopentane	42.08	82.10	0.853
156	Benzene	42.30	78.05	0.812
158	1-methyl-1-cyclopentene	42.46	82.10	0.853
160	C_7-olefin	43.06	98.19	0.874
162	C_2-methyl-3-hexene	43.37	98.19	0.874

TABLE A1.1 *Continued*

Peak No.	New Name	Retention Time	Molecular Mass, MWt	Theoretical Mass, Rf, (C1)
164	3,3-dimethylpentane+5-methyl-1-hexene	43.81	100.21	0.892
166	Cyclohexane	44.07	84.16	0.874
168	Trans-2methyl-3-hexene	44.82	98.19	0.874
170	3,3-dimethyl-1,4-pentadiene	45.44	96.18	0.856
172	*N*-butanol	45.58	74.12	1.500
174	Dimethylcyclopentadiene	45.69	94.17	0.838
176	t,2-ethyl-3-methyl-1-butene	45.97	98.19	0.874
178	4-methyl-1-hexene	46.27	98.19	0.874
180	C_7-olefin	46.55	98.19	0.874
182	3-methyl-1-hexene	46.78	98.19	0.874
184	4-methyl-2-hexene	46.92	98.19	0.874
186	2-methylhexane+C_7-olefin	47.29	100.21	0.892
188	2,3-dimethylpentane	47.51	100.21	0.892
190	Cyclohexene	47.65	82.10	0.853
192	Tert-amyl methyl ether (TAME)	48.10	102.18	1.210
194	C_7-olefin	48.46	98.19	0.874
196	C_7-olefin	48.64	98.19	0.874
198	3-methylhexane	49.05	100.21	0.892
200	C_7-olefin	49.47	98.19	0.874
202	C_7-olefin	49.62	98.19	0.874
204	Trans-1,3-dimethylcyclopentane	49.83	98.19	0.874
206	Cis-1,3-dimethylcyclopentane	50.40	98.19	0.874
208	Trans-1,2-dimethylcyclopentane	51.01	98.19	0.874
210	3-ethylpentane	51.21	100.10	0.892
212	C_7-olefin	51.43	98.19	0.874
214	2,2,4-trimethylpentane	51.61	114.23	0.890
216	C_7-olefin	51.75	98.19	0.874
218	1-heptene	52.05	98.19	0.874
220	C_7-olefin	52.18	98.19	0.874
222	2,3-dimethyl-1,3-pentadiene	52.69	96.18	0.874
224	C_7-diolefin	53.00	96.18	0.856
226	C_7-olefin	53.36	98.19	0.874
228	C_7-diolefin	53.81	96.18	0.856
230	C_7-diolefin	54.13	96.18	0.856
232	C_7-olefin	54.28	98.19	0.874
234	*N*-heptane	54.59	100.21	0.892
236	Cis-3-heptene	54.81	98.19	0.874
238	2-methyl-2-hexene	55.10	98.19	0.874
240	Cis-methyl-3-hexene	55.35	98.19	0.874
242	Trans-3-heptene	55.72	98.19	0.874
244	3-ethyl-2-pentene	55.88	96.18	0.856
246	1,5-dimethylcyclopentene	56.06	96.18	0.856
248	Trans-2-methyl-3-hexene	56.58	98.19	0.874
250	C_7-diolefin+C_7-triolefin	57.01	96.18	0.856
252	2,3-dimethyl-2-pentene	57.35	98.19	0.874
254	3-ethylpentene	57.57	98.19	0.874
256	Methylcyclohexane	57.79	98.19	0.874
258	C_7-olefin	58.28	98.19	0.874
260	1,1,3-trimethylcyclopentane	58.79	112.22	0.874
262	2,2-dimethylhexane	59.29	114.10	0.890
264	2,3,4-trimethyl-1,4-pentadiene	59.45	110.21	0.859
266	3,3-dimethyl-1,5-hexadiene	59.79	110.21	0.859
268	C_8-olefin	60.12	98.19	0.874
270	Ethylcyclopentane	60.60	98.19	0.874
272	3-methylcyclohexene	60.99	96.18	0.856
274	Methylcyclohexadiene	61.14	94.17	0.838
276	2,2,3-trimethylpentane	61.22	114.10	0.890
278	2,5-dimethylhexane+C_8-olefin	61.59	114.23	0.890
280	2,4-dimethylhexane	61.91	114.23	0.890
282	C_7-triolefin+C_8-olefin	62.28	96.18	0.856
284	Trans,cis-1,2,4-trimethylcyclopentane	62.68	112.22	0.874
286	3,3-dimethylhexane+C_8-olefin	63.13	114.23	0.890
288	C_7-triolefin+C_8-olefin	63.39	96.18	0.856
290	C_8-olefin	63.69	112.22	0.874
292	Trans,cis-1,2,3-trimethylcyclopentane	64.27	112.22	0.874
294	C_8-olefin	64.52	112.22	0.874
296	C_8-olefin	64.73	112.22	0.874
298	C_8-olefin	64.82	112.22	0.874
300	2,3,4-trimethylpentane	64.94	114.23	0.890
302	C_7-diolefin	65.25	96.18	0.856
304	Toluene	65.50	92.06	0.821

TABLE A1.1 *Continued*

Peak No.	New Name	Retention Time	Molecular Mass, MWt	Theoretical Mass, Rf, (C1)
306	2,3,3-trimethylpentane	65.76	114.23	0.890
308	C_8-olefin	65.90	112.22	0.874
310	C_8-diolefin	66.12	110.21	0.859
312	C_8-olefin	66.48	112.22	0.874
314	C_8-olefin	66.65	112.22	0.874
316	C_8-olefin	67.08	112.22	0.874
318	C_8-diolefin+C_8-olefin	67.30	110.21	0.859
320	2,3-dimethylhexane	67.47	114.23	0.890
322	2-methyl-3-ethylpentane	67.71	114.23	0.890
324	1,1,2-trimethylcyclopentane+C_7-triolefin	68.04	112.22	0.874
326	C_8-diolefin+C_8-paraffin	68.31	110.21	0.859
328	C_8-olefin	68.41	112.22	0.874
330	C_8-olefin	68.64	112.22	0.874
332	2-methylheptane	68.86	114.23	0.890
334	4-methylheptane	69.11	114.23	0.890
336	C_8-diolefin+C_7-olefin	69.41	112.22	0.874
338	C_8-olefin	69.70	112.22	0.874
340	Cis-1,3-dimethylcyclohexane	69.91	112.22	0.874
342	Trans-1,4-dimethylcyclohexane	70.01	112.22	0.874
344	3-methylheptane	70.23	114.23	0.890
346	3-ethylhexane	70.38	114.23	0.890
348	C_8-diolefin	70.51	110.21	0.874
350	C_8-olefin	70.72	112.22	0.874
352	C_8-olefin	70.92	112.22	0.874
354	1,1-dimethylcyclohexane	71.18	112.22	0.874
356	C_8-olefin	71.43	112.22	0.874
358	C_8-olefin	71.70	112.22	0.874
360	Cis-1-ethyl-3-methylcyclopentane	72.10	112.22	0.874
362	2,2,5-trimethylhexane	72.23	128.26	0.888
364	Trans-1-ethyl-3-methylcyclopentane	72.46	112.22	0.874
366	Trans-1-ethyl-2-methylcyclopentane	72.68	112.22	0.874
368	1-methyl-1-ethylcyclopentane	72.96	112.22	0.874
370	1-octene	73.16	112.22	0.874
372	C_8-olefin	73.26	112.22	0.874
374	Trans-1,2-dimethylcyclohexane	73.36	112.22	0.874
376	C_8-olefin	73.48	112.22	0.874
378	C_8-olefin	73.68	112.22	0.874
380	Trans-3-C_8-Olefin	74.08	112.11	0.874
382	C_8-olefins	74.45	112.22	0.874
384	Trans-1,3-dmcyclohexane	74.66	112.22	0.874
386	Cis-1,4-dmcycloHexane	74.79	112.22	0.874
388	*N*-octane	74.98	114.23	0.890
390	C_8-olefin	75.33	112.22	0.874
392	C_8-olefin	75.49	112.22	0.874
394	Trans-2-octene	75.62	112.22	0.874
396	Isopropylcyclopentane	75.72	112.22	0.874
398	C_9-olefin	75.85	126.24	0.874
400	C_9-olefin	75.89	126.24	0.874
402	C_9-olefin	75.90	126.24	0.874
404	C_9-olefin	76.08	126.24	0.874
406	2,2,4-trimethylhexane	76.31	128.26	0.888
408	2,4,4-trimethylhexane	76.62	128.26	0.888
410	C_9-olefins	76.86	126.24	0.874
412	2,3,5-trimethylhexane	77.29	128.26	0.888
414	Cis-2-octene	77.53	112.22	0.874
416	2,2,3,4-tetramethylpentane	77.77	128.26	0.888
418	2,2-dimethylheptane	78.02	128.26	0.888
420	Cis-1,2-dimethylcyclohexane	78.36	112.22	0.874
422	2,4-dimethylheptane	78.74	128.26	0.888
424	C_9-olefin	78.90	126.24	0.874
426	C_9-olefin	79.08	126.24	0.874
428	Ethylcyclohexane	79.24	112.22	0.874
430	Propylcyclopentane	79.39	112.22	0.874
432	2-methyl-4-ethylhexane	79.59	128.26	0.888
434	2,6-dimethylheptane	79.74	128.26	0.874
436	C_9-olefin	79.85	126.24	0.874
438	1,1,4-trimethylcyclohexane	80.05	126.24	0.874
440	C_9-olefin	80.28	126.24	0.874
442	C_9-olefin	80.38	126.24	0.874
444	1,1,3-trimethylcyclohexane	80.52	126.24	0.874
446	2,5 & 3,5-dimethylheptane	80.69	128.26	0.888

TABLE A1.1 *Continued*

Peak No.	New Name	Retention Time	Molecular Mass, MWt	Theoretical Mass, Rf, (C1)
448	C_9-olefin	80.88	126.24	0.874
450	3,3-DMheptane	81.00	128.26	0.888
452	C_9-paraffin	81.13	128.26	0.888
454	C_9-olefin	81.34	126.24	0.874
456	2,3,3-trimethylhexane	81.56	128.26	0.888
458	C_9-olefin	81.68	126.24	0.874
460	Ethylbenzene	81.96	106.08	0.827
462	C_9-olefin	82.00	126.24	0.874
464	Trans-1,2,4-trimethylcyclohexane	82.31	126.24	0.874
466	C_9-olefin	82.33	126.24	0.874
468	2,3,4-trimethylhexane	82.63	128.26	0.888
470	C_9-olefin	82.73	126.24	0.874
472	3,3,4-trimethylhexane	82.89	128.26	0.888
474	M-Xylene	83.30	106.08	0.827
476	P-Xylene	83.43	106.08	0.827
478	2,3-dimethyheptane	83.57	128.26	0.888
480	3,5-dimethylheptane	83.83	128.26	0.888
482	3,4-dimethylheptane	83.91	128.26	0.888
484	C_9-olefin	84.08	126.24	0.874
486	3-methyl-3-ethylhexane	84.26	128.26	0.888
488	C_9-olefin	84.41	126.24	0.874
490	4-ethylheptane	84.52	128.26	0.888
492	4-methyloctane+C_9-olefin	84.70	128.26	0.888
494	2-methyloctane	84.84	128.26	0.888
496	C_9-olefin	85.01	126.24	0.874
498	C_9-paraffin	85.18	128.26	0.888
500	C_9-olefin	85.36	126.24	0.874
502	3-ethylheptane	85.51	128.26	0.888
504	3-methyloctane	85.69	128.26	0.888
506	C_9-paraffin	85.87	126.24	0.874
508	Cis-1,2,4-trimethylcyclohexane	85.91	126.24	0.874
510	1,1,2-trimethylcyclohexane	86.05	126.24	0.874
512	O-Xylene	86.27	106.08	0.827
514	C_9-olefin	86.47	126.24	0.874
516	C_9-paraffin	86.57	128.26	0.888
518	C_9-paraffin	86.75	128.26	0.888
520	C_9-olefin	86.90	126.24	0.874
522	Trans-1-ethyl-4-methylcyclohexane	87.08	126.24	0.874
524	Cis-1-ethyl-4-methylcyclohexane	87.23	126.24	0.874
526	C_9-paraffin	87.49	128.26	0.888
528	1-nonene	87.79	126.24	0.874
530	Isobutylcyclopentane	88.00	126.24	0.874
532	C_9-paraffin	88.45	128.26	0.888
534	Trans-3-nonene	88.65	126.24	0.874
536	Cis-3-nonene	88.82	126.24	0.874
538	C_9-paraffin	89.09	128.26	0.888
540	*n*-nonane	89.24	128.26	0.888
542	C_{10}-olefin	89.41	140.27	0.874
544	Trans-2-nonene	89.74	126.24	0.874
546	1-methyl-1-ethylcyclohexane	89.61	126.24	0.874
548	1-methyl-2-propylcyclopentane	89.96	126.24	0.874
550	C_{10}-olefin	90.09	140.27	0.874
552	C_{10}-paraffin	90.18	142.28	0.887
554	C_{10}-paraffin	90.29	142.28	0.887
556	Isopropylbenzene	90.46	118.08	0.832
558	Cis-2-nonene	90.78	126.24	0.874
560	Tert-butylcyclopentane	90.80	126.24	0.874
562	C_9-olefins	90.88	126.24	0.874
564	Nonene	91.16	126.24	0.874
566	Isopropylcyclohexane	91.32	126.24	0.874
568	3,3,5-trimethylheptane	91.44	142.28	0.887
570	2,2-dimethyloctane	91.60	142.28	0.887
572	2,4-dimethyloctane	91.67	142.28	0.887
574	1-methyl-4-isopropylcyclohexane	91.82	140.27	0.874
576	Sec-butylcyclopentane	92.20	126.24	0.874
578	Propylcyclohexane	92.40	126.24	0.874
580	2,5-dimethyloctane	92.59	142.28	0.887
582	Butylcyclopentane	92.89	126.24	0.874
584	2,6-dimethyloctane	93.04	142.28	0.887
586	3,6-dimethyloctane	93.43	142.28	0.887
588	1-methyl-2-ethylcyclohexane	93.59	126.24	0.874
590	C_{10}-olefin	93.79	140.27	0.874
592	Propylbenzene	93.96	120.20	0.832

TABLE A1.1 *Continued*

Peak No.	New Name	Retention Time	Molecular Mass, MWt	Theoretical Mass, Rf, (C1)
594	3,3-dimethyloctane	94.27	142.28	0.887
596	3-methyl-5-ethylheptane	94.54	142.28	0.887
598	C_{10}-olefin	94.66	140.27	0.874
600	1-ethyl-3-methylbenzene	94.88	120.20	0.832
602	1-ethyl-4-methylbenzene	95.09	120.20	0.832
604	Naphthene	95.30	140.27	0.874
606	1,3,5-trimethylbenzene	95.73	120.20	0.832
608	2,3-dimethyloctane	95.94	142.28	0.887
610	5-methylnonane	96.13	142.28	0.887
612	4-methylnonane	96.29	142.28	0.887
614	2-methylnonane	96.49	142.28	0.887
616	1-ethyl-2-methylbenzene	96.77	120.20	0.832
618	3-ethyloctane	97.01	142.28	0.887
620	Naphthene	97.14	140.27	0.874
622	3-methylnonane	97.47	142.28	0.887
624	C_{10}-olefin	97.69	140.27	0.874
626	C_{10}-paraffin	97.83	142.28	0.887
628	C_{10}-paraffin	98.16	142.28	0.887
630	1,2,4-trimethylbenzene	98.49	120.20	0.832
632	C_{10}-paraffin	98.74	142.28	0.997
634	C_{10}-paraffin	98.90	142.28	0.887
636	Isobutylcyclohexane	99.10	140.27	0.874
638	C_{10}-paraffin	99.09	142.28	0.887
640	C_{10}-paraffin	99.22	142.37	0.887
642	1-decene	99.52	140.27	0.874
644	C_{10}-paraffin	99.66	142.28	0.887
646	C_{10}-paraffin	99.70	142.28	0.887
648	C_{10}-aromatic	99.75	134.22	0.837
650	C_{10}-paraffin	99.82	142.28	0.887
652	Naphthene	99.93	140.27	0.874
654	Isobutylbenzene	100.06	134.22	0.837
656	Trans-1-methyl-2-propylcyclohexane	100.09	140.27	0.874
658	C_{10}-paraffin	100.19	142.28	0.887
660	Sec-butylbenzene	100.28	134.22	0.837
662	*n*-decane	100.40	142.28	0.887
664	C_{11}-paraffin	100.67	156.32	0.886
666	C_{11}-paraffin	100.85	156.32	0.886
668	1,2,3-trimethylbenzene	101.28	120.20	0.832
670	1-methyl-3-isopropylbenzene	101.40	134.22	0.837
672	C_{11}-paraffin	101.55	156.32	0.886
674	1-methyl-4-isopropylbenzene	101.73	134.22	0.837
676	C_{11}-paraffin	102.06	156.32	0.886
678	C_{11}-paraffin	102.05	156.32	0.886
680	2,3-dihydroindene	102.42	118.17	0.819
682	Sec-butylcyclohexane	102.57	140.27	0.874
684	C_{11}-paraffin	102.87	156.32	0.886
686	1-methyl-2-isopropylbenzene	103.03	134.22	0.837
688	3-ethylnonane	103.26	156.32	0.886
690	C_{11}-paraffin	103.37	156.32	0.886
692	Naphthene	103.55	140.27	0.874
694	C_{11}-paraffin	103.88	126.19	0.886
696	1,3-diethylbenzene	104.08	134.22	0.837
698	1-methyl-3-propylbenzene	104.35	134.22	0.837
700	1,4-diethylbenzene	104.57	134.22	0.837
702	1-methyl-4-propylbenzene	104.73	134.22	0.837
704	Butylbenzene	104.85	134.22	0.837
706	3,5-dimethyl-1-ethylbenzene	105.00	134.22	0.837
708	1,2-diethylbenzene	105.26	134.22	0.837
710	C_{11}-paraffin	105.39	156.32	0.886
712	C_{10}-aromatic	105.49	134.22	0.837
714	C_{10}-aromatic	105.64	134.22	0.837
716	C_{10}-aromatic	105.75	134.22	0.837
718	1-methy-2-propylbenzenes	105.85	134.22	0.837
720	C_{10}-aromatic	105.95	134.22	0.837
722	5-methyldecane	106.11	156.32	0.886
724	4-methyldecane	106.26	156.32	0.886
726	2-methyldecane	106.39	156.32	0.886
728	C_{11}-paraffin	106.55	156.32	0.886
730	1,4-dimethyl-2-ethylbenzene	106.76	134.22	0.837
732	1,3-dimethyl-4-ethylbenzene	106.93	134.22	0.837
734	C_{11}-paraffin	107.06	156.32	0.886
736	3-methyldecane	107.27	156.32	0.886
738	C_1- indane	107.35	132.00	0.837

TABLE A1.1 *Continued*

Peak No.	New Name	Retention Time	Molecular Mass, MWt	Theoretical Mass, Rf, (C1)
740	1,2-dimethyl-4-ethylbenzene	107.46	134.22	0.837
742	C_{11}-paraffin	107.76	156.32	0.886
744	1,3-dimethyl-2-ethylbenzene	108.01	134.22	0.837
746	C_{11}-paraffin	108.58	156.32	0.886
748	C_{11}-paraffin	108.75	156.32	0.886
750	1-methyl-4-tert-butylbenzene	108.98	148.25	0.840
752	1,2-dimethyl-3-ethylbenzene	109.17	134.22	0.837
754	1-ethyl-2-isopropylbenzene	109.50	148.25	0.840
756	*N*-undecane	109.62	156.32	0.886
758	1-ethyl-4-isopropylbenzene	109.80	148.25	0.840
760	C_{12}-paraffin	109.96	170.34	0.885
762	1,2,4,5-tetramethylbenzene	110.15	134.22	0.837
764	2-methylbutylbenzene	110.55	148.25	0.840
766	1,2,3,5-tetramethylbenzene	110.43	134.22	0.837
768	3 methylbutylbenzene	110.64	148.25	0.840
770	C_{11}-aromatic	110.74	148.25	0.840
772	C_{12}-paraffin	110.84	170.34	0.885
774	C_{11}-aromatic	110.94	148.25	0.840
776	C_{11}-aromatic	111.05	148.25	0.840
778	C_{11}-aromatic	111.12	148.25	0.840
780	1-tert-butyl-2-methylbenzene	111.56	148.25	0.840
782	C_{11}-aromatic	111.65	148.25	0.840
784	1-ethyl-2-propylbenzene	111.76	148.25	0.840
786	C_{11}-aromatic	112.00	148.25	0.840
788	C_{11}-aromatic	112.22	148.25	0.840
790	C_{11}-aromatic	112.34	148.25	0.840
792	1-methyl-3-butylbenzene	112.52	148.25	0.840
794	C_{11}-aromatic	112.63	148.25	0.840
796	1,2,3,4-tetramethylbenzene	112.79	148.25	0.840
798	Pentylbenzene	113.17	148.25	0.840
800	Trans-1-methyl-2-(4methylpentyl)-cyclopentane	113.44	168.33	0.874
802	C_{11}-aromatic	113.74	148.25	0.840
804	C_{11}-aromatic	113.85	148.25	0.840
806	C_{11}-aromatic	114.02	148.25	0.840
808	C_{12}-paraffin	114.12	170.34	0.885
810	1,2,3,4-tetrahydronaphthalene	114.17	132.09	0.824
812	1-tert-butyl-3,5-dimethylbenzene	114.32	162.30	0.843
814	Naphthalene	114.65	128.06	0.799
816	1,1-dimethylindane	114.94	146.10	0.829
818	1,2-dimethylindane	115.19	146.10	0.829
820	1,6-dimethylindane	115.33	146.10	0.829
822	C_{11}-aromatic	115.55	148.25	0.885
824	1- ethylindane	115.65	146.10	0.829
826	2- ethylindane	115.88	146.10	0.829
828	Ethyl -1,3,5-trimethylbenzene	116.00	148.25	0.884
830	1,3-dipropylbenzene	116.21	162.34	0.843
832	*n*-dodecane	116.55	170.34	0.885
834	Ethyl -1,2,4-trimethylbenzene	116.69	148.25	0.840
836	C_{11}-aromatic	117.07	148.25	0.840
838	C_{11}-aromatic	117.19	148.25	0.840
840	C_{12}-aromatic+C_2-indane	117.55	162.30	0.843
842	2,4-dimethylindane	117.99	146.10	0.829
844	4-ethylindane	118.13	146.10	0.829
846	1-tert-butyl-4-ethylbenzene	118.59	162.30	0.843
848	1,3-dimethylindane	119.07	146.10	0.829
850	1-methyl-4-pentylbenzene	119.60	162.30	0.843
852	4,7-dimethylindane	119.65	146.10	0.829
854	5,6-dimethylindane	119.70	146.10	0.829
856	C_{12}-aromatic	119.77	162.30	0.843
858	Hexylbenzene	119.87	162.30	0.843
860	C_6-benzene	119.93	162.30	0.843
862	C_6-benzene	119.98	162.30	0.843
864	C_6-benzene	120.20	162.30	0.843
866	4,5-dimethylindane	120.30	146.10	0.829
868	C_6-benzene	120.80	163.30	0.843
870	2-methylnaphthalene	121.42	142.08	0.806
872	C_6-benzene	121.65	162.30	0.843
874	C_6-benzene	121.85	162.30	0.843
876	*n*-tridecane	122.06	184.22	0.884
878	1-methylnaphthalene	122.28	142.08	0.806
880	C_6-benzene	122.40	162.30	0.843
882	C_2-tetralin	122.80	160.20	0.843
884	C_6-benzene	123.20	162.30	0.843

TABLE A1.1 *Continued*

Peak No.	New Name	Retention Time	Molecular Mass, MWt	Theoretical Mass, Rf, (C1)
886	C_6-benzene	124.00	162.30	0.843
888	C_{13}-paraffin	125.60	184.22	0.883
890	Trans-7-decene	126.34	140.20	0.874
892	*n*-tetradecane	126.60	198.34	0.883
895	2,6-dimethylnaphthalene	126.84	156.30	0.812
900	2,7-dimethylnaphthalene	126.97	156.30	0.812
905	*n*-tetradecane	127.10	198.34	0.883
910	1,3-dimethylnaphthalene	127.52	156.30	0.812
915	1,6-dimethylnaphthalene	127.69	156.30	0.812
920	1,5-dimethylnaphthalene	128.44	156.30	0.812
925	1,4-dimethylnaphthalene	128.31	156.30	0.812
930	Acenaphthalene	129.05	156.30	0.801
940	1,2-dimethylnaphthalene	129.92	156.30	0.812
950	*n*-pentadecane	131.10	212.34	0.883

TABLE A1.2 Repeatability and Reproducibility of IHA Determinations

NOTE 1—Brief explanation of header information:
r_{min}—lower 95 % confidence limit of r_{est},
r_{est}—repeatability estimate in percent of concentration,
r_{max}—upper 95 % confidence limit of r_{est},
R_{min}, R_{est}, R_{max}—same as above except for reproducibility,
C_{min}—lower concentration limit that r_{est}, R_{est} is applicable, and
C_{max}—upper concentration limit that r_{est}, R_{est} is applicable.

NOTE 2—Short analyte names were used for the above table and by using the number beside this name, it will correspond to a full name in Annex A1.

NOTE 3—C_2benzene refer to grouping ethylbenzene, M, P, and O-xylene as a group.

NOTE 4—The numbers in the second column were used for the statistical analysis for the round robin for 1996. The numbers beside the names are the new numbers being used in the new presentation of the IHA Method.

GC/MS	No. for RR	IHA No.	IHA/ abbreviated Name	r_{min}	r_{est}	r_{max}	R_{min}	R_{est}	R_{max}	C_{min}	C_{max}
[A]	6	6	iC4	9.8	1.4	17.7	24.9	30.7	37.3	0.04	2.86
[A]	9	9	1C4=	10.4	16.7	25.1	28	36	45.4	0.01	0.14
[A]	11	12	nC4	10	12	14.2	27.1	31.7	36.6	0.92	8.51
[A]	12	14	t2C4=	12.1	15.7	19.8	28.2	36.8	47.1	0.03	0.31
[A]	14	18	c2C4=	14.2	15.4	16.7	25.2	31.1	37.9	0.03	0.29
[A]	20	24	3M1C4=	7.3	9.6	12.3	17.2	19.9	22.7	0.02	0.11
[A]	22	26	iC5	4.6	5.4	6.3	13.4	15.5	17.9	2.39	12.09
[A]	26	32	1C5=	5.9	7.5	9.4	17	20.6	24.7	0.06	0.4
[A]	28	36	2M1C4=	4.4	6.3	8.6	14.5	17.5	20.9	0.14	0.8
[A]	30	38	nC5	4.2	6.2	8.7	13.9	16.1	18.5	1	5.18
[A]	34	42	t2C5=	4.1	6.3	9.1	13	17.3	22.6	0.27	1.08
[A]	38	46	c2C5=	5.2	7.7	11	14.4	18.3	22.9	0.15	0.59
[A]	40	50	2M2C4=	3.9	6.2	9.2	15.2	18.1	21.4	0.44	1.78
[A]	42	52	t13C5=,=	4.5	10.2	19.6	22.1	31.1	42.2	0.01	0.05
[A]	52	62	222DMC4	2.9	3.7	4.7	9.8	12.9	16.6	0.07	2.16
[A]	54	64	cyC5=	4.6	9	15.5	15.6	20.3	25.9	0.07	0.25
[A]	56	66	4M1C5=	11.2	14.8	19	22.6	31.8	43.2	0.02	0.1
[A]	58	68	3M1C5=	8.3	12.1	17	37.1	50.5	66.8	0.04	0.12
[A]	62	72	cyC5	2.5	4.7	7.7	11.8	13.4	15.1	0.07	0.69
[A]	64	74	23DMC4	1.7	2.7	3.9	8.6	9.8	11.1	0.53	1.91
[A]	66	76	MTBE	1.9	3.2	5	9.1	12.3	16.2	0.12	15.73
[A]	70	80	c4M2C5=	5.1	7.1	9.7	27.4	43.7	65.4	0.02	0.09
[A]	74	82	2MC5	2.2	2.9	3.8	9.3	11	12.9	1.03	5.62
[A]	76	84	t4M2C5=	4.9	6.3	7.9	16.9	20.2	23.9	0.05	0.26
[A]	80	88	3MC5	2	2.7	3.5	7.7	9.1	10.7	0.58	3.25
[A]	84	92	2M1C5=	3.6	5.1	7	9.6	12.5	16.1	0.09	0.45
[A]	86	94	1C6=	3.9	6.4	9.9	15.1	19.9	25.7	0.04	0.26
[A]	96	104	nC6	2.5	4.6	7.7	11	13.3	15.8	0.25	3.23
[A]	98	106	c3C6=	4.4	6.5	9.1	12.5	16.3	20.9	0.08	0.48
[A]	102	110	t3C6=+C6=,=	2.9	5.2	8.4	9.4	12.4	15.9	0.17	0.93
[A]	103	112	2M2C5=	2.7	4.7	7.4	9.9	12	14.4	0.15	0.77
[A]	104	114	3McyC5=	7.8	11.3	15.9	22.7	25.2	28	0.02	0.11
[A]	105	116	t3M2C5=	4.3	6.9	10.2	10.1	12.5	15.4	0.1	0.48
[A]	106	118	c2C6=	4.1	6.7	10.2	14.3	17.4	21	0.07	0.4
[A]	109	122	c3M2C5=	3.1	4.5	6.4	9.1	10.5	12.1	0.14	0.75
[A]	112	128	McyC5	2.4	3.3	4.4	9.1	10.1	11.1	0.36	2.34
[A]	116	138	24DMC5	1.8	2.7	3.9	8	10.1	12.4	0.2	1.93
[A]	118	142	223TMC4	0.5	4.1	14.3	20.9	35.2	54.8	0.01	0.06
[A]	124	150	C7=,=	0	3.1	16.6	11.3	19.1	29.9	0.01	0.04
[A]	128	154	methyl-enecyC5	5.5	9.1	14.1	14.9	20.3	26.8	0.01	0.03
[A]	130	156	Benzene	2.6	4.7	7.8	11.5	13.8	16.5	0.15	1.86
[A]	131	158	1McyC5=	4.3	6.3	8.9	18.5	24.1	30.7	0.17	0.92
[A]	133	162	c2M3C6=	0	1.2	6.8	17	29.1	45.9	0.01	0.06
[A]	134	164	33DMC5+5M1C6=	2.3	3.9	6.2	8.5	14.8	23.6	0.02	0.22
[A]	136	166	cyC6	3.3	4.4	5.7	11.3	12.8	14.5	0.04	0.87
[A]	138	168	t2M3C6=	4.2	8.4	14.7	84.2	103.2	124.8	0.02	0.32
[A]	146	176	t2e3m1C4=	3.2	5.7	9.1	20.8	29.6	40.8	0.02	0.19
[A]	148	178	4M1C6=	0.1	2.4	11.5	16.8	29.3	46.6	0.01	0.05
[A]	154	184	4M2C6=	3	4.5	6.4	15.9	18.7	21.8	0.03	0.29
[A]	156	186	2MC6+C7=	1.4	2.1	3	6.2	7.7	9.5	1.09	3.54
[A]	160	190	cyC6=	3.9	7.2	12.1	30.1	45.4	65.2	0.02	0.13
[A]	166	198	3MC6	1.3	2	2.8	8.5	9.9	11.5	0.36	2.38
[A]	172	204	t13DMcyC5	1.7	2.4	3.3	10.5	11.3	12.2	0.12	0.6
[A]	174	206	c13DMcyC5	1.9	2.7	3.6	9.8	10.7	11.6	0.09	0.49
[A]	176	208	t12DMcyC5	2.2	3.2	4.3	7.6	9.1	10.8	0.05	0.46
[A]	180	210	3EC5	2.8	4.8	7.6	10	13.4	17.6	0.02	0.21

TABLE A1.2 *Continued*

GC/MS	No. for RR	IHA No.	IHA/ abbreviated Name	r_{min}	r_{est}	r_{max}	R_{min}	R_{est}	R_{max}	C_{min}	C_{max}
^{A}	184	212	5M-1-C6=	1.8	5	10.6	24.1	35.2	49.1	0.03	0.19
^{A}	186	214	224TMC5	2.3	3.4	4.9	7.6	13.2	21.1	0.09	23.25
^{A}	188	218	1C7=	4.3	6.8	10.1	15.8	20.9	26.9	0.02	0.13
^{A}	189	220	C7=	5.2	7.8	11.1	15.1	18.3	22	0.02	0.13
^{A}	194	226	C7=	3.3	4.8	6.8	16.6	20.7	25.2	0.02	0.16
^{A}	196	228	C7=,=	3.7	5	6.5	12.5	17.2	22.8	0.04	0.31
^{A}	197	230	C7=,=	5.6	7.3	9.3	19.5	23	26.9	0.04	0.26
^{A}	198	232	C7=	3.8	4.7	5.7	42.9	60.4	82.1	0.05	0.45
^{A}	200	234	nC7	1.5	2.2	3.2	7.4	8.9	10.7	0.13	1.55
^{A}	202	236	c3C7=	2.1	3	4.2	14.2	18.2	23	0.04	0.36
^{A}	204	238	2M2C6=	2.1	3	4.3	14.4	16.5	18.7	0.05	0.43
^{A}	206	240	c3M3C6=	3.3	4.5	6.1	21	24.9	29.3	0.03	0.29
^{A}	208	242	t3C7=	1.8	2.7	4	12.9	15.2	17.8	0.04	0.35
^{A}	210	244	3E2C5=	0.1	1.2	5.4	13.4	16.6	20.4	0.02	0.13
^{A}	212	246	1,5DMcyC5=	3	5	7.8	10.3	16.2	24	0.03	0.27
^{A}	214	248	t2M3C6=	2.8	3.6	4.7	13.8	17.9	22.9	0.04	0.33
^{A}	218	252	23DM2C5=	3.1	4	5	9.1	13	17.8	0.04	0.56
^{A}	222	256	McyC6	1.9	2.6	3.6	8.5	9.9	11.5	0.16	1.44
^{A}	224	260	113TMCyC5	1.7	5.1	11.5	10.8	14.4	18.7	0.01	0.09
^{A}	226	262	22DMC6	4.7	9.2	15.9	12.9	23.2	38.1	0.01	0.07
^{A}	234	270	EcyC5	2.5	3.6	5	9.6	13.5	18.4	0.04	0.3
^{A}	240	276	223TMC5	2.2	4.9	9.3	14.1	27.3	46.7	0.02	0.54
^{A}	245	278	25DMC6+C8=	1.5	2.8	4.7	6.3	8.1	10.3	0.17	1.58
^{A}	250	280	24DMC6	1.8	2.9	4.5	6.1	8.1	10.4	0.25	2.19
^{A}	260	284	tc124TMcyC5	2.4	3.7	5.4	10.8	15.1	20.5	0.03	0.16
^{A}	265	286	3,3DMC6+C8=	1.3	5.4	14.1	8.7	14.8	23.2	0.01	0.07
^{A}	278	292	tc123TMcyC5	6.1	11.5	19.5	40.9	70	110.3	0.03	0.09
^{A}	290	298	C8='S	0.3	3.2	11.8	15.5	20.3	26.1	0.02	0.23
^{A}	292	300	234TMC5	1.9	3.2	5	8.7	12	16	0.09	9.14
^{A}	294	302	C7=,=	2.9	4.2	5.8	19.2	41.1	75.2	0.06	0.51
^{A}	300	304	Toluene	1.7	3.1	5.3	8.7	16.6	28.2	2.52	13.14
^{A}	312	316	C8=	3.9	6	8.7	26	35.7	47.6	0.02	0.2
^{A}	314	320	23DMC6	2.2	3.5	5.2	16.1	30.6	51.9	0.18	2.06
^{A}	316	322	2M3EC5	2.3	4.5	7.9	21.3	40	67.2	0.03	0.31
^{A}	318	324	112TMcyC5+C7=,=	0.4	3.3	11.8	26.6	33.7	42	0.02	0.23
^{A}	326	332	2MC7	3.3	4.4	5.9	8.4	11.2	14.5	0.14	0.93
^{A}	328	334	4MC7	3.5	5.6	8.3	12.5	24.4	42.4	0.15	0.5
^{A}	334	340	c13DMcyC6	3.7	4.8	6.2	18.7	32.6	52.1	0.04	0.25
^{A}	336	344	3MC7	2.3	3.3	4.5	17.8	21.9	26.5	0.15	1.04
^{A}	338	346	3EC6	4.1	6.4	9.4	34.8	53	76.7	0.04	0.21
^{A}	352	360	c1E3McyC5	3.1	4.3	5.7	8.6	23.2	48.7	0.09	2.32
^{A}	356	364	t1E3McyC5	3.8	5.1	6.7	24.4	35.5	49.7	0.03	0.21
^{A}	360	366	t1E2McyC5	4.5	7.7	12.3	32.3	54.1	84.1	0.02	0.11
^{A}	362	368	1M1EcyC5	0.2	3.1	12.5	24.1	33.3	44.7	0.01	0.08
^{A}	366	372	C8=	7.2	9.9	13.3	27.1	37	49	0.01	0.08
^{A}	368	374	t12DMcyC6	2.2	4.8	9	63.9	97.3	140.6	0.02	0.15
^{A}	372	378	C8='S	3.4	5.3	7.9	109.3	124.4	141	0.02	0.26
^{A}	374	380	t-3-C8=	0	1.5	9.4	50.8	67.2	86.9	0.02	0.12
^{A}	380	382	C8=	3.6	5.4	7.9	21.1	38.9	64.7	0.03	0.33
^{A}	385	384	t13DMcyC6	3.1	5.4	8.4	34.1	48.5	66.5	0.04	0.31
^{A}	400	388	nC8	3	3.7	4.5	8.8	11.9	15.6	0.1	0.89
^{A}	406	394	t2C8=	3	6.5	12.2	45.6	72.5	108.4	0.02	0.28
^{A}	408	396	iPrcyC5	5.8	7.4	9.3	31.7	50.8	76.5	0.03	0.36
^{A}	416	404	C9=	0.3	2.9	9.9	46.9	63.8	84.4	0.02	0.14
^{A}	422	410	C9='S	4.8	8	12.4	30.5	43.2	58.9	0.02	0.17
^{A}	432	420	c12DMcyC6	3.4	4.9	6.8	22.1	39.3	63.8	0.04	0.39
^{A}	434	422	24DMC7	5.6	9.9	15.9	54.5	105.5	181.2	0.02	0.09
^{A}	436	424	C9=	1.9	6	13.7	34.7	47.5	63.1	0.01	0.07
^{A}	438	426	C9=	4.1	6.6	10	19	27.7	38.7	0.02	0.11
^{A}	440	428	EcyC6	2.7	5	8.2	14.1	22	32.5	0.03	0.28
^{A}	444	432	2M4EC6	7.7	11.1	15.3	20.2	27.4	36	0.01	0.03
^{A}	446	434	26DMC7	5.9	7.3	8.9	21.9	27.7	34.4	0.03	0.14
^{A}	450	438	114TMcyC6	5.9	8.2	11	28	42.1	60.3	0.03	0.21
^{A}	458	446	25&35DMc7	3.7	5.9	8.7	10.5	14.9	20.5	0.07	0.25
^{A}	460	448	C9='S	3.3	8.4	17.1	40.1	56.4	76.6	0.01	0.07
^{A}	462	450	33DMC7	0.1	3.3	15.7	25	44	70.9	0.01	0.05
^{A}	475	460	EBenzene	2.8	3.9	5.4	7.2	8.9	10.9	0.66	3.12
^{A}	480	464	t124TMcyC6	6.9	10.9	16.3	84.7	109.3	138.2	0.02	0.15
^{A}	500	474	M-Xylene	2.7	3.7	5	7.5	9.2	11	1.67	7.93
^{A}	502	476	P-Xylene	3.1	4.4	5.9	8.8	11.6	14.8	0.63	3.26
^{A}	503	478	23DMC7	5.1	7.6	10.9	45.3	73.5	111.5	0.03	0.16
^{A}	504	480	35DMC7	7.2	9.8	13	44.1	82.8	139.2	0.02	0.07

TABLE A1.2 *Continued*

GC/MS	No. for RR	IHA No.	IHA/ abbreviated Name	r_{min}	r_{est}	r_{max}	R_{min}	R_{est}	R_{max}	C_{min}	C_{max}
[A]	506	482	34DMC7	6.5	10.1	15	42.5	67.7	101.4	0.02	0.07
[A]	510	486	3M3EC6	6.3	10	15	38	61	92	0.02	0.14
[A]	518	492	4MC8+C9=	4.1	5.9	8.1	12.4	14.3	16.3	0.05	0.3
[A]	520	494	2MC8	4.4	5.9	7.7	12.4	15.9	20.1	0.07	0.38
[A]	522	496	C9=	6.8	10.6	15.7	22.3	33.3	47.4	0.01	0.1
[A]	528	502	3EC7	4.5	6.8	9.8	24.7	34.4	46.3	0.02	0.11
[A]	530	504	3MC8	5	8	12	12.4	17.9	24.9	0.08	0.45
[A]	550	512	O-Xylene	2.1	3	4.1	7.7	9.8	12.3	0.92	4.18
[A]	564	518	C9P	3.1	6.6	12	31.1	50.4	76.3	0.01	0.37
[A]	568	522	t1E4McyC6	6.5	9.7	13.8	26.3	46.1	74.1	0.02	0.13
[A]	570	524	c1E4McyC6	4.7	7.4	10.8	22.1	35.8	54.2	0.02	0.15
[A]	572	526	C9P	4.5	7.2	10.7	28.7	55.7	95.9	0.03	0.6
[A]	582	532	C9P	7.5	11.1	15.6	16.9	23.1	30.8	0.02	0.24
[A]	586	534	t3C9=	4.6	9.1	16	27.3	38.8	53.2	0.01	0.16
[A]	590	536	c3C9=	7.1	11.1	16.4	23.5	36.1	52.7	0.01	0.17
[A]	600	540	nC9	5.8	7.2	8.7	18.3	30	45.8	0.1	0.51
[A]	606	546	1M1EcyC6	0.4	3.1	10.7	46.2	75.8	116	0.02	0.11
[A]	608	548	1M2PrcyC5	0.2	3	12.2	19.2	30.1	44.5	0.01	0.1
[A]	616	556	iPrbenz	4.3	6.9	10.4	11.2	18.9	29.6	0.04	0.41
[A]	626	566	iPrcyC6	4.4	7.7	12.4	21.8	40.2	66.9	0.01	0.35
[A]	636	576	sBucyC5	0.5	4.5	16.1	22.9	36.7	55.1	0.01	0.06
[A]	638	578	PrcyC6	4	7.3	12	77.9	96.8	118.6	0.02	0.12
[A]	644	584	26DMC8	4.6	8.6	14.4	41.2	68.2	105	0.03	0.23
[A]	646	586	36DMC8	4.5	7.7	12.3	31.6	40.4	50.8	0.03	0.11
[A]	651	592	nPrbenz	3.5	5.8	9	11.6	17.3	24.6	0.21	0.83
[A]	655	600	1E3Mbenz	2.8	4.5	6.9	6.5	8.3	10.3	0.85	2.8
[A]	656	602	1E4Mbenz	3.1	4.5	6.3	7.8	9.7	11.9	0.36	1.26
[A]	658	606	135TMbenz	3.4	5.8	9.1	8.5	12.5	17.7	0.46	1.53
[A]	660	610	5MC9	10.9	12.9	15.1	76.7	104.7	138.8	0.02	0.13
[A]	661	612	4MC9	7.1	10.2	14	29.7	44.5	63.5	0.02	0.13
[A]	662	614	2MC9	4.4	7.1	10.9	14.9	24.2	36.6	0.1	2.07
[A]	663	616	1E2Mbenz	3.6	5.5	8.1	10.3	15.9	23.2	0.3	1.1
[A]	668	622	3MC9	7.2	12.9	21	41.8	59	80.3	0.04	0.19
[A]	671	626	C10-P	0.5	5.4	19.5	30.3	52.1	82.6	0.01	0.47
[A]	673	630	124TMbenz	2.8	4.7	7.4	9.3	12.5	16.4	1.29	4.65
[A]	674	632	C10-P	7.1	12.9	21.4	35.6	81.2	155.1	0.01	0.32
[A]	675	634	C10P	2.6	6.2	12.3	25.2	55.1	102.4	0.01	0.34
[A]	684	648	C10A	5.2	9.3	15.1	22.8	38.2	59.4	0.01	0.3
[A]	688	652	naphthene	4.8	7.5	11	40.2	63.2	93.7	0.03	0.27
[A]	700	662	nC10	7.3	8.9	10.7	14.3	29.5	52.8	0.07	0.29
[A]	705	668	123TMbenz	4	6.3	9.2	18.2	23.2	29.1	0.28	1.15
[A]	708	674	1M4iPrbenz	3	6.6	12.1	22	34.2	50.1	0.01	0.08
[A]	709	676	C11P	5.1	8.9	14.1	34.9	68.2	118.1	0.02	0.12
[A]	712	680	indan	4	6.6	10.1	15.7	23.6	33.8	0.15	0.4
[A]	714	682	sBucyC6	8.7	12.7	17.6	46.7	70.2	100.5	0.01	0.06
[A]	718	686	1M2iPrbenz	4.6	8.4	13.7	48	88.1	146	0.02	0.33
[A]	723	694	C11P	5	7.8	11.4	29.6	60.7	108.3	0.02	0.19
[A]	724	696	13DEbenz	4.6	6.1	8	11.1	19.5	31.5	0.07	0.22
[A]	725	698	1M3Prbenz	3.5	5.2	7.3	8.5	13	18.8	0.18	0.71
[A]	727	702	1M4Prbenz	4.8	7.8	11.7	16.7	22.8	30.2	0.1	0.35
[A]	728	704	Bubenz	7.2	11	16.1	15.8	21.8	29.3	0.04	0.14
[A]	729	706	35DM1EBenz	3.5	6.4	10.5	9.1	14	20.3	0.18	0.56
[A]	730	708	12DEbenz	6.4	9.7	14	38.6	57.4	81.4	0.02	0.09
[A]	740	718	1M2PrBenz	6.8	10.7	15.8	27.3	41.7	60.4	0.06	0.21
[A]	746	722	5MC10	7.1	11.5	17.5	30.8	44.5	61.8	0.02	0.08
[A]	748	724	4MC10	4.2	6.9	10.4	15.3	32.1	57.9	0.01	0.68
[A]	750	726	2MC10	6.5	9.5	13.3	52.7	68.9	88.2	0.02	0.15
[A]	756	730	14DM2Ebenz	4.1	6.1	8.7	17.4	26.3	37.9	0.12	0.42
[A]	758	732	13DM4Ebenz	4.5	6.2	8.3	18.5	22.9	27.8	0.12	0.54
[A]	762	736	3MC10	10.9	15.7	21.7	35.8	54.5	78.8	0.02	0.17
[A]	764	740	12DM4Ebenz+C1indane	3.1	5.3	8.5	8.2	12.5	18.2	0.27	0.75
[A]	768	744	13DM2Ebenz	6.2	9.6	14	37.9	68.9	113.3	0.03	0.35
[A]	780	750	1M4tBubenz	6.1	10.3	16.1	45.8	83.5	137.7	0.03	0.11
[A]	785	752	12DM3Ebenz	4.1	7.3	11.7	28.2	45.3	68.2	0.09	0.2
[A]	800	756	nC11	8.7	11.1	13.9	31.2	40.2	50.6	0.04	0.21
[A]	806	762	1245tertMbenz	5.4	6.8	8.6	12.3	16.8	22.2	0.12	0.39
[A]	810	766	1235tertMbenz	4.7	7.7	11.6	12.7	19.9	29.3	0.16	0.56
[A]	824	782	C11A	8.7	11.3	14.2	32.9	55.6	86.9	0.02	0.07
[A]	826	784	1E2Prbenz?	5	7.5	10.7	14.2	25.2	40.8	0.09	0.44

TABLE A1.2 *Continued*

GC/MS	No. for RR	IHA No.	IHA/ abbreviated Name	r_{min}	r_{est}	r_{max}	R_{min}	R_{est}	R_{max}	C_{min}	C_{max}
[A]	828	786	C11A	8.5	11.8	15.7	23.4	35.1	50.3	0.02	0.1
[A]	830	788	C11A	8.8	12.3	16.7	35.7	49.9	67.5	0.02	0.1
[A]	832	790	C11A	9.7	13.4	17.8	22.9	39.6	63	0.02	0.1
[A]	834	792	1M3Bubenz	5.6	7.9	10.9	11.1	14.8	19.2	0.08	0.35
[A]	836	796	1234tetraMbenz +C11A	6.8	9.3	12.5	24.4	36.5	52.1	0.1	0.28
[A]	840	800	t1M2(4MC5)cyC5	10.2	15.5	22.3	41	56.7	75.8	0.02	0.11
[A]	844	804	C11A	9.1	13.5	19	34	54.7	82.5	0.02	0.07
[A]	846	806	C11A	9.6	13.6	18.5	65.6	96.4	135.5	0.02	0.08
[A]	854	812	1tBu35DMbenz	11.2	15.5	20.7	36.6	62.3	97.7	0.02	0.1
[A]	858	814	naphthalene	4.9	6.7	8.9	15.3	25.8	40.3	0.12	0.52
[A]	862	817	C11A	9.7	14.4	20.5	46.5	66.5	91.4	0.02	0.16
[A]	870	820	16DMINDANE	9	12.3	16.3	25.7	42.6	65.8	0.02	0.17
[A]	875	822	C11A	15.6	19.4	23.8	43.8	68.4	100.9	0.02	0.09
[A]	884	824	2ETHYL INDANE	5.8	9.8	15.4	18.4	29	42.9	0.03	0.19
[A]	888	826	2ETHYL135TMBZ	7.9	12.8	19.5	39.4	59.9	86.6	0.01	0.07
[A]	895	832	nC12	13.4	16.7	20.6	53.4	73.9	99.1	0.02	0.15
[A]	915	842	24DMINDANE	10.3	16.3	24.2	27.2	40	56.2	0.02	0.05
[A]	925	846	1tBu4Ebenz	7.7	13.1	20.7	60.2	101.8	159.2	0.04	0.16
[A]	930	848	13DM INDANE	5.3	10.3	17.9	31.3	43	57.3	0.01	0.18
[A]	940	858	HEXYLbenz	9.8	15.1	21.9	61.2	96	141.8	0.01	0.13
[A]	942	870	2Mnaphthalene	6.4	8.9	12.1	17	21.6	27	0.04	0.64
[A]	947	879	1Mnaphthalene	7.5	11.6	16.9	25	29.8	35.2	0.02	0.27

[A] The components that have been checked by GCMS by one of the participants on one of the samples that was used in the 1996 ASTM round robin.

TABLE A1.3 Group Summaries for the Gasolines Run in the 1996 ASTM Interlaboratory Cooperative Study

Name	r_{min}	r_{est}	r_{max}	R_{min}	R_{est}	R_{max}	C_{min}	C_{max}
Paraffin	0.0562	0.0646	0.08	0.125	0.186	0.373	1	20
Isoparaffin	0.0209	0.024	0.03	0.047	0.065	0.102	20	65
C_2Benzene	0.0334	0.0384	0.05	0.057	0.073	0.102	3	20
Oxygenates	0.0418	0.0491	0.06	0.104	0.141	0.221	3	20

A2. OXYGENATE LINEARITY STUDY

A2.1 This information is presented in Tables A2.1-A2.7 and Figs. A2.1-A2.13.

A2.2 Tables A2.2-A2.7 show comparisons between this test method and other methods for several compound types. Multidimensional PIONA is included since it tends to give reasonable peak compound type groupings for total olefins, total paraffins, and total naphthenes. The differences for benzene and toluene among the indicated methods are well within the reproducibilities of the methods. The sample numbers refer to the interlaboratoy cooperative study samples. It should be noted that the interlaboratory cooperative study samples included only spark ignition fuels and different results may be obtained with pure blending components.

TABLE A2.1 Oxygenates Relative Response Factors

NOTE—All RRF relative to N-C_7= 1.000; this also applies to the cooperative study.

	Laboratory No. 1	Laboratory No. 2	Laboratory No. 3	Laboratory No. 4	Laboratory No. 5	Laboratory No. 6	Laboratory No. 7	Average RRF	Standard Deviation	% Standard Deviation
Methanol	2.921	2.957	2.903	2.795	3.085	3.391	2.923	2.996	.194	6.465
Ethanol	1.997	2.043	2.003	2.057	2.138	2.354	2.014	2.087	.127	6.1
t-butanol	1.274	1.282	1.329	1.305	1.297	1.429	1.2	1.302	.069	5.281
MTBE	1.508	1.523	1.552	1.791	1.508	1.658	1.498	1.577	.109	6.932
ETBE	1.352	1.349	1.406	1.543	1.369	1.509	1.319	1.407	.086	6.108
TAME	1.308	1.323	1.342	1.451	1.336	1.471	1.264	1.356	.076	5.593

TABLE A2.2 Benzene

Sample	Benzene (weight %)	
	D 5580	D 6729
2	1.52	1.61
6	1.05	1.12
8	1.10	1.16
10	1.13	1.18
13	0.14	0.16
14	0.62	0.70
Average	0.93	0.99

TABLE A2.3 Toluene

Sample	Toluene (weight %)	
	D 5580	D 6729
2	4.3	4.6
6	2.1	1.9
8	10.1	11.4
10	5.0	6.1
13	3.3	2.9
14	4.4	5.3
Average	4.9	5.4

TABLE A2.4 Total Aromatics

Sample	Total Aromatics (weight %)		
	D 5580	PIONA[A]	D 6729
2	30.3	28.2	32.6
6	18.9	18.7	20.0
8	49.1	49.0	51.0
10	23.9	24.5	25.4
13	19.7	19.8	22.4
14	23.8	24.6	27.5
Average	27.6	27.5	29.8

[A] Multidimensional PIONA.

TABLE A2.5 Total Olefins

Sample	Total Olefins (weight %)	
	PIONA[A]	D 6729
2	7.1	4.4
6	9.8	9.4
8	6.6	6.2
10	15.1	13.7
13	11.1	11.1
14	24.6	22.2
Average	12.4	11.2

[A] Multidimensional PIONA.

TABLE A2.6 Total Oxygenates

Sample	Total Oxygenates (weight %)	
	PIONA[A]	Procedure B
2[B]	15.3	16.1
6[B]	7.0	8.1
8[B]	4.2	4.5
10[C]	>8	10.0
13[B]	20.5	19.9
14[B]	2.8	3.2
Average	N/A	10.3

[A] Multidimensional PIONA.
[B] Major oxygenate = MTBE.
[C] Major oxygenate = Ethanol.

TABLE A2.7 Total Paraffins and Total Napthenes

Sample	Total Paraffins (weight %)		Total Naphthenes (weight %)	
	PIONA[A]	D 6729	PIONA[A]	D 6729
8	35.6	35.0	2.2	2.8
10	41.1	42.3	5.6	6.7
13	42.6	43.0	1.3	3.5
14	34.1	37.9	5.9	7.6
Average	38.4	39.6	3.8	5.2

[A] Multidimensional PIONA.

Spl(mass%)						Avg RF	RRF
MEOH	1.01	5.05	10.02	20.01	29.83		
	37792	201545	406795	816960	1208524		
	38002	200204	409233	820596	1225686		
avg	37897	200874.5	408014	818778	1217105		
RF	2.67E-05	2.51E-05	2.46E-05	2.44E-05	2.45E-05	2.51E-05	2.920678
Spl(mass%)						Avg RF	RRF
ETOH	1	5	10.1	20.15	30.18		
	56107	288820	604107	1214248	1807248		
	52935	285869	597366	1223531	1830666		
avg	54521	287344.5	600736.5	1218890	1818957		
RF	1.83E-05	1.74E-05	1.68E-05	1.65E-05	1.66E-05	1.71E-05	1.997164
Spl(mass%)						Avg RF	RRF
TBA	0.964	4.9692	9.9583	19.8768	29.7953		
	89751	443262	899170	1830312	2742339		
	92269	441843	893544	1820174	2765568		
avg	91010	442552.5	896357	1825243	2753954		
RF	1.06E-05	1.12E-05	1.11E-05	1.09E-05	1.08E-05	1.09E-05	1.273649
Spl(mass%)						Avg RF	RRF
MTBE	0.9992	5.0362	9.9724	20.0248	30.0471		
	76166	391956	765248	1537935	2332931		
	77640	399654	761273	1535598	2332734		
avg	76903	395805	763260.5	1536767	2332833		
RF	1.3E-05	1.27E-05	1.31E-05	1.3E-05	1.29E-05	1.29E-05	1.507996
Spl(mass%)						Avg RF	RRF
ETBE	0.9851	4.9255	9.8707	19.6724	29.5727		
	86770	420851	852468	1689595	2515456		
	85993	420221	867050	1690395	2506966		
avg	86381.5	420536	859759	1689995	2511211		
RF	1.14E-05	1.17E-05	1.15E-05	1.16E-05	1.18E-05	1.16E-05	1.352309
Spl(mass%)						Avg RF	RRF
TAME	0.9997	4.9788	9.8883	19.153	29.7144		
	90368	443934	876234	1740744	2576420		
	88502	444981	874999	1762466	2584069		
avg	89435	444457.5	875616.5	1751605	2580245		
RF	1.12E-05	1.12E-05	1.13E-05	1.09E-05	1.15E-05	1.12E-05	1.308241
Spl(mass%)						Avg RF	RRF
Nc7	8.475	8.44	8.4525	8.4525	8.695		
	994302	951197	991971	982424	1006023		
	997469	983612	990664	1002009	1006083		
avg	995885.5	967404.5	991317.5	992216.5	1006053		
RF	8.51E-06	8.72E-06	8.53E-06	8.52E-06	8.64E-06	8.58E-06	1

FIG. A2.1 IHA Method Oxygenates Linearity Cooperative Study–Laboratory 1

Spl(mass%)						Avg RF	RRF
MEOH	1.01	5.05	10.02	20.01	29.83		
	44097	236256	478801	985095	1454605		
	44051	237455	480020	992190	1465533		
avg	44074	236855.5	479410.5	988642.5	1460069		
RF	2.29E-05	2.13E-05	2.09E-05	2.02E-05	2.04E-05	2.12E-05	2.956773
Spl(mass%)						Avg RF	RRF
ETOH	1	5	10.1	20.15	30.18		
	63749	332568	698238	1430974	2178293		
	62784	332799	701430	1431363	2204197		
avg	63266.5	332683.5	699834	1431169	2191245		
RF	1.58E-05	1.5E-05	1.44E-05	1.41E-05	1.38E-05	1.46E-05	2.04331
Spl(mass%)						Avg RF	RRF
TBA	0.964	4.9692	9.9583	19.8768	29.7953		
	108001	526541	1055347	2147710	3316200		
	110407	524386	1061356	2163089	3322481		
avg	109204	525463.5	1058352	2155400	3319341		
RF	8.83E-06	9.46E-06	9.41E-06	9.22E-06	8.98E-06	9.18E-06	1.282428
Spl(mass%)						Avg RF	RRF
MTBE	0.9992	5.0362	9.9724	20.0248	30.0471		
	90887	473216	910349	1794640	2777855		
	91715	476896	904173	1794196	2780266		
avg	91301	475056	907261	1794418	2779061		
RF	1.09E-05	1.06E-05	1.1E-05	1.12E-05	1.08E-05	1.09E-05	1.523223
Spl(mass%)						Avg RF	RRF
ETBE	0.9851	4.9255	9.8707	19.6724	29.5727		
	103792	516002	1020170	2007710	2980345		
	104863	518258	1035091	2007448	2983391		
avg	104327.5	517130	1027631	2007579	2981868		
RF	9.44E-06	9.52E-06	9.61E-06	9.8E-06	9.92E-06	9.66E-06	1.349418
Spl(mass%)						Avg RF	RRF
TAME	0.9997	4.9788	9.8883	19.153	29.7144		
	103829	523120	1050222	2077446	3083066		
	104085	517930	1057409	2115710	3084788		
avg	103957	520525	1053816	2096578	3083927		
RF	9.62E-06	9.56E-06	9.38E-06	9.14E-06	9.64E-06	9.47E-06	1.322771
Spl(mass%)						Avg RF	RRF
Nc7	8.475	8.44	8.4525	8.4525	8.695		
	1198960	1190806	1178498	1177607	1195493		
	1198844	1190899	1178015	1176611	1212114		
avg	1198902	1190853	1178257	1177109	1203804		
RF	7.07E-06	7.09E-06	7.17E-06	7.18E-06	7.22E-06	7.15E-06	1

FIG. A2.2 IHA Method Oxygenates Linearity Cooperative Study–Laboratory 2

Spl(mass%)						Avg RF	RRF
MEOH	1.01	5.05	10.02	20.01	29.83		
	151533	864732	1741799	3589766	5293556		
	164863	854798	1759435	3746174	5368227		
avg	158198	859765	1750617	3667970	5330892		
RF	6.38E-06	5.87E-06	5.72E-06	5.46E-06	5.6E-06	5.81E-06	2.903282
Spl(mass%)						Avg RF	RRF
ETOH	1	5	10.1	20.15	30.18		
	245820	1078429	2521533	5099484	7899031		
	257618	1197628	2511218	5200823	8259533		
avg	251719	1138029	2516376	5150154	8079282		
RF	3.97E-06	4.39E-06	4.01E-06	3.91E-06	3.74E-06	4.01E-06	2.002794
Spl(mass%)						Avg RF	RRF
TBA	0.964	4.9692	9.9583	19.8768	29.7953		
	399808	1793750	3184446	7393280	11429736		
	409171	1908282	3579163	7370104	11664000		
avg	404489.5	1851016	3381805	7381692	11546868		
RF	2.38E-06	2.68E-06	2.94E-06	2.69E-06	2.58E-06	2.66E-06	1.32856
Spl(mass%)						Avg RF	RRF
MTBE	0.9992	5.0362	9.9724	20.0248	30.0471		
	353648	1719976	3016380	5400167	9756443		
	365624	1734192	3207775	6049396	9486117		
avg	359636	1727084	3112078	5724782	9621280		
RF	2.78E-06	2.92E-06	3.2E-06	3.5E-06	3.12E-06	3.1E-06	1.55197
Spl(mass%)						Avg RF	RRF
ETBE	0.9851	4.9255	9.8707	19.6724	29.5727		
	368857	1916504	3651460	6366342	8631784		
	370528	1990928	3698002	6858897	9781590		
avg	369692.5	1953716	3674731	6612620	9206687		
RF	2.66E-06	2.52E-06	2.69E-06	2.97E-06	3.21E-06	2.81E-06	1.405891
Spl(mass%)						Avg RF	RRF
TAME	0.9997	4.9788	9.8883	19.153	29.7144		
	373564	1867693	3846963	7398715	9605677		
	364642	1876735	4016568	7511412	10394700		
avg	369103	1872214	3931766	7455064	10000189		
RF	2.71E-06	2.66E-06	2.51E-06	2.57E-06	2.97E-06	2.68E-06	1.342326
Spl(mass%)						Avg RF	RRF
Nc7	8.475	8.44	8.4525	8.4525	8.695		
	3E+06	4E+06	312404	4E+06	4E+06		
	4E+06	4E+06	4E+06	5E+06	4E+06		
avg	3691763	4064455	2253742	4516374	4371883		
RF	2.3E-06	2.08E-06	3.75E-06	1.87E-06	1.99E-06	2E-06	1

FIG. A2.3 IHA Method Oxygenates Linearity Cooperative Study–Laboratory 3

Spl(mass%)						Avg RF	RRF
MEOH	1.01	5.05	10.02	20.01	29.83		
	658639	3389850	6670376	13542502	18749414		
	601443	3019715	6368637	13051539	17165160		
avg	630041	3204783	6519507	13297021	17957287		
RF	1.6E-06	1.58E-06	1.54E-06	1.5E-06	1.66E-06	1.58E-06	2.794957
Spl(mass%)						Avg RF	RRF
ETOH	1	5	10.1	20.15	30.18		
	826854	4450557	9154374	18060524	28066595		
	734856	4082467	8580584	17505672	28072314		
avg	780855	4266512	8867479	17783098	28069455		
RF	1.28E-06	1.17E-06	1.14E-06	1.13E-06	1.08E-06	1.16E-06	2.056683
Spl(mass%)						Avg RF	RRF
TBA	0.964	4.9692	9.9583	19.8768	29.7953		
	1578407	4266396	14460028	29135138	43225116		
	1435170	6337881	13565261	27794630	42612348		
avg	1506789	5302139	14012645	28464884	42918732		
RF	6.4E-07	9.37E-07	7.11E-07	6.98E-07	6.94E-07	7.36E-07	1.305022
Spl(mass%)						Avg RF	RRF
MTBE	0.9992	5.0362	9.9724	20.0248	30.0471		
	1252485	5941164	10848222	17786018	23089928		
	1255790	6142349	10162313	17011562	22404206		
avg	1254138	6041757	10505268	17398790	22747067		
RF	7.97E-07	8.34E-07	9.49E-07	1.15E-06	1.32E-06	1.01E-06	1.791283
Spl(mass%)						Avg RF	RRF
ETBE	0.9851	4.9255	9.8707	19.6724	29.5727		
	1310455	6926229	12417871	20398546	27031106		
	1306372	7052557	12595757	19329114	26122426		
avg	1308414	6989393	12506814	19863830	26576766		
RF	7.53E-07	7.05E-07	7.89E-07	9.9E-07	1.11E-06	8.7E-07	1.542526
Spl(mass%)						Avg RF	RRF
TAME	0.9997	4.9788	9.8883	19.153	29.7144		
	1400316	6820054	13673677	22152636	28646506		
	1357511	6857019	13936737	22286660	27439076		
avg	1378914	6838537	13805207	22219648	28042791		
RF	7.25E-07	7.28E-07	7.16E-07	8.62E-07	1.06E-06	8.18E-07	1.450677
Spl(mass%)						Avg RF	RRF
Nc7	8.475	8.44	8.4525	8.4525	8.695		
	15260819	15252480	14899327	15397626	14345822		
	14816484	14876828	14956987	15670374	15233576		
avg	15038652	15064654	14928157	15534000	14789699		
RF	5.64E-07	5.6E-07	5.66E-07	5.44E-07	5.88E-07	5.64E-07	1

FIG. A2.4 IHA Method Oxygenate Linearity Cooperative Study–Laboratory 4

Spl(mass%)						Avg RF	RRF
MEOH	1.01	5.05	10.02	20.01	29.83		
avg	130.85	729.625	1474.483	3103.843	4600.484		
RF	0.007719	0.006921	0.006796	0.006447	0.006484	0.006873	3.08498
Spl(mass%)						Avg RF	RRF
ETOH	1	5	10.1	20.15	30.18		
avg	195.402	1054.59	2115.254	4301.374	6707.759		
RF	0.005118	0.004741	0.004775	0.004685	0.004499	0.004763	2.138015
Spl(mass%)						Avg RF	RRF
TBA	0.964	4.9692	9.9583	19.8768	29.7953		
avg	347.107	1725.706	3442.236	6695.103	10183.1		
RF	0.002777	0.00288	0.002893	0.002969	0.002926	0.002889	1.296638
Spl(mass%)						Avg RF	RRF
MTBE	0.9992	5.0362	9.9724	20.0248	30.0471		
avg	290.368	1518.529	3008.79	6043.303	8800.898		
RF	0.003441	0.003316	0.003314	0.003314	0.003414	0.00336	1.508054
Spl(mass%)						Avg RF	RRF
ETBE	0.9851	4.9255	9.8707	19.6724	29.5727		
avg	308.613	1630.908	3253.559	6580.098	9806.89		
RF	0.003192	0.00302	0.003034	0.00299	0.003016	0.00305	1.369041
Spl(mass%)						Avg RF	RRF
TAME	0.9997	4.9788	9.8883	19.153	29.7144		
avg	322.928	1631.466	3351.751	6693.316	10161.7		
RF	0.003096	0.003052	0.00295	0.002862	0.002924	0.002977	1.336026
Spl(mass%)						Avg RF	RRF
Nc7	8.475	8.44	8.4525	8.4525	8.695		
avg	3915.73	3733.39	3714.828	3835.85	3889.013		
RF	0.002164	0.002261	0.002275	0.002204	0.002236	0.002228	1
note: average area counts are the average of two runs							

FIG. A2.5 IHA Method Oxygenate Linearity Cooperative Study–Laboratory 5

Spl(mass%)						Avg RF	RRF
MEOH	1.01	5.05	10.02	20.01	29.83		
avg	128.825	795.291	1607.186	3383.189	5800.591		
RF	0.00784	0.00635	0.006234	0.005915	0.005143	0.006296	3.390586
Spl(mass%)						Avg RF	RRF
ETOH	1	5	10.1	20.15	30.18		
avg	212.988	1149.503	2305.626	4688.498	7300.836		
RF	0.004695	0.00435	0.004381	0.004298	0.004134	0.004371	2.354003
Spl(mass%)						Avg RF	RRF
TBA	0.964	4.9692	9.9583	19.8768	29.7953		
avg	378.347	1881.019	3752.037	7297.662	11045.72		
RF	0.002548	0.002642	0.002654	0.002724	0.002697	0.002653	1.428645
Spl(mass%)						Avg RF	RRF
MTBE	0.9992	5.0362	9.9724	20.0248	30.0471		
avg	316.501	1655.196	3279.581	6587.2	9660.288		
RF	0.003157	0.003043	0.003041	0.00304	0.00311	0.003078	1.657594
Spl(mass%)						Avg RF	RRF
ETBE	0.9851	4.9255	9.8707	19.6724	29.5727		
avg	336.388	1777.69	3546.379	7172.307	10609.51		
RF	0.002928	0.002771	0.002783	0.002743	0.002787	0.002803	1.509178
Spl(mass%)						Avg RF	RRF
TAME	0.9997	4.9788	9.8883	19.153	29.7144		
avg	351.991	1778.298	3653.409	7295.715	11076.25		
RF	0.00284	0.0028	0.002707	0.002625	0.002683	0.002731	1.47059
Spl(mass%)						Avg RF	RRF
Nc7	8.475	8.44	8.4525	8.4525	8.695		
avg	4698.033	4477.402	4454.942	4601.379	4665.706		
RF	0.001804	0.001885	0.001897	0.001837	0.001864	0.001857	1
note: average area counts are an average of three runs							

FIG. A2.6 IHA Method Oxygenate Linearity Cooperative Study–Laboratory 6

Spl(mass%)						Avg RF	RRF
MEOH	1.01	5.05	10.02	20.01	29.83		
	35419	207968	408281	807253	1208115		
	36040	195967	408281	874729	1301947		
avg	35729.5	201967.5	408281	840991	1255031		
RF	2.83E-05	2.5E-05	2.45E-05	2.38E-05	2.38E-05	2.51E-05	2.922508
Spl(mass%)						Avg RF	RRF
ETOH	1	5	10.1	20.15	30.18		
	45510	292874	642031	1234541	1824287		
	50885	281463	594198	1259869	2005196		
avg	48197.5	287168.5	618114.5	1247205	1914742		
RF	2.07E-05	1.74E-05	1.63E-05	1.62E-05	1.58E-05	1.73E-05	2.014392
Spl(mass%)						Avg RF	RRF
TBA	0.964	4.9692	9.9583	19.8768	29.7953		
	93315	475528	979360	2031219	2865032		
	102421	476914	888766	1840517	2928378		
avg	97868	476221	934063	1935868	2896705		
RF	9.85E-06	1.04E-05	1.07E-05	1.03E-05	1.03E-05	1.03E-05	1.200454
Spl(mass%)						Avg RF	RRF
MTBE	0.9992	5.0362	9.9724	20.0248	30.0471		
	75952	405208	705631	1548681	2380261		
	77415	417553	757750	1580147	2408423		
avg	76683.5	411380.5	731690.5	1564414	2394342		
RF	1.3E-05	1.22E-05	1.36E-05	1.28E-05	1.25E-05	1.29E-05	1.497693
Spl(mass%)						Avg RF	RRF
ETBE	0.9851	4.9255	9.8707	19.6724	29.5727		
	83107	436772	890514	1713524	2609194		
	85993	442601	917344	1720724	2604325		
avg	84550	439686.5	903929	1717124	2606760		
RF	1.17E-05	1.12E-05	1.09E-05	1.15E-05	1.13E-05	1.13E-05	1.31875
Spl(mass%)						Avg RF	RRF
TAME	0.9997	4.9788	9.8883	19.153	29.7144		
	89539	455171	900734	1836776	2713677		
	90145	461944	915196	1883508	2658665		
avg	89842	458557.5	907965	1860142	2686171		
RF	1.11E-05	1.09E-05	1.09E-05	1.03E-05	1.11E-05	1.08E-05	1.264195
Spl(mass%)	20%	5%	1%	10%	30%	Avg RF	RRF
Nc7	8.475	8.44	8.4525	8.4525	8.695		
	1034198	1392371	989383	983168	1077830		
	889948	935398	1051329	1067382	1010624		
avg	962073	1163885	1020356	1025275	1044227		
RF	8.81E-06	7.25E-06	8.28E-06	8.24E-06	8.33E-06	8.18E-06	1

FIG. A2.7 IHA Method Oxygenate Linearity Cooperative Study–Laboratory 7

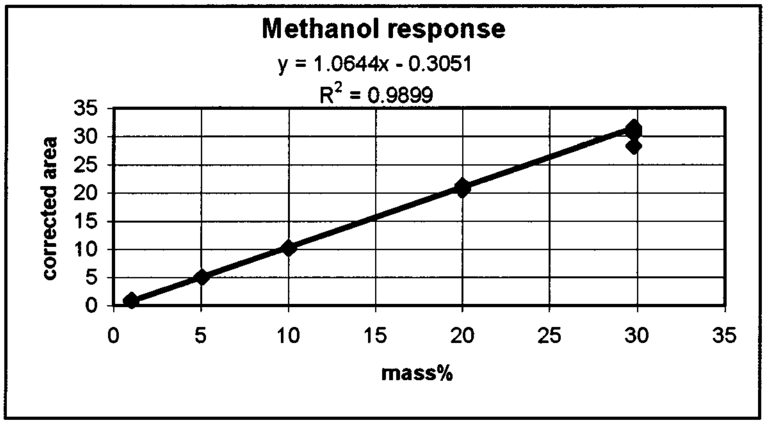

FIG. A2.8 Determination of Calculated Oxygenate Response from IHA Method–Methanol

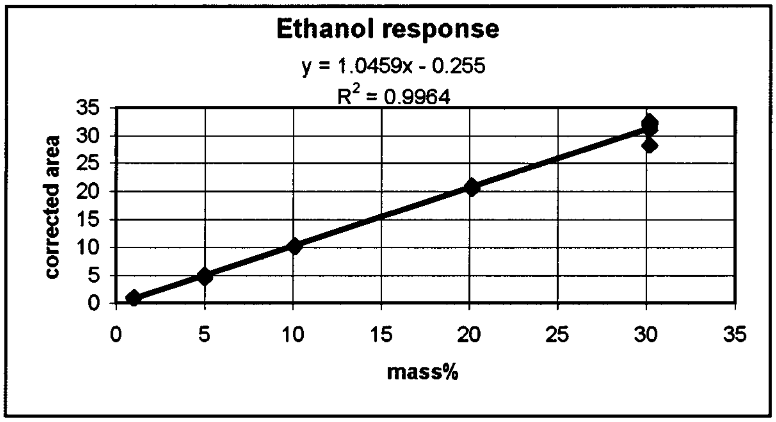

FIG. A2.9 Determination of Calculated Oxygenate Response from IHA Method–Ethanol

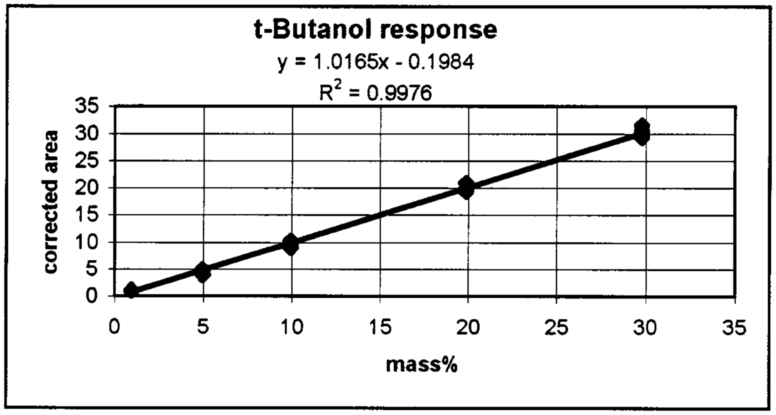

FIG. A2.10 Determination of Calculated Oxygenate Response from IHA Method–t-Butanol

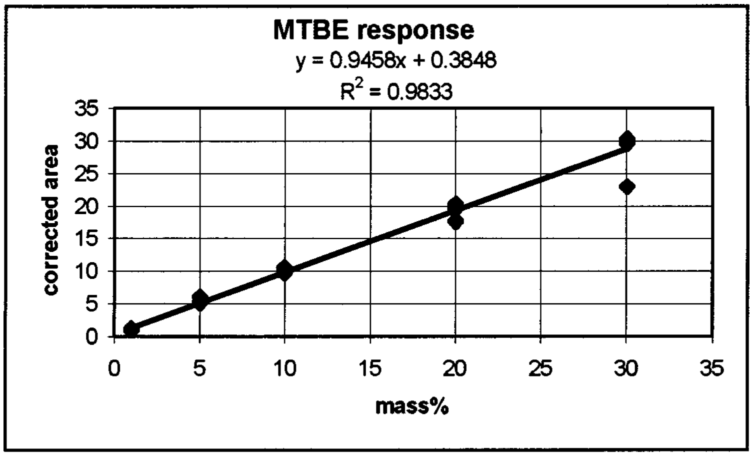

FIG. A2.11 Determination of Calculated Oxygenate Response from IHA Method–MTBE

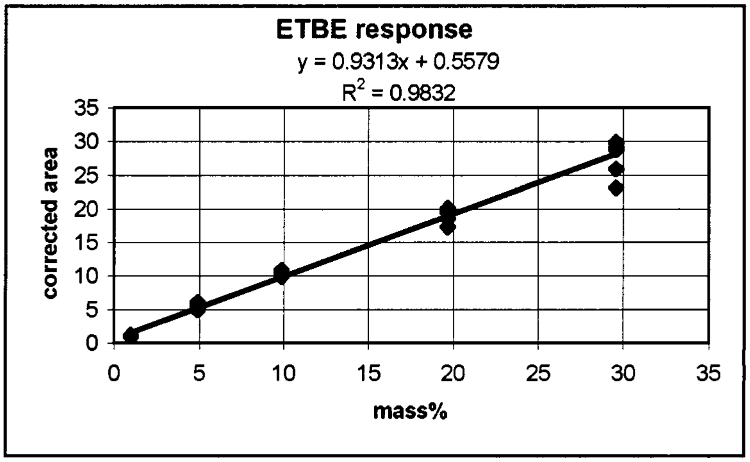

FIG. A2.12 Determination of Calculated Oxygenate Response from IHA Method–ETBE

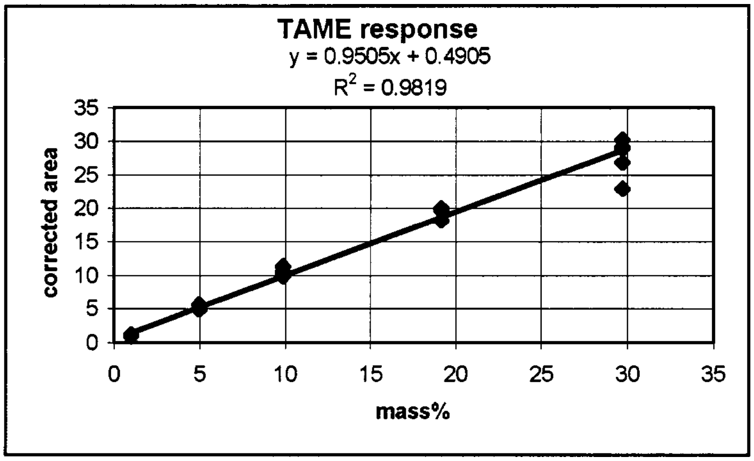

FIG. A2.13 Determination of Calculated Oxygenate Response from IHA Method–TAME

APPENDIX

(Nonmandatory Information)

X1. BIBLIOGRAPHY

X1.1 The following publications on DHA analyses may be useful as background and are recommended to the user of these test procedures:

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X1.1.3 Kopp, V.R., Bones, C.J., Doerr, D.G., Ho, S.P., and Schubert, A.J., "Heavy Hydrocarbon/Volatility Study: Fuel Blending and Analysis for the Auto/Oil Air Quality Improvement Research Program," SAE Paper No. 930143, March 1993

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