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An American National Standard

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

This standard is issued under the fixed designation D 6623; 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.

INTRODUCTION

This test method consists of three individual procedures designated as A, B, and C. Procedure A (Detailed Hydrocarbon Analysis-DHA) was the first procedure submitted to be tested and developed by ASTM. Procedure B (Individual Hydrocarbon Analysis-IHA) is derived from the revised Canadian CAN/CGSB-3.0 No. 14-3-94 test method. Procedure C (DHC) is derived and is consistent with the French Standard NF M07-086. Procedures A and B employ 100 metre poly (dimethyl) siloxane open tubular capillary columns and procedure C employs a 50 metre poly (dimethyl) siloxane capillary column. In addition, Procedure A requires the use of a short precolumn (injector end) located in the GC oven and connected to the 100 metre capillary column. The precolumn is used to optimize separation selectivity. Similar samples were used to obtain the precision statements for Procedures A and B while the precision for Procedure C was obtained with a different sample set. All three procedures used similar ASTM approved statistical procedures for the calculation of the precision statements. Although the three procedures share similar instrumentation requirements and practice of the gas chromatographic art, the scope as indicated, apparatus description, reagents and materials, system optimization, calibration, calculation and precision sections are presented separately for each procedure to allow the user to perform effectively each procedure as practiced in the original interlaboratory cooperative study. It is very important that the user of this test method specify clearly which procedure (A, B, or C) was used when comparing results with other laboratories or reporting results. Appendix X1 of this test method contains comparison data for Procedures A and B for several interlaboratory cooperative study samples with other types of test methods for several selected oxygenates and hydrocarbon types. Comparison data for Procedure C is not available since it used a different set of gasolines in the round robin.

1. Scope

1.1 *Procedures A and B*:

1.1.1 Test Procedures A and B provide for 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.

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

1.1.3 Test Procedures A and B also determine 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 in Procedure B only.

1.1.4 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, or both (for example, virgin naphthas) constituents above *N*-octane may reflect significant errors in PONA type

[1] This test method is under the jurisdiction of ASTM Committee D02 on Petroleum Products and Lubricants and is the direct responsibility of Subcommittee D.02.04.0L on Hydrocarbon Analysis.

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groupings. Based on the gasoline samples in the interlaboratory cooperative study, these procedures are applicable to concentrations of olefins to less than 25 mass %. However, some interfering coelution with the olefins above C7 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. Appendix X1 of this test method compares results of the test procedures 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 analysis can be obtained by using the specific test methods listed in the reference section.

1.1.4.1 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 multidimentional PONA type of instruments.

1.1.5 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 Test Method D 5623 for sulfur compounds or equivalent.

1.2 *Procedure C*:

1.2.1 Test Procedure C provides for the determination of individual hydrocarbon components of spark-ignition engine fuels 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. The tables related to Procedure C enumerate the components reported. Component concentrations are determined in the range of 0.10 to 15 mass %. The procedure may be applicable to higher and lower concentrations for the individual components; however, the user shall verify the accuracy if the procedures are used for components with concentrations outside the specified ranges.

1.2.2 This test method is applicable also to spark-ignition engine fuel blends containing oxygenated components. However, in this case, the oxygenate content shall be determined by Test Methods D 5599 or D 4815.

1.2.3 Benzene co-elutes with 1-methylcyclopentene. Benzene content shall be determined by Test Method D 3606 or D 5580.

1.2.4 Toluene co-elutes with 2,3,3-trimethylpentane. Toluene content shall be determined by Test Method D 3606 or D 5580.

1.2.5 Although a majority of the individual hydrocarbons present are determined, some co-elution of compounds is encountered. If this procedure 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 (for example, cracked naphthas) or naphthenic, or both (for example, virgin naphthas) constituents above *N*-octane may reflect significant errors in PONA type groupings. Based on the interlaboratory cooperative study, this procedure is applicable to concentrations of olefins to less than 20 mass %. However, some interfering coelution with the olefins above normal heptane 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. Since many of the olefins in spark ignition fuels are at a concentration below 0.10 %, they are not reported by this test method and may bias the total olefin results low.

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

1.2.6 If water is or is suspected of being present, its concentration may be determined, if desired, by the use of Test Method D 1744. Other compounds containing 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 Method D 5623 for sulfur compounds.

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

1.4 *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 3606 Test Method for Determination of Benzene and Toluene in Finished Motor and Aviation Gasoline by Gas Chromatography[4]

D 3700 Practice for Containing Hydrocarbon Fluid Samples Using a Floating Piston Cylinder[4]

D 4057 Practice for Manual Sampling of Petroleum and Petroleum Products[4]

D 4177 Practice for Automatic Sampling of Petroleum and Petroleum Products[4]

D 4307 Practice for Preparation of Liquid Blends for Use as Analytical Standards[4]

D 4420 Test Method for Aromatics in Finished Gasoline by Gas Chromatography[4]

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

[3] Discontinued; see 2000 *Annual Book of ASTM Standards*, Vol 05.01.

[4] *Annual Book of ASTM Standards*, Vol 05.02.

D 4626 Practice for Calculation of Gas Chromatographic Response Factors[4]
D 4815 Test Method for Determination of MTBE, ETBE, TAME, DIPE, *tertiary*-Amyl Alcohol and C_1 to C_4 Alcohols in Gasoline by Gas Chromatography[4]
D 5580 Test Method for Determination of Benzene, Toluene, Ethylbenzene, *p/m*-Xylene, *o*-Xylene, C_9 and Heavier Aromatics and Total Aromatics in Finished Gasoline by Gas Chromatography[5]
D 5599 Test Method for Determination of Oxygenates in Gasoline by Gas Chromatography and Oxygen Selective Flame Ionization Detection[5]
D 5623 Test Method for Sulfur Compounds in Light Petroleum Liquids by Gas Chromatography and Sulfur Selective Detection[5]
E 355 Practice for Gas Chromatography Terms and Relationships[6]
E 594 Practice for Testing Flame Ionization Detectors Used in Gas or Supercritical Fluid Chromatography[6]
E 1510 Practice for Installing Fused Silica Open Tubular Capillary Columns in Gas Chromatographs[6]

2.2 *Other Standard:*

CAN/CGSB-3.0 No. 14-3-99 Test Method for Individual Hydrocarbon Component Analysis (IHA) in Spark Ignition Engine Fuels by Gas Chromatography[7]

3. Terminology

3.1 *Definitions:*

3.1.1 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 specified stationary phase(s). 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 those 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. In Procedures A and B, the unknown components are reported individually as well as a summary total.

5. Significance and Use

5.1 Knowledge of the 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.

PROCEDURE A – DETAILED HYDROCARBON ANALYSIS

6. Apparatus

6.1 *Gas Chromatograph*— Instrumentation capable of column oven temperature programming, from subambient (5°C) to at least 200°C, in 0.1°C/min or less rate increments, is required. Multi-step column oven temperature programming is required, consisting of an initial hold time, an initial temperature program followed by an isothermal temperature hold and another programmed temperature rise. A heated flash vaporizing injector designed to provide a linear sample split injection (that is, 200:1) is required for proper sample introduction. The associated carrier gas controls must be of sufficient precision to provide reproducible column flows and split ratios in order to maintain analytical integrity. A hydrogen flame ionization detector, with associated gas controls and electronics, designed for optimum response with open tubular columns, shall conform to the specifications as described in Practice E 594, as well as having an operating temperature range of up to at least 250°C.

6.2 *Sample Introduction*—Manual or automatic liquid sample injection to the splitting injector may be employed. Micro-syringes, auto-syringe samplers, or valves capable of 0.1 to 0.5 µL injections are suitable. It should be noted that some syringes and improper injection techniques as well as inadequate splitter design could result in sample fractionation. This must be determined in accordance with Section 10.

6.3 *Electronic Integrator*—Any electronic integration device used for quantitating these analyses shall meet or exceed these minimum requirements:

6.3.1 Capacity to handle 400 or more peaks each analysis.

6.3.2 Normalized area percent calculation with response factors.

6.3.3 Noise and spike rejection.

6.3.4 Accurate area determination of fast (1 to 2 s) peaks (10 Hz or greater sampling rate).

6.3.5 Maintain peak detection sensitivity for narrow and broad peaks.

6.3.6 Positive and negative sloping baseline correction.

6.3.7 Perpendicular drop and tangent skimming as needed.

6.3.8 Display of baseline used to ensure correct peak area determination.

6.4 *Open Tubular Column*—The column used for this test method consists of a primary (100 m) analytical column and a precolumn. The ability to provide the required component separations is dependent on the precise control of the column selectivity, which is typically slightly more than that exhibited by current commercially available columns. Some older columns, and columns that have a sample residue from repeated use without conditioning, may exhibit the required selectivity. Until adequate columns are commercially available, the currently used dimethylpolysiloxane columns can be modified or *tuned* to meet the method column specifications. See Section

[5] *Annual Book of ASTM Standards*, Vol 05.03.
[6] *Annual Book of ASTM Standards*, Vol 14.02.
[7] Available from Canadian General Standards Board (CGSB), Ottawa, Canada K1A 1G6, Methods of Testing Petroleum and Associated Products.

10 for a description of the column specifications and Annex A1 for a description of the column modification procedure.

6.4.1 The primary gas chromatographic column used for this test method will meet the following specifications.

Column Specifications:
Material
fus
Ed silica
Length
10
0 metres
Internal diameter
0.2
5 millimetre
Liquid phase
di
Methylpolysiloxane
Film thickness
0.5
0 micrometre
Theoretical plates, n, pentane at 35°C
~
400 000 to 500 000
Retention Factor, k, pentane at 35°C
0.4
5 to 0.50
Resolution, R, *t*-butanol and 2-methylbutene-2 at 35°C
3.2
5 to 5.25
Peak Symmetry, *t*-butanol at 35°C
>
1.0 to < 5.0

6.4.2 *Precolumn*—A variable length (1 to 4 metres) of 5 % phenyl methyl silicone fused silica open tubular column (0.25 mm inside diameter) is added to the front (injector) end of the 100 m column, as described in Annex A1.

7. Reagents and Materials

7.1 *Carrier Gas*—Helium, 99.999 % pure. (**Warning**—Helium, air, nitrogen, compressed gas under high pressure.)

7.2 *Oxidant*—Air, 99.999 % pure. (**Warning**—see 7.1).

7.3 *Detector Makeup Gas*—Nitrogen, 99.999 % pure. (**Warning**—see 7.1).

7.4 *Fuel Gas*—Hydrogen, 99.999 % pure. (**Warning**—Hydrogen, flammable gas under high pressure.)

7.5 *Reference Standards*:

7.5.1 *Purity of Reagents*—Reagent grade chemicals shall be used in all tests. Unless otherwise indicated, it is intended that all reagents conform to the specifications of the Committee on Analytical Reagents of the American Chemical Society[8] where such specifications are available. Other grades may be used, provided it is first ascertained that the reagent is of sufficiently high purity to permit its use without lessening the accuracy of the determination.

7.5.2 *Methanol*—(**Warning**—These materials are flammable and may be harmful or fatal, if ingested or inhaled.)

7.5.3 *Ethanol*—Only absolute ethanol of 99.5 minimum % meets the requirements of this test method. (**Warning**—see 7.5.2).

7.5.4 *Hydrocarbon and Other Component References*—Individual and mixed component reference materials are commercially available and may be used to establish qualitative and quantitative calibration. (**Warning**—see 7.5.2).

7.5.5 *System and Column Evaluation Mixture*—A quantitatively prepared mixture, complying with Practice D 4307, of individual hydrocarbons and oxygenates of interest is used for system and column evaluation. (**Warning**—7.5.2). Fig. 1 is a chromatogram of the recommended mixture in Table 1.

8. Sampling

8.1 Hydrocarbon liquids with Reid vapor pressures of 110 kPa (16 psi) or less may be sampled either into a floating piston cylinder or into an open container (Test Methods D 4057 and D 4177). If the sample as received does not meet the upper boiling range requirements of 1.1.1, it may be necessary to extend the analysis time and raise the upper column temperature of this test method to ensure complete elution of higher boiling range sample material from the column.

8.1.1 *Piston Cylinder Sampling*—Refer to Practice D 3700 for instructions on transferring a representative sample of a hydrocarbon fluid from a source into a floating piston cylinder. Add inert gas to the ballast side of the floating piston cylinder to achieve a pressure of 350 kPa (45 psi) above the vapor pressure of the sample.

8.1.2 *Open Container Sampling*—Refer to Practice D 4057 for instructions on manual sampling from bulk storage into open containers. Stopper the container immediately after taking a sample.

8.2 Preserve the sample by cooling to approximately 4°C and maintaining that temperature prior to analysis.

8.3 Transfer an aliquot of the cooled sample to a pre-cooled septum vial and seal immediately.

8.4 Obtain the test specimen for analysis directly from the sealed septum vial, for either manual or automatic injection.

9. Preparation of Apparatus

9.1 Install the 100m column and, if required, a precolumn in accordance with the manufacturer's or supplier's instructions and Annex A1. See Practice E 1510 for recommended installation procedures.

9.2 Determine the required length of the precolumn in accordance with Annex A1. Adjust the operating conditions of the gas chromatograph to those listed in Table 2 or as determined by Section 12 and Annex A1.

9.3 During setup and when not performing analyses it is advisable to turn off the cryogenic operation and set the column oven temperature at 35°C. Attach the column outlet to the flame ionization detector inlet and check for leaks throughout the system. If leaks are found, tighten or replace fittings before proceeding.

9.4 Confirm or adjust, or both, the column carrier gas flow rate by making injections of methane or natural gas. *The methane retention time shall be 7.00 ± 0.02 min with the column oven temperature at 35°C*, which results in an average linear velocity of 24 cm/s, as determined using Eq 1. This will result in a methane retention time of 6.53 min at 5°C. Raising or lowering the carrier gas pressure to the injector makes flow rate adjustment. A starting point of 277 kPa (40 psig) helium

[8] *Reagent Chemicals, American Chemical Society Specifications*, American Chemical Society, Washington, DC. For suggestions on the testing of reagents not listed by the American Chemical Society, see *Analar Standards for Laboratory Chemicals*, BDH Ltd., Poole, Dorset, U.K., and the *United States Pharmacopeia and National Formulary*, U.S. Pharmaceutical Convention, Inc. (USPC), Rockville, MD.

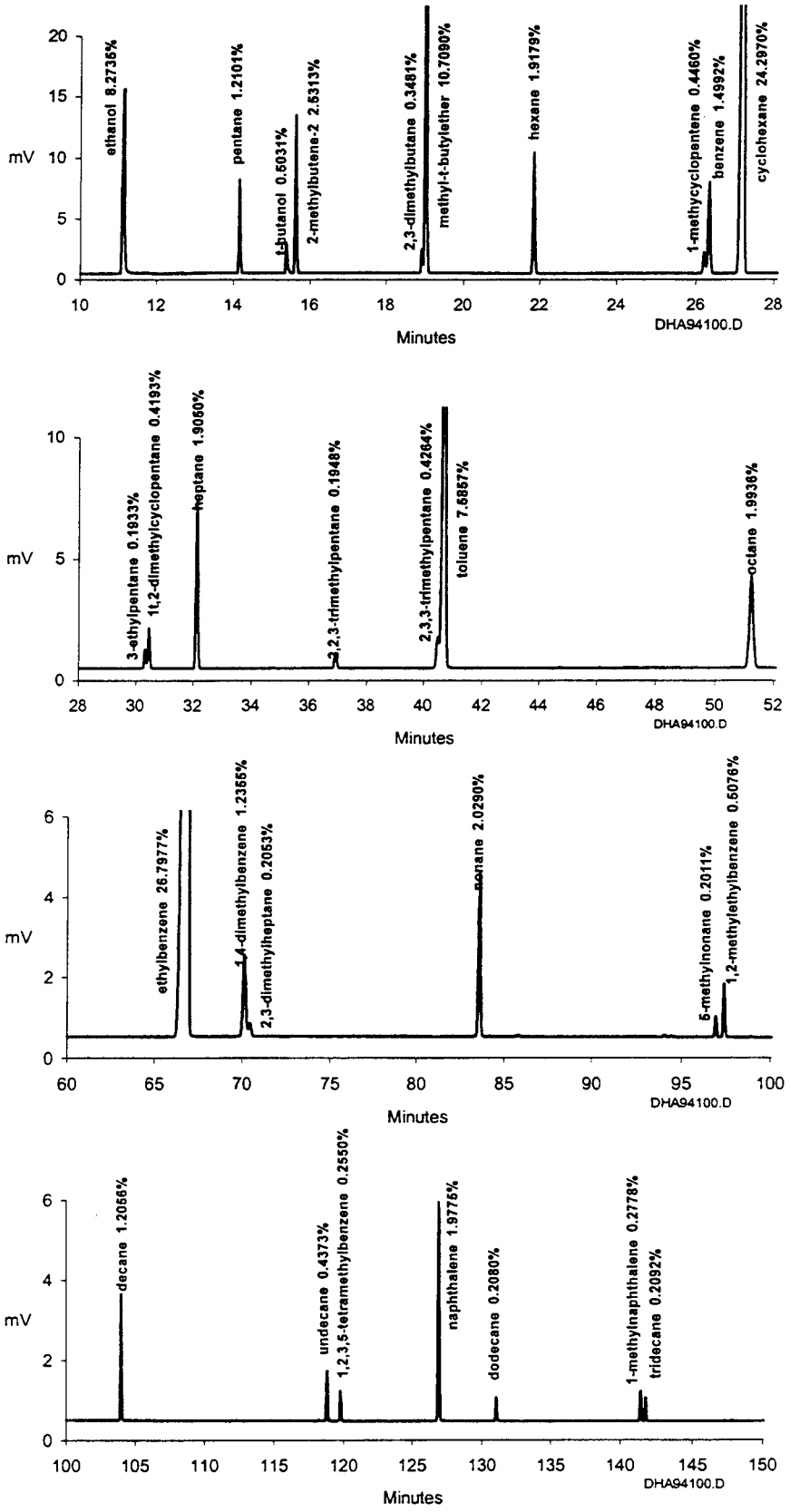


FIG. 1 DHA Speciation Analysis - System and Column Evaluation Mixture

TABLE 1 System and Column Evaluation Mixture (mass%)

Ethanol	8.00 %	*N*-octane	2.00 %
N-pentane	2.00 %	ethylbenzene	25.00 %
t-butanol	0.50 %	p-xylene	1.00 %
2-methylbutene-2	2.50 %	2,3-dimethylheptane	0.20 %
2,3-dimethylbutane	0.50 %	*N*-nonane	2.00 %
methyl-t-butyl ether	10.00 %	5-methylnonane	0.20 %
N-hexane	2.00 %	1-methyl-2-ethylbenzene	0.50 %
1-methylcyclopentene	0.50 %	*N*-decane	1.00 %
benzene	1.00 %	*N*-undecane	0.50 %
cyclohexane	28.90 %	1,2,3,5-tetramethylbenzene	0.25 %
3-ethylpentane	0.20 %	naphthalene	0.50 %
1,2t-dimethylcyclopentane	0.50 %	*N*-dodecane	0.25 %
N-heptane	2.00 %	1-methylnaphthalene	0.25 %
2,3,3-trimethylpentane	0.50 %	*N*-tridecane	0.25 %
toluene	7.00 %		

TABLE 2 Gas Chromatograph Operating Conditions

Column Temperature Program	
Initial temperature	5°C
Initial time	10 min
First program rate	5.0°/min
First hold temperature	50°C
First hold time	to the elution of ethylbenzene (~50 min.)
Second program rate	1.5°/min
Final temperature	200°C
Final hold time	5 min
Injector	
Temperature	250°C
Split ratio	150:1
Sample size	0.1-0.2 µL
Detector	
Type	flame ionization
Temperature	250°C
[A]Fuel gas	hydrogen at 30 mL/min
Oxidant	air at 300 mL/min
Make-up gas, where required	nitrogen at 20 mL/min
Carrier Gas	
Type	helium
Pressure	~277 kPa (40 psig)
Average linear velocity	24 cm/s at 35°C

[A] Use manufacturer's recommended detector gas flows or:

pressure is recommended, although columns requiring as high as 332 kPa (48 psig) helium have been encountered.

$$\text{average linear gas velocity: } u_{ave}\ (\text{cm/s}) = \text{column length (cm)}/t_{M(s)} \quad (1)$$

9.5 After final adjustment of the carrier gas flow rate, note the carrier gas inlet pressure. Measure and, if necessary, readjust the injector split flow rate to give the specified or desired split ratio. Calculate the column outlet flow rate using 9.5.1 and the split ratio using 9.5.2.

9.5.1 *Column Carrier Gas Flow Rate (at outlet)*:

where:
P = (head pressure (psig) + ambient pressure)/ambient pressure,
j = compressibility factor = $3/2((P^2 - 1)/(P^3 - 1))$,
u_o = u_{ave}/j = column outlet velocity,
A_c = $\text{pi}(r)^2$ = column cross-sectional area (cm^2),

where:
r = column internal radius (cm), and
flow rate (cm^3/min) = $u_o \times A_c \times 60$.

9.5.2 *Injection Split Ratio*—(split flow rate + column flow rate)/column flow rate (Section 7).

9.5.3 *Example*—Using a 100 m × 0.25 mm capillary column:

where:
u_{ave} = $100 \times 100/6.98 \times 60 = 23.88$ cm/s,
P = 40psig + 12.0/12.0 = 4.33,
j = 3/2((18.778-1)/(81.370-1)) = 0.33,
u_o = 23.88/0.33 = 71.96 cm/s,
A_c = $\text{pi}(0.025/2)^2 = 4.9 \times 10^{-4}\text{cm}^2$,
flow rate = $71.96 \times 4.9 \times 10^{-4} \times 60 = 2.12\ \text{cm}^3$/min., and
split ratio = (192 + 2.12)/2.12 = 91.6:1.

9.6 Make a blank analysis (no sample injection) run to ensure proper instrument operation and further condition the column and instrumentation. If stray peaks or a rising baseline signal is observed, the column oven shall be kept at the upper temperature until the baseline becomes steady and returns to within approximately 5 % of the starting temperature detector signal.

9.7 After any extended conditioning period, or if the instrument has been shut down, it is advisable to repeat 9.4, 9.5, and 9.6 to ensure proper carrier gas flows are being used and the column is clean.

10. Split Injection Linearity

10.1 Splitting injector linearity must be established to determine proper quantitative parameters and limits. The split ratio used is dependent upon the split linearity characteristics of the particular injector and the sample retention factor of the column. The retention factor of a particular column for a sample component is proportional to the amount of liquid phase (loading or film thickness) and the ratio of the column temperature to the component boiling point (vapor pressure). Overloading of the column may cause loss of resolution for some components and, since overloaded peaks are skewed, variance in retention times. This can lead to erroneous component identification. During column evaluations and split linearity studies, be aware of any peaks that may appear front skewed, indicating column overload. Note the component size and avoid conditions leading to this problem during actual analyses.

10.2 Set the injector temperature and split ratio to the values in Fig. 2 and for each set of conditions inject the listed quantities of the System and Column Evaluation Mixture (see 7.5.5), using the operating conditions listed in Table 2 or as determined in Section 12.

10.3 Compare the calculated concentrations to the known standard concentrations after calculating the corrected area normalization using the response factors from 13.2.

$$\%\ \text{relative error} = 100 \times (\textit{concentration determined} - \textit{concentration known})/\text{concentration known} \quad (2)$$

10.4 Report and use only those combinations of conditions from 10.2 that result in 3 % or less relative error. This is the splitter linearity range.

11. Column Evaluation

11.1 In order to establish that a column will perform as required, the following specifications shall be determined for

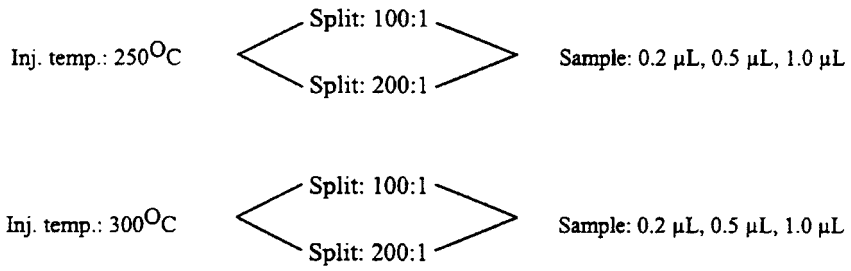


FIG. 2 Split Ratio Values

new column acceptability and are useful for periodic evaluation of column deterioration. These specification determinations can be made with or without a precolumn, since the precolumn will have little effect on their values. See Annex A1, Figure A1.1, for examples of these determinations. After performing the steps in Sections 9 and 10, analyze the column performance mixture (7.5.5) at 35°C isothermal, at least through heptane. The remainder of the analysis may be ignored, but the remaining components must be eluted from the column prior to performing another analysis. Setting the column temperature to 220°C for an additional 20 min will be sufficient.

11.2 Calculate the retention factor (k) for pentane at 35°C:

$$k = (t_R - t_M)/t_M \quad (3)$$

where:
t_M = gas holdup time (methane), and
t_R = retention time for pentane, min.

The retention factor must be between 0.45 and 0.50 for proper application of this test method.

11.3 Calculate the column efficiency using the pentane peak:

$$n = 5.545\,(t_R/w^1_{\frac{1}{2}h})^2 \quad (4)$$

where:
n = column efficiency (theoretical plates),
t_R = retention time of pentane, and
$w^{1}/_{2}h$ = peak width at half height.

The column efficiency must be at least 400 000 plates for proper application of this test method.

11.4 The selectivity of apparently identical columns toward hydrocarbons may vary regarding oxygenated compounds, either due to extraneous materials in the liquid phase, or due to activity of the column wall surface. The addition of a precolumn has little, if any, affect on the selectivity toward oxygenates (see Annex A1, Fig. A1.4). The relative resolution of oxygenates is inherent to the quality of the primary 100 m column, and is specified by the resolution of t-butanol from 2-methylbutene-2 at 35°C. Calculate the resolution:

$$R = 2(t_{R2-M-Butene-2} - t_{R_{TBA}})/1.699(w^1_{\frac{1}{2}h_{2-M-Butene-2}} + w^1_{\frac{1}{2}h_{TBA}}) \quad (5)$$

The resolution for this pair at 35°C must be between 3.25 and 5.25.

11.5 Extraneous column effects or instrumental effects, such as an active injector liner, may cause adsorption of oxygenated compounds commonly seen and referred to as *tailing*, and may increase their retention. If this effect is caused by instrumental activity the problem should be corrected. If the column is inherently active, a new column should be obtained. A measure of the tailing can be made and specified by applying a *skewness* calculation, which determines a ratio of the distances from the peak apex perpendicular to the front and back of the peak at 5 % of the peak height. See Annex A1, Fig. A1.3 for an example of this calculation.

$$\text{skewness} = B/A \quad (6)$$

This test shall be made using the *t*-butanol peak (0.5 %) in the analysis of the column performance mixture (7.5.5) at 35°C isothermal. The skewness ratio must be greater than 1.0 and not more than 5.0.

12. Optimization of Instrument Operating Conditions

12.1 The column temperature programming profile is dependent upon the individual column characteristics. Table 2 lists the programming profile determined for a 100 m methyl silicone column with a precolumn as determined in Annex A1. The profile is determined by establishing satisfactory separations for the sets of sample components listed in 12.3. It is not practical to expect complete separation of all components, so the optimum for each column may contain some compromises, also dependent upon any particular other separations deemed important.

12.2 The use of retention indices to numerically express the relative location of components among themselves and to surrounding normal paraffins is a convenient convention. The indices are also useful in providing a system of component identification with complex analyses such as this. There are several schemes for calculating retention indices, the first of which is the Kovats method, developed to express the logarithmic relationship of retention times of a homologous series of compounds when chromatographed isothermally. While this test method is not an isothermal column temperature procedure, it does contain isothermal steps and the longer temperature program step is a slow rate. The use of the Kovats indices provides a closer relationship to previous work in this field than using the linear index format.

12.2.1 The formula for the calculation of Kovats retention indices is:

$$RI_i = 100 \times (n + (\log(t_i) - \log(t_n))/(\log(t_{n+1}) - \log(t_n))) \quad (7)$$

where:
RI = retention index,
n = carbon number of *N*-paraffin,
t_i = retention time of component,
t_n = retention time of preceding *N*-paraffin, and
t_{n+1} = retention time of next *N*-paraffin.

12.3 The following examples show the key or critical

separations required for this analysis. Typical retention indices are given, and a description of the effect of instrumental conditions on the separation is provided.

12.3.1 *i-butane/methanol and ethanol/3-methyl-butene-1*—The initial starting temperature of 5°C is dictated by these separations. A lower starting temperature is not necessary and a higher temperature would effect the next set. The retention indices should be about 380 for methanol and 456.5 for ethanol. See Fig. 3.

12.3.2 *i-propanol/2-methylbutene-1* and *t-butanol/2-methylbutene-2*—*i*-propanol will appear resolved between pentene-1 and 2-methyl-butene-1, *t*-butanol will appear resolved between c-pentene-2 and 2-methylbutene-2. See Fig. 4.

12.3.2.1 Higher temperatures will move the alcohols into the peaks ahead of them. At 35°C the alcohols will be located ahead of the pentene-1 and *c*-pentene-2, respectively.

12.3.3 *2,3-dimethylbutane/methyl-t-butylether*—This separation is critical and the 5°C hold for 10 min determines its success. The retention indices should be about 569.5, 571.5, and 574.0 for 2,3-dimethylbutane, MTBE, and 2-methylpentane, respectively. If the MTBE is too close to the 2,3-DMC_4, use a 9 min initial hold. If too close to the 2-MC_5, use an 11 min hold. See Fig. 5.

12.3.4 *1-methylcyclopentene/benzene*—This is a key separation that is used to specify the column selectivity. Changing column temperature produces only slight differences in this resolution. See Fig. 6.

12.3.4.1 The 50°C column temperature is held isothermal until the elution of ethylbenzene. This is variable due to slight differences in the column retention factor.

12.3.5 *2,3,3-trimethylpentane/toluene*—This is a key separation that is used to specify the column selectivity. Column temperature has very little effect on this resolution, which is controlled by the column selectivity for aromatics. See Fig. 7.

12.3.6 *p-xylene/2,3-dimethylheptane*—This is a key separation which limits the maximum length of the precolumn. If the column selectivity is too great the aromatics are retained and this separation is not achieved. If this resolution is excessive and the separation in 12.3.5 is insufficient, the precolumn should be lengthened slightly. Lowering the 50°C hold temperature to 48°C will increase this separation. See Fig. 8.

12.3.7 *I17 (unknown)/1,2-methylethylbenzene*—The unknown isoparaffin (I17) appears to be a component of alkylate and must be resolved from the aromatic. If the resolution is incomplete, the final column temperature program rate of 1.5°/min. is adjusted to provide sufficient separation. Increase the rate in 0.1°/min. increments to increase the resolution. This rate is also dictated by the separation requirements in 12.3.8. The proper rate will provide for both separations. See Fig. 9.

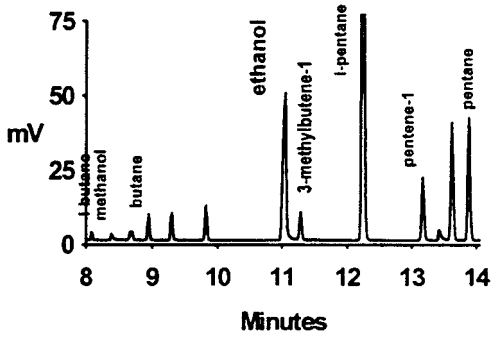


FIG. 3 Separation of i-butane/methanol and ethanol/3–methyl-butene-1

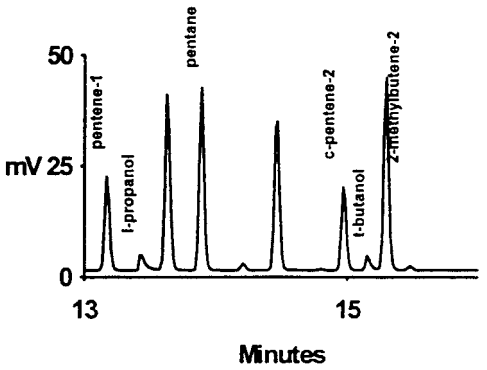


FIG. 4 Separation of i-propanol/2–methylbutene-1 and t-butanol/2–methylbutene-2

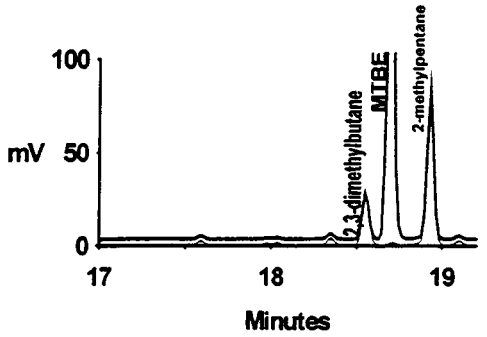


FIG. 5 Separation Between 2,3–dimethylbutane and methyl-t-butylether

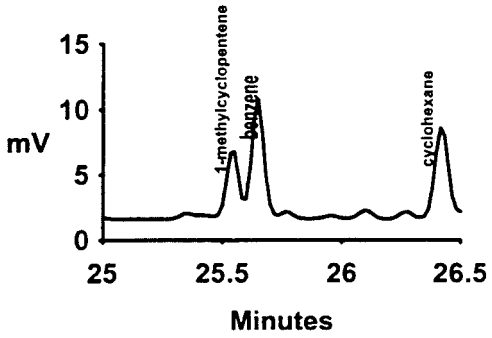


FIG. 6 Separation Between 1–methylcyclopentene and benzene

12.3.8 *1-methylnaphthalene/tridecane*—The recommended final column temperature program rate of 1.5°/min. should also provide this separation. If the 1-MeNaph/*N*-C_{13} resolution is incomplete, this rate may be adjusted to provide sufficient separation. Lower the rate in 0.1°/min. increments to increase the resolution. See Fig. 10.

13. Calibration

13.1 *Qualitative*—Determine the retention times of components by analyzing known reference mixtures or samples under identical conditions. Calculate retention indices from these data using 12.2. Table A1.1 provides a listing of typical values for this test method.

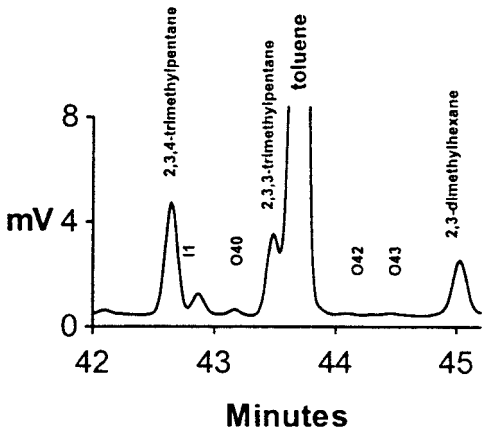


FIG. 7 Separation Between 2, 3, 3–trimethylpentane and toluene

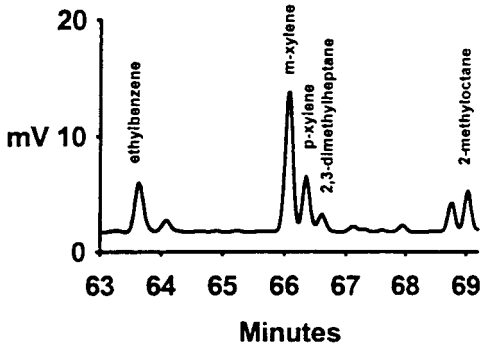


FIG. 8 Separation Between p-xylene and 2,3–dimethylheptane

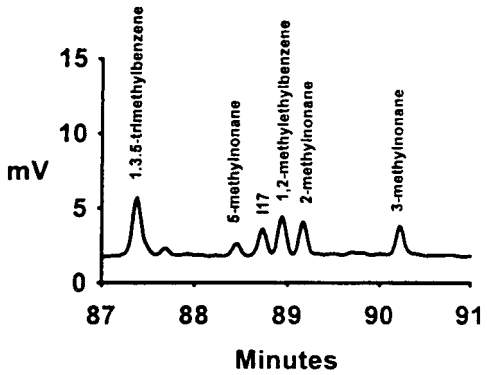


FIG. 9 Separation Between Unknown isoparaffin (I17) and 1,2–methylethylbenzene

13.2 *Quantitative, Hydrocarbons*—Use theoretical response factors for correction of the detector response of hydrocarbons determined by this test method, unless response factors have been determined experimentally. The response of an FID to hydrocarbons is determined by the ratio of the molecular weight of the carbon in the analyte to the total molecular weight of the analyte. If experimentally determined response factors are to be used they must be determined using known purity individual standards and calculated using Practice D 4626. The response factors, as listed in Table 3, are relative to that calculated for heptane. Calculations are based on the following equation:

$$F_i = ((((C_{aw} \times C_n) + (H_{aw} \times H_n))/C_n) \times 0.83905)/C_{aw} \quad (8)$$

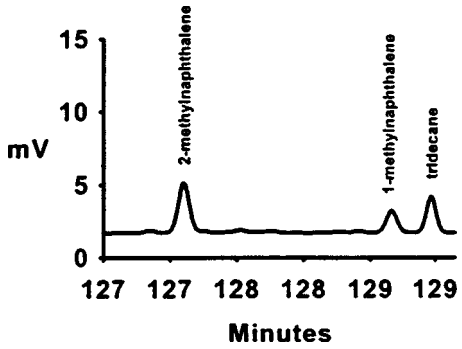


FIG. 10 Separation Between 1–methylnaphthalene and tridecane

TABLE 3 Theoretical FID Relative Response Factors

Carbon Number	Saturated Aromatics Paraffins	Unsaturated Paraffins	Saturated Naphthenes	Unsaturated Naphthenes	
1	1.1207	-	-	-	-
2	1.0503	-	-	-	-
3	1.0268	0.9799	-	-	-
4	1.0151	0.9799	-	-	-
5	1.0080	0.9799	0.9799	0.9517	-
6	1.0034	0.9799	0.9799	0.9564	0.9095
7	1.0000	0.9799	0.9799	0.9598	0.9195
8	0.9975	0.9799	0.9799	0.9623	0.9271
9	0.9955	0.9799	0.9799	0.9642	0.9329
10	0.9940	0.9799	0.9799	0.9658	0.9376
11	0.9927	0.9799	0.9799	0.9671	0.9415
12	0.9916	0.9799	0.9799	0.9681	0.9447
13	0.9907	0.9799	0.9799	0.9690	0.9474
14	0.9899	0.9799	0.9799	0.9698	0.9497
15	0.9893	0.9799	0.9799	0.9705	0.9517

where:

F_i = relative response factor for a hydrocarbon type group of a particular carbon number,
C_{aw} = atomic weight of carbon, 12.011,
C_n = number of carbon molecules in the group,
H_{aw} = atomic weight of hydrogen, 1.008,
H_n = number of hydrogen molecules in the group,
0.83905 = the correction factor with heptane as unity (1.0000), and
0.7487 = used with methane as unity.

13.3 *Quantitative, Oxygenates*—Determine response factors for methanol, ethanol, and other oxygenated compounds experimentally. The principles in Practice D 4626 should be applied when determining these response factors. The response of the flame ionization detector for oxygenated compounds is not directly (theoretically) related to mass concentration. A study has indicated that the FID response is linear for the conditions of this test method (see Fig. 11). Each individual apparatus must be calibrated using gravimetrically prepared standards, covering the sample concentration ranges expected and the scope of this method. Standards used must comply with the requirements in Section 7. Fig. 11 and Fig. 12 presents calibration data for six oxygenates as determined in a preliminary cooperative study report for calibration of this test method. Precision data will be prepared when more data becomes available.

14. Sample Analysis Procedure

14.1 Adjust the instrument operating variables to the values

Oxygenates Relative Response Factors

	Lab1	Lab 2	Lab 3	Lab4	Ave.	Std. Dev	%SD	Auto/Oil RRF
Methanol	3.0760	3.0477	2.9779	2.9230	3.0062	0.0691	2.30	3.0965
Ethanol	2.1888	2.0797	2.1755	2.0640	2.1270	0.0642	3.02	2.0953
t-Butanol	1.2975	1.3189	1.3312	1.2989	1.3116	0.0163	1.24	1.3368
MTBE	1.5279	1.5590	1.4860	1.5024	1.5188	0.0318	2.09	1.5016
ETBE	1.3848	1.3720	1.3804	1.3720	1.3773	0.0064	0.46	1.4032
TAME	1.3383	1.2993	1.3598	1.3340	1.3329	0.0250	1.88	1.3775

DHA Method Oxygenate Linearity Cooperative Study - peak area

Laboratory 4

Spl							Ave. RF	RRF
MeOH	0.0100	1.0100	5.0500	10.0200	20.0100	29.8300		
	0.4037	34.7643	174.8862	340.9069	717.4781	1046.1427		
	0.3599	33.8017	179.9043	353.4087	717.1507	980.1586		
ave.	0.3818	34.2830	177.3953	347.1578	717.3144	1013.1496		
RF	0.0262	0.0295	0.0285	0.0289	0.0279	0.0294	0.0288	2.9230
EtOH	0.0100	1.0000	5.0000	10.1000	20.1500	30.1800		
	0.2883	50.5190	237.7223	495.9717	987.7886	1526.2755		
	0.4095	46.7438	242.3003	500.4514	1007.0434	1537.3776		
ave.	0.3489	48.6314	240.0113	498.2116	987.4161	1531.8265		
RF	0.0287	0.0206	0.0208	0.0203	0.0204	0.0197	0.0204	2.0640
TBA	0.0099	0.9640	4.9692	9.9583	19.8768	29.7953		
	1.0363	77.5423	408.5969	757.2307	1546.4197	2241.0530		
	1.1869	72.7672	392.8649	775.5192	1550.7498	2346.4085		
ave.	1.1116	75.1548	400.7309	766.3749	1548.5847	2293.7307		
RF	0.0089	0.0128	0.0124	0.0130	0.0128	0.0130	0.0128	1.2989
MTBE	0.0100	0.9992	5.0362	9.9724	20.0248	30.0471		
	0.7645	66.0865	345.4606	713.3773	1332.2089	2041.1591		
	0.5690	65.8994	325.8215	679.7792	1348.4042	2052.4822		
ave.	0.6767	65.9929	335.6411	696.5783	1340.3055	2046.8206		
RF	0.0148	0.0151	0.0150	0.0143	0.0149	0.0147	0.0148	1.5024
ETBE	0.0099	0.9851	4.9255	9.8707	19.6724	29.5727		
	0.4527	69.3251	374.3939	732.8740	1537.9746	2144.9023		
	0.6242	72.7316	374.7065	695.3345	1462.4055	2173.4412		
ave.	0.5384	71.0283	374.5502	714.1042	1500.1901	2159.1718		
RF	0.0183	0.0139	0.0132	0.0138	0.0131	0.0137	0.0135	1.3720
TAME	0.0100	0.9997	4.9788	9.8883	19.1530	29.7144		
	0.3702	75.3456	363.7452	762.9970	1488.8628	2346.1907		
	0.0072	75.1503	380.0280	763.6254	1420.3514	2230.3657		
ave.	0.1887	75.2480	371.8866	763.3112	1454.6070	2288.2782		
RF	0.0530	0.0133	0.0134	0.0130	0.0132	0.0130	0.0132	1.3340
C6	8.5050	8.4750	8.4400	8.4525	8.4525	8.6950		
	890.3467	843.5383	836.5459	803.1739	843.6532	847.7344		
	847.7681	854.2333	840.8679	834.8488	841.6083	802.3011		
ave.	869.0574	848.8858	838.7069	819.0113	842.6307	825.0177		
RF	0.0098	0.0100	0.0101	0.0103	0.0100	0.0105	0.0101	1.0262
C7	8.5050	8.4750	8.4400	8.4525	8.4525	8.6950		
	893.5123	847.7426	868.0640	834.6944	880.9965	869.8032		
	846.4708	858.0901	862.0443	871.7571	882.1653	834.0419		
ave.	869.9916	852.9164	865.0541	853.2258	881.5809	851.8225		
RF	0.0098	0.0099	0.0098	0.0099	0.0096	0.0102	0.0099	1.0000
C8	8.5050	8.4750	8.4400	8.4525	8.4525	8.6950		
	889.7205	846.6591	877.1065	838.8929	890.2631	873.8851		
	839.2188	855.2006	852.7846	884.2601	895.4804	854.5747		
ave.	864.4697	850.9298	869.9455	861.5765	892.8718	864.2299		
RF	0.0098	0.0100	0.0097	0.0098	0.0095	0.0101	0.0098	0.9944
C9	8.5050	8.4750	8.4400	8.4525	8.4525	8.6950		
	883.5337	843.1968	870.7139	832.1808	883.3178	868.7531		
	829.0626	849.0969	854.1742	881.9661	889.9074	860.0512		
ave.	856.2982	846.1469	862.4440	857.0734	886.6126	864.4021		
RF	0.0099	0.0100	0.0098	0.0099	0.0095	0.0101	0.0099	1.0003

FIG. 11 Determination of Oxygenate Response - DHA Speciation Analysis

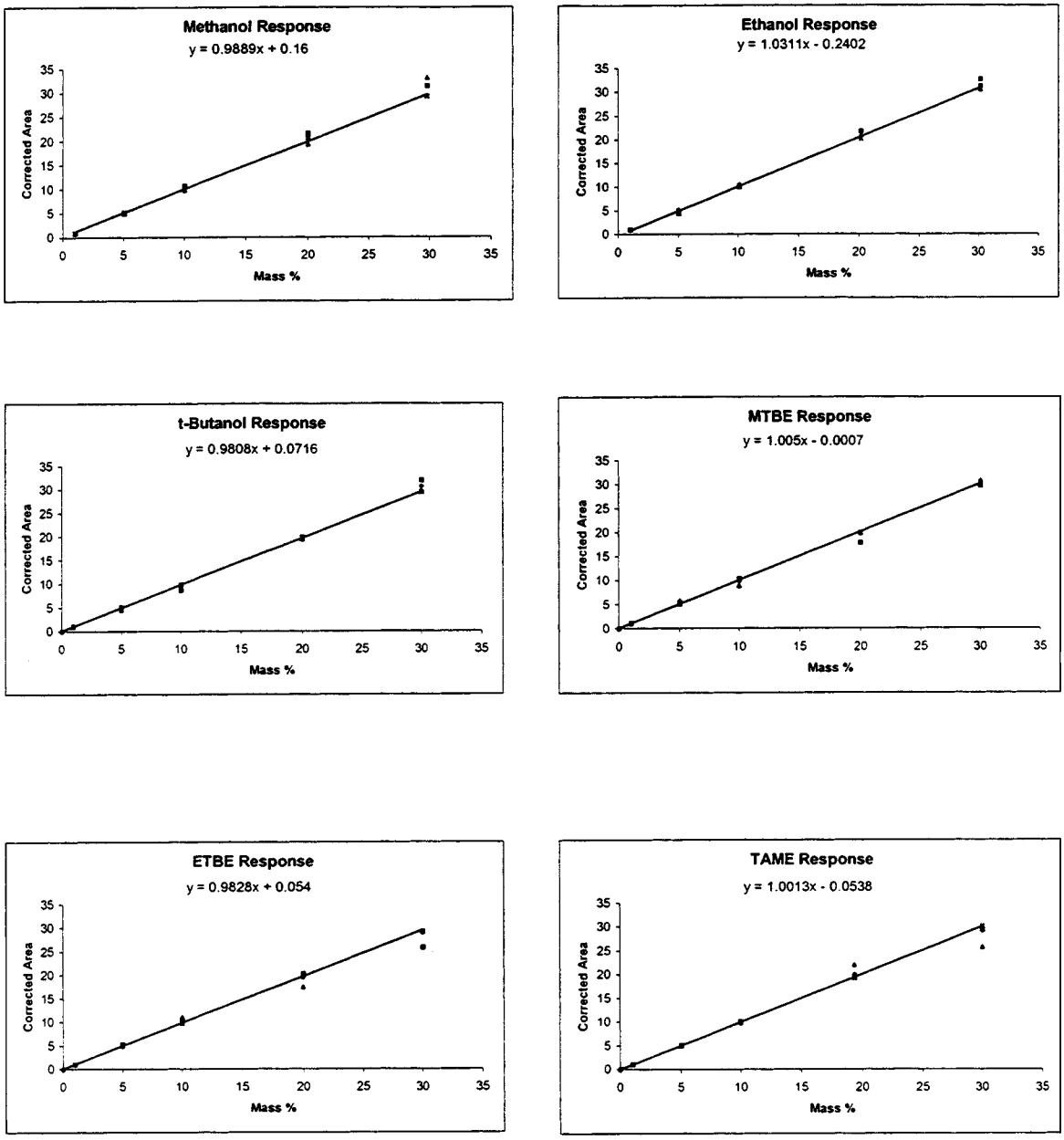


FIG. 12 Determination of Oxygenate Response for Procedure A — Speciation Analysis

specified in Table 2 or as determined in Section 12.

14.2 Set the recorder and/or integration device for accurate presentation and collection of the data.

14.3 Inject an appropriate size sample (as determined in Section 10) into the injection port and start the analysis. Obtain a chromatogram and a peak integration report.

15. Calculation of Results

15.1 Identify each peak by matching retention indices (or retention times) with those for known reference standards or sample components. If a computing integrator is used, examine the chromatographic data for proper peak integration. Examine the report to ensure peaks are properly identified.

15.1.1 Proper component identification using retention indices requires the use of *windows* surrounding each retention index (RI) value in order to account for the analysis to analysis variations. The following windows have been found to provide satisfactory identification for this test method.

Indices	Window
100 - 300	± 15
300 - 400	± 2.6
400 - 500	± 1.5
500 - 885	± 0.6
885 - 900	± 0.5
> 900	± 0.6

15.2 Obtain the area for each peak. Multiply each peak area by its appropriate response factor, taken from Table 3 or determined separately with standards, to obtain corrected peak areas. Use a response factor of 1.000 for unknown peaks.

15.3 If required, determine the concentration of water in the sample using Test Method D 1744, or an equivalent method. The total concentration of any other materials not determined by this test method should also be obtained.

15.4 The corrected peak areas are normalized to 100 % or to 100 % minus the concentrations determined in 15.3.

component % (m/m) = corrected peak area × (100 – % undetected)/total corrected peak area

16. Expression of Results

16.1 Report the concentration of each component as mass percent, % (m/m), to the nearest 0.001 % (m/m).

16.2 These individual component data may be 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 calculation of other properties of petroleum liquids. See the warning in 5.3.

17. Precision and Bias [9]

17.1 *Repeatability*— The difference in two test results obtained by the same operator with the same apparatus in a given laboratory under constant operating conditions on test samples taken from the same laboratory sample should, in the long run, in the normal and correct operation of the test method not exceed the values given in Table 4 and Table 5 for the gasoline components.

17.2 *Reproducibility*— The difference between two single and independent measurements on test samples taken from the same bulk sample should, in the long run, in the normal and correct operation of the test method, not exceed the values given in Table 4 and Table 5 for the gasoline components.

17.3 *Bias*—No information can be presented on the bias of the procedure in Test Method D 6623 for measuring hydrocarbon concentrations because no material having an accepted reference value is available.

18. Keywords

18.1 detailed hydrocarbon analysis; DHA; DHC; gas chromatography; hydrocarbons; IHA; open tubular column; oxygenates; PIANO; PONA

[9] Supporting data describing the interlaboratory cooperative study to determine precision has been filed at ASTM headquarters and may be obtained by requesting research report RR:D02-1505.

TABLE 4 Repeatability and Reproducibility of DHA Determinations

NOTE 1—The following is a partial list of precision data which has been prepared by statisticians of CS94 in accordance with research report RR:D02-1007, and represents their best estimate of the cooperative study data. The complete precision data set appears in Annex A1, Table A1.3.

NOTE 2—For each analyte to qualify for a precision statement, it must be present in at least six samples, and detected by at least six labs, at least once. 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.

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} – for reproducibility
C_{min} – lower concentration limit that r_{est}, R_{est} is applicable
C_{max} – upper concentration limit that r_{est}, R_{est} is applicable

Component	Ave. RI	r_{min}	r_{est}	r_{max}	R_{min}	R_{est}	R_{max}	C_{min}	C_{max}
n-butane	400.00	6.8	9.9	13.9	15.3	32.4	59.1	1.02	3.75
i-pentane	477.45	5.9	7.2	8.7	8.5	14.8	23.8	2.48	13.38
pentene-1	490.83	5.2	7.5	10.5	9.7	13.8	19	0.06	0.43
n-pentane	500.00	5.2	6.5	8.1	7.1	10.4	14.8	1.06	3.49
cyclopentane	566.84	3.8	4.9	6.2	7	10.1	14	0.07	0.59
2,3-dimethylbutane	569.24	2.9	3.2	3.5	5.1	8.5	13.1	0.7	1.91
n-hexane	600.00	2	2.4	2.9	3.6	5.1	6.9	0.33	2.52
methylcyclopentane	625.86	2.2	2.6	3.1	4.5	6.4	8.7	0.37	2.35
1-methylcyclopentene	648.71	1.9	2.7	3.7	7.9	8.7	9.6	0.17	0.82
benzene	649.92	2.6	3.6	4.8	5.5	9	13.7	0.17	1.58
cyclohexane	657.81	2.7	3.7	4.9	8.2	14.8	24.3	0.07	0.9
2-methylhexane	667.61	1.6	2.2	2.9	5.1	6.1	7.2	0.39	1.09
2,2,4-trimethylpentane	688.48	2.4	3.2	4.1	7.4	11.4	16.7	0.1	11.26
n-heptane	700.00	2.5	3.4	4.5	7.7	10.8	14.7	0.21	1.06
methylcyclohexane	717.89	2.8	3.4	4	4.1	5.9	8.2	0.11	1.2
2,3,4-trimethylpentane	746.83	2.3	3.8	6	5.8	7.8	10.3	0.08	4.26
toluene	751.77	1.9	2.7	3.8	10.8	13.5	16.5	1.99	10.34
2-methylheptane	764.14	3.5	4.9	6.6	4.8	6.1	7.5	0.15	0.63
n-octane	800.00	2.2	3.6	5.5	6.5	15.7	30.9	0.14	0.75
ethylbenzene	854.65	2.2	3.2	4.4	7.2	10.6	14.9	0.62	2.62
1,3-dimethylbenzene	864.22	2.6	3.3	4.2	9.7	12.5	15.7	1.55	6.66
3-methyloctane	880.24	5.1	8.5	13	8.7	15.5	24.9	0.07	0.29
n-nonane	900.20	3.9	6.4	9.8	8.6	10.3	12.2	0.06	0.34
n-propylbenzene	946.33	2.8	5	8.1	7.6	11.9	17.7	0.21	0.77
1,4-methylethylbenzene	956.22	3.5	5.3	7.7	5.1	7.7	11.1	0.32	1.19
1,3,5-trimethylbenzene	961.92	3.7	5.5	7.7	5.4	8.3	12.1	0.39	1.21
2-methylnonane	971.77	6.5	10.6	16.2	17.5	25.9	36.6	0.03	0.19
1,2,4-trimethylbenzene	983.40	4.2	5.7	7.5	7.8	10.6	13.9	1.19	4.32
n-decane	1000.20	7.5	9.2	11.1	12.1	17.9	25.3	0.03	0.25
1,2,3-trimethylbenzene	1006.88	3.8	5.8	8.5	7.2	8.5	10	0.28	0.96
n-undecane	1100.00	8.6	13.9	21	24.4	40	61.2	0.03	0.18
1,2,3,5-tetramethylbenzene	1108.79	6.4	7.8	9.3	10.2	13.9	18.3	0.21	0.51
naphthalene	1168.01	6.1	8.5	11.3	12.9	16.9	21.5	0.13	0.4
n-dodecane	1200.00	12.2	16.7	22.1	20.2	32.9	50	0.01	0.11
2-methylnaphthalene	1282.57	7.6	11.1	15.4	17.5	22.3	28	0.05	0.5

TABLE 5 Repeatability and Reproducibility of DHA Determinations

NOTE 1—The following data has been prepared by statisticians of CS94 in accordance with RR:D02-1007, and represents their best estimate of the cooperative study data. Not all of the data qualified for this evaluation since:
(a) For each analyte to qualify for a precision statement, it must be present in at least six samples, and detected by at least six labs, at least once.
(b) 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.

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} – for reproducibility
C_{min} – lower concentration limit that r_{est}, R_{est} is applicable
C_{max} – upper concentration limit that r_{est}, R_{est} is applicable

Component	Ave. RI	r_{min}	r_{est}	r_{max}	R_{min}	R_{est}	R_{max}	C_{min}	C_{max}
i-butane	366.15	5.6	10.1	16.4	22.8	46.1	81.5	0.06	0.38
butene-1	390.72	6.4	11.1	17.6	31.2	64.5	115.8	0.01	0.14
n-butane	400.00	6.8	9.9	13.9	15.3	32.4	59.1	1.02	3.75
2,2-dimethylpropane	415.10	3.3	8.8	18.6	32.1	50.1	73.7	0.01	0.02
i-pentane	477.45	5.9	7.2	8.7	8.5	14.8	23.8	2.48	13.38
pentene-1	490.83	5.2	7.5	10.5	9.7	13.8	19.0	0.06	0.43
2-methylbutene-1	496.66	4.9	6.9	9.4	8.3	12.9	19.0	0.14	0.86
n-pentane	500.00	5.2	6.5	8.1	7.1	10.4	14.8	1.06	3.49
t-pentene-2	510.56	4.5	6.5	9.0	7.2	10.3	14.4	0.28	1.16
c-pentene-2	519.53	4.7	6.3	8.1	7.6	13.2	20.9	0.16	0.63
2-methylbutene-2	524.92	4.3	6.0	8.1	7.8	11.4	15.9	0.50	1.85
1t,3-pentadiene	527.97	6.7	14.0	25.3	17.0	25.3	35.9	0.01	0.06
2,2-dimethylbutane	540.54	3.1	4.7	6.8	6.4	9.9	14.6	0.08	2.18
cyclopentene	557.21	4.0	5.8	8.1	7.6	10.5	13.9	0.07	0.27
4-methylpentene-1	562.02	2.7	4.2	6.1	8.9	11.3	14.0	0.02	0.09
3-methylpentene-1	562.81	3.5	5.0	6.9	6.1	8.8	12.0	0.03	0.12
cyclopentane	566.84	3.8	4.9	6.2	7.0	10.1	14.0	0.07	0.59
2,3-dimethylbutane	569.24	2.9	3.2	3.5	5.1	8.5	13.1	0.70	1.91
2-methylpentane	573.70	2.5	2.9	3.4	5.1	6.6	8.4	1.06	5.80
4-methyl-t-pentene-2	575.47	6.5	8.7	11.3	18.1	28.0	41.1	0.08	0.28
3-methylpentane	585.52	2.6	2.9	3.2	4.0	5.6	7.5	0.60	2.50
2-methylpentene-1	590.19	2.3	2.7	3.2	3.8	5.4	7.4	0.11	0.45
hexene-1	591.06	3.1	4.2	5.5	5.9	8.2	10.9	0.06	0.26
n-hexane	600.00	2.0	2.4	2.9	3.6	5.1	6.9	0.33	2.52
t-hexene-3	602.83	1.9	3.2	4.9	7.4	11.8	17.7	0.08	0.35
t-hexene-2	605.44	2.5	2.8	3.2	4.5	6.4	8.9	0.16	0.71
2-methylpentene-2	607.86	2.4	3.0	3.8	6.1	13.1	24.1	0.22	0.97
3-methyl-c-pentene-2	610.54	2.1	2.5	2.9	5.3	6.9	8.7	0.11	0.48
3-methylcyclopentene	611.61	3.0	4.6	6.8	10.1	12.8	15.9	0.02	0.10
c-hexene-2	614.67	2.6	3.3	4.1	4.8	5.4	6.1	0.09	0.40
3,3-dimethylpentene-1	620.91	1.9	2.5	3.1	4.3	5.7	7.5	0.17	0.75
2,2-dimethylpentane	624.17	3.3	4.3	5.5	4.4	8.2	13.7	0.01	0.09
methylcyclopentane	625.86	2.2	2.6	3.1	4.5	6.4	8.7	0.37	2.35

TABLE 5 *Continued*

Component	Ave. RI	r_{min}	r_{est}	r_{max}	R_{min}	R_{est}	R_{max}	C_{min}	C_{max}
2,4-dimethylpentane	630.60	1.6	2.5	3.8	4.2	5.3	6.6	0.20	1.94
2,2,3-trimethylbutane	634.86	3.2	7.1	13.1	12.5	20.4	31.1	0.02	0.08
3,4-dimethylpentene-1	642.87	5.5	14.7	30.6	9.7	22.3	43.0	0.01	0.03
4,4-dimethyl-c-pentene-2	646.65	3.8	5.6	8.0	6.1	11.0	17.9	0.01	0.11
2,4-dimethylpentene-1	647.67	3.8	6.7	10.8	11.9	13.5	15.3	0.01	0.04
1-methylcyclopentene	648.71	1.9	2.7	3.7	7.9	8.7	9.6	0.17	0.82
benzene	649.92	2.6	3.6	4.8	5.5	9.0	13.7	0.17	1.58
5-methylhexene-1	655.56	5.3	7.5	10.1	18.0	30.4	47.6	0.01	0.22
cyclohexane	657.81	2.7	3.7	4.9	8.2	14.8	24.3	0.07	0.90
2-methyl-t-hexene-3	661.03	3.2	6.3	11.0	16.8	23.4	31.6	0.03	0.14
2-ethyl-3-methylbutene-1	662.60	4.1	8.9	16.5	89.5	117.0	149.7	0.01	0.04
4-methylhexene-1	663.81	2.5	4.5	7.2	11.7	14.7	18.3	0.02	0.09
4-methyl-t/c-hexene-2	666.23	2.1	3.2	4.7	5.4	7.3	9.5	0.05	0.28
2-methylhexane	667.61	1.6	2.2	2.9	5.1	6.1	7.2	0.39	1.09
2,3-dimethylpentane	668.84	1.6	2.3	3.2	5.4	6.4	7.5	0.33	3.16
3-methylhexane	675.89	1.9	2.8	4.0	4.7	5.6	6.7	0.37	1.08
3,4-dimethyl-c-pentene-2	679.46	3.6	5.9	9.1	11.6	23.4	41.2	0.02	0.14
1c,3-dimethylcyclopentane	681.68	1.7	2.7	4.0	5.4	7.5	10.1	0.11	0.56
1t,3-dimethylcyclopentane	684.37	1.7	2.8	4.4	5.4	7.7	10.5	0.08	0.48
3-ethylpentane	685.98	3.1	3.7	4.3	5.6	8.3	11.9	0.08	0.26
2,2,4-trimethylpentane	688.48	2.4	3.2	4.1	7.4	11.4	16.7	0.10	11.26
3-methyl-c-hexene-3	694.82	3.2	6.5	11.6	7.3	12.9	20.8	0.03	0.17
t-heptene-3	698.39	2.6	3.2	3.8	5.0	8.1	12.3	0.11	0.67
n-heptane	700.00	2.5	3.4	4.5	7.7	10.8	14.7	0.21	1.06
3-methyl-c-hexene-2	702.30	1.5	2.5	4.0	4.6	7.2	10.6	0.13	0.75
3-methyl-t-hexene-3	702.99	2.2	4.1	6.7	8.1	10.1	12.3	0.05	0.26
t-heptene-2	704.58	2.6	4.2	6.4	5.9	7.1	8.4	0.06	0.34
3-ethylpentene-2	705.96	4.7	8.3	13.4	14.5	17.9	21.8	0.03	0.16
c-heptene-2	708.82	1.9	3.2	5.0	7.0	7.8	8.7	0.12	0.63
2,3-dimethylpentene-2	712.07	2.4	3.7	5.5	7.8	9.1	10.5	0.06	0.57
O29	715.67	6.8	11.5	18.0	15.7	22.6	31.3	0.01	0.08
1c,2-dimethylcyclopentane	717.13	2.4	3.7	5.3	9.5	11.6	13.9	0.05	0.20
methylcyclohexane	717.89	2.8	3.4	4.0	4.1	5.9	8.2	0.11	1.20
2,2-dimethylhexane	720.70	4.2	7.2	11.3	10.2	15.4	22.3	0.02	0.10
2,5-dimethylhexane	730.05	2.5	3.0	3.5	4.9	6.2	7.7	0.16	1.12
2,4-dimethylhexane	731.84	3.5	4.3	5.2	6.5	9.0	12.1	0.29	1.39
1c,2t,4-trimethylcyclopentane	737.11	3.0	4.2	5.6	6.9	7.9	9.0	0.03	0.17
2,3,4-trimethylpentane	746.83	2.3	3.8	6.0	5.8	7.8	10.3	0.08	4.26
I1	747.91	2.2	6.2	13.4	10.1	21.1	38.1	0.09	0.59
toluene	751.77	1.9	2.7	3.8	10.8	13.5	16.5	1.99	10.34
2,3-dimethylhexane	757.87	2.2	3.7	5.7	5.0	6.9	9.2	0.22	1.23
1,1,2-trimethylcyclopentane	760.33	7.6	13.5	21.8	13.6	25.7	43.4	0.02	0.26
O44	761.73	4.2	9.4	17.7	12.7	20.5	30.8	0.03	0.24
2-methylheptane	764.14	3.5	4.9	6.6	4.8	6.1	7.5	0.15	0.63
4-methylheptane	765.62	4.1	6.2	9.1	7.1	9.1	11.5	0.05	0.29
3-methyl-3-ethylpentane	766.62	5.4	7.1	9.3	11.0	15.8	21.8	0.05	0.10
3-methylheptane	771.78	2.1	3.4	5.3	4.4	5.1	5.9	0.13	0.71
1c,2t,3-trimethylcyclopentane	772.98	3.4	4.4	5.7	5.9	7.4	9.1	0.06	0.29
3-ethylhexane	773.76	6.9	10.8	15.9	13.1	23.8	39.1	0.01	0.07
1t,4-dimethylcyclohexane	774.89	9.8	18.0	29.8	22.2	49.5	93.1	0.01	0.11
2,2,5-trimethylhexane	782.93	3.1	4.3	5.7	5.7	8.0	10.8	0.14	2.21
3c-ethylmethylcyclopentane	784.35	5.7	12.1	22.1	9.7	22.2	42.5	0.05	0.21
3t-ethylmethylcyclopentane	786.55	7.4	9.7	12.4	8.4	22.1	46.0	0.02	0.11
2t-ethylmethylcyclopentane	787.86	8.9	11.4	14.2	12.6	26.7	48.7	0.02	0.12

TABLE 5 *Continued*

Component	Ave. RI	r_{min}	r_{ave}	r_{max}	R_{min}	R_{ave}	R_{max}	C_{min}	C_{max}
1t,2-dimethylcyclohexane	792.77	3.7	6.7	11.0	7.0	10.1	14.0	0.04	0.29
t-octene-4	794.21	12.7	14.5	16.6	16.7	21.9	28.1	0.02	0.18
1c,2c,3-trimethylcyclopentane	797.25	3.5	6.0	9.4	6.3	9.2	12.9	0.07	0.51
1t,3-dimethylcyclohexane	798.80	6.8	9.3	12.4	11.9	16.3	21.7	0.02	0.10
n-octane	800.00	2.2	3.6	5.5	6.5	15.7	30.9	0.14	0.75
octene-2	804.40	4.9	8.2	12.7	11.1	20.1	32.9	0.03	0.23
I2	806.39	4.7	10.9	20.9	8.7	19.7	37.4	0.05	0.36
i-propylcyclopentane	808.06	4.1	10.7	22.0	8.4	19.8	38.4	0.03	0.18
2,3,4-trimethylhexane	818.10	2.5	5.0	8.9	5.1	7.2	9.8	0.05	0.37
N2	819.93	7.7	11.5	16.4	6.8	17.4	35.7	0.01	0.06
N3	822.29	8.0	13.3	20.7	11.3	23.2	41.5	0.01	0.09
2,3,5-trimethylhexane	827.51	3.9	5.4	7.1	7.5	31.4	82.4	0.07	0.12
1,1,4-trimethylcyclohexane	832.56	8.6	17.1	29.9	21.7	36.0	55.6	0.03	0.26
2,2,3-trimethylhexane	834.96	8.4	13.1	19.2	14.8	20.3	27.0	0.05	0.09
2,5-dimethylheptane	842.63	6.8	8.8	11.1	7.8	12.3	18.2	0.11	0.18
ethylbenzene	854.65	2.2	3.2	4.4	7.2	10.6	14.9	0.62	2.62
1,3-dimethylbenzene	864.22	2.6	3.3	4.2	9.7	12.5	15.7	1.55	6.66
1,4-dimethylbenzene	865.20	3.6	4.2	5.0	10.4	14.1	18.5	0.62	2.97
I5	870.95	6.6	11.5	18.3	13.8	28.4	50.9	0.02	0.13
4-methyloctane	873.81	4.4	7.6	12.0	5.9	11.2	18.9	0.05	0.20
2-methyloctane	874.76	4.6	8.2	13.3	6.0	10.4	16.6	0.07	0.35
3-ethylheptane	879.11	8.5	13.4	20.1	27.7	38.7	52.5	0.02	0.09
3-methyloctane	880.24	5.1	8.5	13.0	8.7	15.5	24.9	0.07	0.29
1,2-dimethylbenzene	883.47	2.1	3.2	4.7	8.8	11.5	14.8	0.83	3.85
I6	885.34	10.2	17.0	26.4	23.3	44.5	75.8	0.02	0.06
I7	886.38	6.5	9.0	12.0	7.8	21.1	44.7	0.05	0.32
N22	895.99	7.9	16.5	29.6	16.7	29.4	47.2	0.03	0.22
N23/c-nonene-2	897.24	5.7	15.9	34.2	26.1	48.7	81.6	0.02	0.15
I10	898.70	4.5	12.3	26.0	9.3	31.1	73.3	0.04	0.44
n-nonane	900.20	3.9	6.4	9.8	8.6	10.3	12.2	0.06	0.34
i-propylbenzene	912.28	3.2	5.0	7.3	8.3	15.1	24.9	0.04	0.33
N27	914.45	3.6	12.3	29.2	9.0	21.1	40.8	0.02	0.14
I12	921.30	4.4	11.0	22.2	8.7	21.2	42.2	0.03	0.34
2,4-dimethyloctane	924.39	6.1	12.1	21.3	16.8	26.0	38.1	0.03	0.11
2,6-dimethyloctane	930.83	7.0	14.6	26.4	15.4	27.7	45.3	0.02	0.10
2,5-dimethyloctane	932.66	5.6	11.2	19.6	15.3	22.0	30.4	0.04	0.13
3,3-dimethyloctane	942.30	4.3	10.4	20.6	7.5	17.5	34.0	0.03	0.11
n-propylbenzene	946.33	2.8	5.0	8.1	7.6	11.9	17.7	0.21	0.77
3,6-dimethyloctane	948.31	7.6	14.9	25.7	18.1	38.9	71.4	0.01	0.04
1,3-methylethylbenzene	954.42	3.7	5.2	7.2	7.6	10.2	13.3	0.81	2.61
1,4-methylethylbenzene	956.22	3.5	5.3	7.7	5.1	7.7	11.1	0.32	1.19
1,3,5-trimethylbenzene	961.92	3.7	5.5	7.7	5.4	8.3	12.1	0.39	1.21
2-methylnonane	971.77	6.5	10.6	16.2	17.5	25.9	36.6	0.03	0.19
3-methylnonane	977.26	7.5	13.5	22.1	23.5	41.0	65.5	0.03	0.16
I18	980.12	7.3	15.7	28.8	14.9	30.0	52.9	0.04	0.82
1,2,4-trimethylbenzene	983.40	4.2	5.7	7.5	7.8	10.6	13.9	1.19	4.32
I21	987.40	6.9	18.6	39.3	16.9	49.6	109.2	0.03	0.27
I24	994.53	6.9	12.2	19.6	18.9	31.1	47.7	0.04	0.36
n-decane	1000.20	7.5	9.2	11.1	12.1	17.9	25.3	0.03	0.25
N38	1003.39	9.7	19.8	35.2	25.8	47.6	79.3	0.01	0.12
1,2,3-trimethylbenzene	1006.88	3.8	5.8	8.5	7.2	8.5	10.0	0.28	0.96
2-3-dihydroindene	1019.44	5.2	7.8	11.3	8.8	10.8	13.0	0.18	0.37
I30	1024.82	7.5	13.9	23.3	20.4	61.8	138.4	0.01	0.15
1,2-methyl-i-propylbenzene	1027.73	17.3	19.5	22.0	66.4	99.4	141.9	0.02	0.08

TABLE 5 *Continued*

Component	Ave. RI	r_{min}	r_{ave}	r_{max}	R_{min}	R_{ave}	R_{max}	C_{min}	C_{max}
?	1038.53	6.8	16.0	31.1	16.8	37.4	70.2	0.02	0.16
1,3-diethylbenzene	1039.97	5.0	7.3	10.1	9.9	13.7	18.5	0.08	0.22
1,3-methyl-n-propylbenzene	1042.60	4.0	6.4	9.5	6.7	13.5	23.6	0.30	0.68
1,4-methyl-n-propylbenzene	1046.40	4.6	8.7	14.7	7.8	12.7	19.4	0.16	0.32
1,3-dimethyl-5-ethylbenzene	1049.78	3.4	6.0	9.8	7.6	10.6	14.3	0.22	0.51
1,2-methyl-n-propylbenzene	1057.87	6.3	9.3	13.2	20.9	30.3	42.1	0.11	0.20
		4.5	11.4	23.2	14.4	36.1	73.1	0.06	0.56
I38	1065.53	7.9	16.6	30.0	28.4	37.4	48.2	0.02	0.09
1,4,dimethyl-2-ethylbenzene	1068.05	4.1	6.7	10.3	15.3	27.8	45.7	0.15	0.38
1,2-dimethyl-4-ethylbenzene	1075.25	5.1	7.0	9.3	13.8	18.7	24.6	0.29	0.71
undecene-1	1090.45	8.2	17.8	32.9	20.5	35.4	56.1	0.01	0.09
1,2-dimethyl-3-ethylbenzene	1093.12	6.8	10.3	14.8	15.2	18.4	22.1	0.09	0.19
1,2-ethyl-i-propylbenzene	1097.22	14.3	31.3	58.2	51.7	74.6	103.4	0.02	0.06
n-undecane	1100.00	8.6	13.9	21.0	24.4	40.0	61.2	0.03	0.18
1,2,4,5-tetramethylbenzene	1104.83	6.1	8.3	11.1	12.5	16.0	20.1	0.15	0.36
1,2,3,5-tetramethylbenzene	1108.79	6.4	7.8	9.3	10.2	13.9	18.3	0.21	0.51
5-methylindan	1127.35	6.6	9.2	12.4	7.5	9.3	11.4	0.06	0.34
I43	1131.42	9.1	15.0	23.0	18.8	30.8	47.1	0.02	0.35
4-methylindan	1133.70	8.0	13.8	21.9	15.3	20.9	27.6	0.02	0.10
1,2-ethyl-n-propylbenzene	1136.52	7.4	12.0	18.3	25.3	39.6	58.4	0.02	0.11
2-methylindan	1138.11	5.6	7.7	10.2	6.4	8.9	12.0	0.08	0.34
1,3-di-i-propylbenzene	1142.70	7.9	9.5	11.2	16.2	17.9	19.7	0.06	0.18
1,2-di-i-propylbenzene	1153.16	13.9	22.4	34.0	21.3	36.0	56.2	0.01	0.06
?	1157.64	12.8	20.7	31.4	24.5	44.1	71.9	0.02	0.06
1,4-di-i-propylbenzene	1159.52	11.1	18.6	28.8	18.6	35.6	60.8	0.01	0.09
naphthalene	1168.01	6.1	8.5	11.3	12.9	16.9	21.5	0.13	0.40
1,4-ethyl-t-butylbenzene	1173.72	9.8	12.0	14.5	18.0	28.1	41.3	0.04	0.30
I48	1187.14	9.1	14.3	21.1	16.8	30.7	50.8	0.01	0.09
1,3-di-n-propylbenzene	1188.64	9.9	14.4	19.9	18.9	24.2	30.4	0.02	0.08
A5	1190.24	11.5	19.2	29.8	26.7	30.3	34.2	0.02	0.06
A6	1198.52	13.7	23.3	36.7	28.1	39.5	53.5	0.01	0.05
n-dodecane	1200.00	12.2	16.7	22.1	20.2	32.9	50.0	0.01	0.11
1,4-methyl-n-pentylbenzene	1241.71	8.2	14.1	22.3	16.5	31.2	52.7	0.01	0.14
1,2,3,4,5-pentamethylbenzene	1274.04	11.4	13.9	16.7	23.1	29.7	37.5	0.01	0.11
2-methylnaphthalene	1282.57	7.6	11.1	15.4	17.5	22.3	28.0	0.05	0.50
1-methylnaphthalene	1297.72	7.3	11.0	15.8	14.0	21.0	30.1	0.02	0.22

PROCEDURE B – INDIVIDUAL HYDROCARBON ANALYSIS

19. Apparatus

19.1 *Gas Chromatograph*— A gas chromatograph equipped with cryogenic column oven cooling and capable of producing repeatable oven ramps from 0°C 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 21.1 and 21.2.

19.2 *Inlet*—A capillary split/splitless inlet system operated in the split mode is recommended. It must be operated in its linear range. Refer to 21.4 to determine the proper split ratio.

19.2.1 *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.

19.2.2 *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.

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

19.3 *Column*—A fused silica capillary column, 100 m in length by 0.25 mm inside diameter, coated with a 0.5 µm film of bonded dimethylpolysiloxane. The column must meet the resolution requirements expressed in 21.3. Columns from two different commercial sources were used in the interlaboratory cooperative study.

19.4 *Data System*—A computer based chromatography data system capable of accurately and repeatedly measuring the

retention time and areas of eluting peaks. The system must 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 21.3.

19.4.1 *Electronic Integrators*—Must be capable of storing up to 400 components in the peak table. Must be able to acquire the data at 10 Hz or faster speeds. They must be capable of integrating peaks having peak width at half height which are 1.0 s 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.

19.5 *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.

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

20. Reagents and Materials

20.1 *Calibrating Standard Mixture*—A spark ignition engine fuel standard of known composition and concentration by mass may be used. In order to corroborate the identification of the sample, a typical chromatogram (Fig. 13), was obtained from reference sample ARC96OX[10]

20.2 *Gas Chromatograph Gases*—All of the following gases shall have a purity of 99.999 % (V/V) or greater. (**Warning**—Gases are compressed. Some are flammable and all gases are under high pressure.

20.2.1 *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.

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

21. Instrument Check Out Prior to Analysis

21.1 *Setting, Linear Gas Velocity*—If the gas chromatograph is equipped with an electronic flow readout device, set the flow to 1.8mL/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 min. ± 0.05. 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.

21.1.1 If the gas chromatograph is not equipped with an electronic flow readout device, calculate the linear gas velocity in cm/s using Eq 9.

$$\text{linear gas velocity} = V = \frac{\text{column length (cm)}}{\text{Retention time of methane(s)}} \quad (9)$$

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.

21.2 *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 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 the equations below.

$$\text{column flow rate} = F = \frac{(60\ \pi\ r^2)\ L\ (T_{ref})\ 2(P_i - P_o)}{(T)3(P_{ref})(P_i^2 - P_o^2)\mu} \quad (10)$$

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 atmosphere,
T = temperature of the column oven,
T_{ref} = temperature at the column outlet, and
μ = linear velocity in cm/s.

$$\text{split ratio} = S = \frac{\text{split vent flow} + F}{F} \quad (11)$$

The column flow rate is calculated by the use of Eq 10. Use the results obtained from Eq 11 to adjust the split flow until a split flow of approximately 200:1 is achieved.

21.3 *Evaluation of Column Performance*:

21.3.1 Prior to using the column described in Table 6, measure the resolution of the column under the conditions of Table 7. Check that the resolution for the following pairs of components is obtained as follows. Use the following equation to calculate the resolution of a pair of components.

$$R = \frac{(t_{R2} - t_{R1})^2}{1.699\ (W_{h1} + W_{h2})} \quad (12)$$

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.

Column resolution should be checked frequently by examining the resolution of these compounds. (See Table 8 for an example.)

21.3.2 *Evaluation of the Baseline*—Carry out a blank baseline utilizing no solvent injection, by setting the GC in accordance with conditions of Table 5.

21.3.3 Subtract the baseline from a sample chromatogram and verify that the residual signal at the beginning of the

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

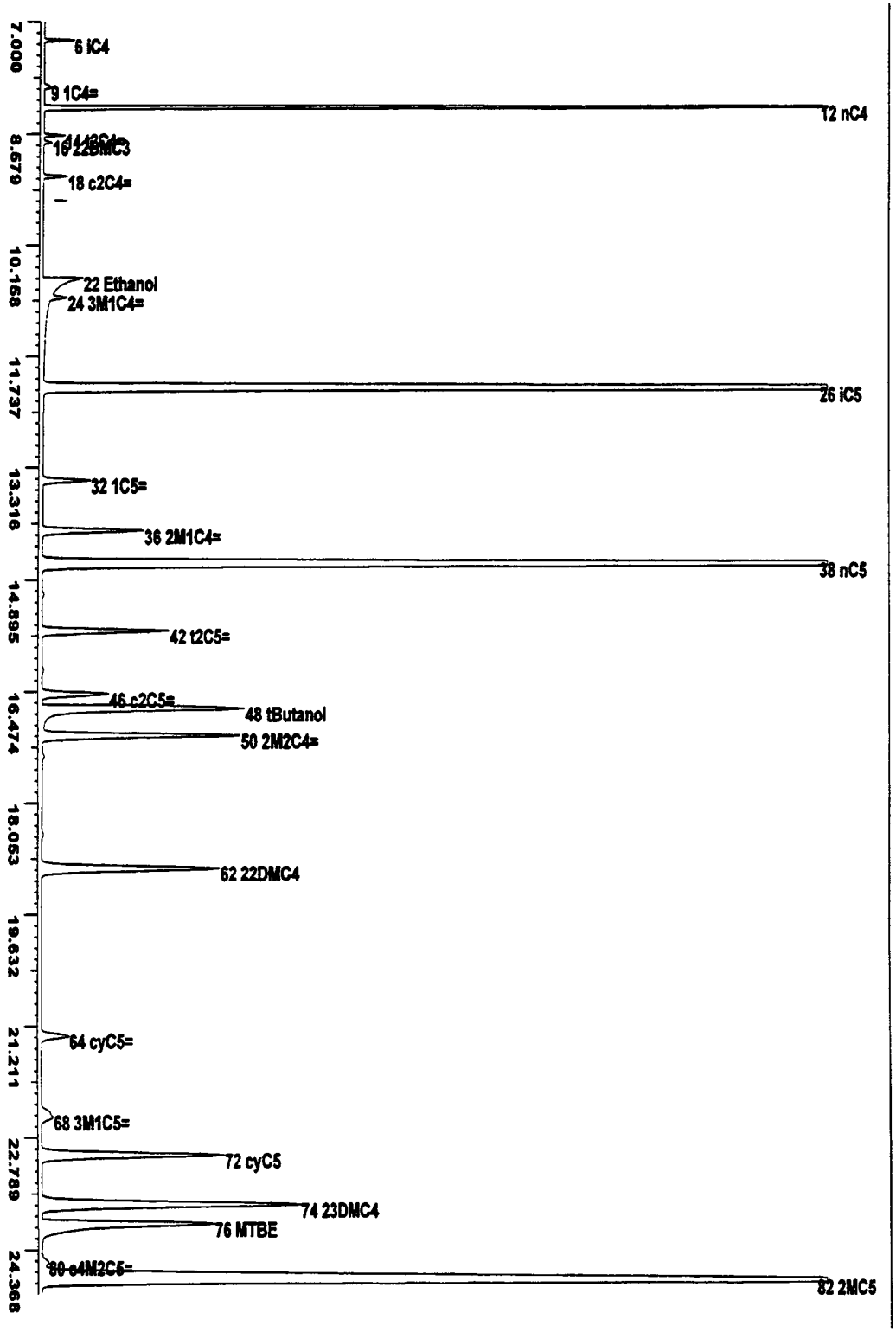


FIG. 13 Chromatogram for Reference Spiked Gasoline

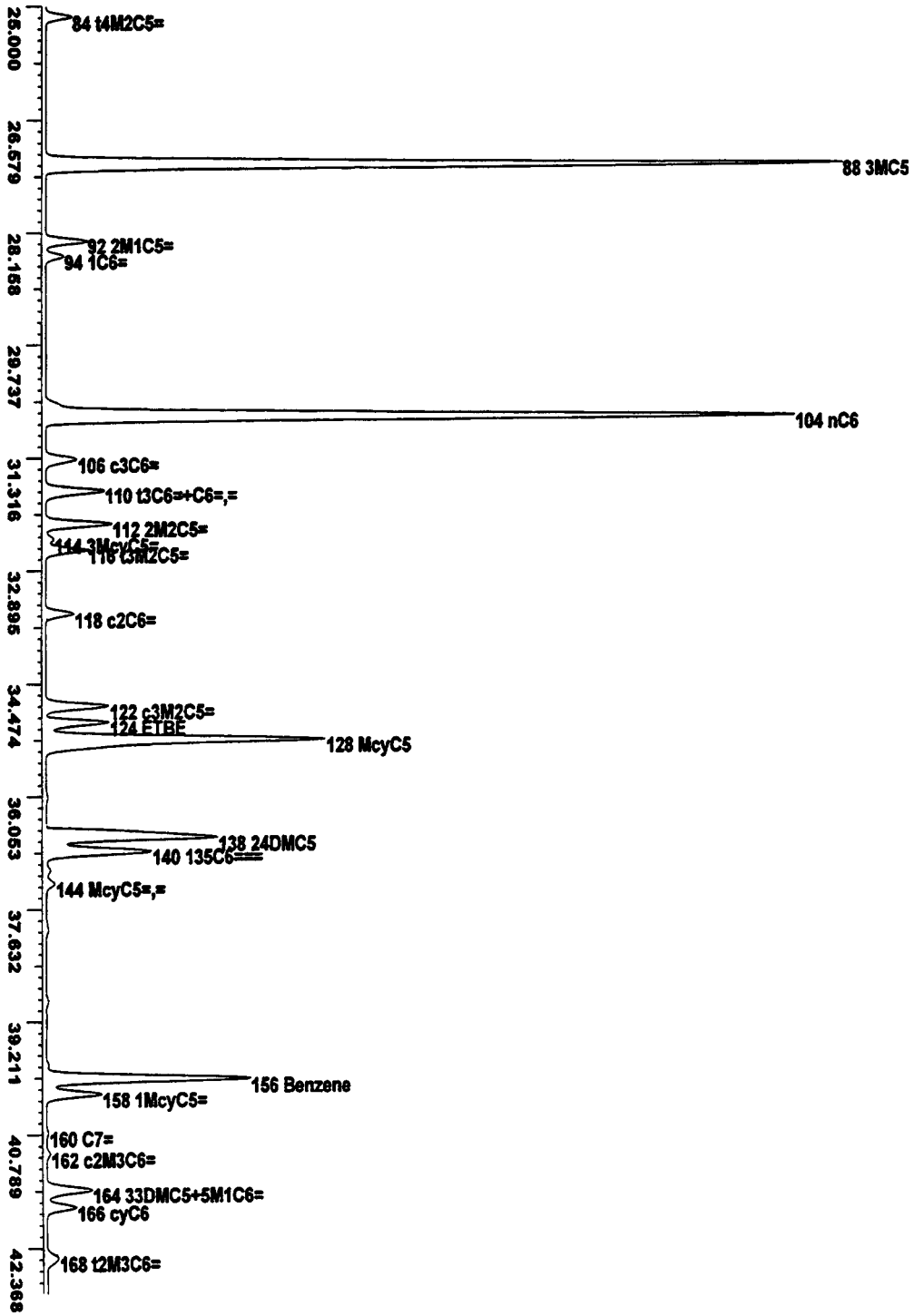


FIG. 13 Chromatogram for Reference Spiked Gasoline *(continued)*

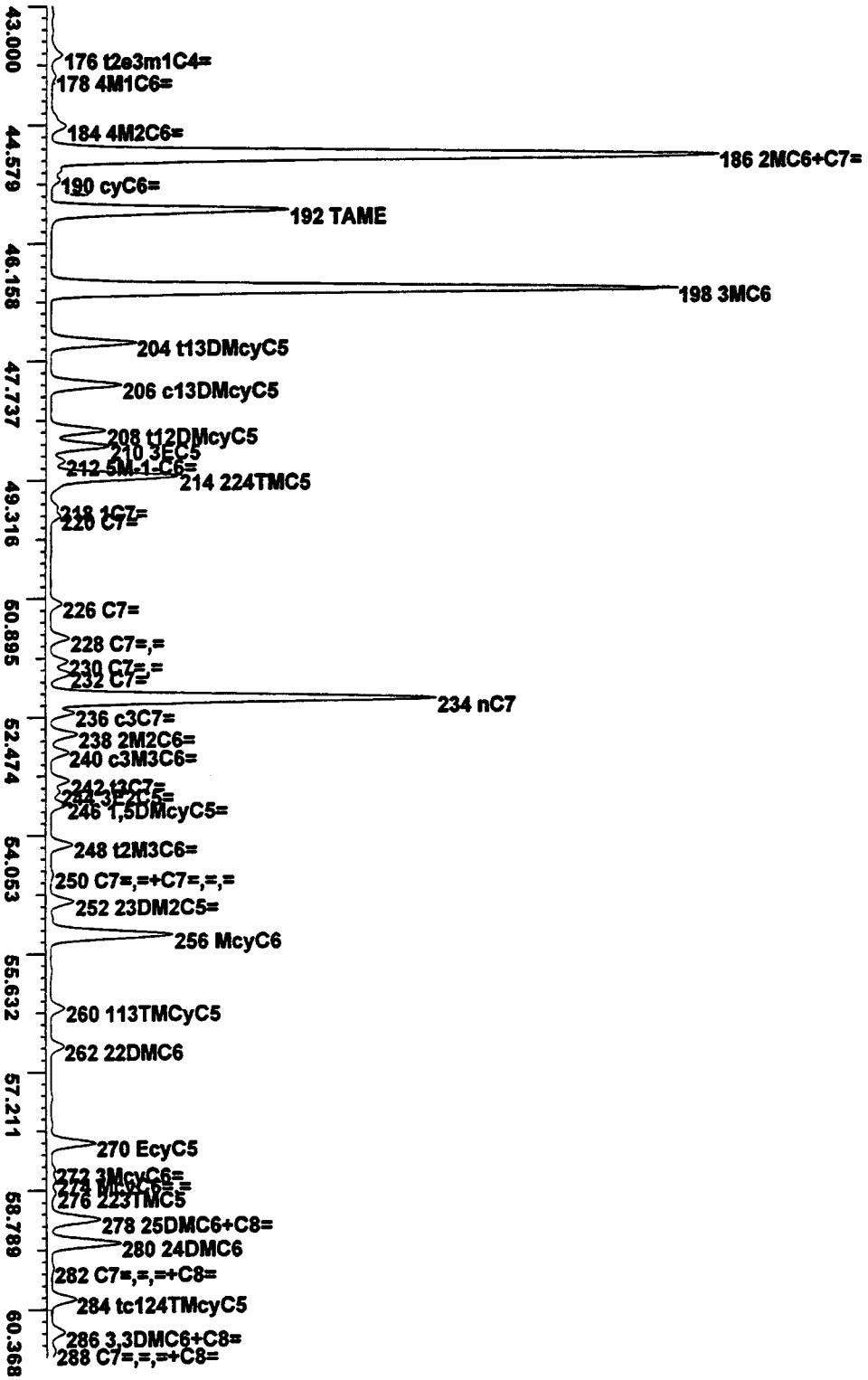


FIG. 13 Chromatogram for Reference Spiked Gasoline *(continued)*

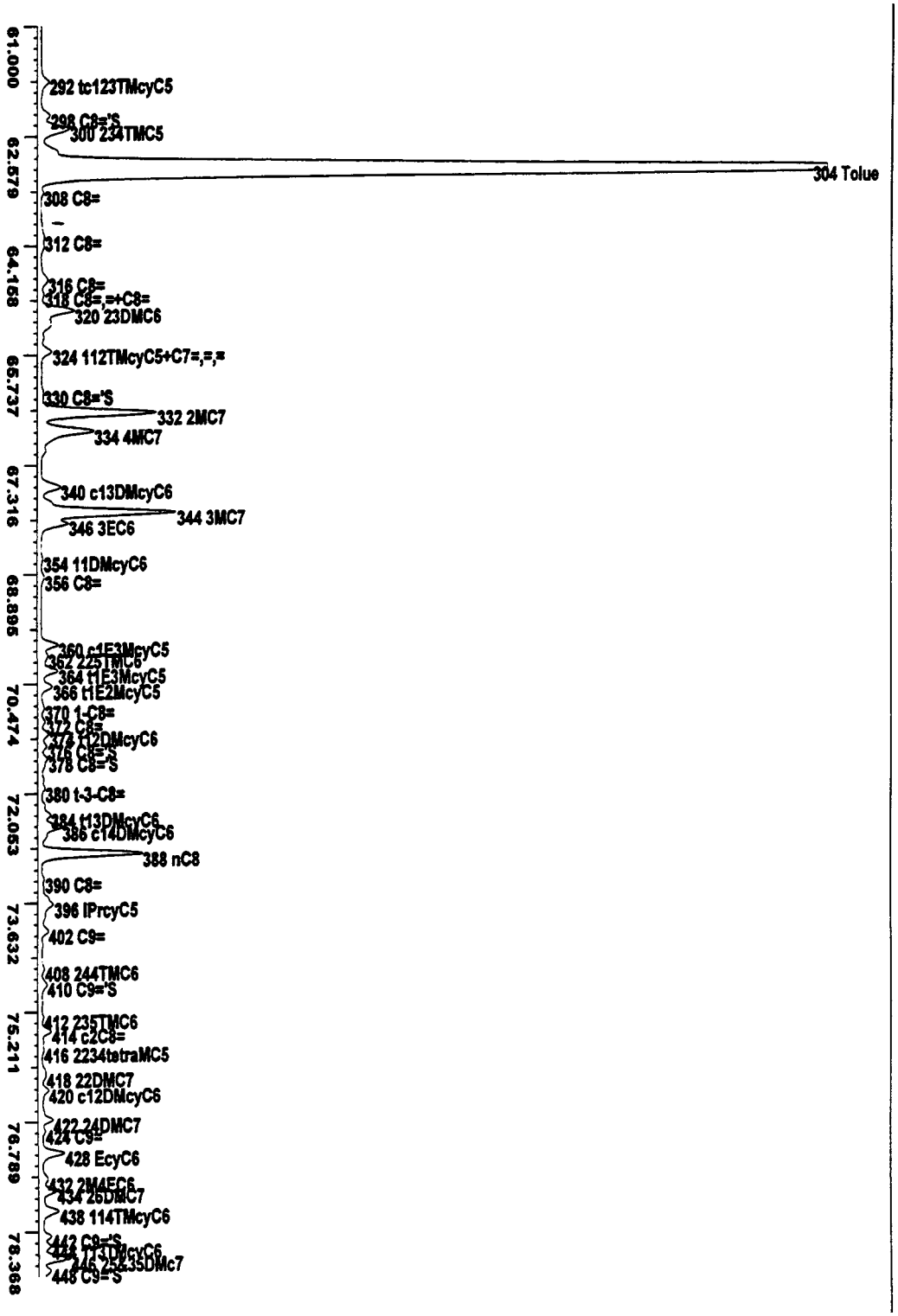


FIG. 13 Chromatogram for Reference Spiked Gasoline *(continued)*

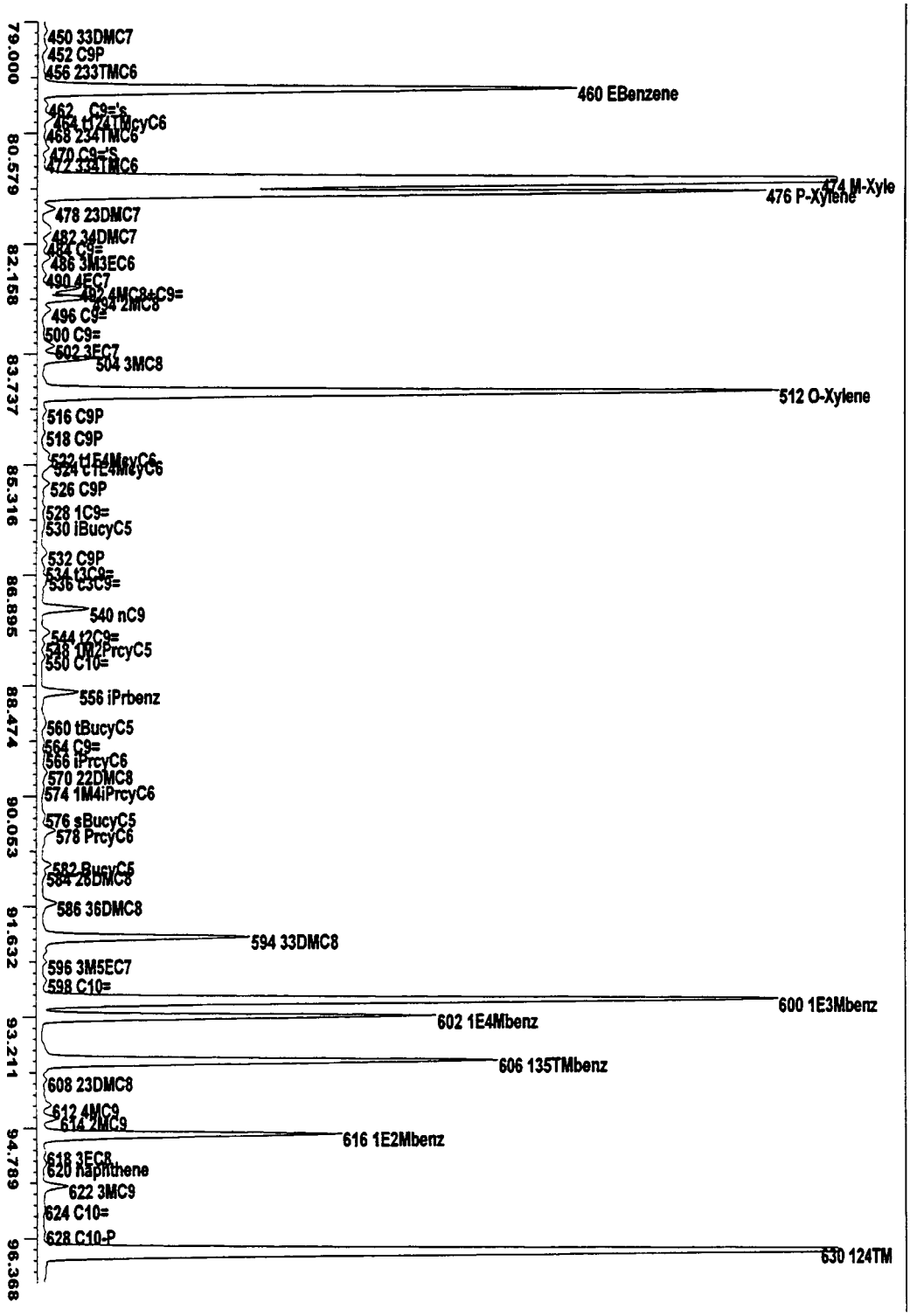


FIG. 13 Chromatogram for Reference Spiked Gasoline *(continued)*

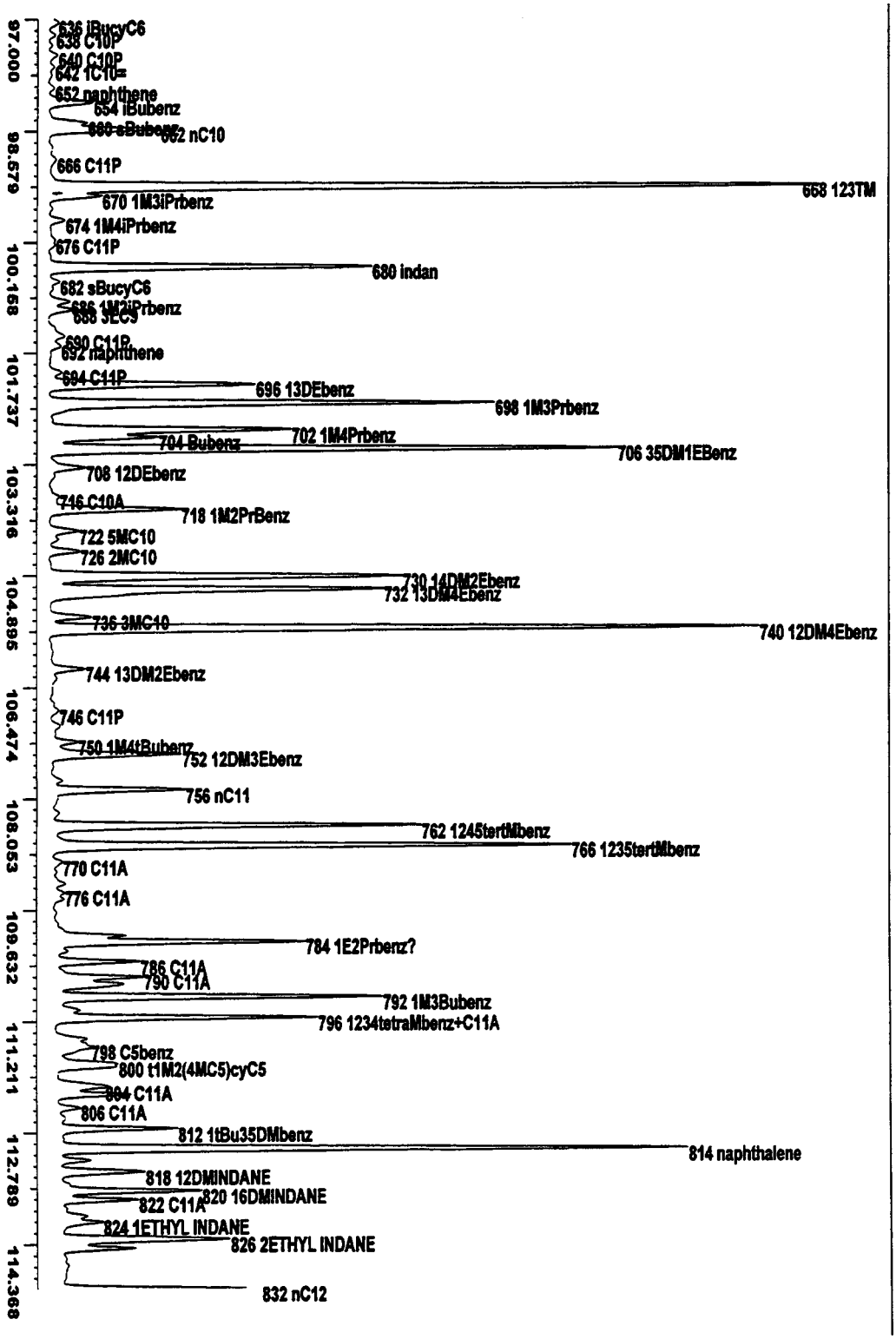


FIG. 13 Chromatogram for Reference Spiked Gasoline *(continued)*

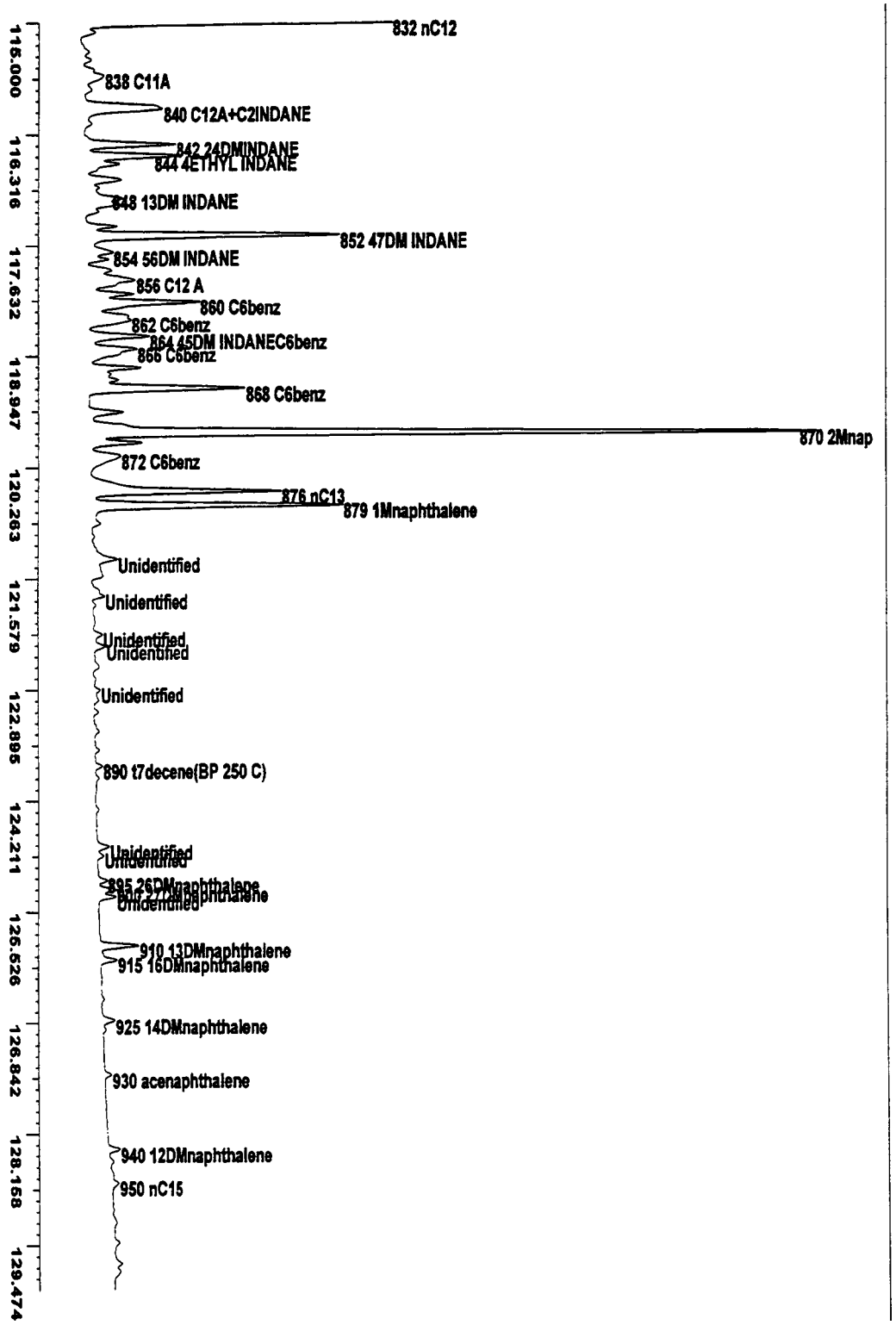


FIG. 13 Chromatogram for Reference Spiked Gasoline *(continued)*

TABLE 6 Chromatographic Operating Conditions, Column Requirements, and Data Acquisition Requirements

Chromatographic Conditions	Requirements
Injector settings	
Injector temperature	250°C
Split ratio	175:1 - 275:1
Liner	deactivated glass
Injection volume	0.2 - 0.5 µl
Detector settings	
FID detector temperature[A]	300° - 350°C
Gas flows	
Hydrogen[B]	30 - 40 mL/min
Air	300 - 450 mL/min
Nitrogen make up	30 mL/min
Column oven settings	
Initial temperature	0°C
Initial time	15 min
First ramp rate	1°C/min
Final temperature	50°C
Final time	0 min.
Second ramp rate	2°C/min
Final temperature	130°C
Final time	0 min
Third ramp rate	4.0°C/min
Final temperature	270°C
Final time[C]	0 min
Column requirements	
Length	100 m
Inside diameter	0.25 mm
Liquid phase	100 % dimethylpolysiloxane
Film thickness	0.5 µ
Pressure	40 - 50 psig
Flow	1.7-2.0 mL/min
Linear gas velocity	24.5 cm/s
Data acquisition	10 -20 Hz
Total analysis time	140-150 min

[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 7 Column Resolution

Component Pair	Resolution, min	Concentration of each Compenent, 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

chromatogram does not differ from the end of the chromatogram by more than 2 %.

21.4 *Evaluation of Splitter Linearity*—Using the reference gasoline sample, inject this sample according to the schedule listed in Table 9. Select from the chromatogram about 10 to 15 components, which have concentrations in the range of .01 to 30-wt. %. 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 %.

22. Procedure

22.1 Set the operating conditions of the gas chromatograph as shown in Table 5. These conditions will elute all components up to and including pentadecane (nC15).

TABLE 8 Operating Conditions

Temperatures	Method 1	Method 2
Column initial isotherme	35°C	10°C
Initial hold time	10 min.	15 min.
Rate 1	1.1°C/min.	1.3°C/min
Final temperature 1	114°C	70°C
Hold time 2	0 min.	0 min.
Rate 2	1.7°C/min.	1.7°C/min
Final temperature 2	250°C	250°C
Final hold time 2	5 min.	20 minutes
Injector	250°C	250°C
Détector	280°C	280°C
Carrier gas helium		
Pressure	207kPa (30psi)	190 kP(27 psi)
Flow rate (initial isotherme)	0.9 mL/min.	0.7 mL/min.
Average linear velocity	22 cm/s	21.5 cm/s
Injection		
Sample size	0.5µL	0.3µL
Splitter vent - flow out	250 mL/min.	200 mL/min.

TABLE 9 Schedule of Splitler Linearity Injections

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

22.2 All of the parameters in Table 5 can be marginally changed to optimize for sample types and optimize for characteristics of each gas chromatographic system. The final boiling point of samples should not exceed nC15 and the column resolution (*R*) performance requirements listed in Table 6 should not be compromised.

22.3 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.

22.4 *Preparation/Storage*:

22.4.1 *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.

22.4.2 *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°. Store pressure containers in accordance with manufacturer's instructions.

22.5 It is recommended that a quality assurance (QA) sample similar to the reference material gasoline sample be run at regular intervals (See Fig. 13). An interval of once a 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.

23. Data Analysis

23.1 *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.

23.2 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.

$$(R1)_i = n100 + 100\left(\frac{\log(Ti) - \log(Tn)}{\log(TN) - \log(Tn)}\right) \quad (13)$$

where:

$(R\ 1)_i$ = retention index of component I bracketed by the *N*-paraffin, *n* in its lower boundary and *N*-paraffin N in its upper boundary,
Ti = adjusted retention time of component i, (Retention time of component *i* minus the retention time of methane),
Tn = adjusted retention time of *N*-paraffin n, and
TN = retention time of *N*-paraffin N.

23.3 Determine the hydrocarbon response factors by using the following equation.[11]

$$RRF_{CH4} = \frac{MW_i}{N_c} \times \frac{1}{MW_{CH4}} \quad (14)$$

where:

RRF_{CH4} = relative response factor of each component with respect to methane (RRF_{CH4}= 1.000),
MW_i = the molecular weight of the component, i
N_c = the number of carbon atoms in the molecule, and
MW_{CH4} = the molecular weight of methane (16.04276).

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

$$A_{c_i} = (A)_I (RRF)_I \quad (15)$$

where:

$(Ac)_i$ = the corrected area,
A_i = acquired area for an individual component, and
RRF = the relative response factor (weight basis).

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

$$\%\ Wi = \frac{(Ac)_i}{\sum_{i=1}^{i=n} A_{c_i}} \times 100 \quad (16)$$

where:

$\%\ W_i$ = the % weight of the component *i* in the mixture, and
$\sum_{i=1}^{i=n} A_{c_i}$ = the summation of all the corrected areas for the components analyzed.

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

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

24. Oxygenates

24.1 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 concentrations ranges from 1.0 up to 30 mass % (Annex A2 Oxygenate Linearity Study). The average relative response factors for the oxygenates were calculated from the study and are listed in Table 10. 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 research report RR:D02-1007. Therefore the statistical data for MTBE should be taken from Table A2.2.

25. Expression of Results

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

25.2 The data for individual components may be 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 calculation of other properties of petroleum liquids. See the warning in 5.2.

26. Precision and Bias [8]

26.1 The repeatability and reproducibility precision estimates are quoted in Table A2.2.

26.2 *Precision Statement Outline*—analyte qualification process:

26.2.1 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 research report RR:D02-1007 requirement.

26.2.2 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. The summaries for the paraffins, isoparaffins, C_2 benzene, and oxygenates follow the same procedure that was used for the analytes and are at the end of analyte Table A2.2.

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

27. Keywords

27.1 gas chromatograph; gasoline; individual hydrocarbon

TABLE 10 Response Factors of Oxygenated Compounds

Analytes	Relative Response Factors	
	RRF C7 = 1.000	*RRF CH4 = 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

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

analysis; oxygenated fuels; spark-ignition engine fuels

PROCEDURE C – DETAIL HYDROCARBON CHARACTERIZATION (DHC)

28. Apparatus

28.1 *Instrumentation*— A gas chromatograph capable of operating under the conditions outlined in Table 11, equipped with a split injector, a carrier gas pressure control and a flame ionization detector are required.

28.2 *Sample Introduction System*—Manual or automatic liquid syringe sample injection may be employed.

28.3 *Data Acquisition System*—Any data system can be used with a requirement:

28.3.1 Sampling rate of 10 hz or more with a storage of sampling data for later processing.

28.3.2 Capacity for at least 400 peaks/analysis.

28.3.3 *Identification of Individual Components from Retention Time*—Software can be used to automatically identify the peaks with the index system determined from Table A3.1, or A3.2.

28.4 *Sampling*—2 mL or more crimp top vials and aluminum caps with polytetrafluoroethylene (PTFE)-lined septa are used to transfer the sample.

28.5 *Capillary Column*— A 50 m fused silica capillary column with an internal diameter of 0.2 mm, containing a 0.5µm film thickness of bonded dimethylpolysiloxane phase is used. The features must be respected to reproduce the separation of the reference chromatogram. The column must meet the criteria of efficiency, resolution and polarity defined in Section 32.

29. Reagents and Materials

29.1 *Carrier Gas and Make-up*—Helium, 99.99 mol % pure (**Warning**—Compressed gas under high pressure).

29.2 *Fuel Gas*—Hydrogen, hydrocarbon free, 99.99 mol % pure (**Warning**—Compressed gas under high pressure. Extremely flammable).

TABLE 11 Predominant Compounds and Identified Coeluting Compounds[A]

NOTE 1—The response factor of the predominant compound will be used for the analyte and this analyte will be used for the calculations.

Peak Number	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 TMC_5.

29.3 *Oxiding Gas*—Air, 99 mol % (**Warning**—Compressed gas under high pressure).

29.4 *N-Pentane*—99 + mol % pure (**Warning**—Extremely Flammable. Harmful if inhaled).

29.5 *N-Hexane*, 99 + % mol % pure (**Warning**—Extremely Flammable. Harmful if inhaled).

29.6 *N-Heptane*—99 + mol % pure (**Warning**—Extremely Flammable. Harmful if inhaled).

29.7 *2-Methylheptane*— 99+ mol % pure (**Warning**—Extremely Flammable. Harmful if inhaled).

29.8 *4-Methylheptane*— 99+ mol % pure (**Warning**—Extremely Flammable. Harmful if inhaled).

29.9 *N-Octane*—99 + mol % pure (**Warning**—Extremely Flammable. Harmful if inhaled).

29.10 *N-Dodecane*—99 + mol % pure (**Warning**—Extremely Flammable. Harmful if inhaled).

29.11 *Toluene*—99 + mol % pure (**Warning**—Extremely Flammable. Harmful if inhaled).

29.12 *System Performance Mixture*—Weigh an equal amount of *N*-pentane, *N*-heptane, *N*-octane, *N*-dodecane, 2-methylheptane, 4-methylheptane and toluene. Dilute this mixture in *N*-hexane to obtain a concentration of 2 mass % for each compound.

30. Sampling

30.1 *Container Sampling*—Samples shall be taken as described in Practice D 4057 for instructions on manual sampling into open container.

30.2 The sample and a 2 mL vial must be cooled at 4°C. Part of sample is transfered to *the vial up to 80 %* of its volume and aluminium cap with septum is crimped.

31. Preparation of Apparatus

31.1 *Installation*— Install and condition column in accordance with supplier's instruction.

31.2 *Operating Conditions*—Two sets of operating conditions are proposed in the Table 8, the first with an initial column temperature above the ambient temperature, the second with a subambient column temperature profile. Adjust the operating conditions of the gas chromatograph to conform to the first or second method.

31.3 *Carrier Gas Pressure*—Set a correct carrier gas pressure using the system performance mixture such that the retention time of *N*-Heptane, *N*-Octane and *N*-Dodecane are between the values given in Table 12.

32. System Performance Evaluation

32.1 Evaluation of the column and linearity of the split injection are carried out with a system performance mixture defined in 29.12 and with the column temperature conditions defined as follows:

TABLE 12 Reference Retention Times of Normal Paraffins (min. and one tenth of a minute)

	Method 1	Method 1	Method 1	Method 2	Method 2	Method 2
N-Paraffins	Lower Time	Reference Time	Upper Time	Lower Time	Reference Time	Upper Time
N-Heptane	18.5	19.4	20.3	39.5	40.7	42.0
N-Octane	32.0	33.0	34.0	57.0	57.8	59.0
N-Dodecane	92.8	94.0	95.2	106.4	107.6	108.8

initial temperature	35°C
hold time	50 min.
final temperature	220°C
hold time	20 min.
rate	3°C/min.

32.2 *Column Evaluation*— To perform the required separation, the column must meet three criteria of separation – efficiency, resolution, and polarity.

32.2.1 *Efficiency*— The number of theoretical plates is calculated with the normal octane peak using Eq.

$$n = 5.545(Rt/W_{0.5})^2 \quad (17)$$

where:

n = number of theoretical plates,
Rt = retention time of normal octane, and
$W_{0.5}$ = mid-height peak width of normal octane in the same unit as retention time.

The number of theoretical plates must be greater than 200 000.

32.2.2 *ResolutioN*— Resolution is determined between the peaks of 2-methylheptane and 4-methylheptane using Eq 18.

$$R = \frac{2(Rt_{(a)} - Rt_{(b)})}{1.699(W_{0.5(a)} + W_{0.5(b)})} \quad (18)$$

where:

$Rt_{(a)}$ = retention time of 4-methylheptane,
$Rt_{(b)}$ = retention time of 2-methylheptane,
$W_{0.5(a)}$ = mid-height peak width of 4-methylheptane in the same unit as retention time, and
$W_{0.5(b)}$ = the mid-height peak width of 2-methylheptane in the same unit as retention time.

The resolution must be equal or greater than 1.20

32.2.3 *Polarity*—Polarity is defined by the Mc Reynolds constant of toluene, using Eq 19.

$$Rn_{tol} = Ki_{ana} - Ki_{squalane} \quad (19)$$

where:

$Ki_{squalane}$ = toluene Kovats index on Squalane at 35°C = 742.6, and
Ki_{ana} = toluene Kovats index on the analytical column at 35°C.

Toluene Kovats index is calculated using Eq 20.

$$Ki_{ana} = 700 + 100\left(\frac{\log T'_{R(t)} - \log T'_{R(h)}}{\log T'_{R(o)} - \text{Log } T'_{R(h)}}\right) \quad (20)$$

where:

$T'_{R(t)}$ = the adjusted retention time for toluene,
$T'_{R(h)}$ = the adjusted retention time for *N*-heptane, and
$T'_{R(o)}$ = the adjusted retention time for *N*-octane.

Adjusted retention time of a peak is determined by subtracting the retention time of an unretained compound (air or methane) from the retention time of the peak. The McReynolds constant must be less than 10.

32.2.4 *Base Line Stability*—Base line stability is calculated with the difference between area slices at the beginning and at the end of analysis, divided by the maximum area slice of *N*-octane obtained with the system performance mixture.

32.2.4.1 *Measurement of the Stability*—Carry out one temperature programming defined in 32.1 without injecting any sample. Subtract the area slices at the start of the analysis with those corresponding to 120 min. (average of three slices).

32.2.4.2 *Stability Standardization*—Standardization is carried out using the system performance mixture defined in 29.12 with the column temperature conditions defined in 32.1. The value obtained in 32.2.4.1 is divided by the maximum area slice of *N*-octane and multiplied by 100. The value obtained must be less than 2 %. If this is not the case, check for possible leaks, or recondition the column according to the manufacturer's recommendations.

32.3 *Evaluation of the Linearity of the Split Injector*— Evaluation is carried out using the system performance mixture defined in 29.12 with the column temperature conditions defined in 32.1. The % (m/m) of each compound is determined from the corrected area % using the response factors for each compound given in Annex CA Table C1A or CA2. The relative % error is determined from the known mixture concentrations according to Eq 21.

Relative Error

$$\text{relative \% error} = \frac{100(\text{calculated concentration} - \text{known concentration})}{\text{known concentration}} \quad (21)$$

The relative error must not exceed 3 %.

33. Response Factor

33.1 Theoretical response factors are used for correction of the detector response of hydrocarbons. The response factor for each compound is relative to that of benzene taken equal to unity and are listed in Tables 11 and 12. For peaks corresponding to the co-elution of compounds with benzene, toluene and oxygenates, the response factor is the one of the co-eluted compound of % (m/m). Co-eluted compounds are footnoted in A3.1and A3.2.

34. Procedure

34.1 *Preparation of Apparatus*—After optimization of the carrier gas pressure (Section 31.3) and evaluation of apparatus (Section 32), set the temperature program corresponding to the selected method (Table 8).

34.2 *Injection of Sample*—Inject with a 5 or 10 µL syringe, manually or by autosampler, the size corresponding to the method (Table 8).

34.3 *Integration of Chromatogram*—Integration codes must be selected to obtain a horizontal baseline with a perpendicular drop to the baseline for partially resolved peaks. An example of correct baseline is given in Figs. A3.1 and A3.2.

34.4 *Identification*— Each peak is identified by matching the retention time with that of compounds listed in Table 11 or Table 12 and standard chromatogram given in Fig. A3.1 or A3.2. A specific software using the data of Table 11 or Table 12 can be employed. If an oxygenate has been determined by Test Methods D 4815 or D 5599 and is not in the table, it is necessary to prepare a mixture of a weighed amount of this oxygenate in a known spark-ignition engine fuel to know its retention time and to determine its response factor and then add it to the table.

35. Calculation of Results

35.1 *Calculation of % (m/m) of Each Compound Without*

Co-elution and Not Corrected for Co-elutions— % (m/m) of each component without co-elution and no corrected co-elutions is calculated according to the Eq 22.

$$C_{i'} = \frac{Ai\ Bi}{\sum_{i=0}^{i=n} (Ai\ Bi + A_{int}\ B_{int})} 100 \quad (22)$$

where:

$C_{i'}$ = % (m/m) of compound *i* without co-elution and no correction of co-elutions,
Ai = peak area of compound *i* without co-elution (benzene, toluene, and oxygenates),
A_{int} = peak area of compounds co-eluting (benzene, toluene and oxygenates),
B_i = response factor for component *i* (given in Tables A3.1 or A3.2), and
B_{int} = response factor for components co-eluted with benzene, toluene, and oxygenates.

35.2 *Calculation of Components Co-eluted with Benzene, Toluene, and Oxygenates*—Benzene, toluene contents are determined by Test Methods D 3606 or D 4420 or Test Method D 5580 oxygenates contents are determined by Test Methods D 4815 or D 5599. The % (m/m) of components coeluted with benzene, toluene and oxygenates is calculated according the Eq 23.

$$C_{coeluted} = C_{int.}\ 0.01\left[100 - \sum\left(C_{ext.} - C_{ext.} \times \frac{B_{int.}}{B_{ext.}}\right)\right] - C_{ext.} \times \frac{B_{int.}}{B_{ext.}} \quad (23)$$

where:

$C_{coeluted}$ = % (m/m) of component eluted with benzene, toluene, or oxygenates,
C_{int} = % (m/m) calculated with the Eq 22 for the peak with co-elution,
C_{ext} = % (m/m) of benzene, toluene, or oxygenates determined by other method, and
B_{ext} = response factor of benzene, toluene or oxygenates.

35.3 *Calculation of Other Components*—% (m/m) of other components is calculated using Eq 24.

$$C_i = C_{i'} \frac{100 - \sum C_{coeluted} - \sum C_{ext.}}{\sum C_{i'}} \quad (24)$$

36. Report

36.1 Report the content of each component as % (m/m) to the nearest 0.01 %.

37. Precision [8]

37.1 *Individual Components*—The precision of this test method was determined by a statistical analysis of interlaboratory test results. It applies only to a range of 0.1 to 15 % (m/m), for all components with a resolution greater than 1.0 and without co-elution with oxygenate components. When two components of the same hydrocarbon type have a resolution less than 1.0, the precision can be applied by adding the concentration of two components. The precision is the same for all:

37.1.1 Light components (saturates and olefins) with a carbon number of C_4 and C_5

37.1.2 Saturates and olefins with a range of carbon number of C_6 to C_{12} aromatics.

37.1.3 This precision is as follows:

37.1.3.1 *Repeatability*— The difference between successive test results, obtained by the same operator with the same apparatus under constant operating conditions on identical test material, in the normal and correct operation of the test method, would exceed the value given in the Table 12 in only one case in twenty.

37.1.3.2 *Reproducibility*—The difference between two single and independent results, obtained by different operators in different laboratories on nominally identical test material, in the normal and correct operation of the test method, would exceed the values given in the Table 13 in only one case in twenty.

38. Keywords

38.1 detailed hydrocarbon analysis; DHA; gas chromatography; gasoline; hydrocarbons; open tubular; oxygenates; spark ignition engine fuels

TABLE 13 Repeatability and Reproducibility for Individual Components

	Range of Carbon	Range % (m/m)	Repeatability X (% (m/m))	Reproducibility X (% (m/m))
Light components	C_4- C_5	0.1 - 14	0.04 × X	0.16 × X
Paraffins	C_6- C_{12}	0.1 - 11.5	0.01 + 0.03 × X	0.04 + 0.07 × X
Naphthenes	C_6- C_8	0.1 - 3		
Olefins	C_6- C_8	0.1 - 1		
Aromatics	C_6- C_{12}	0.1 - 14	0.05 + 0.02× X	0.1 + 0.06 × X

ANNEXES

(Mandatory Information)

A1. PROCEDURE FOR ADJUSTING THE SELECTIVITY OF A DHA DIMETHYLPOLYSILOXANE OPEN TUBULAR COLUMN

A1.1 The successful application of this test method is highly dependent upon the selectivity of the column used. New 100 m × 0.25 mm 0.5 µm 100 % dimethylpolysiloxane open tubular fused silica columns will likely not have sufficient selectivity for aromatics to function properly. Critical to the successful analysis of *reformulated* and oxygenated spark engine motor fuels is column inertness and component selectivity. Inertness of the primary 100 m column affects the retention and adsorption of the oxygenates such as alcohols and ethers, while selectivity for the aromatic compounds is controlled by the liquid phase. Until adequate commercial columns are available, it will be necessary to slightly increase the column selectivity, which is accomplished by the addition of a short precolumn containing a moderately selective liquid phase.

A1.2 Prior to making any precolumn additions to the 100 m 100 % dimethylpolysiloxane capillary column, determine that the main column meets the column specifications outlined in 6.4.1 and determined in Section 9. Section 9 describes the preliminary evaluation of the 100 m 100 % dimethylpolysiloxane capillary column, using a 35° isothermal analysis to determine the basic column characteristics of efficiency, retention factor, inertness, and selectivity. Figs. A1.1-A1.3 provide examples of the column quality specification determinations. These determinations may also be made with a precolumn attached, since the precolumn has little if any affect on the results. Fig. A1.4 illustrates that the addition of different lengths of precolumn has negligible influence on the retention characteristics of oxygenated compounds. Poor peak shape and resolution of these the result of an active injector liner or packing, or both, material in the injector liner. An increase in retention of the oxygenates is likely due to column activity. The relative position of the oxygenates to the hydrocarbons is dependent upon column temperature, thus a faulty column oven temperature control could also result in shifted peaks.

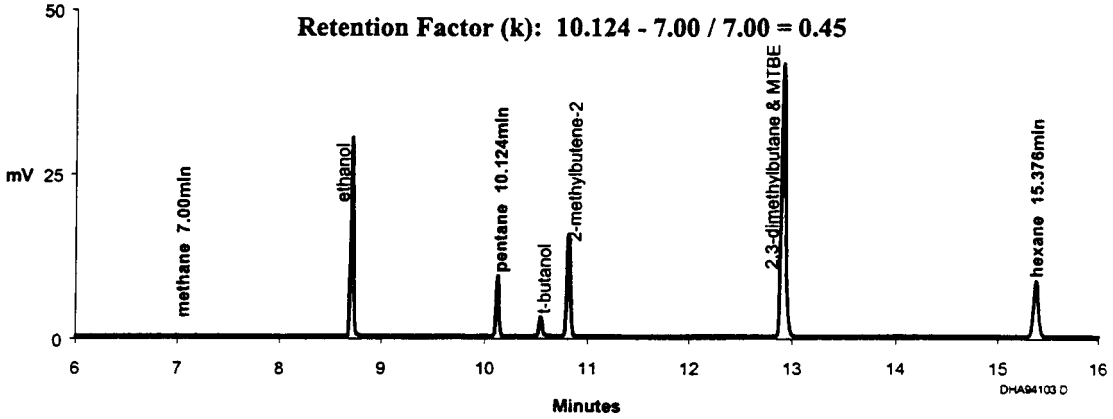
A1.3 When necessary, a precolumn is added to the primary 100 m column to adjust the column selectivity for aromatic compounds. Precolumns that have been used successfully are variable lengths of 0.25 mm internal diameter fused silica open tubular column containing a 1.0 µm film thickness of 5 % phenyl dimethylpolysiloxane. The film thickness is likely not critical, only the total amount of phase. Lengths ranging from one to more than 3 m have been necessary to provide sufficient selectivity, depending on the initial selectivity of the methyl silicone column used. One meter of 1.0 µm precolumn is equivalent to a 100 m column with 0.5 µm of 0.1 % phenyl methyl silicone liquid phase.

A1.4 Figs. A1.5-A1.8 illustrate the resolution of the methylcyclopentene-1 and benzene pair with a new column and 1, 2, and 3 m of precolumn. The key segment of the chromatogram is expanded to better illustrate the resolution of this component pair.

A1.5 The preliminary evaluation of the 100 m column will provide the user with information regarding the initial length of precolumn with which to start the tuning process. Dependent upon the methylcyclopentene-1 and benzene resolution, an initial precolumn of between 1 and 4 m is selected; which ever provides a resolution greater than 1.2.

A1.6 The final tuning will consist of reducing the precolumn length, probably in increments of 0.25 m, until the proper resolution is achieved between 2,3,3-trimethylpentane and toluene, and 1,4-dimethylbenzene and 2,3-dimethylheptane; using the actual analysis temperature conditions.

A1.7 Fig. A1.9 illustrates graphically the effect of different lengths of precolumn attached to the same 100 m column. The



NOTE 1—Efficiency (n): $5.545\ (10.124/0.032)^2 = 555\ 016$

FIG. A1.1 Column Retention Factor Calculation (9.1)

Efficiency (n): 5.545 (10.124 / 0.032)^2 = 555,016

Resolution (R): 2(10.817 - 10.547) / 1.699(0.034+0.034) = 4.673

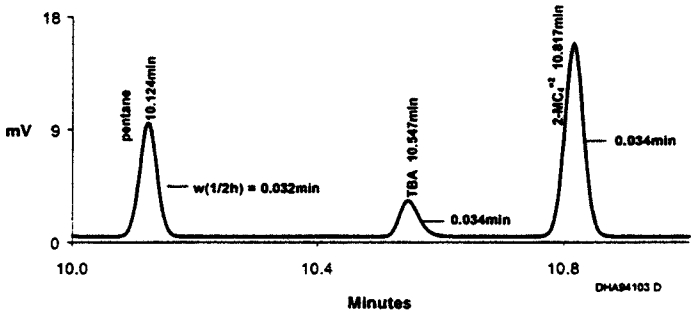


FIG. A1.2 Column Efficiency and Resolution Calculations (9.2 and 9.3)

Skew: ratio of B / A = 3.5 / 2.2 = 1.59

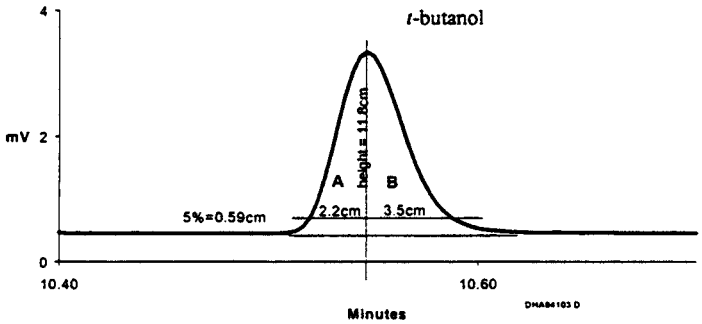


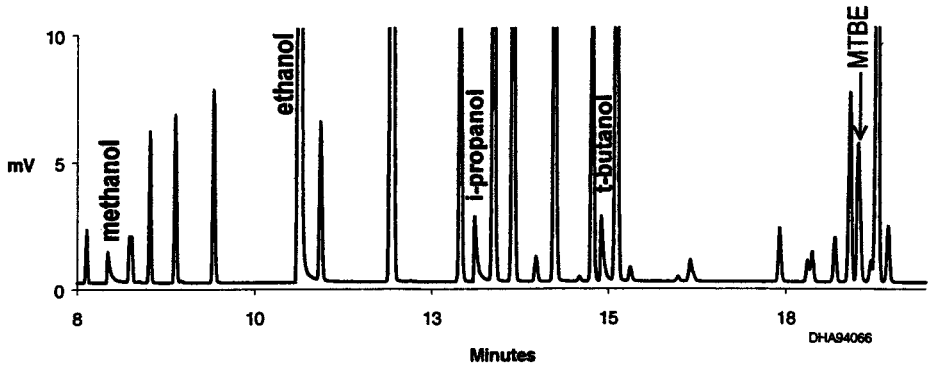
FIG. A1.3 Column Inertness – Peak Skewness Calculation (11.5)

key component separations are shown. These analyses were made using the conditions given in Table 3. In this case, the use of the 1.25 m precolumn provides the best compromise for the three key separations.

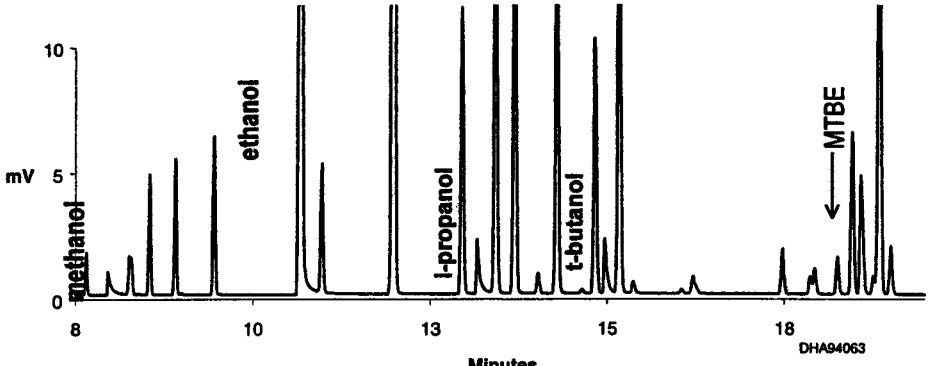
A1.8 Fig. A1.10 illustrates the use of different lengths of precolumn to achieve the specified selectivity for three different 100 m columns. The final precolumn length will provide adequate resolution of all three of the key separations.

A1.9 Figs. A1.11-A1.17 illustrate typical chromatographic elution.

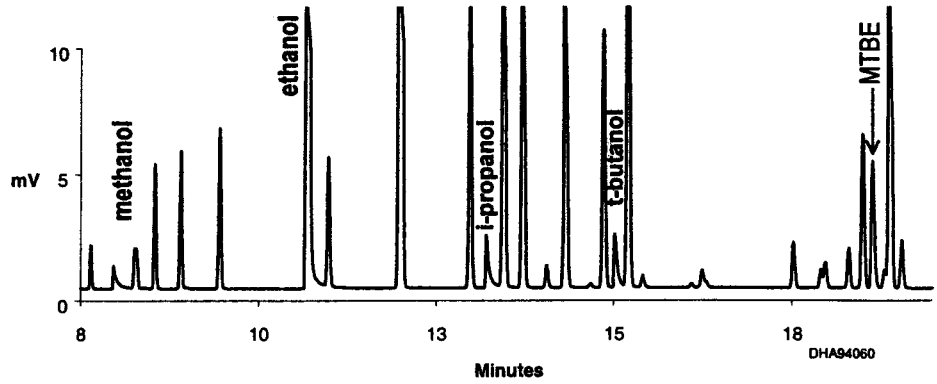
A1.10 Table A1.1 provides the data for the physical constants used in the cooperative study. Table A1.2 presents data on the analyses of various refinery samples.



Petrocol DH100 0.5μm_{df} methylsilicone column + **1.25m** 1μm_{df} DB5 precolumn



Petrocol DH100 0.5μm_{df} methylsilicone column + **1.5m** 1μm_{df} DB5 precolumn



Petrocol DH100 0.5μm_{df} methylsilicone column + **2.0m** 1μm_{df} DB5 precolumn

FIG. A1.4 Oxygenates Separations – Effect of Different Precolumn Lengths

$$R = 2(21.658 - 21.590) / 1.699(0.08 + 0.08) = 0.500$$

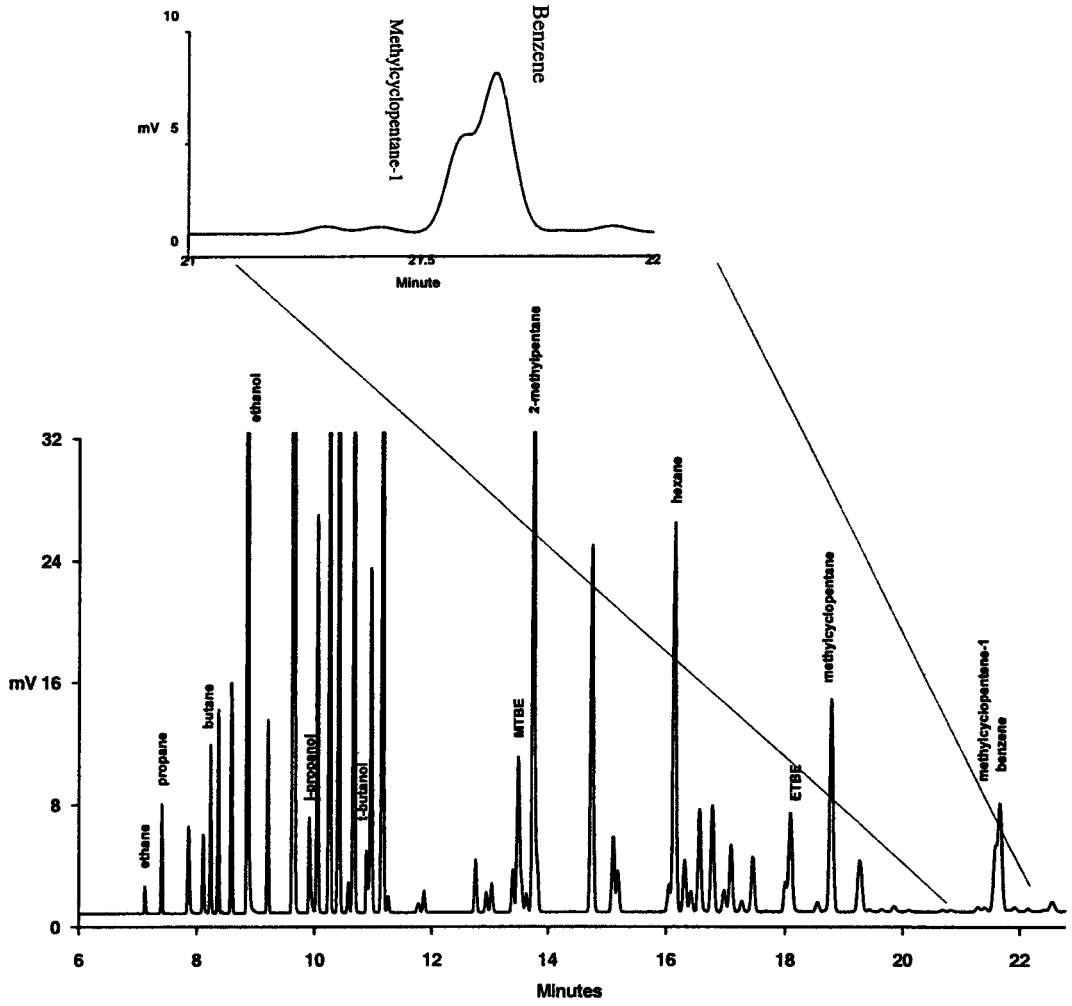


FIG. A1.5 PONA-V Standard – Analysis through Benzene (New DHA Column Analyzed at 35°C Isothermal)

$$R = 2(21.025 - 20.925) / 1.699(0.076 + 0.081) = 0.750$$

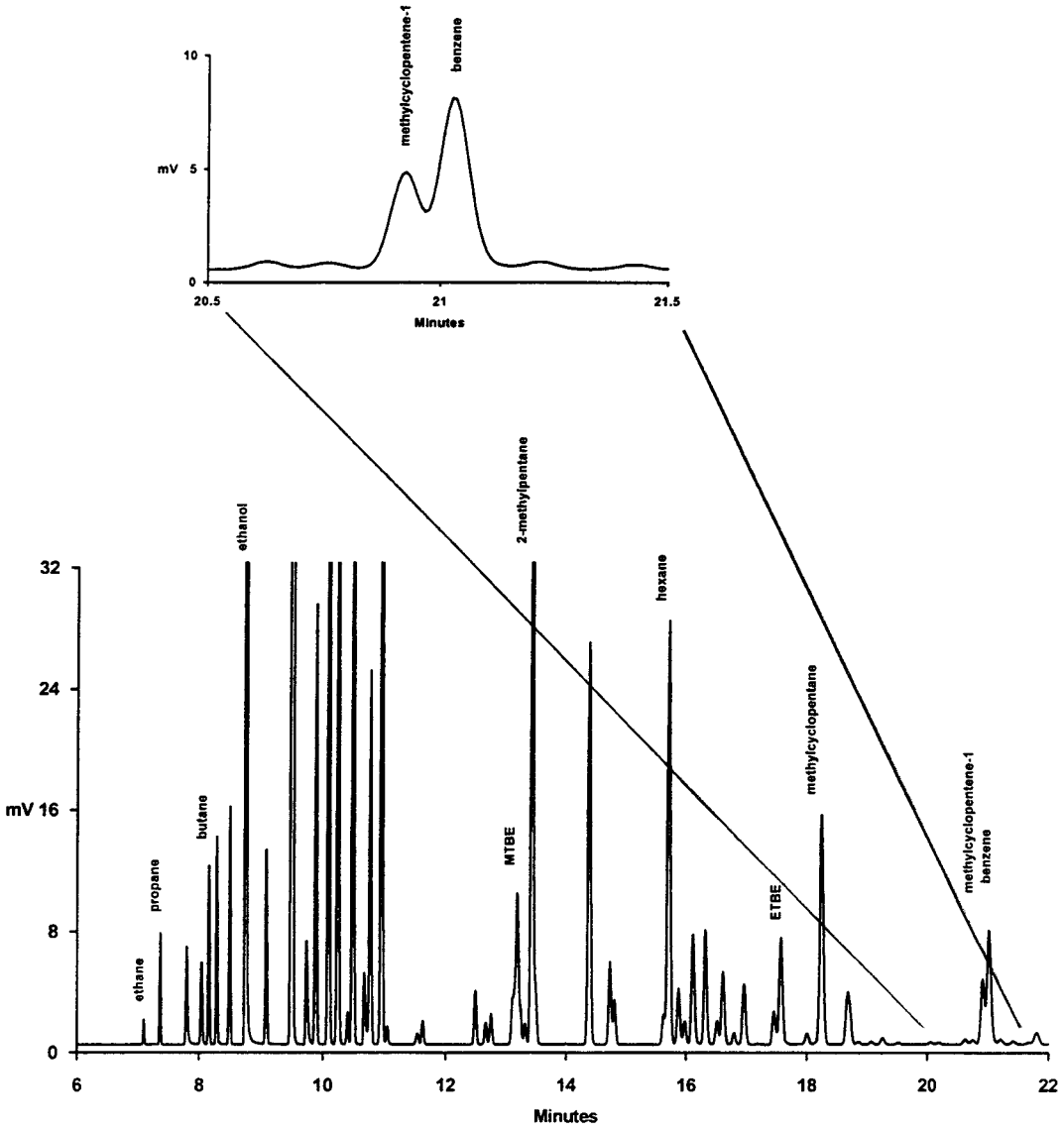


FIG. A1.6 PONA-V Standard – Analysis through Benzene (New DHA Column plus 1 m × 0.25 mm 1 µm DB5 Precolumn Analyzed at 35°C Isothermal)

$$R = 2(21.258 - 21.125) / 1.699(0.079 + 0.081) = 0.978$$

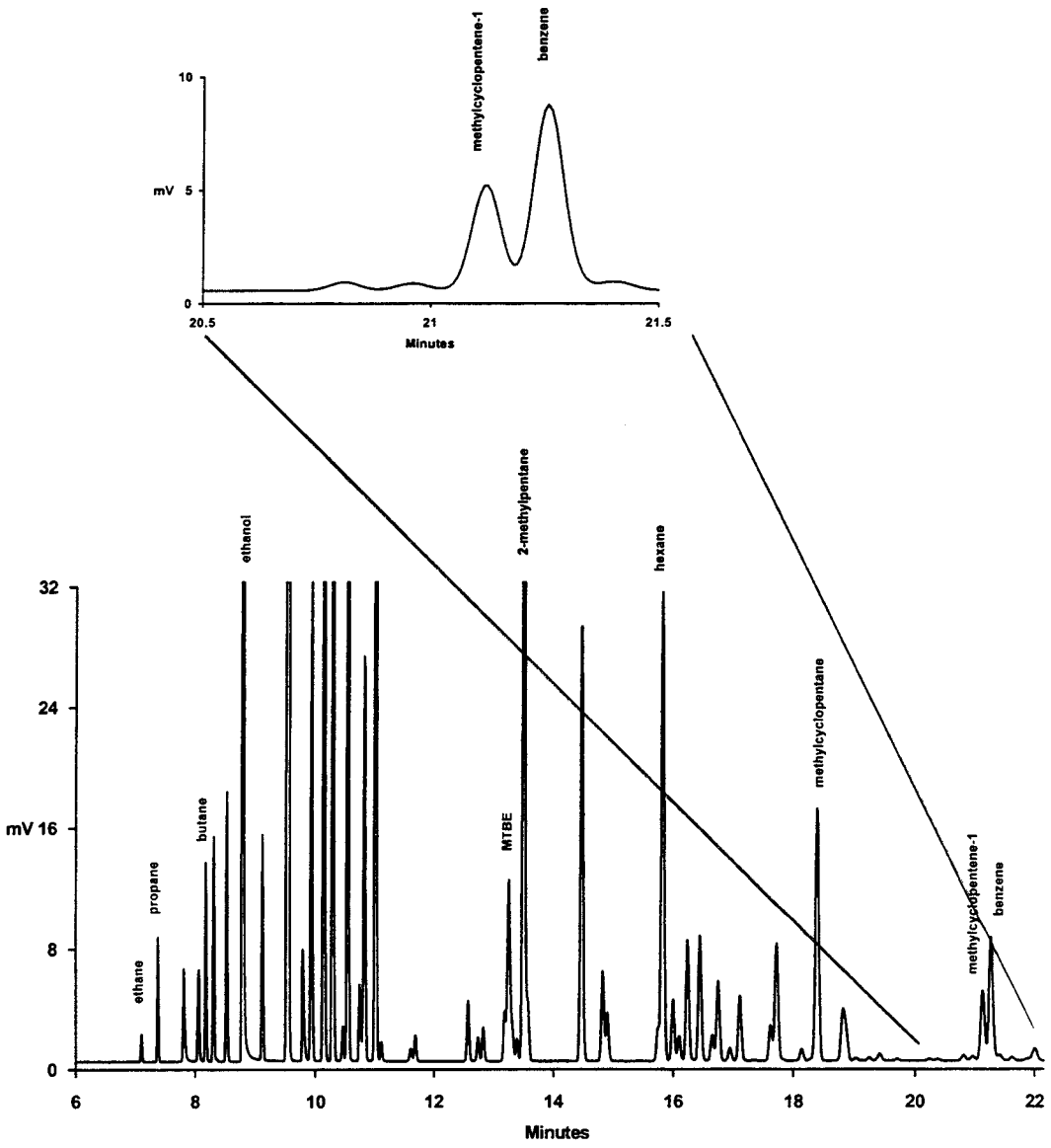


FIG. A1.7 PONA-V Standard – Analysis through Benzene (New DHA Column plus 2 m × 0.25 mm 1 µm DB5 Precolumn Analyzed at 35°C Isothermal)

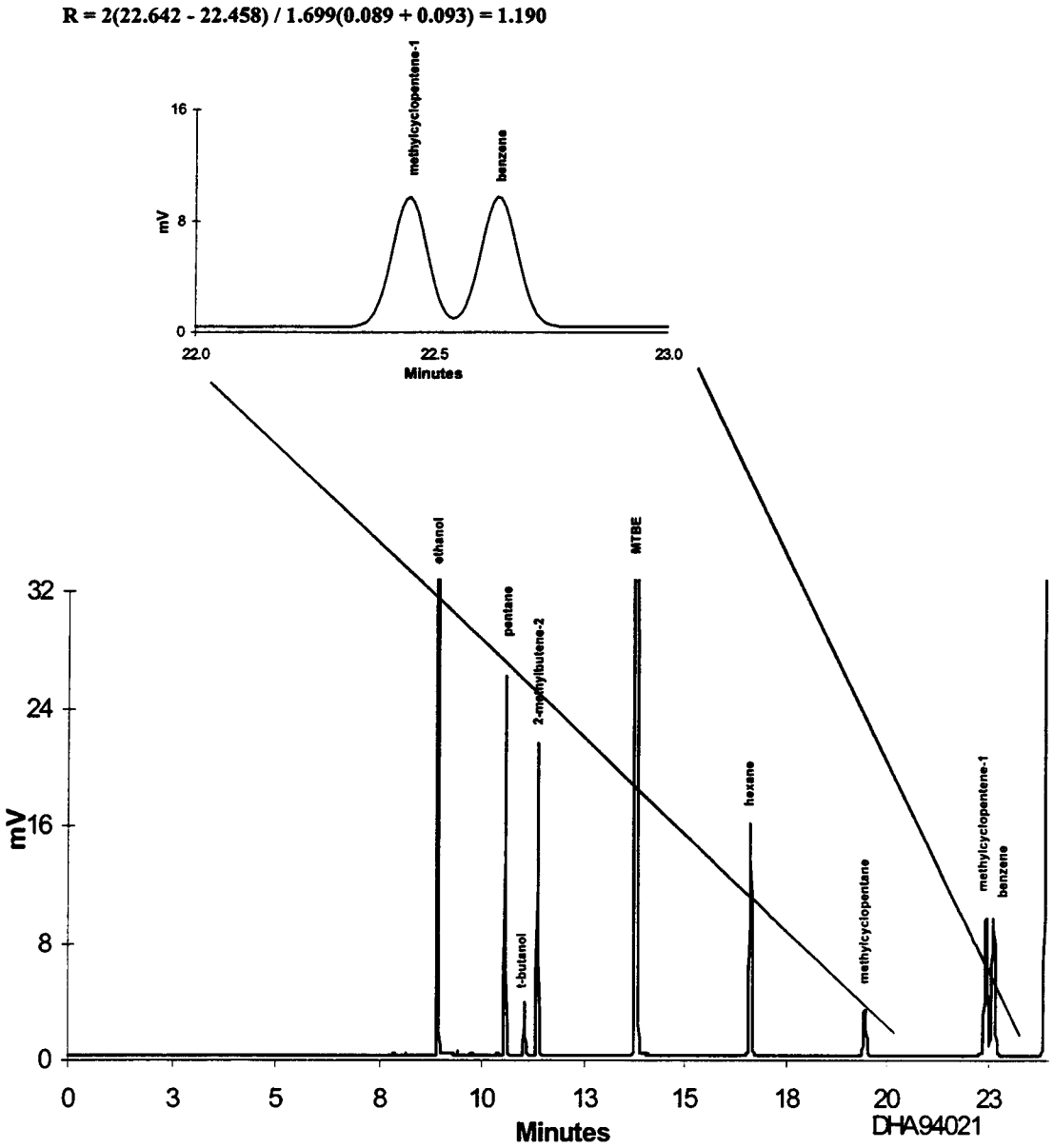


FIG. A1.8 DHA Calibration Standard – Analysis through Benzene (New DHA Column plus 3 m × 0.25 mm 1 µm DB5 Precolumn Analyzed at 35°C Isothermal)

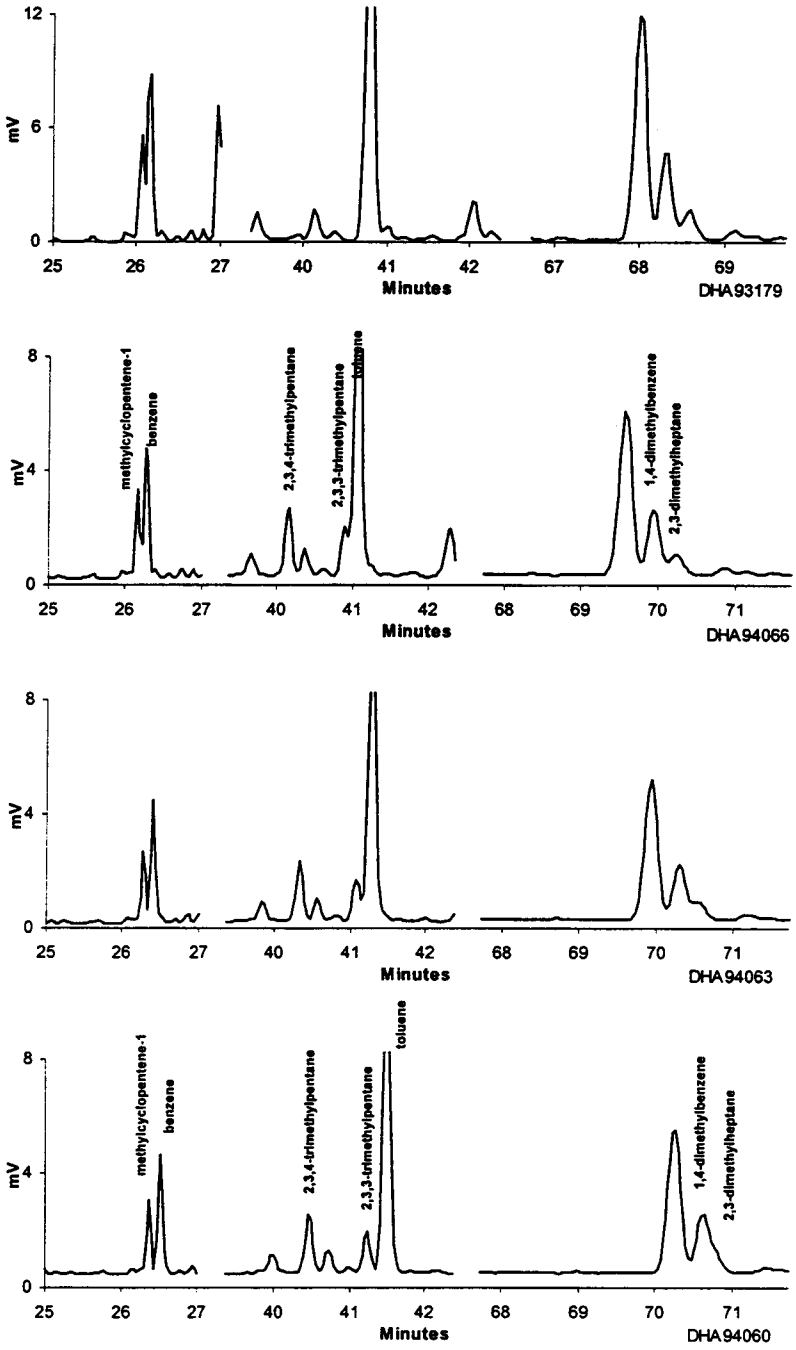
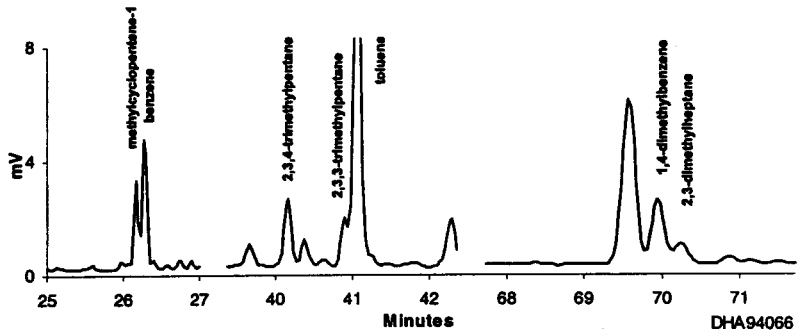
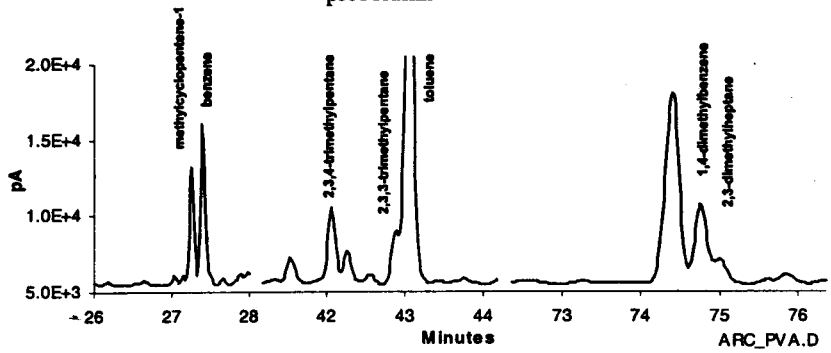


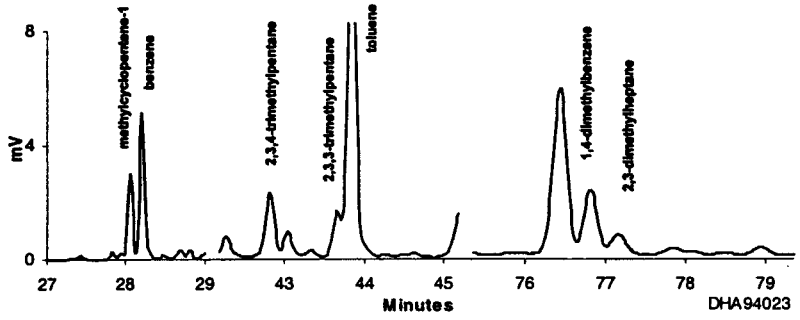
FIG. A1.9 Key Separations – Effect of Different Precolumn Lengths (Same Primary Column. Conditions according to Table 3 Top to Bottom - 1.00m, 1.25m, 1.50m, and 2.00m DB5 precolumn)



(Old) Petrocol DH100 0.5μm_{df} methylsilicone column + 1.25m 1μm_{df} DB5 precolumn



Petrocol DH100 0.5μm_{df} methylsilicone column + 2.4m 1μm_{df} DB5 precolumn



100m x 0.25mm HP 0.5μm_{df} methylsilicone column + 3.0m 1μm_{df} DB5 precolumn

FIG. A1.10 Key Separations – Tuning of Different Columns (Conditions according to Table A3 Table ? - DHA Component Data)

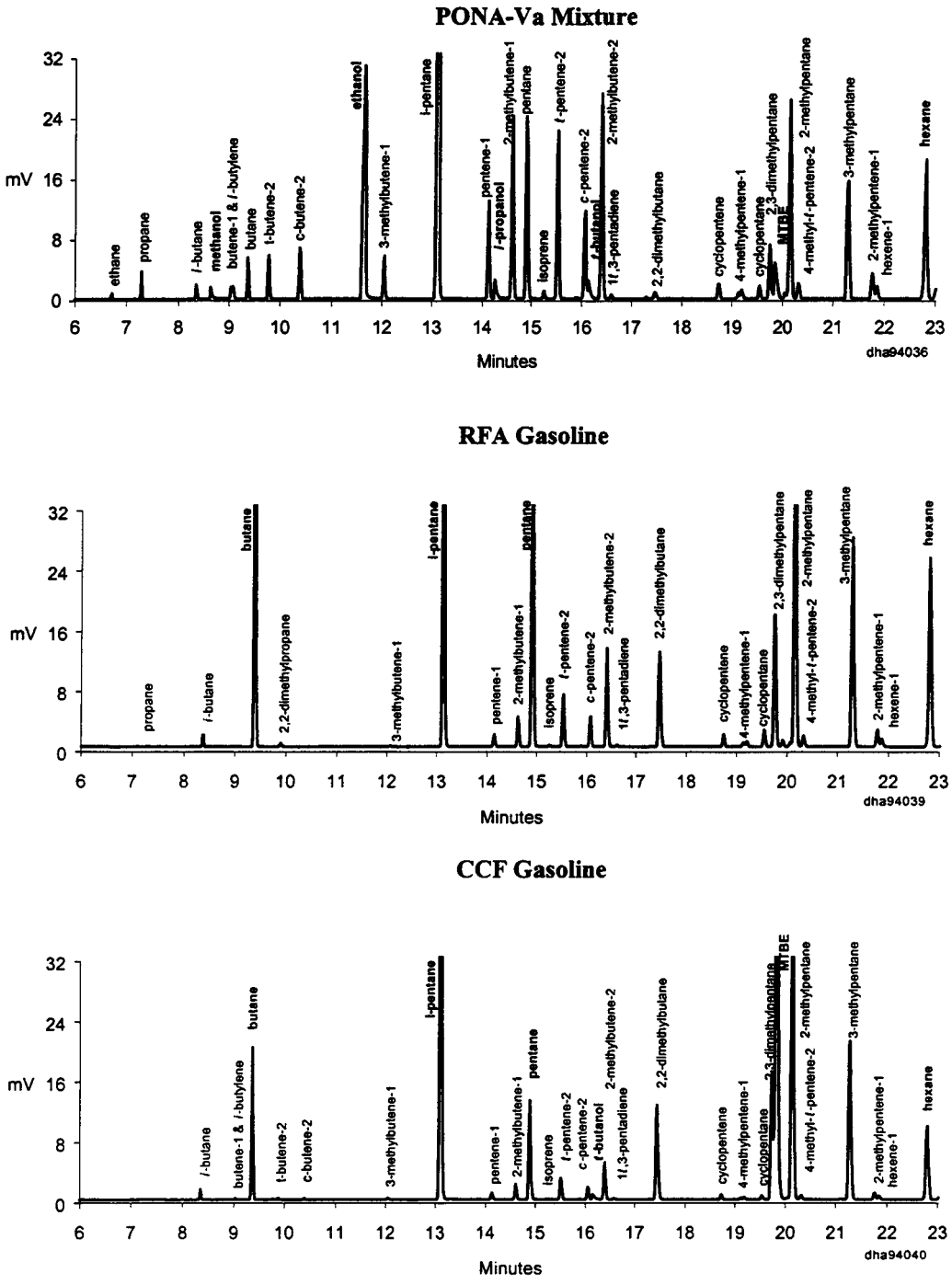


FIG. A1.11 DHA Analyses – Methane through Hexane

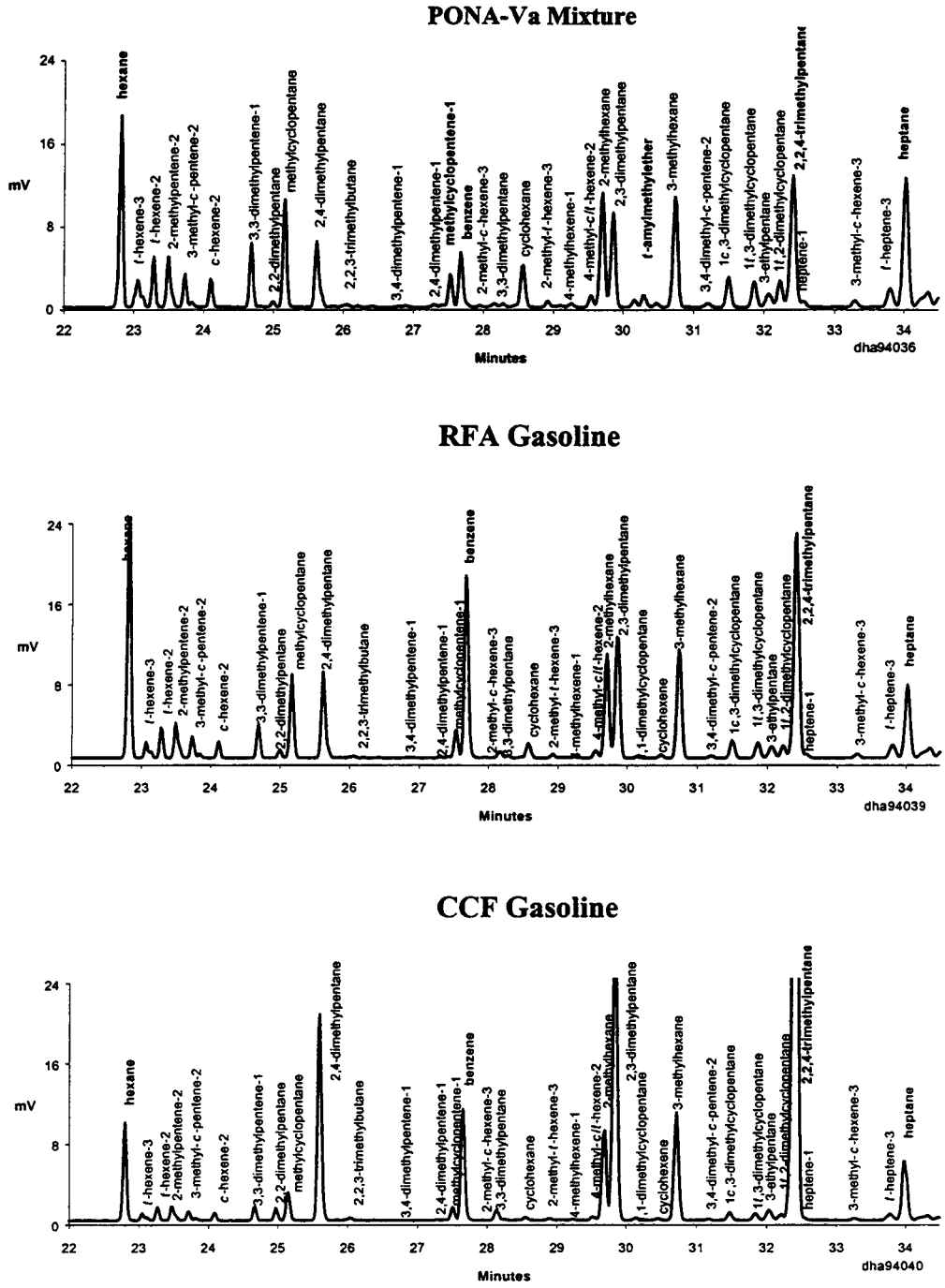


FIG. A1.12 DHA Analyses – Heptane through Heptane

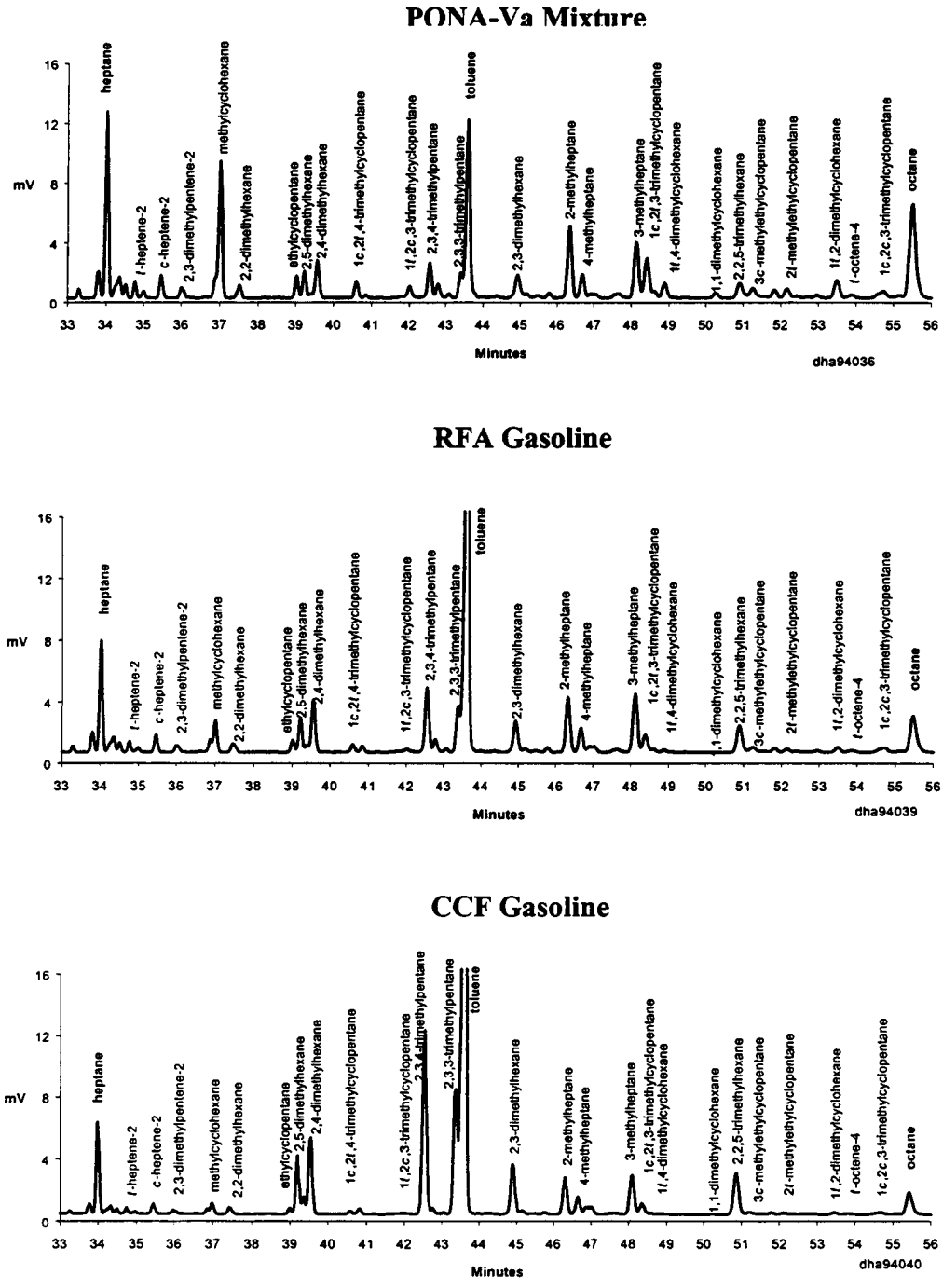


FIG. A1.13 DHA Analyses – Heptane through Octane

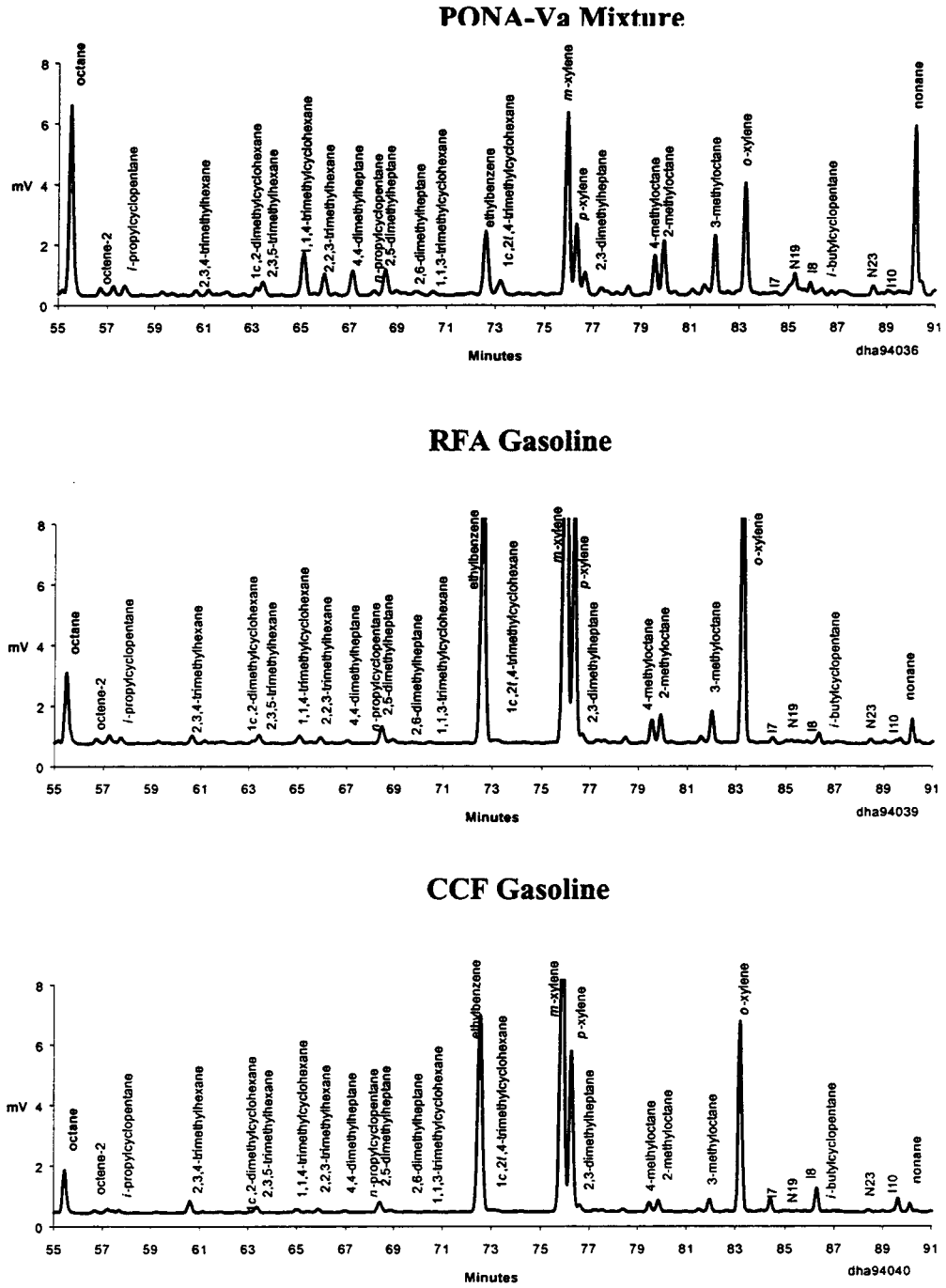
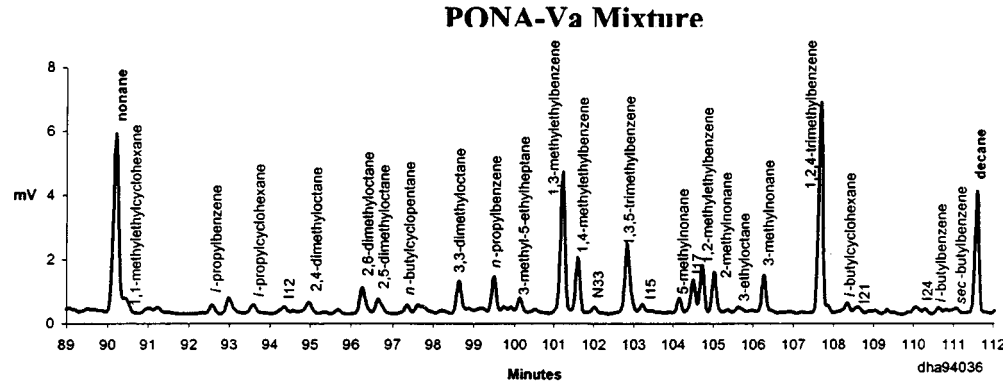
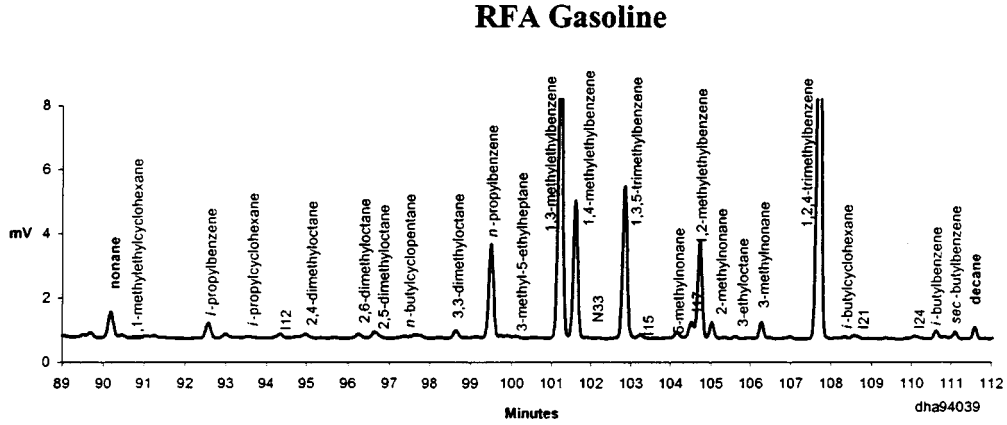


FIG. A1.14 DHA Analyses – Octane through Nonane





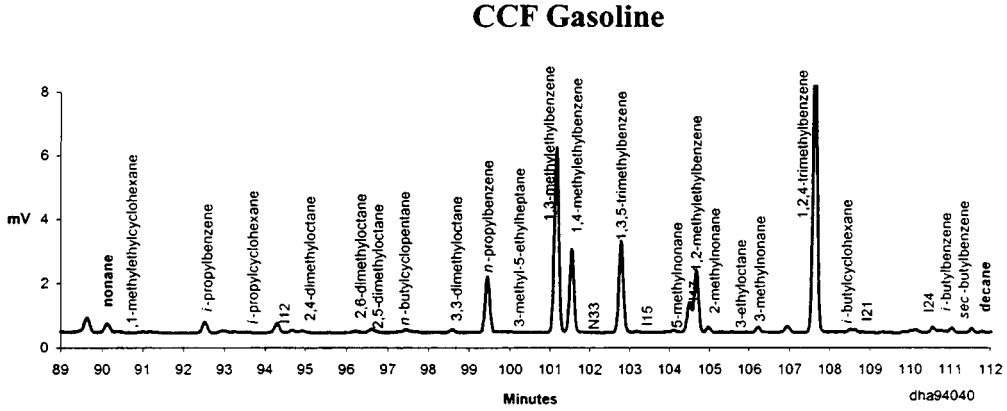
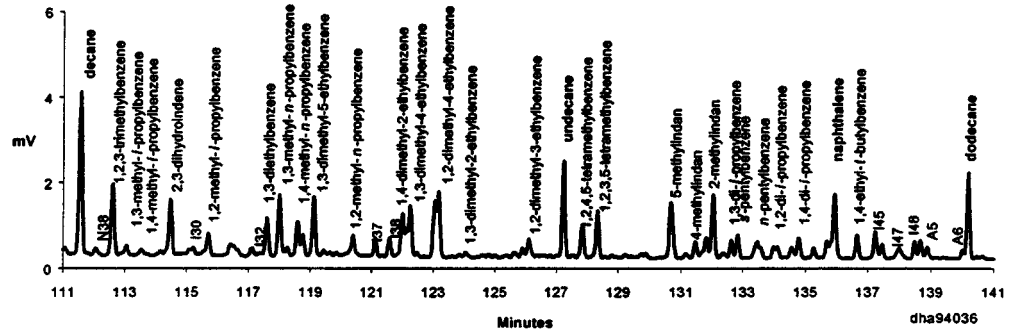
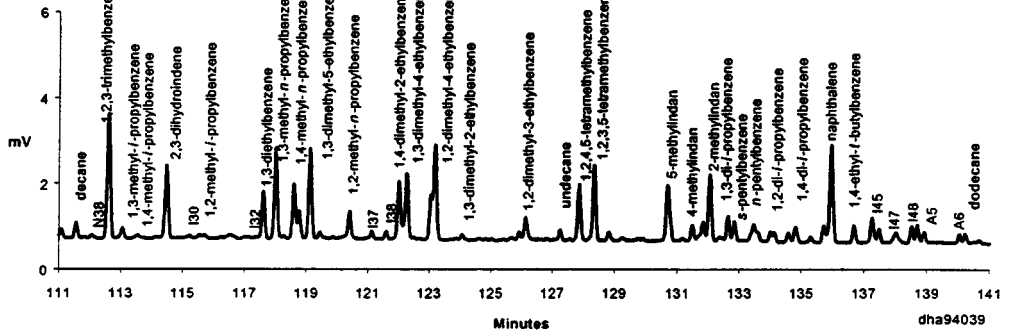


FIG. A1.15 DHA Analyses – Nonane through Decane

PONA-Va Mixture



RFA Gasoline



CCF Gasoline

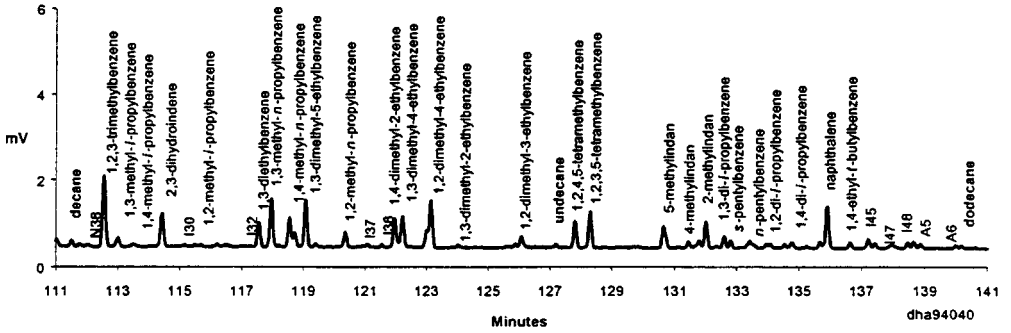
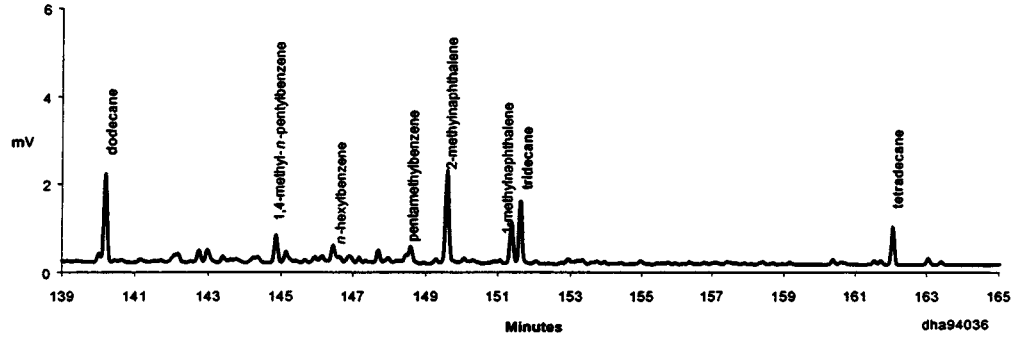
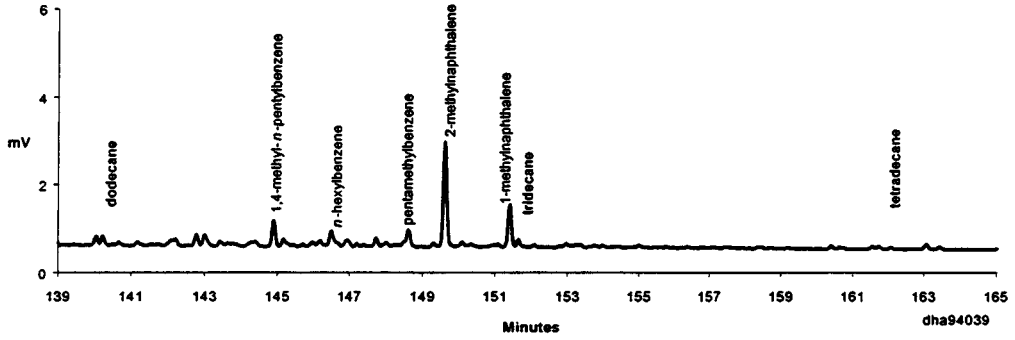


FIG. A1.16 DHA Analyses – Decane through Dodecane

PONA-Va Mixture



RFA Gasoline



CCF Gasoline

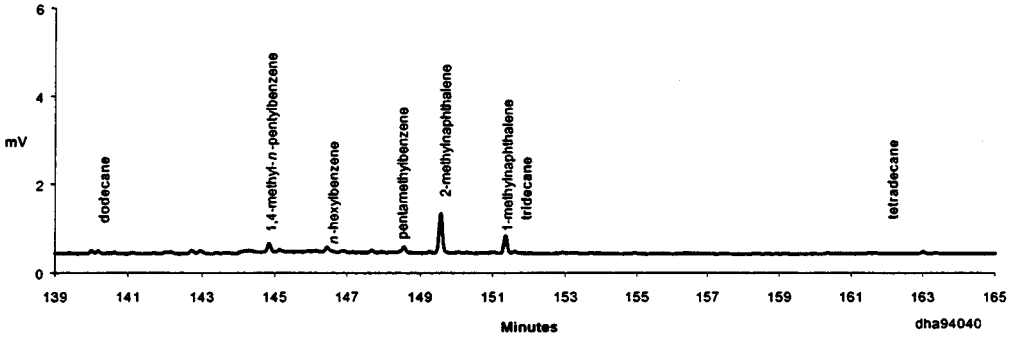


FIG. A1.17 DHA Analyses – Dodecane through Tetradecane

TABLE A1.1 DHA Component Data

NOTE 1—These data consist of the current physical constants used in the cooperative study. The average retention index are those accumulated in a ruggedness test of the "tuning" process. The RFA and CCF gasoline data are the averages determined in the cooperative study. RFA is an industry average regular gasoline and CCF is a California Certification Fuel (reformulated gasoline).

NOTE 2—Components known to co-elute are indicated with an asterisk preceding the name. Unknown components whose group type are known are named with a letter (that is, O for olefin and a consecutive number. If consecutive numbers are missing, they have been identified by name.

					RFA Gasoline			CCF Gasoline		
Component	Ave. RI	RRF	MW	Rel. Den.	Min.	INDEX	Mass%	Min.	INDEX	Mass%
methane	100.00	1.121	16.043	0.2600						
ethylene	178.10	0.980	28.054	0.3000						
ethane	200.00	1.050	30.070	0.3399						
propylene	284.00	0.980	42.081	0.5053				7.173	293.43	0.000
propane	300.00	1.027	44.097	0.5005	7.270	300.32	0.003	7.266	299.79	0.003
i-butane	366.15	1.015	58.124	0.5572	8.266	365.46	0.088	8.262	365.29	0.078
methanol	378.82	3.148	32.040	0.7914				8.506		0.021
butene-1	390.72	0.980	56.108	0.5951				8.893	390.31	0.019
isobutylene	391.51	0.980	56.108	0.5951						
1,3-butadiene	394.93	0.945	54.092	0.6211						
n-butane	400.00	1.015	58.124	0.5788	9.195	400.00	4.637	9.193	400.00	1.201
vinyl acetylene	409.00	1.100	54.090	0.6500						
t-butene-2	412.09	0.980	56.108	0.6042	9.441	411.72	0.002	9.567	412.10	0.013
2,2-dimethylpropane	415.10	1.008	72.151	0.5910	9.670	415.09	0.036	9.666	415.05	0.017
c-butene-2	427.74	0.980	56.108	0.6213	9.983	427.70	0.004	10.128	427.73	0.018
1,2-butadiene	450.00	0.945	54.092	0.6520						
ethanol	455.33	2.193	46.070	0.7890	11.063	452.52	0.006			
3-methylbutene-1	460.84	0.980	70.135	0.6272	11.670	460.81	0.010	11.665	460.76	0.020
O1	469.00	0.980	70.135	0.6300	12.030	470.03	0.005			
O2	474.00	0.980	70.135	0.6300						
i-pentane	477.45	1.008	72.151	0.6196	12.653	477.15	4.773	12.650	477.13	7.163
*acetone	477.55	1.850	58.080	0.7899				12.649		0.134
1,4-pentadiene	481.18	0.952	68.119	0.6607				13.464	482.77	0.005
?	483.00				13.122	486.32	0.014	12.675	482.80	0.003
butyne-2	488.00	0.945	54.092	0.6910						
pentene-1	490.83	0.980	70.135	0.6405	13.616	490.86	0.152	13.613	490.85	0.091
i-propanol	493.38	1.400	60.110	0.8000						
2-methylbutene-1	496.66	0.980	70.135	0.6504	14.074	496.73	0.334	14.071	496.72	0.185
n-pentane	500.00	1.008	72.151	0.6262	14.341	500.00	3.627	14.339	500.00	1.094
isoprene	506.02	0.952	68.119	0.6809	14.666	506.00	0.013	14.664	505.98	0.009
?	508.00				14.644	508.07	0.003			
t-pentene-2	510.56	0.980	70.135	0.6482	14.917	510.41	0.653	14.916	510.41	0.285
3,3-dimethylbutene-1	516.79	0.980	70.135	0.6500	15.277	516.60	0.011	15.141	516.58	0.004
c-pentene-2	519.53	0.980	70.135	0.6556	15.439	519.25	0.378	15.438	519.28	0.160
t-butanol	521.64	1.154	74.120	0.7887				15.468	522.58	0.065
?	522.40							16.198	522.66	0.038
2-methylbutene-2	524.92	0.980	70.135	0.6623	15.765	524.49	1.100	15.763	524.51	0.461
1t,3-pentadiene	527.97	0.952	68.119	0.6760	15.960	527.59	0.022	15.956	527.56	0.015
3-methylbutadiene-1,2	535.00	0.952	68.120	0.6500						

TABLE A1.1 *Continued*

					RFA Gasoline			CCF Gasoline		
Component	**Ave. RI**	**RRF**	**MW**	**Rel. Den.**	**Min.**	**INDEX**	**Mass%**	**Min.**	**INDEX**	**Mass%**
cyclopentadiene	538.05	0.938	67.100	0.6500	16.478	537.58	0.004	16.475	537.57	0.003
2,2-dimethylbutane	540.54	1.004	86.178	0.6491	16.779	539.78	1.102	16.776	539.75	1.106
1c,3-pentadiene	541.90	0.952	68.119	0.6910						
?	543.00				16.895	543.44	0.006			
O5	547.70	0.980	70.135	0.6500						
O6	549.70	0.980	70.135	0.6500						
cyclopentene	557.21	0.952	68.119	0.7720	18.026	556.65	0.160	18.025	556.67	0.070
n-propanol	560.00	1.400	60.110	0.8035						
4-methylpentene-1	562.02	0.980	84.162	0.6673	18.411	561.26	0.050	18.402	561.42	0.021
3-methylpentene-1	562.81	0.980	84.162	0.6637	18.468	562.21	0.083	18.469	562.26	0.032
cyclopentane	566.84	0.980	70.135	0.7454	18.811	566.40	0.216	18.813	566.45	0.052
2,3-dimethylbutane	569.24	1.004	86.178	0.6616	19.003	568.67	1.723	19.001	568.69	1.655
methyl-t-butylether	570.65	1.417	88.150	0.7405				19.110	570.03	11.282
4-methyl-c-pentene-2	571.00	0.980	84.162	0.6741	19.154	570.47	0.113			
2,3-dimethylbutene-1	572.67	0.980	84.162	0.6830	19.306	572.01	0.048	19.520	572.52	0.028
2-methylpentane	573.70	1.004	86.178	0.6531	19.388	573.19	5.145	19.389	573.23	3.967
4-methyl-t-pentene-2	575.47	0.980	84.162	0.6736	19.542	574.94	0.167	19.546	575.03	0.083
O8	578.00	0.980	84.162	0.6736	20.042		0.002	19.893		0.002
2-methyl-1,4-pentadiene	579.00	0.956	82.146	0.6940	20.078		0.002			
?	581.00							20.002		0.002
1,5-hexadiene	581.90	0.956	82.146	0.6923	20.123	581.47	0.002	20.210		0.011
?	583.90				20.250	583.99	0.002			
3-methylpentane	585.52	1.004	86.178	0.6643	20.477	585.25	2.589	20.476	585.25	2.189
2-methylpentene-1	590.19	0.980	84.162	0.6848	20.933	590.01	0.241	20.934	590.05	0.103
hexene-1	591.06	0.980	84.162	0.6780	21.021	590.91	0.127	21.021	590.94	0.059
O11	592.00	0.980	84.162	0.6780						
i-butanol	593.50	1.337	74.120	0.8030						
?	596.00				21.474	596.35	0.007			
1c/t,4-hexadiene	597.14	0.956	84.146	0.7000	21.571	597.22	0.004			
2-ethylbutene-1	598.95	0.980	84.162	0.6944						
n-hexane	600.00	1.004	86.178	0.6594	21.937	600.00	2.598	21.935	600.00	1.057
diisopropylether	601.90	1.100	102.180	0.7241						
t-hexene-3	602.83	0.980	84.162	0.6821	22.169	602.83	0.191	22.170	602.86	0.080
c-hexene-3	603.56	0.980	84.162	0.6847	22.258	603.60	0.063	22.234	603.65	0.028
t-hexene-2	605.44	0.980	84.162	0.6827	22.382	605.40	0.347	22.383	605.43	0.157
2-methylpentene-2	607.86	0.980	84.162	0.6912	22.583	607.77	0.462	22.584	607.80	0.193
4-methylcyclopentene	609.00				21.685	608.90	0.113	22.589	608.65	0.047
3-methyl-c-pentene-2	610.54	0.980	84.162	0.6980	22.816	610.51	0.240	22.817	610.54	0.102
3-methylcyclopentene	611.61	0.956	82.146	0.7622	22.920	611.74	0.055	22.921	611.77	0.025
O13	613.08	0.980	84.162	0.6920						
c-hexene-2	614.67	0.980	84.162	0.6920	23.171	614.60	0.194	23.172	614.63	0.088
O14	617.06	0.980	84.162	0.6920	23.007	617.10	0.004	23.088	617.08	0.002
ethyl-t-butylether	619.00	1.342	102.180	0.7519						
3,3-dimethylpentene-1	620.91	0.980	98.189	0.7019	23.722	620.77	0.371	23.723	620.80	0.158
3-methyl-t-pentene-2	622.11	0.980	84.162	0.7023	23.603	622.17	0.006	23.480	622.19	0.003
2-butanol	622.40	1.295	74.120	0.8080						
4,4-dimethyl-t-pentene-2	623.10	0.980	98.189	0.6936						

TABLE A1.1 *Continued*

					RFA Gasoline			CCF Gasoline		
Component	Ave. RI	RRF	MW	Rel. Den.	Min.	INDEX	Mass%	Min.	INDEX	Mass%
2,2-dimethylpentane	624.17	1.000	100.205	0.6738	24.025	624.11	0.084	24.024	624.12	0.128
methylcyclopentane	625.86	0.980	84.162	0.7486	24.189	625.88	0.963	24.190	625.91	0.355
cyclic diolefin or triolefin	627.00	0.957	82.140	0.7092						
2,4-dimethylpentane	630.60	1.000	100.205	0.6727	24.622	630.47	1.036	24.623	630.48	2.437
2,3,3-trimethylbutene-1	631.00	0.980	98.189	0.7092						
cyclic diolefin or triolefin	632.90	0.957	82.140	0.7092	24.846	632.82	0.010	24.844	632.80	0.008
?	634.20				25.835	634.14	0.009			
2,2,3-trimethylbutane	634.86	1.000	100.205	0.6901	25.049	634.91	0.031	25.050	634.93	0.038
?	636.30				25.186	636.30	0.007	25.091	636.33	0.004
cyclic diolefin or triolefin	638.30	0.957	82.140	0.7092	25.380	638.26	0.008	25.378	638.27	0.005
O17	641.97	0.980	84.160	0.7039	25.745	641.92	0.005	25.622	642.14	0.002
3,4-dimethylpentene-1	642.87	0.980	98.189	0.7022	25.846	642.92	0.014	25.845	642.92	0.008
4,4-dimethyl-c-pentene-2	646.65	0.980	98.189	0.7039	26.223	646.57	0.024	26.224	646.61	0.011
2,4-dimethylpentene-1	647.67	0.980	98.189	0.6988	26.332	647.63	0.021	26.334	647.65	0.011
diolefin	647.70	0.957	82.140	0.6988						
1-methylcyclopentene	648.71	0.957	82.146	0.7795	26.443	648.69	0.374	26.444	648.72	0.180
benzene	649.92	0.910	78.114	0.8789	26.580	649.98	1.969	26.579	649.99	1.242
3-ethylpentene-1	650.00	0.980	98.189	0.7005						
*n-butanol	650.02	1.295	74.120	0.8000						
3-methylhexene-1	650.95	0.980	98.189	0.6959	26.420	651.56	0.029	26.434	651.55	0.015
2-methyl-c-hexene-3	652.60	0.980	98.189	0.6980	27.081	652.56	0.018	27.059	652.59	0.009
3,3-dimethylpentane	654.43	1.000	100.205	0.6932	27.057	654.47	0.094	27.055	654.46	0.139
5-methylhexene-1	655.56	0.980	98.189	0.6965	27.198	655.83	0.031	26.985	656.10	0.016
?	656.93				28.233	656.74	0.014	27.752	656.78	0.007
cyclohexane	657.81	0.980	84.162	0.7785	27.440	657.97	0.225	27.445	658.05	0.050
2-methyl-t-hexene-3	661.03	0.980	98.189	0.6941	27.763	660.87	0.057	27.766	660.91	0.027
diolefin (hexadiene)	661.30	0.980	98.189	0.6941	27.946	661.74	0.007	27.794		0.003
2-ethyl-3-methylbutene-1	662.60	0.980	98.189	0.7135	27.941	662.47	0.018	27.944	662.51	0.009
4-methylhexene-1	663.81	0.980	98.189	0.7030	28.087	663.77	0.040	28.089	663.80	0.019
4-methyl-t/c-hexene-2	666.23	0.980	98.189	0.7040	28.357	666.13	0.107	28.361	666.18	0.051
2-methylhexane	667.61	1.000	100.205	0.6786	28.510	667.45	1.342	28.518	667.54	1.236
2,3-dimethylpentane	668.84	1.000	100.205	0.6951	28.663	668.79	1.635	28.673	668.88	4.375
5-methyl-t-hexene-2	669.80	0.980	98.189	0.6971						
1,1-dimethylcyclopentane	671.25	0.980	98.189	0.7545	28.958	671.32	0.045	28.961	671.35	0.042
t-amylmethylether	672.48	1.318	102.180	0.7517				28.973		0.002
cyclohexene	673.69	0.956	82.146	0.8110	29.254	673.82	0.058	29.255	673.84	0.032
3-methylhexane	675.89	1.000	100.205	0.6871	29.496	675.82	1.449	29.497	675.83	1.450
1,6-heptadiene	677.40	0.960	98.190	0.7500						
3,4-dimethyl-c-pentene-2	679.46	0.980	98.189	0.7180	29.935	679.42	0.043	29.938	679.46	0.021
5-methyl-c-hexene-2	680.00	0.980	98.189	0.7060						
1c,3-dimethylcyclopentane	681.68	0.980	98.189	0.7448	30.225	681.78	0.261	30.228	681.82	0.114
1t,3-dimethylcyclopentane	684.37	0.980	98.189	0.7488	30.567	684.51	0.228	30.572	684.54	0.104
3-ethylpentane	685.98	1.000	100.205	0.6981	30.751	685.96	0.202	30.757	686.01	0.169
1t,2-dimethylcyclopentane	687.07	0.980	98.189	0.7514	30.911	687.21	0.185	30.921	687.30	0.085
2,2,4-trimethylpentane	688.48	0.998	114.232	0.6919	31.086	688.57	3.273	31.115	688.81	9.481
heptene-1	688.60	0.980	98.189	0.6970						
2-ethylpentene-1	689.58	0.980	98.189	0.6970	31.231	689.58	0.059			

TABLE A1.1 *Continued*

					RFA Gasoline			CCF Gasoline		
Component	Ave. RI	RRF	MW	Rel. Den.	Min.	INDEX	Mass%	Min.	INDEX	Mass%
1,5-heptadiene	691.60	0.960	93.168	0.7500						
O25	692.89	0.980	98.189	0.6900	31.502	692.93	0.007	31.422	692.95	0.004
3-methyl-c-hexene-3	694.82	0.980	98.189	0.7181	31.912	694.87	0.070	31.913	694.88	0.034
?	696.80							31.826	696.87	0.004
t-heptene-3	698.39	0.980	98.189	0.7026	32.392	698.43	0.250	32.393	698.44	0.126
n-heptane	700.00	1.000	100.205	0.6837	32.605	700.00	1.164	32.604	700.00	0.996
c-heptene-3	701.00	0.980	98.189	0.7028						
2-methyl-2-hexene	701.30	0.980	98.189	0.7126						
3-methyl-c-hexene-2	702.30	0.980	98.189	0.7126	32.916	702.07	0.283	32.917	702.08	0.139
3-methyl-t-hexene-3	702.99	0.980	98.189	0.6941	33.064	703.05	0.103	33.065	703.06	0.049
t-heptene-2	704.58	0.980	98.189	0.7057	33.306	704.63	0.124	33.307	704.64	0.063
3-ethylpentene-2	705.96	0.980	98.189	0.7249	33.526	706.06	0.065	33.527	706.07	0.030
c-heptene-2	708.82	0.980	98.189	0.7116	33.974	708.92	0.221	33.990	709.04	0.129
3-methyl-t-hexene-2	709.50	0.980	98.189	0.7188						
O28	710.53	0.980	98.189	0.7188						
2,3-dimethylpentene-2	712.07	0.980	98.189	0.7322	34.488	712.18	0.123	34.488	712.17	0.059
3-ethylcyclopentene	713.22	0.980	96.173	0.7830	34.789	713.45	0.010	34.562	713.41	0.004
O29	715.67	0.980	98.189	0.7190	35.083	715.85	0.018	35.084	715.86	0.009
1c,2-dimethylcyclopentane	717.13	0.980	98.189	0.7322	35.329	717.35	0.138	35.331	717.36	0.060
methylcyclohexane	717.89	0.980	98.189	0.7694	35.451	718.09	0.380	35.452	718.09	0.139
O30	719.00	0.980	98.189	0.7322	35.359	720.75	0.079			
2,2-dimethylhexane	720.70	0.998	114.232	0.6953	35.884	720.70	0.117	35.854	720.51	0.099
*1,1,3-trimethylcyclopentane	720.72	0.980	112.216	0.7482						
O32	721.00	0.980	98.189	0.7322						
O33	722.00	0.980	112.216	0.7322						
O34	723.00	0.980	112.216	0.7322						
O35	724.35	0.980	98.189	0.7322	36.531	724.50	0.013	36.398	724.50	0.005
O36	726.26	0.980	98.189	0.7322	36.872	726.47	0.010	36.652	725.97	0.010
?	727.00							36.637	726.09	0.003
ethylcyclopentane	728.90	0.980	98.189	0.7664	37.342	729.16	0.146	37.381	729.09	0.072
2,5-dimethylhexane	730.05	0.998	114.232	0.6935	37.522	730.17	0.422	37.523	730.17	0.693
2,2,3-trimethylpentane	730.90	0.998	114.232	0.7160	37.775	730.96	0.064	37.682	731.06	0.188
2,4-dimethylhexane	731.84	0.998	114.232	0.7003	37.846	731.99	0.697	37.848	731.98	1.056
?	733.53				38.081	733.63	0.011	37.823		0.007
O37	735.18	0.980	98.189	0.7322	38.047	735.41	0.004	38.027	735.34	0.003
1c,2t,4-trimethylcyclopentane	737.11	0.980	112.216	0.7634	38.824	737.36	0.102	38.825	737.35	0.046
3,3-dimethylhexane	738.39	0.998	114.232	0.7100	39.052	738.59	0.077	39.053	738.59	0.075
O38	740.43	0.980	98.189	0.7322	39.432	740.61	0.005	38.887	740.62	0.004
?	742.18				39.825	742.27	0.007	39.387	742.53	0.003
?	743.20				40.364	743.28	0.024	40.227	743.50	0.015
?	743.80				39.701	744.00	0.033	39.868	743.90	0.014
1t,2c,3-trimethylcyclopentane	744.21	0.980	112.216	0.7704	40.162	744.46	0.077	40.163	744.44	0.033
O39	745.34	0.980	98.189	0.7322				40.019	744.72	0.005
2,3,4-trimethylpentane	746.83	0.998	114.232	0.7190	40.667	747.06	0.862	40.678	747.11	2.585
I1	747.91	0.998	114.232	0.7190	40.874	748.12	0.195	40.876	748.11	0.093
O40	749.37	0.980	98.189	0.7322	41.157	749.56	0.058	41.160	749.54	0.032

TABLE A1.1 *Continued*

					RFA Gasoline			CCF Gasoline		
Component	Ave. RI	RRF	MW	Rel. Den.	Min.	INDEX	Mass%	Min.	INDEX	Mass%
2,3,3-trimethylpentane	750.84	0.998	114.232	0.7262	41.539	751.10	0.525	41.470	751.10	1.716
toluene	751.77	0.920	92.143	0.8670	41.666	752.08	6.421	41.688	752.18	8.999
O41	752.20	0.980	112.220	0.7322						
O42	753.63	0.980	112.220	0.7322	42.037	753.73	0.030	42.362	753.75	0.014
?	754.63				42.054	754.65	0.009	42.183	754.77	0.020
O43	755.33	0.980	112.220	0.7322	42.351	755.48	0.049	42.334	755.36	0.031
2,3-dimethylhexane	757.87	0.998	114.232	0.7121	42.890	758.08	0.508	42.898	758.11	0.812
2-methyl-3-ethylpentane	759.04	0.998	114.232	0.7121	43.139	759.28	0.060	43.149	759.31	0.062
1,1,2-trimethylcyclopentane	760.33	0.980	112.216	0.7725	43.380	760.44	0.045	43.379	760.42	0.025
O44	761.73	0.980	112.220	0.7322	43.709	761.99	0.076	43.712	761.97	0.041
O45	762.20	0.980	112.220	0.7322						
O46	763.00	0.980	112.220	0.7322						
2-methylheptane	764.14	0.998	114.232	0.6979	44.199	764.29	0.831	44.198	764.26	0.571
*2-ethylhexene-1	764.20	0.980	112.220	0.7650						
4-methylheptane	765.62	0.998	114.232	0.7046	44.521	765.78	0.362	44.521	765.75	0.266
3-methyl-3-ethylpentane	766.62	0.998	114.232	0.7121	44.753	766.83	0.084	44.750	766.80	0.104
3,4-dimethylhexane	767.18	0.998	114.232	0.7192	44.865	767.35	0.086	44.867	767.33	0.114
1c,2c,4-trimethylcyclopentane	768.95	0.980	112.216	0.7620	45.430	769.91	0.090	45.427	769.88	0.041
1c,3-dimethylcyclohexane	769.80	0.980	112.216	0.7625						
3-methylheptane	771.78	0.998	114.232	0.7058	45.880	771.92	0.911	45.877	771.88	0.651
1c,2t,3-trimethylcyclopentane	772.98	0.980	112.216	0.7704	46.135	773.05	0.291	46.127	772.98	0.185
3-ethylhexane	773.76	0.998	114.232	0.7136	46.360	774.03	0.055	46.362	774.01	0.022
1t,4-dimethylcyclohexane	774.89	0.980	112.216	0.7625	46.689	775.16	0.059	46.621	775.15	0.024
?	775.65				46.439	775.62	0.009			
1,3-octadiene	777.16	0.962	110.200	0.7650	47.117	777.33	0.011	46.298	777.29	0.006
O48	778.50	0.980	112.220	0.7322	46.756	779.08	0.004	46.542	779.02	0.003
1,1-dimethylcyclohexane	780.48	0.980	112.216	0.7809	47.922	780.76	0.009	47.413	780.75	0.005
2,2,5-trimethylhexane	782.93	0.996	128.259	0.7072	48.473	783.08	0.470	48.473	783.04	0.740
3c-ethylmethylcyclopentane	784.35	0.980	112.216	0.7670	48.831	784.57	0.130	48.833	784.53	0.060
2,6-dimethylheptene-1	785.55	0.980	126.240	0.7196	49.152	785.64	0.018	49.046	785.66	0.010
3t-ethylmethylcyclopentane	786.55	0.980	112.216	0.7670	49.366	786.75	0.081	49.369	786.74	0.036
2t-ethylmethylcyclopentane	787.86	0.980	112.216	0.7690	49.679	788.03	0.071	49.682	788.00	0.036
*octene-1	787.87	0.980	112.220	0.7650						
1,1-methylethylcyclopentane	788.78	0.980	112.216	0.7809	49.894	788.90	0.028	49.896	788.89	0.013
?	789.88				49.436	789.88	0.013	50.166	789.96	0.013
2,2,4-trimethylhexane	790.75	0.996	128.259	0.7392	50.384	790.88	0.046	50.386	790.86	0.020
1t,2-dimethylcyclohexane	792.77	0.980	112.216	0.7760	50.911	792.96	0.096	50.915	792.94	0.045
t-octene-4	794.21	0.980	112.216	0.7185	51.252	794.31	0.052	51.259	794.31	0.029
3,5,5-trimethylhexene-1	795.00	0.980	126.240	0.7196	50.669		0.002			
t-octene-3	796.00	0.980	112.216	0.7196						
1c,2c,3-trimethylcyclopentane	797.25	0.980	112.216	0.7792	52.033	797.34	0.151	52.042	797.34	0.080
1t,3-dimethylcyclohexane	798.80	0.980	112.216	0.7760	52.443	798.90	0.033	52.450	798.89	0.017
n-octane	800.00	0.998	114.232	0.7025	52.733	800.00	0.811	52.740	800.00	0.502
1c,4-dimethylcyclohexane	801.05	0.980	112.216	0.7828						
3,3-dimethylheptene-1	802.50	0.980	126.240	0.7196						
octene-2	804.40	0.980	112.216	0.7196	53.872	804.52	0.065	53.885	804.54	0.035
O50	805.50	0.980	112.216	0.7196						

TABLE A1.1 *Continued*

					RFA Gasoline			CCF Gasoline		
Component	Ave. RI	RRF	MW	Rel. Den.	Min.	INDEX	Mass%	Min.	INDEX	Mass%
I2	806.39	0.996	128.259	0.7300	54.389	806.51	0.112	54.406	806.56	0.052
?	807.00							54.600	807.29	0.020
i-propylcyclopentane	808.06	0.980	112.216	0.7765	54.822	808.20	0.074	54.840	808.23	0.035
2,4,4-trimethylhexane	808.50	0.996	128.259	0.7392						
O52	810.62	0.980	126.240	0.7196	55.508	810.81	0.011	55.545	810.84	0.006
O53	813.47	0.980	126.240	0.7196	56.268	813.67	0.035	56.295	813.72	0.016
N1	815.02	0.980	112.216	0.7800	56.655	815.09	0.012	55.395	814.95	0.007
?	815.60				55.673		0.006			
2,2,3,4-tetramethylpentane	816.45	0.996	128.259	0.7389	57.221	816.59	0.009	56.554	816.50	0.005
2,3,4-trimethylhexane	818.10	0.996	128.259	0.7392	57.536	818.33	0.081	57.567	818.38	0.127
N2	819.93	0.980	112.216	0.7800	58.170	820.20	0.034	58.093	820.25	0.014
?	820.85				58.049	821.28	0.014	57.612	821.13	0.007
?	821.10				59.376	820.70	0.014	59.939	821.10	0.009
N3	822.29	0.980	112.216	0.7800	58.668	822.41	0.039	58.725	822.55	0.022
2,3,3-trimethylhexene-1	824.74	0.980	126.240	0.6826	59.404	824.98	0.017	59.582	825.08	0.010
?	825.00									
1c,2-dimethylcyclohexane	826.48	0.980	112.216	0.7962	59.179	826.84	0.023			
2,3,5-trimethylhexane	827.51	0.996	128.259	0.7219	60.088	827.38	0.122	60.141	827.50	0.084
?	828.95				60.649	828.50	0.006			
?	829.20							59.422		0.002
2,2-dimethylheptane	829.76	0.996	128.259	0.7105	59.233	829.20	0.012	59.294	829.15	0.005
?	831.80							60.231		0.004
1,1,4-trimethylcyclohexane	832.56	0.980	126.243	0.7722	61.689	832.81	0.104	61.744	832.94	0.049
N4	834.07	0.980	112.216	0.7800	62.028	833.97	0.021	62.098	834.13	0.014
?	834.40				60.862		0.013	60.851		0.008
2,2,3-trimethylhexane	834.96	0.996	128.259	0.7153	62.399	835.22	0.074	62.472	835.37	0.043
2,4-dimethylheptane	836.47	0.996	128.259	0.7153	62.878	836.79	0.011	61.246	836.60	0.005
4,4-dimethylheptane	838.68	0.996	128.259	0.7153	63.454	838.68	0.048	63.530	838.83	0.024
ethylcyclohexane	840.20	0.980	112.216	0.7839	62.675		0.004	62.624		0.003
n-propylcyclopentane	841.38	0.980	112.216	0.7763	64.307	842.00	0.008	62.897	841.45	0.004
*1c,3c,5-trimethylcyclohexane	841.40	0.980	126.243	0.7697						
2,5-dimethylheptane	842.63	0.996	128.259	0.7167	64.762	842.88	0.208	64.855	843.09	0.132
3,3-dimethylheptane	843.96	0.996	128.259	0.7256	65.189	844.25	0.059	65.283	844.44	0.032
3,5-dimethylheptane	845.02	0.996	128.259	0.7225	65.042	844.55	0.015	64.178		0.002
?	845.60							64.526		0.002
2,6-dimethylheptane	846.47	0.996	128.259	0.7089	65.987	846.73	0.023	64.434	846.51	0.007
?	847.00							64.667		0.002
1,1,3-trimethylcyclohexane	848.43	0.980	126.243	0.7870	66.612	848.67	0.024	66.718	848.90	0.011
2,4-dimethylheptene-1	849.43	0.980	126.240	0.6826	66.462	848.89	0.006	65.309	849.56	0.005
N7	850.89	0.980	112.216	0.7800	66.993	850.52	0.008	65.931	851.33	0.005
N8	852.36	0.980	112.216	0.7800	68.017	852.57	0.017	67.247	852.64	0.010
N10	853.04	0.980	126.240	0.7800						
ethylbenzene	854.65	0.927	106.168	0.8670	68.687	854.92	3.131	68.809	855.18	2.395
N11	854.70	0.980	126.240	0.7800	67.693		0.015			
1c,2t,4t-trimethylcyclohexane	856.34	0.980	126.243	0.7800	69.261	856.61	0.060	69.377	857.03	0.037
I3	858.51	0.996	128.259	0.7300	70.138	858.77	0.016	68.290	858.74	0.011
?	859.00							68.711		0.002
2-methyloctene-1	859.80	0.980	126.240	0.6826	70.172	859.99	0.021	70.169	859.87	0.015

TABLE A1.1 *Continued*

					RFA Gasoline			CCF Gasoline		
Component	Ave. RI	RRF	MW	Rel. Den.	Min.	INDEX	Mass%	Min.	INDEX	Mass%
?	860.50							69.131		0.002
I4	860.89	0.996	128.259	0.7300	70.240	860.78	0.011	69.125	861.19	0.008
?	861.40				69.536		0.005	69.853		0.002
2-methyloctene-2	862.14	0.980	126.240	0.6826	71.310	862.00	0.014	69.565	862.44	0.009
N12	863.00	0.980	126.243	0.7800	72.374	863.22	0.017	70.111		0.005
N13	863.77	0.980	126.243	0.7800						
1,3-dimethylbenzene	864.22	0.927	106.168	0.8642	72.171	864.48	5.181	72.190	864.82	3.649
1,4-dimethylbenzene	865.20	0.927	106.168	0.8610	72.389	865.45	2.299	72.556	865.82	1.698
2,3-dimethylheptane	866.02	0.996	128.259	0.7260	71.154	866.59	0.111	72.052	866.55	0.088
3,4-dimethylheptane	867.94	0.996	128.259	0.7314	73.307	868.00	0.040	73.490	868.38	0.025
?	868.00							72.160		0.002
3,4-dimethylheptane	868.78	0.996	128.259	0.7314	73.584	868.75	0.041	73.782	869.18	0.023
N14	869.70	0.980	126.243	0.7800	74.035	869.96	0.018	72.336	870.12	0.009
I5	870.95	0.996	128.259	0.7300	74.478	871.15	0.073	74.658	871.53	0.036
4-ethylheptane	872.73	0.996	128.259	0.7202	75.147	872.96	0.016	75.560	873.30	0.010
4-methyloctane	873.81	0.996	128.259	0.7202	75.557	874.05	0.237	75.727	874.35	0.104
2-methyloctane	874.76	0.996	128.259	0.7134	75.918	874.99	0.298	76.089	875.30	0.128
?	875.00							75.116		0.002
N15	876.00	0.980	126.243	0.7800	76.402	876.26	0.023	74.595	876.35	0.010
1c,2t,3-trimethylcyclohexane	877.98	0.980	126.243	0.7580	76.601	878.00	0.016	76.726	878.30	0.007
?	878.00				77.313	878.27	0.040	75.982		0.005
3-ethylheptane	879.11	0.996	128.259	0.7265	77.373	879.55	0.075	77.742	879.58	0.031
3-methyloctane	880.24	0.996	128.259	0.7205	78.034	880.47	0.336	78.185	880.70	0.144
?	881.04				80.286	881.32	0.016	76.824	881.25	0.004
1c,2t,4c-trimethylcyclohexane	881.67	0.980	126.243	0.7722	78.628	881.99	0.019	78.869	882.43	0.020
1,1,2-trimethylcyclohexane	882.78	0.980	126.243	0.8000	78.917	882.72	0.015			
1,2-dimethylbenzene	883.47	0.927	106.168	0.8802	79.328	883.76	2.652	79.453	883.89	1.784
?	884.87				77.949	884.74	0.015	77.734	884.66	0.004
I6	885.34	0.996	128.259	0.7300	80.135	885.49	0.022	80.257	885.89	0.023
?	885.88				79.109		0.008			
I7	886.38	0.996	128.259	0.7300	80.474	886.61	0.062	80.608	886.75	0.139
N18	887.87	0.980	126.243	0.7800	81.060	888.07	0.038	81.621	888.18	0.017
N19	888.36	0.980	126.243	0.7800	81.279	888.60	0.030	81.398	888.69	0.011
nonene-1	889.00	0.980	126.240	0.7684						
?	889.40				81.509	889.16	0.040	80.759	889.21	0.016
I8	889.78	0.996	128.259	0.7300	81.888	890.09	0.024	81.476	889.94	0.011
N20	890.51	0.980	126.243	0.7800	85.070	890.70	0.111	86.286	890.45	0.010
I9	891.29	0.996	128.259	0.7300	82.375	891.28	0.102	82.454	891.24	0.235
i-butylcyclopentane	892.11	0.980	126.243	0.7809	82.743	892.17	0.017	82.390	892.18	0.008
N21	892.96	0.980	126.243	0.7800	83.054	892.92	0.030	82.938	892.86	0.015
?	893.20				83.607	893.23	0.030	83.590	893.22	0.009
?	894.00				80.659	893.15	0.033	81.076	893.14	0.015
t-7-methyloctene-3	895.10	0.980	126.241	0.6826						
N22	895.99	0.980	126.243	0.7800	84.408	896.11	0.057	84.519	896.14	0.029
?	896.76				84.742	896.88	0.014	84.855	896.93	0.007
N23/c-nonene-2	897.24	0.980	126.243	0.7800	84.967	897.41	0.035	85.075	897.44	0.018
t-nonene-3	897.94	0.980	126.241	0.6826						

TABLE A1.1 *Continued*

Component	Ave. RI	RRF	MW	Rel. Den.	RFA Gasoline			CCF Gasoline		
					Min.	INDEX	Mass%	Min.	INDEX	Mass%
?	898.44				84.255	898.49	0.034			
I10	898.70	0.996	128.259	0.7300	85.566	898.78	0.051	85.709	898.90	0.147
?	899.19				87.478	898.94	0.046			
n-nonane	900.20	0.996	128.259	0.7176	86.082	900.00	0.214	86.186	900.01	0.086
1,1-methylethylcyclohexane	901.39	0.980	126.243	0.8062	86.378	901.62	0.035	86.476	901.59	0.016
3,7-dimethyloctene-1	903.40	0.980	140.270	0.7013						
?	904.38				86.929	904.59	0.023	87.029	904.57	0.012
N25	905.50	0.980	126.243	0.7900	87.138	905.71	0.026	87.239	905.70	0.010
t-2,2,5,5-tetramethylhexene-3	906.68	0.980	140.270	0.7013	87.352	906.86	0.012	85.841	906.79	0.006
i-propylbenzene	912.28	0.933	120.195	0.8618	88.419	912.54	0.112	88.510	912.51	0.082
N26	913.43	0.980	126.243	0.7900						
N27	914.45	0.980	126.243	0.7900	88.839	914.76	0.045	88.957	914.88	0.029
c-nonene-3	915.00	0.980	126.240	0.6826	88.198		0.004			
I11	916.40	0.994	142.286	0.7300				89.216	916.24	0.010
i-propylcyclohexane	917.51	0.980	126.243	0.8022	89.365	917.50	0.020	88.849	917.53	0.009
?	918.60				90.523	918.03	0.006			
I12	921.30	0.994	142.286	0.7300	90.138	921.53	0.042	90.227	921.50	0.082
2,2-dimethyloctane	922.59	0.994	142.286	0.7245	89.707		0.018	90.591	923.41	0.025
2,4-dimethyloctane	924.39	0.994	142.286	0.7264	90.743	924.65	0.061	90.829	924.62	0.026
N28	926.32	0.980	126.243	0.7900	89.078	926.37	0.005	90.227		0.003
N29	927.99	0.980	126.243	0.7900	91.453	928.31	0.008	88.997	928.03	0.005
2,6-dimethyloctane	930.83	0.994	142.286	0.7276	91.999	931.09	0.038	92.075	931.02	0.018
2,5-dimethyloctane	932.66	0.994	142.286	0.7302	92.361	932.90	0.065	92.438	932.86	0.034
?	934.00							92.042		0.002
?	934.50				92.053		0.004			
n-butylcyclopentane	936.13	0.980	126.243	0.7846	93.070	936.48	0.022			
I13	937.41	0.994	142.286	0.7300	93.309	937.65	0.033	93.261	937.01	0.045
?	937.60							92.567		0.002
N30	938.04	0.980	140.270	0.8000	92.877	938.25	0.025	93.516	938.28	0.011
I14	940.39	0.994	142.286	0.7300	93.378	940.53	0.009	91.869	940.47	0.005
?	941.00				93.027		0.005			
3,3-dimethyloctane	942.30	0.994	142.286	0.7390	94.291	942.54	0.064	94.358	942.50	0.028
N31	943.42	0.980	140.270	0.8000	92.409	943.48	0.006	92.497	943.66	0.004
?	944.55				98.078	945.10	0.018	97.967	945.45	0.006
?	944.95				92.576	944.76	0.019	92.740	944.90	0.009
n-propylbenzene	946.33	0.933	120.195	0.8620	95.116	946.61	0.627	95.182	946.55	0.401
?	947.54				93.127	947.53	0.020	93.521	947.53	0.008
3,6-dimethyloctane	948.31	0.994	142.286	0.7363	95.496	948.44	0.023	95.564	948.39	0.011
3-methyl-5-ethylheptane	949.41	0.994	142.286	0.7264	95.692	949.41	0.022	95.536	949.35	0.010
?	950.00				95.233		0.002	95.262		0.002
N32	951.22	0.980	140.270	0.8000	96.296	951.32	0.018	95.351		0.002
?	951.50				95.460		0.004	95.442		0.002
?	953.00				95.589		0.003	95.580		0.002
1,3-methylethylbenzene	954.42	0.933	120.195	0.8645	96.789	954.72	2.027	96.840	954.63	1.276
1,4-methylethylbenzene	956.22	0.933	120.195	0.8612	97.157	956.49	0.878	97.212	956.42	0.571
?	957.40				94.626	957.43	0.011	96.594		0.005
N33	958.16	0.980	140.270	0.8000						
?	958.90				95.762	958.89	0.008	96.900		0.003

TABLE A1.1 *Continued*

Component	Ave. RI	RRF	MW	Rel. Den.	RFA Gasoline			CCF Gasoline		
					Min.	INDEX	Mass%	Min.	INDEX	Mass%
?	960.80				96.911		0.006			
1,3,5-trimethylbenzene	961.92	0.933	120.195	0.8652	98.348	962.16	0.996	98.400	962.09	0.638
2,3-dimethyloctane	961.99	0.994	142.286	0.7379						
I15	963.67	0.994	142.286	0.7400	98.713	963.86	0.043	98.765	963.81	0.019
N34	964.76	0.980	140.270	0.8000						
?	965.40				98.438		0.003			
I16	966.53	0.994	142.286	0.7400	97.299	966.78	0.011	97.660	966.93	0.007
?	967.10				103.953	967.90	0.018	98.644		0.004
5-methylnonane	967.89	0.994	142.286	0.7326	99.600	968.02	0.051	99.652	967.98	0.023
I17	969.41	0.994	142.286	0.7400	99.944	969.61	0.116	100.383	969.77	0.216
1,2-methylethylbenzene	970.33	0.933	120.195	0.8807	100.146	970.57	0.605	100.194	970.52	0.447
2-methylnonane	971.77	0.994	142.286	0.7264	100.431	971.87	0.115	100.479	971.83	0.048
?	973.00				100.210	973.37	0.017	99.457	973.29	0.011
3-ethyloctane	974.47	0.994	142.286	0.7399	101.009	974.55	0.022	100.826	974.53	0.010
?	975.05							100.504		0.003
N35	975.89	0.980	140.270	0.8000	101.669	976.12	0.018	99.640	976.08	0.006
3-methylnonane	977.26	0.994	142.286	0.7334	101.629	977.38	0.119	101.675	977.35	0.046
?	978.30				101.271	978.34	0.011	100.504	978.16	0.007
N36	979.33	0.980	140.270	0.8000	100.066	979.21	0.008	99.919	979.30	0.005
3-ethyl-2-methylheptene-2	979.35	0.980	140.270	0.7013						
I18	980.12	0.994	142.286	0.7400	102.306	980.46	0.029	102.362	980.49	0.065
I19	981.56	0.994	142.286	0.7400	101.282	981.67	0.007	99.704	981.50	0.007
1,2,4-trimethylbenzene	983.40	0.933	120.195	0.8758	103.003	983.63	2.813	103.032	983.55	1.829
*t-butylbenzene	983.42	0.933	120.200	0.8665						
I20	985.82	0.994	142.286	0.7400	103.376	985.29	0.014	102.881	985.32	0.011
i-butylcyclohexane	986.27	0.980	140.270	0.7960	103.606	986.32	0.023	103.402	986.29	0.010
I21	987.40	0.994	142.286	0.7400	103.819	987.26	0.044	103.845	987.19	0.025
?	987.60							104.866	987.79	0.026
I22	988.00	0.994	142.286	0.7400	105.334	988.43	0.018	102.938	987.84	0.019
?	988.60				102.239	988.63	0.009	102.157	988.55	0.005
I23	989.12	0.994	142.286	0.7400	103.648	989.04	0.011	103.593		0.002
N37	990.53	0.980	140.270	0.8000	104.581	990.68	0.015	104.365	990.61	0.006
?	991.24				104.174	991.37	0.010	103.370	991.29	0.005
decene-1	992.81	0.980	140.270	0.7408	103.762	992.78	0.009	103.952	992.90	0.004
1t-methyl-2-n-propylcyclohexane	993.55	0.980	140.270	0.8000						
2,3-dimethyloctene-2	993.56	0.980	140.270	0.7400						
I24	993.70	0.994	142.286	0.7400	105.255	993.65	0.053	105.375	993.99	0.041
?	994.20							107.662	994.18	0.029
i-butylbenzene	995.95	0.938	134.222	0.8532	105.781	995.97	0.063	105.813	995.95	0.046
I25	996.84	0.994	142.286	0.7400	105.356	996.81	0.021	105.398	996.72	0.024
sec-butylbenzene	997.79	0.938	134.222	0.8620	106.237	997.97	0.054	106.270	997.95	0.040
?	998.70				105.784		0.005	105.732		0.002
?	999.30							105.862		0.004
n-decane	1000.20	0.994	142.286	0.7300	106.708	999.99	0.080	106.737	999.97	0.038
I26	1001.71	0.993	156.313	0.7400	106.952	1001.70	0.011	106.990	1001.72	0.016
N38	1003.39	0.980	140.260	0.8000	107.189	1003.32	0.028	107.218	1003.28	0.017
1,2,3-trimethylbenzene	1006.88	0.933	120.195	0.8944	107.705	1006.91	0.539	107.732	1006.87	0.323

TABLE A1.1 *Continued*

					RFA Gasoline			CCF Gasoline		
Component	Ave. RI	RRF	MW	Rel. Den.	Min.	INDEX	Mass%	Min.	INDEX	Mass%
1,3-methyl-i-propylbenzene	1009.84	0.938	134.222	0.8610	108.117	1009.73	0.058	108.144	1009.70	0.048
N39	1011.33	0.980	154.290	0.8000						
1,4-methyl-i-propylbenzene	1013.24	0.938	134.222	0.8573	108.602	1013.08	0.034	108.638	1013.12	0.025
I27	1014.33	0.993	156.313	0.7400	106.759	1014.42	0.005	105.253	1014.26	0.002
I28	1015.86	0.993	156.313	0.7400	112.126	1016.63	0.012	113.222	1016.31	0.010
I29	1017.87	0.993	156.313	0.7400	107.874	1017.86	0.012	106.471	1017.20	0.009
2-3-dihydroindene	1019.44	0.918	118.179	0.9640	109.504	1019.21	0.341	109.532	1019.21	0.163
?	1022.40				109.027		0.006	109.056		0.002
sec-butylcyclohexane	1023.07	0.980	140.270	0.8140	107.271	1022.40	0.008	108.837	1022.14	0.007
I30	1024.82	0.993	156.313	0.7400	110.213	1023.97	0.028	110.225	1023.86	0.013
?	1026.50				108.990	1026.17	0.022	107.795	1026.59	0.011
1,2-methyl-i-propylbenzene	1027.73	0.938	134.222	0.8766	110.677	1027.07	0.031	110.675	1026.86	0.017
?	1028.40				110.218		0.002			
3-ethylnonane	1029.40	0.993	156.313	0.7440	110.240		0.003	110.276		0.002
?	1031.13				111.214	1030.68	0.011	111.238	1030.69	0.015
N40	1032.29	0.980	154.290	0.8000						
I31	1033.20	0.993	156.313	0.7400	111.495	1032.55	0.048	111.515	1032.54	0.020
I32	1036.92	0.993	154.290	0.8000	112.055	1036.34	0.021	111.809	1036.22	0.008
?	1038.53				112.295	1037.88	0.012	112.295	1037.71	0.008
1,3-diethylbenzene	1039.97	0.938	134.222	0.8639	112.538	1039.49	0.205	112.563	1039.49	0.112
1,3-methyl-n-propylbenzene	1042.60	0.938	134.222	0.8609	112.944	1042.17	0.400	112.967	1042.18	0.232
I33	1044.35	0.993	156.313	0.7400	112.500	1044.04	0.020	112.163	1043.97	0.008
1,4-diethylbenzene	1045.25	0.938	134.222	0.8620						
1,4-methyl-n-propylbenzene	1046.40	0.938	134.222	0.8584	113.528	1046.00	0.237	113.550	1046.00	0.135
n-butylbenzene	1047.48	0.938	134.222	0.8610	113.688	1047.04	0.121	113.710	1047.05	0.063
1,3-dimethyl-5-ethylbenzene	1049.78	0.938	134.222	0.8800	114.044	1049.36	0.392	114.064	1049.35	0.218
1,2-diethylbenzene	1051.72	0.938	134.222	0.8799	114.349	1051.35	0.043	114.372	1051.36	0.024
I34	1051.80	0.993	156.313	0.7400				113.736		0.003
t-decahydronaphthalene	1053.12	0.980	154.290	0.8000	110.769	1052.71	0.004	110.626	1052.67	0.002
N41	1054.60	0.980	154.290	0.8000	114.769	1054.07	0.017	111.829	1054.53	0.008
?	1055.80							114.310		0.007
?	1056.50				115.938	1056.62	0.013	114.197	1056.55	0.007
1,2-methyl-n-propylbenzene	1057.87	0.938	134.222	0.8736	115.304	1057.54	0.150	115.324	1057.56	0.078
I35	1058.87	0.993	156.313	0.7400	114.740		0.004	114.800		0.003
?	1059.00				114.838		0.002			
?	1059.50				114.918		0.003			
I36	1060.15	0.993	156.313	0.7400	115.058		0.008	115.622	1061.18	0.013
I37	1062.62	0.993	156.313	0.7400	116.030	1062.17	0.045	116.044	1062.16	0.020
?	1063.96				113.810	1063.86	0.006	115.398		0.005
I38	1065.53	0.993	156.313	0.7400	116.492	1065.12	0.038	116.508	1065.12	0.015
1,4,dimethyl-2-ethylbenzene	1068.05	0.938	134.222	0.8772	116.905	1067.76	0.264	116.920	1067.77	0.140
A3	1068.90	0.938	134.222	0.8594						
1,3-dimethyl-4-ethylbenzene	1069.53	0.938	134.222	0.8594	117.158	1069.36	0.307	117.173	1069.38	0.158
I39	1071.12	0.993	156.313	0.7400	114.335	1071.04	0.015	114.937	1071.08	0.005
?	1072.49				113.681	1072.50	0.003	116.744		0.006
?	1073.00				116.736		0.005			
I40	1074.39	0.993	156.313	0.7400	117.933	1074.24	0.178	118.598	1073.91	0.068

TABLE A1.1 *Continued*

Component	Ave. RI	RRF	MW	Rel. Den.	RFA Gasoline			CCF Gasoline		
					Min.	INDEX	Mass%	Min.	INDEX	Mass%
1,2-dimethyl-4-ethylbenzene	1075.25	0.938	134.222	0.8745	118.068	1075.08	0.426	118.079	1075.09	0.250
?	1076.00				117.400		0.002			
?	1077.00							117.638		0.003
?	1078.00				115.592	1078.25	0.007	114.048	1078.31	0.005
I41	1079.65	0.993	156.313	0.7400	118.759	1079.41	0.012	117.600	1079.52	0.006
1,3-dimethyl-2-ethylbenzene	1080.68	0.938	134.222	0.8904	118.945	1080.60	0.031	118.958	1080.62	0.017
I42	1081.60	0.993	156.313	0.7400	114.969	1081.44	0.003	114.988	1081.58	0.003
?	1083.35							118.280		0.002
?	1083.60							118.402		0.003
I43	1084.18	0.993	156.313	0.7400	119.495	1084.00	0.016	118.753	1084.00	0.008
?	1085.30				118.946	1085.34	0.009	116.463	1085.44	0.004
?	1086.54				119.122	1086.45	0.009	118.927		0.006
?	1087.50							117.379	1088.22	0.004
?	1088.80				120.278	1088.86	0.011	117.484	1088.96	0.004
undecene-1	1090.45	0.980	154.300	0.7503	120.533	1090.42	0.022	120.544	1090.44	0.012
1,4-methyl-t-butylbenzene	1092.00	0.942	148.240	0.8500	120.778	1091.92	0.038	120.788	1091.96	0.018
1,2-dimethyl-3-ethylbenzene	1093.12	0.938	134.222	0.8921	120.985	1093.18	0.113	120.993	1093.22	0.058
?	1094.89				117.966	1094.87	0.008	117.921	1094.88	0.004
?	1095.78				118.105	1095.78	0.013	118.273	1095.78	0.007
1,2-ethyl-i-propylbenzene	1097.22	0.942	148.240	0.8900	121.661	1097.33	0.011	119.139	1097.36	0.005
?	1098.54				118.119	1098.85	0.009	119.095	1098.88	0.003
?	1099.00				120.899		0.005	125.366	1099.10	0.004
n-undecane	1100.00	0.993	156.313	0.7440	122.105	1100.03	0.053	122.106	1100.03	0.020
1,4-ethyl-i-propylbenzene	1102.50	0.942	148.240	0.8900	122.417	1102.56	0.012	121.163	1102.56	0.006
1,2,4,5-tetramethylbenzene	1104.83	0.938	134.222	0.8875	122.718	1104.99	0.234	122.720	1105.00	0.116
1,2-methyl-n-butylbenzene	1107.30	0.942	148.240	0.8900						
1,2,3,5-tetramethylbenzene	1108.79	0.938	134.222	0.8903	123.207	1108.93	0.319	123.208	1108.94	0.158
?	1110.82				119.539	1110.82	0.006	122.376		0.005
?	1112.39				122.367		0.002			
?	1113.53				123.033	1112.50	0.047	123.661	1112.56	0.007
?	1115.92				126.210	1113.03	0.045	122.689		0.003
?	1117.49				124.100	1116.08	0.023	123.509	1115.99	0.008
?	1119.00				120.791	1117.53	0.007	124.824	1116.58	0.011
?	1119.50							123.251		0.001
?	1120.13				124.606	1120.12	0.017	124.435	1120.07	0.006
?	1121.30				124.756	1121.30	0.015	123.419	1121.29	0.005
1,2-methyl-t-butylbenzene	1122.80	0.942	148.240	0.8900						
?	1124.62				123.227	1124.59	0.006	124.027		0.006
?	1126.18				127.869	1126.31	0.007			
5-methylindan	1127.35	0.938	132.200	0.8900	125.539	1127.50	0.300	125.538	1127.50	0.122
?	1127.30				124.651		0.002			
I43	1131.42	0.992	170.340	0.7530	126.032	1131.37	0.020	125.747	1131.30	0.008
4-methylindan	1133.70	0.938	132.200	0.8900	126.337	1133.74	0.072	126.333	1133.72	0.031
?	1134.90				134.919	1134.95	0.032	135.048	1134.95	0.013
1,2-ethyl-n-propylbenzene	1136.52	0.942	148.240	0.8900	126.698	1136.56	0.105	126.692	1136.53	0.043
2-methylindan	1138.11	0.938	132.200	0.9034	126.908	1138.22	0.289	126.903	1138.20	0.121
1,3-methyl-n-butylbenzene	1140.67	0.942	148.240	0.8900	127.238	1140.79	0.029	127.233	1140.74	0.012

TABLE A1.1 *Continued*

					RFA Gasoline			CCF Gasoline		
Component	Ave. RI	RRF	MW	Rel. Den.	Min.	INDEX	Mass%	Min.	INDEX	Mass%
1,3-di-i-propylbenzene	1142.70	0.945	162.272	0.8900	127.496	1142.79	0.103	127.490	1142.77	0.050
s-pentylbenzene	1144.27	0.942	148.240	0.8900	127.697	1144.35	0.084	127.692	1144.33	0.033
?	1146.90				129.097	1146.97	0.008	126.758		0.004
n-pentylbenzene	1149.04	0.942	148.240	0.8900	128.303	1149.00	0.123	128.297	1148.99	0.053
?	1149.83				127.775	1149.87	0.039	129.737	1149.75	0.015
1t-M-2-(4-MP)cyclopentane	1151.80	0.980	168.320	0.8000						
1,2-di-i-propylbenzene	1153.16	0.945	162.272	0.8900	128.847	1153.19	0.045	128.839	1153.17	0.019
?	1154.09				128.970	1154.13	0.046	128.961	1154.11	0.019
?	1155.98				127.861		0.005	127.862		0.004
?	1157.64				129.427	1157.63	0.051	128.886	1157.45	0.021
?	1158.00							130.655	1158.06	0.023
1,4-di-i-propylbenzene	1159.52	0.945	162.272	0.8900	129.675	1159.53	0.079	129.666	1159.51	0.033
tetrahydronaphthalene	1163.30	0.924	132.206	0.9695	130.166	1163.27	0.034	130.156	1163.24	0.013
?	1165.13				128.975		0.004	128.924		0.002
?	1166.34				129.516	1166.43	0.076	130.568	1166.34	0.030
naphthalene	1168.01	0.896	128.174	1.0253	130.803	1168.08	0.438	130.792	1168.05	0.190
?	1168.50				129.780		0.004	129.802		0.006
1-t-butyl-3,5-dimethylbenzene	1169.25	0.945	162.272	0.8900	140.612	1169.00	0.013			
1,4-ethyl-t-butylbenzene	1173.72	0.945	162.272	0.8900	131.554	1173.75	0.083	131.544	1173.73	0.030
I45	1177.88	0.942	170.300	0.7530	132.112	1177.91	0.124	132.101	1177.89	0.047
I46	1179.46	0.942	170.300	0.7530	132.325	1179.51	0.062	132.313	1179.48	0.022
?	1181.20				131.043		0.003	131.107		0.003
I47	1183.44	0.942	170.300	0.7530	132.864	1183.52	0.083	132.850	1183.47	0.032
I48	1187.14	0.942	170.300	0.7530	133.358	1187.20	0.071	133.347	1187.17	0.027
1,3-di-n-propylbenzene	1188.64	0.945	162.272	0.8900	133.560	1188.67	0.077	133.547	1188.66	0.032
A5	1190.24	0.945	162.272	0.8900	133.778	1190.29	0.052	133.765	1190.26	0.023
?	1191.00				132.431		0.009	132.415		0.005
dodecene-1	1192.19	0.980	168.330	0.7584	129.949	1192.19	0.012	132.673		0.005
?	1193.83				130.211	1193.93	0.012	130.350	1193.95	0.004
?	1194.60				132.870	1194.59	0.011			
?	1196.00				129.167	1196.71	0.006	133.044		0.003
A6	1198.52	0.945	162.272	0.8900	134.904	1198.56	0.040	134.888	1198.53	0.016
n-dodecane	1200.00	0.992	170.340	0.7530	135.106	1200.07	0.046	135.089	1200.03	0.016
?	1202.51				135.377	1202.51	0.013	135.454	1202.41	0.007
?	1204.12				132.955	1204.05	0.025	132.926	1204.09	0.009
?	1205.70				132.109	1205.60	0.002	134.038		0.004
?	1208.41				136.041	1208.47	0.029	136.025	1208.45	0.010
1,3,5-triethylbenzene	1211.79	0.945	162.272	0.8897	136.427	1211.94	0.015	135.785	1211.76	0.005
?	1212.90				132.913	1213.33	0.015	132.196	1213.37	0.007
?	1213.71				135.006	1213.74	0.017	139.107	1214.01	0.006
?	1215.50				147.556	1215.90	0.028	141.394	1215.65	0.014
?	1216.27				137.053	1217.68	0.059	137.053	1217.63	0.020
?	1217.50				135.296		0.036			
?	1220.12				133.673	1220.92	0.007	135.640		0.005
?	1220.90				135.780	1220.94	0.009	131.628	1220.92	0.002
?	1222.36				137.009	1222.52	0.057	136.986	1222.46	0.021
?	1223.70				144.395	1223.59	0.051	144.409	1223.50	0.020

TABLE A1.1 *Continued*

					RFA Gasoline			CCF Gasoline		
Component	Ave. RI	RRF	MW	Rel. Den.	Min.	INDEX	Mass%	Min.	INDEX	Mass%
?	1225.08				137.897	1225.05	0.061	137.878	1224.99	0.023
?	1228.60				138.310	1228.69	0.031	138.291	1228.66	0.011
?	1230.00				136.676		0.020	136.675		0.008
1,2,4-triethylbenzene	1230.83	0.945	162.272	0.8897	138.551	1230.60	0.019	137.335	1230.73	0.008
?	1232.23				139.172	1232.17	0.027	136.248	1232.12	0.009
?	1235.00				149.881	1235.00	0.008	137.282		0.013
?	1236.42				140.655	1236.40	0.030	141.732	1236.33	0.013
?	1237.42				136.485	1237.39	0.038	136.151	1237.46	0.014
?	1238.00				150.631	1238.00	0.009	137.580		0.002
1,4-methyl-n-pentylbenzene	1241.71	0.945	162.272	0.8897	139.782	1241.65	0.111	139.761	1241.62	0.041
?	1242.50				151.463	1243.85	0.047			
?	1244.15				140.120	1244.60	0.040	140.045	1244.10	0.018
?	1245.00				142.998	1246.66	0.013	136.979	1245.15	0.005
?	1246.48				140.387	1246.86	0.016	140.890	1246.61	0.006
?	1248.73				140.651	1249.22	0.015	139.999	1248.99	0.006
?	1251.16				140.918	1251.54	0.033	140.895	1251.51	0.012
n-hexylbenzene	1252.85	0.945	162.272	0.8897	141.130	1253.37	0.048	141.107	1253.34	0.019
?	1254.25				137.178	1254.09	0.006	139.194		0.003
?	1255.61				138.479	1255.85	0.108	136.643	1255.74	0.042
?	1257.39				144.513	1257.88	0.040	146.044	1257.31	0.030
?	1259.54				138.912	1259.82	0.053	138.882	1259.85	0.020
?	1262.15				142.153	1262.20	0.020	142.129	1262.17	0.007
?	1262.55				139.337	1263.68	0.017	137.487	1263.60	0.006
?	1264.03				144.425	1265.33	0.014	149.847	1265.65	0.008
?	1265.92				142.689	1266.78	0.043	142.663	1266.76	0.016
?	1266.71				155.002	1268.55	0.025	154.983	1268.25	0.010
?	1269.02				139.934	1269.13	0.031	139.907	1269.18	0.011
I49	1270.79	0.991	184.370	0.7560	143.152	1270.72	0.016	138.284	1270.93	0.005
?	1271.58				140.243	1271.91	0.011	138.379	1271.81	0.004
?	1273.13				143.553	1273.26	0.020	143.558	1273.31	0.009
1,2,3,4,5-pentamethylbenzene	1274.04	0.942	148.240	1.0000	143.534	1273.98	0.094	143.510	1273.98	0.035
?	1276.70							141.702		0.004
?	1277.23				143.318	1277.27	0.007			
?	1279.96				144.231	1279.89	0.023	144.205	1279.88	0.008
2-methylnaphthalene	1282.57	0.903	143.170	1.0200	144.522	1282.34	0.431	144.494	1282.33	0.171
?	1286.59				144.932	1285.80	0.034	142.460	1285.86	0.014
?	1287.50				157.493	1285.55	0.036	152.473	1286.23	0.013
?	1288.77				145.273	1288.67	0.032	144.965	1288.52	0.013
tridecene-1	1290.10	0.980	182.350	0.7658				143.309		0.002
?	1292.41				150.934	1292.15	0.015	143.429		0.002
?	1293.81				145.906	1293.96	0.020	144.668	1293.93	0.007
?	1295.08				142.847	1295.31	0.019	142.817	1295.36	0.008
1-methylnaphthalene	1297.72	0.903	143.170	1.0200	146.330	1297.50	0.175	146.303	1297.49	0.074
n-tridecane	1300.00	0.991	184.370	0.7564	146.635	1300.11	0.040	146.604	1300.09	0.013
C14+	1300.50						0.361			0.127

TABLE A1.2 Analyses of Naphtha, Reformate, Alkylate, and other Refinery Streams

NOTE 1—These data consist of analyses of various refinery samples and the purpose for this table is to illustrate that the DHA test method is equally applicable to other refinery samples as well as to the analysis of spark-ignition engine gasolines. The table presents the retention times and retention indices of the components covering a range of different concentrations as well as the actual analyses.

	Coop. Study	File: DHA94096.D Sample: PONA-Va "NJ" Reference Mixture			File: DHA94099.D Sample: HFLA C-Matrix Auto/Oil C-Matrix Alkylate			File: DHA94101.D Sample: Platformate Auto/Oil C-Matrix Reformate			File: DHA94105.D Sample: #1 Ref Naphtha ASTM #1 Reference Sample			File: DHA94108.D Sample: ASTM Indolene Std ASTM D.02 Reference Std		
Component	Ave. RI	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%
methane	100.00															
ethylene	178.10															
ethane	200.00	6.70	201.5	0.033												
propylene	284.00															
propane	300.00	7.20	300.0	0.166												
i-butane	366.15	8.13	366.0	0.099				8.15	366.1	0.036				8.15	366.0	0.350
methanol	378.62	8.42	378.6	0.362												
butene-1	390.72	8.74	390.6	0.087										8.75	390.6	0.007
isobutylene	391.51	8.76	391.5	0.090												
1,3-butadiene	394.93	8.87	395.1	0.005												
n-butane	400.00	9.02	400.0	0.315	9.02	400.0	0.155	9.04	400.0	0.596				9.04	400.0	1.844
vinyl acetylene	409.00															
t-butene-2	412.09	9.38	412.0	0.353				9.40	412.0	0.003				9.40	412.1	0.005
2,2-dimethylpropane	415.10	9.46	414.6	0.005										9.49	414.7	0.024
c-butene-2	427.74	9.92	427.5	0.438				9.94	427.6	0.004				9.95	427.6	0.012
1,2-butadiene	450.00															
ethanol	455.33	11.13	454.8	6.914												
3-methylbutene-1	460.84	11.43	460.5	0.418				11.46	460.6	0.005				11.47	460.6	0.021
O1	469.00															
O2	474.00															
i-pentane	477.45	12.43	477.2	9.757	12.43	477.2	11.716	12.45	477.1	3.248	12.45	477.1	0.158	12.46	477.1	5.163
*acetone	477.55															
1,4-pentadiene	481.18	12.70	481.1	0.004												
butyne-2	488.00															
pentene-1	490.83	13.40	490.8	0.951				13.43	490.9	0.007				13.44	490.9	0.041
i-propanol	493.38	13.58	493.1	0.310												
2-methylbutene-1	496.66	13.87	496.7	1.811				13.90	496.8	0.029				13.91	496.8	0.099
n-pentane	500.00	14.14	500.0	1.850	14.14	500.0	0.599	14.17	500.0	2.693	14.17	500.0	0.428	14.18	500.0	2.875
isoprene	506.02	14.47	506.0	0.072												
t-pentene-2	510.56	14.74	510.7	1.641				14.77	510.9	0.022				14.78	510.8	0.090
3,3-dimethylbutene-1	516.79	15.09	516.8	0.016												
c-pentene-2	519.53	15.27	519.7	0.888				15.30	519.9	0.012				15.31	519.8	0.055
t-butanol	521.64	15.37	521.4	0.250												
2-methylbutene-2	524.92	15.61	525.2	1.980	15.61	525.3	0.005	15.64	525.3	0.060				15.65	525.2	0.165
1t,3-pentadiene	527.97	15.81	528.3	0.042												
3-methylbutadiene-1,2	535.00															
cyclopentadiene	538.05	16.48	538.3	0.015												
2,2-dimethylbutane	540.54	16.64	540.7	0.087	16.64	540.6	0.005	16.67	540.6	0.185	16.67	540.6	0.067	16.68	540.6	0.330
1c,3-pentadiene	541.90															
O5	547.70															
O6	549.70															
cyclopentene	557.21	17.91	557.5	0.157										17.94	557.5	0.020
n-propanol	560.00															
4-methylpentene-1	562.02	18.31	562.5	0.062										18.35	562.5	0.011
3-methylpentene-1	562.81	18.37	563.2	0.097										18.41	563.2	0.013
cyclopentane	566.84	18.70	567.1	0.140	18.70	567.1	0.007	18.72	567.1	0.094	18.72	567.0	0.190	18.73	567.1	0.232
2,3-dimethylbutane	569.24	18.91	569.6	0.611	18.90	569.5	2.601	18.93	569.6	0.346	18.94	569.6	0.228	18.95	569.6	1.522
methyl-t-butylether	570.65	19.01	570.8	0.731												
4-methyl-c-pentene-2	571.00							19.09	571.4	0.008				19.10	571.4	0.018
2,3-dimethylbutene-1	572.67	19.21	573.1	0.061										19.25	573.0	0.009
2-methylpentane	573.70	19.30	574.1	2.213	19.29	573.9	0.754	19.32	574.1	1.878	19.33	574.0	1.857	19.34	574.0	2.536
4-methyl-t-pentene-2	575.47	19.46	575.9	0.175				19.49	575.9	0.012				19.50	575.9	0.027
O8	578.00															
2-methyl-1,4-pentadiene	579.00															
1,5-hexadiene	581.90															
3-methylpentane	585.52	20.38	585.7	1.450	20.37	585.6	0.356	20.40	585.7	1.441	20.41	585.7	1.332	20.42	585.7	1.831
2-methylpentene-1	590.19	20.83	590.4	0.288				20.86	590.4	0.015				20.88	590.4	0.041
hexene-1	591.06	20.92	591.2	0.157				20.95	591.3	0.005				20.97	591.2	0.020
O11	592.00															
i-butanol	593.50															
1c/t,4-hexadiene	597.14															
2-ethylbutene-1	598.95															
n-hexane	600.00	21.83	600.0	1.754				21.85	600.0	1.735	21.86	600.0	3.609	21.87	600.0	2.573
diisopropylether	601.90															

TABLE A1.2 *Continued*

		PONA-Va			Alkylate			Reformate			Naphtha			Indolene		
Component	Ave. RI	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%
t-hexene-3	602.83	22.06	602.9	0.323				22.09	603.0	0.010				22.11	603.0	0.035
c-hexene-3	603.56	22.11	603.6	0.076				22.15	603.8	0.002						
t-hexene-2	605.44	22.27	605.5	0.436				22.30	605.6	0.014				22.32	605.5	0.049
2-methylpentene-2	607.86	22.47	608.0	0.547				22.50	608.0	0.028				22.52	608.0	0.073
4-methylcyclopentene																
3-methyl-c-pentene-2	610.54	22.68	610.6	0.308				22.71	610.7	0.018				22.73	610.6	0.041
3-methylcyclopentene	611.61	22.76	611.5	0.040										22.81	611.5	0.007
O13	613.08	22.90	613.2	0.003												
c-hexene-2	614.67	23.04	614.8	0.250				23.07	614.8	0.008				23.08	614.8	0.028
O14	617.06	23.23	617.1	0.005												
ethyl-t-butylether	619.00															
3,3-dimethylpentene-1	620.91	23.58	621.1	0.602				23.60	621.1	0.026				23.63	621.1	0.053
3-methyl-t-pentene-2	622.11	23.70	622.4	0.009												
2-butanol	622.40															
4,4-dimethyl-t-pentene-2	623.10															
2,2-dimethylpentane	624.17	23.86	624.3	0.053	23.86	624.0	0.006	23.88	624.2	0.118	23.89	624.2	0.104	23.91	624.2	0.174
methylcyclopentane	625.86	23.99	625.7	1.057				24.02	625.7	0.310	24.03	625.7	2.226	24.04	625.7	0.982
cyclic diolefin or triolefin	627.00															
2,4-dimethylpentane	630.60	24.45	630.8	0.768	24.47	630.8	8.169	24.47	630.7	0.243	24.48	630.7	0.192	24.50	630.7	1.039
2,3,3-trimethylbutene-1	631.00															
cyclic diolefin or triolefin	632.90	24.67	633.1	0.013												
2,2,3-trimethylbutane	634.86	24.83	634.9	0.046	24.83	634.7	0.057	24.86	634.9	0.010	24.87	634.8	0.027	24.88	634.8	0.091
	636.38	25.00	636.6	0.010												
cyclic diolefin or triolefin	638.30	25.16	638.4	0.011												
O17	641.97	25.52	642.0	0.006												
3,4-dimethylpentene-1	642.87	25.60	642.9	0.017												
4,4-dimethyl-c-pentene-2	646.65	25.99	646.8	0.029				26.00	646.6	0.005				26.04	646.8	0.006
2,4-dimethylpentene-1	647.67	26.06	647.6	0.021												
diolefin	647.70															
1-methylcyclopentene	648.71	26.18	648.7	0.328										26.24	648.7	0.042
benzene	649.92	26.29	649.8	0.541				26.32	649.8	1.786	26.33	649.7	0.445	26.35	649.8	1.506
3-ethylpentene-1	650.00															
*n-butanol	650.02															
3-methylhexene-1	650.95	26.42	651.0	0.038												
2-methyl-c-hexene-3	652.60	26.60	652.8	0.020				26.61	652.7	0.003						
3,3-dimethylpentane	654.43	26.77	654.4	0.049	26.77	654.2	0.009	26.80	654.5	0.109	26.81	654.4	0.073	26.82	654.4	0.161
5-methylhexene-1	655.56	26.91	655.8	0.038				26.95	656.0	0.007				26.97	655.8	0.007
cyclohexane	657.81	27.10	657.6	0.513				27.13	657.7	0.040	27.14	657.5	1.886	27.16	657.6	0.717
2-methyl-t-hexene-3	661.03	27.49	661.2	0.078				27.51	661.2	0.006				27.54	661.2	0.011
diolefin (hexadiene)	661.30															
2-ethyl-3-methylbutene-1	662.60	27.65	662.7	0.014												
4-methylhexene-1	663.81	27.77	663.9	0.049										27.84	663.9	0.008
4-methyl-t/c-hexene-2	666.23	28.05	666.4	0.138				28.08	666.4	0.012				28.09	666.2	0.020
2-methylhexane	667.61	28.19	667.7	1.337	28.23	667.8	0.310	28.22	667.7	1.382	28.23	667.6	1.464	28.25	667.7	1.452
2,3-dimethylpentane	668.84	28.32	668.8	1.179	28.37	669.0	13.267	28.35	668.8	0.484	28.37	668.8	0.539	28.38	668.8	1.229
5-methyl-t-hexene-2	669.80															
1,1-dimethylcyclopentane	671.25	28.58	671.1	0.085				28.61	671.1	0.048	28.62	671.0	0.508	28.64	671.1	0.130
t-amylmethylether	672.48	28.71	672.3	0.200												
cyclohexene	673.69	28.85	673.5	0.050										28.91	673.4	0.009
3-methylhexane	675.89	29.13	675.9	1.351	29.13	675.7	0.310	29.17	676.0	1.743	29.17	675.8	1.775	29.20	675.9	1.771
1,6-heptadiene	677.40															
3,4-dimethyl-c-pentene-2	679.46	29.55	679.5	0.049				29.59	679.6	0.005				29.61	679.5	0.012
5-methyl-c-hexene-2	680.00															
1c,3-dimethylcyclopentane	681.68	29.79	681.5	0.376				29.83	681.6	0.076	29.84	681.4	1.014	29.86	681.6	0.279
1t,3-dimethylcyclopentane	684.37	30.12	684.2	0.331				30.15	684.3	0.081	30.16	684.1	0.950	30.18	684.2	0.255
3-ethylpentane	685.98	30.34	686.0	0.189	30.36	686.0	0.009	30.34	685.8	0.175	30.36	685.7	0.169	30.38	685.9	0.183
1t,2-dimethylcyclopentane	687.07	30.44	686.9	0.359				30.48	686.9	0.097	30.49	686.8	1.785	30.51	686.9	0.446
2,2,4-trimethylpentane	688.48	30.63	688.4	1.852	30.75	689.1	30.506				30.66	688.2	0.006	30.71	688.6	5.212
heptene-1	688.60															
2-ethylpentene-1	689.58	30.78	689.6	0.071												
1,5-heptadiene	691.60	30.97	691.2	0.002										31.05	691.3	0.003
O25	692.89															
3-methyl-c-hexene-3	694.82	31.45	694.9	0.087				31.48	694.9	0.009				31.51	694.9	0.013
t-heptene-3	698.39	31.90	698.4	0.289				31.94	698.5	0.017				31.97	698.5	0.035
n-heptane	700.00	32.11	700.0	1.810				32.14	700.0	1.304	32.17	700.0	4.808	32.18	700.0	1.914
c-heptene-3	701.00															
2-methyl-2-hexene	701.30															
3-methyl-c-hexene-2	702.30	32.41	702.1	0.355				32.45	702.2	0.032				32.48	702.1	0.043
3-methyl-t-hexene-3	702.99	32.55	703.1	0.130				32.59	703.1	0.012				32.62	703.1	0.016
t-heptene-2	704.58	32.78	704.7	0.170				32.82	704.7	0.009				32.85	704.7	0.017
3-ethylpentene-2	705.96	32.99	706.1	0.074				33.03	706.1	0.005				33.06	706.1	0.010
c-heptene-2	708.82	33.40	708.8	0.252				33.44	708.9	0.020				33.48	708.9	0.041
3-methyl-t-hexene-2	709.50															

TABLE A1.2 *Continued*

		PONA-Va			Alkylate			Reformate			Naphtha			Indolene		
Component	Ave. RI	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%
O28	710.53															
2,3-dimethylpentene-2	712.07	33.90	712.1	0.160				33.96	712.5	0.014				33.97	712.1	0.014
3-ethylcyclopentene	713.22															
O29	715.67	34.43	715.5	0.015												
1c,2-dimethylcyclopentane	717.13	34.75	717.6	1.667				34.68	717.0	0.028						
methylcyclohexane	717.89				34.74	717.4	0.005	34.78	717.6	0.094	34.82	717.6	5.093	34.82	717.6	1.113
O30	719.00															
2,2-dimethylhexane	720.70	35.21	720.5	0.174	35.19	720.1	0.008	35.23	720.4	0.126	35.27	720.4	0.748	35.28	720.5	0.199
*1,1,3-trimethylcyclopentane	720.72															
O32	721.00															
O33	722.00															
O34	723.00															
O35	724.35	35.82	724.3	0.019												
O36	726.26	36.14	726.2	0.014												
ethylcyclopentane	728.90	36.56	728.7	0.254				36.59	728.7	0.066	36.61	728.6	0.373	36.64	728.7	0.112
2,5-dimethylhexane	730.05	36.78	730.0	0.386	36.80	729.9	2.941	36.82	730.1	0.211	36.84	729.9	0.258	36.87	730.1	1.326
2,2,3-trimethylpentane	730.90															
2,4-dimethylhexane	731.84	37.08	731.8	0.480	37.10	731.7	3.098	37.12	731.9	0.387	37.14	731.7	0.295	37.17	731.9	0.849
	733.53	37.37	733.5	0.015												
O37	735.18															
1c,2t,4-trimethylcyclopentane	737.11	37.97	737.0	0.208				38.01	737.0	0.052	38.03	736.8	0.703	38.06	737.0	0.137
3,3-dimethylhexane	738.39	38.20	738.3	0.045				38.24	738.3	0.084	38.26	738.1	0.098	38.29	738.3	0.088
O38	740.43	38.60	740.5	0.008												
	742.18	38.91	742.2	0.015												
	743.20	39.07	743.1	0.019												
1t,2c,3-trimethylcyclopentane	744.21	39.24	744.0	0.196				39.28	744.1	0.035	39.30	743.9	0.871	39.33	744.1	0.156
O39	745.34															
2,3,4-trimethylpentane	746.83	39.73	746.7	0.497	39.79	746.8	8.132	39.77	746.8	0.016	39.79	746.6	0.052	39.84	746.8	2.781
I1	747.91	39.95	747.9	0.198				40.01	748.0	0.009	40.02	747.8	0.004			
O40	749.37	40.21	749.3	0.060												
2,3,3-trimethylpentane	750.84	40.47	750.6	0.302	40.52	750.7	6.021							40.58	750.8	2.818
toluene	751.77	40.64	751.5	2.306				40.78	752.1	12.895	40.70	751.4	1.930	40.77	751.8	7.664
O41	752.20															
O42	753.63	41.03	753.6	0.031												
O43	755.33	41.35	755.3	0.060												
2,3-dimethylhexane	757.87	41.86	757.8	0.417	41.86	757.6	2.284	41.92	758.0	0.263	41.94	757.8	0.472	41.96	757.9	0.856
2-methyl-3-ethylpentane	759.04	42.08	759.0	0.065	42.09	758.8	0.099	42.14	759.1	0.045	42.15	758.8	0.136	42.19	759.1	0.062
1,1,2-trimethylcyclopentane	760.33	42.36	760.4	0.055												
O44	761.73	42.59	761.5	0.074												
O45	762.20															
O46	763.00															
2-methylheptane	764.14	43.12	764.1	1.092	43.10	763.8	0.075	43.17	764.2	0.836	43.20	764.0	2.228	43.22	764.1	0.785
*2-ethylhexene-1	764.20															
4-methylheptane	765.62	43.42	765.6	0.359	43.41	765.3	0.022	43.47	765.7	0.433	43.50	765.5	0.524	43.52	765.6	0.305
3-methyl-3-ethylpentane	766.62	43.64	766.7	0.056	43.60	766.2	0.229	43.67	766.6	0.070	43.69	766.4	0.064	43.71	766.6	0.100
3,4-dimethylhexane	767.18	43.71	767.0	0.061	43.72	766.8	0.267	43.78	767.2	0.073	43.80	766.9	0.096	43.83	767.1	0.107
1c,2c,4-trimethylcyclopentane	768.95							44.23	769.3	0.024	44.27	769.2	0.100	44.28	769.3	0.028
1c,3-dimethylcyclohexane	769.80	44.27	769.7	0.128												
3-methylheptane	771.78	44.71	771.7	0.873	44.70	771.5	0.064	44.76	771.8	1.057	44.79	771.6	1.166	44.81	771.8	0.718
1c,2t,3-trimethylcyclopentane	772.98	44.92	772.7	0.734	44.92	772.5	0.009	44.98	772.9	0.299	45.00	772.6	1.845	45.02	772.8	0.412
3-ethylhexane	773.76										45.17	773.4	0.192			
1t,4-dimethylcyclohexane	774.89	45.33	774.6	0.241				45.39	774.7	0.013	45.41	774.5	0.662	45.44	774.7	0.107
1,3-octadiene	777.16	45.89	777.2	0.016												
O48	778.50										46.16	777.9	0.002			
1,1-dimethylcyclohexane	780.48	46.55	780.2	0.099							46.62	780.0	0.291	46.67	780.3	0.047
2,2,5-trimethylhexane	782.93	47.16	782.9	0.274	47.19	782.8	3.951	47.22	783.0	0.010	47.25	782.8	0.030	47.28	783.0	1.175
3c-ethylmethylcyclopentane	784.35	47.44	784.1	0.199				47.50	784.2	0.037	47.52	784.0	0.216	47.56	784.2	0.054
2,6-dimethylheptene-1	785.55	47.64	785.0	0.034												
3t-ethylmethylcyclopentane	786.55	47.95	786.4	0.154				48.01	786.4	0.034	48.03	786.2	0.192	48.07	786.4	0.049
2t-ethylmethylcyclopentane	787.86	48.26	787.7	0.172				48.32	787.8	0.037	48.34	787.5	0.484	48.38	787.7	0.094
*octene-1	787.87															
1,1-methylethylcyclopentane	788.78	48.54	788.9	0.039	48.70	789.3	0.050	48.79	789.8	0.012	48.82	789.5	0.065	48.83	789.7	0.026
	789.88	48.73	789.7	0.023												
2,2,4-trimethylhexane	790.75	49.00	790.8	0.053												
1t,2-dimethylcyclohexane	792.77	49.41	792.6	0.314				49.47	792.7	0.021	49.49	792.4	0.902	49.52	792.6	0.141
t-octene-4	794.21	49.83	794.3	0.075												
3,5,5-trimethylhexene-1	795.00															
t-octene-3	796.00															
1c,2c,3-trimethylcyclopentane	797.25	50.57	797.3	0.200				50.61	797.3	0.018				50.68	797.3	0.014
1t,3-dimethylcyclohexane	798.80	50.91	798.7	0.051							50.94	798.3	0.031	50.97	798.5	0.006
n-octane	800.00	51.23	800.0	1.978				51.27	800.0	0.837	51.36	800.0	5.227	51.34	800.0	1.159
1c,4-dimethylcyclohexane	801.05															
3,3-dimethylheptene-1	802.50															

TABLE A1.2 *Continued*

		PONA-Va			Alkylate			Reformate			Naphtha			Indolene		
Component	Ave. RI	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%
octene-2	804.40	52.33	804.5	0.082												
O50	805.50															
I2	806.39	52.79	806.3	0.109	52.92	806.6	0.119							53.06	806.9	0.041
i-propylcyclopentane	808.06	53.21	808.0	0.123				53.28	808.1	0.019	53.36	808.0	0.125	53.25	807.7	0.028
2,4,4-trimethylhexane	808.50															
O52	810.62	53.85	810.5	0.013												
	812.50										54.39	812.1	0.013			
O53	813.47	54.60	813.4	0.044												
N1	815.02	54.93	814.6	0.031							55.04	814.5	0.073	55.08	814.8	0.013
2,2,3,4-tetramethylpentane	816.45	55.35	816.2	0.014												
2,3,4-trimethylhexane	818.10	55.77	817.8	0.057	55.75	817.5	0.585	55.83	817.6	0.022	55.87	817.7	0.049	55.90	817.9	0.207
N2	819.93	56.21	819.4	0.063				56.25	819.4	0.014	56.30	819.3	0.067	56.33	819.4	0.017
	820.85	56.45	820.3	0.016												
N3	822.29	56.89	821.9	0.069				56.96	822.0	0.028	57.00	821.8	0.107	57.02	822.0	0.036
2,3,3-trimethylhexene-1	824.74	57.55	824.3	0.024										57.58	824.0	0.003
1c,2-dimethylcyclohexane	826.48	57.95	825.7	0.084							58.04	825.6	0.174	58.10	825.9	0.030
2,3,5-trimethylhexane	827.51	58.23	826.8	0.172	58.20	826.4	0.116	58.28	826.8	0.094	58.35	826.7	0.304	58.37	826.8	0.095
2,2-dimethylheptane	829.76										59.00	829.0	0.059			
1,1,4-trimethylcyclohexane	832.56	59.66	831.8	0.530	59.60	831.4	0.006	59.71	831.8	0.030	59.79	831.7	1.549	59.81	831.9	0.264
N4	834.07	60.06	833.1	0.031	60.05	832.9	0.012	60.12	833.2	0.022	60.17	833.1	0.033	60.19	833.2	0.020
2,2,3-trimethylhexane	834.96	60.42	834.4	0.263	60.40	834.1	0.056	60.49	834.5	0.059	60.55	834.3	0.862	60.57	834.5	0.183
2,4-dimethylheptane	836.47	60.80	835.6	0.030							60.91	835.6	0.061			
4,4-dimethylheptane	838.68	61.43	837.8	0.323	61.41	837.5	0.020				61.55	837.7	1.205	61.58	837.9	0.175
ethylcyclohexane	840.20															
n-propylcyclopentane	841.38	62.20	840.4	0.076	62.20	840.2	0.011				62.33	840.3	0.156	62.35	840.5	0.027
*1c,3c,5-trimethylcyclohexane	841.40															
2,5-dimethylheptane	842.63	62.68	841.9	0.326	62.66	841.7	0.192	62.74	842.0	0.179	62.80	841.9	0.421	62.84	842.1	0.212
3,3-dimethylheptane	843.96	63.09	843.3	0.086	63.04	842.9	0.020	63.16	843.4	0.062	63.23	843.3	0.101	63.27	843.5	0.069
3,5-dimethylheptane	845.02	63.30	843.9	0.038							63.46	844.0	0.100			
2,6-dimethylheptane	846.47	63.79	845.5	0.083							63.93	845.5	0.188	63.95	845.7	0.033
1,1,3-trimethylcyclohexane	848.43	64.40	847.5	0.070							64.51	847.4	0.095	64.55	847.6	0.022
2,4-dimethylheptene-1	849.43															
N7	850.89															
N8	852.36	65.77	851.8	0.046							65.98	852.0	0.103	66.03	852.2	0.020
N10	853.04															
ethylbenzene	854.65	66.41	853.7	0.728	66.43	853.7	0.032	66.64	854.3	7.364	66.54	853.7	0.797	66.61	854.0	2.653
N11	854.70															
1c,2t,4t-trimethylcyclohexane	856.34	66.91	855.3	0.222	66.90	855.1	0.049				67.04	855.3	0.580	67.08	855.5	0.106
I3	858.51	67.63	857.5	0.032							67.75	857.4	0.042			
2-methyloctene-1	859.80	68.01	858.6	0.030												
I4	860.89	68.51	860.1	0.033							68.61	859.9	0.030			
2-methyloctene-2	862.14	69.05	861.7	0.021												
N12	863.00	69.25	862.3	0.016												
N13	863.77															
1,3-dimethylbenzene	864.22	69.69	863.6	1.828				69.96	864.3	10.485	69.81	863.5	1.833	69.94	863.9	5.660
1,4-dimethylbenzene	865.20	70.06	864.6	0.693				70.31	865.2	4.479	70.18	864.6	0.558	70.28	864.9	2.475
2,3-dimethylheptane	866.02	70.36	865.5	0.261	70.32	865.3	0.127				70.47	865.4	0.560			
3,4-dimethylheptane	867.94	70.99	867.3	0.102	70.93	867.0	0.019	71.09	867.5	0.029	71.11	867.2	0.207	71.15	867.4	0.049
3,4-dimethylheptane	868.78	71.30	868.2	0.042	71.23	867.9	0.021	71.38	868.3	0.029	71.36	868.0	0.065	71.48	868.4	0.032
N14	869.70	71.62	869.1	0.033							71.74	869.0	0.048	71.82	869.3	0.012
I5	870.95	72.11	870.5	0.106				72.23	870.7	0.053	72.21	870.3	0.131	72.28	870.6	0.051
4-ethylheptane	872.73	72.83	872.5	0.025												
4-methyloctane	873.81	73.19	873.5	0.393				73.27	873.6	0.217	73.30	873.4	0.557	73.34	873.6	0.187
2-methyloctane	874.76	73.55	874.4	0.560	73.53	874.3	0.006	73.63	874.6	0.215	73.66	874.4	0.822	73.69	874.5	0.222
N15	876.00	73.95	875.5	0.045							74.05	875.4	0.072	74.10	875.7	0.018
1c,2t,3-trimethylcyclohexane	877.96	74.66	877.5	0.073							74.76	877.4	0.208	74.86	877.7	0.033
3-ethylheptane	879.11	75.19	878.9	0.135				75.24	878.9	0.063	75.29	878.8	0.206	75.32	878.9	0.066
3-methyloctane	880.24	75.62	880.0	0.577				75.68	880.1	0.288	75.72	879.9	1.004	75.75	880.1	0.280
1c,2t,4c-trimethylcyclohexane	881.67	76.05	881.2	0.061	76.23	881.6	0.042				76.17	881.1	0.090	76.40	881.6	0.124
1,1,2-trimethylcyclohexane	882.78	76.49	882.3	0.065	76.49	882.3	0.007				76.60	882.3	0.158	76.64	882.5	0.014
1,2-dimethylbenzene	883.47	76.83	883.2	1.011	76.86	883.2	0.062	76.98	883.5	5.364	76.92	883.1	0.970	76.99	883.4	3.212
	884.87	77.43	884.8	0.022							77.56	884.8	0.021	77.48	884.6	0.003
I6	885.34				77.60	885.2	0.044				77.91	885.7	0.020	77.76	885.4	0.082
I7	886.38	77.99	886.2	0.054	77.97	886.1	0.296				78.08	886.1	0.022	78.13	886.3	0.141
N18	887.87															
N19	888.36	78.70	888.1	0.323				78.62	887.8	0.011	78.80	888.0	0.990	78.83	888.1	0.172
nonene-1	889.00	78.91	888.6	0.036							79.02	888.5	0.059			
	889.40	79.08	889.0	0.051							79.15	888.9	0.109			
I8	889.78	79.32	889.6	0.112							79.41	889.5	0.332	79.45	889.7	0.047
N20	890.51	79.81	890.9	0.083	79.80	890.8	0.442				79.90	890.8	0.030	79.95	890.9	0.141
I9	891.29	80.20	891.8	0.033							80.26	891.6	0.057	80.30	891.8	0.011
n-butylcyclopentane	892.11	80.54	892.7	0.091							80.70	892.7	0.116	80.69	892.8	0.024
N21	892.96															

TABLE A1.2 *Continued*

		PONA-Va			Alkylate			Reformate			Naphtha			Indolene		
Component	Ave. RI	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%
	894.00													81.25	894.2	0.003
t-7-methyloctene-3	895.10															
N22	895.99	81.89	896.0	0.113							81.81	895.5	0.068			
	896.76	82.22	896.8	0.019												
											82.22	896.5	0.010			
N23/c-nonene-2	897.24	82.46	897.4	0.070							82.57	897.3	0.083	82.61	897.5	0.016
t-nonene-3	897.94															
	898.44										83.04	898.5	0.029			
I10	898.70	82.93	898.5	0.081	83.01	898.7	0.242				83.26	899.0	0.140	83.15	898.8	0.110
	899.19	83.17	899.1	0.026	83.33	899.4	0.007									
n-nonane	900.20	83.55	900.0	1.495				83.57	900.0	0.224	83.68	900.0	4.771	83.64	900.0	0.691
1,1-methylethylcyclohexane	901.39															
3,7-dimethyloctene-1	903.40															
N24	904.38	84.17	903.4	0.033							84.27	903.2	0.078			
N25	905.50	84.43	904.9	0.108							84.54	904.7	0.056	84.58	905.1	0.013
t-2,2,5,5-tetramethylhexene-3	906.68															
	911.02	85.55	910.9	0.008							85.60	910.5	0.019			
i-propylbenzene	912.28	85.80	912.3	0.061				85.83	912.3	0.295	85.87	911.9	0.132	85.90	912.3	0.207
N26	913.43															
N27	914.45	86.15	914.1	0.145	86.27	914.7	0.020				86.22	913.8	0.493	86.25	914.1	0.068
c-nonene-3	915.00															
I11	916.40				86.50	915.9	0.015									
i-propylcyclohexane	917.51	86.75	917.3	0.086				86.79	917.4	0.009	86.82	917.0	0.234	86.85	917.4	0.036
	918.60	87.06	919.0	0.011							87.07	918.3	0.025			
I12	921.30	87.53	921.4	0.098	87.51	921.2	0.130	87.57	921.4	0.013	87.60	921.1	0.228	87.64	921.5	0.093
2,2-dimethyloctane	922.59				87.86	923.1	0.037							88.00	923.4	0.016
2,4-dimethyloctane	924.39	88.13	924.6	0.135	88.11	924.4	0.017	88.16	924.5	0.029	88.20	924.2	0.274	88.21	924.5	0.042
N28	926.32	88.49	926.4	0.018							88.56	926.1	0.051			
N29	927.99	88.75	927.8	0.037							88.82	927.5	0.101	88.85	927.8	0.014
2,6-dimethyloctane	930.83	89.33	930.7	0.221	89.36	930.8	0.006	89.39	930.8	0.014	89.40	930.5	0.800	89.43	930.8	0.107
2,5-dimethyloctane	932.66	89.75	932.9	0.144	89.72	932.7	0.021	89.78	932.8	0.038	89.81	932.6	0.245	89.84	932.9	0.050
	934.50				90.51	936.7	0.053									
n-butylcyclopentane	936.13	90.38	936.1	0.078							90.44	935.8	0.212	90.48	936.2	0.028
I13	937.41	90.68	937.7	0.078				90.71	937.6	0.015	90.76	937.4	0.179	90.66	937.1	0.031
														90.78	937.7	0.028
N30	938.04	90.83	938.4	0.059				90.84	938.2	0.016	90.93	938.3	0.125			
I14	940.39	91.21	940.3	0.042							91.26	939.9	0.121			
3,3-dimethyloctane	942.30	91.66	942.5	0.295	91.62	942.3	0.011	91.68	942.4	0.039	91.73	942.3	1.121	91.75	942.6	0.158
N31	943.42										92.15	944.4	0.241			
	944.55	92.07	944.6	0.077										92.18	944.7	0.015
	944.95													92.27	945.2	0.011
n-propylbenzene	946.33	92.43	946.4	0.242				92.46	946.3	1.417	92.49	946.1	0.203	92.52	946.4	0.863
	947.54	92.70	947.7	0.056				92.73	947.6	0.009	92.76	947.4	0.190	92.80	947.8	0.024
3,6-dimethyloctane	948.31	92.85	948.5	0.051				92.89	948.4	0.007	92.92	948.2	0.069			
3-methyl-5-ethylheptane	949.41	93.08	949.6	0.125							93.15	949.4	0.669	93.18	949.6	0.063
N32	951.22	93.39	951.1	0.058							93.48	951.0	0.158			
1,3-methylethylbenzene	954.42	94.07	954.4	0.925				94.16	954.6	4.421	94.13	954.1	0.725	94.19	954.6	2.428
1,4-methylethylbenzene	956.22	94.44	956.2	0.359				94.51	956.2	1.972	94.50	955.9	0.300	94.55	956.3	1.063
N33	958.16	94.79	957.9	0.066							94.86	957.7	0.383	94.89	957.9	0.037
1,3,5-trimethylbenzene	961.92	95.63	961.9	0.544				95.69	961.9	2.101	95.70	961.7	0.985	95.73	962.0	1.370
2,3-dimethyloctane	961.99				95.72	962.2	0.019									
I15	963.67	96.05	963.9	0.081				96.08	963.7	0.025	96.11	963.7	0.144	96.14	963.9	0.025
N34	964.76	96.20	964.6	0.024							96.27	964.4	0.158			
I16	966.53															
5-methylnonane	967.89	96.93	968.1	0.159				96.96	967.9	0.023	97.00	967.9	0.262	97.03	968.1	0.033
I17	969.41	97.25	969.6	0.219	97.26	969.5	0.417				97.32	969.4	0.604			
1,2-methylethylbenzene	970.33	97.39	970.2	0.306				97.43	970.1	1.356	97.45	970.0	0.218	97.49	970.3	1.308
2-methylnonane	971.77	97.75	971.9	0.294				97.78	971.7	0.051	97.82	971.7	0.700	97.84	971.9	0.082
	973.13	98.04	973.3	0.049							98.07	972.9	0.100			
3-ethyloctane	974.47	98.33	974.6	0.080				98.35	974.4	0.013	98.40	974.4	0.255	98.43	974.7	0.027
N35	975.89	98.57	975.7	0.059							98.65	975.6	0.120			
3-methylnonane	977.26	98.93	977.4	0.260				98.96	977.2	0.060	99.00	977.2	0.622	99.03	977.4	0.077
	978.30	99.14	978.3	0.030												
N36	979.33										99.55	979.8	0.028			
3-ethyl-2-methylheptene-2	979.35															
I18	980.12	99.51	980.0	0.048	99.57	980.2	0.116				99.78	980.8	0.069	99.67	980.4	0.111
I19	981.56				99.79	981.2	0.005	99.92	981.5	0.010	99.99	981.8	0.049			
					100.12	982.6	0.006									
1,2,4-trimethylbenzene	983.40	100.22	983.2	1.286	100.33	983.6	0.042	100.32	983.3	5.960	100.28	983.1	1.477	100.34	983.4	3.921
*t-butylbenzene	983.42															
	984.20										100.45	983.9	0.266			
I20	985.82	100.72	985.5	0.035	100.63	985.0	0.007									
i-butylcyclohexane	986.27	100.87	986.2	0.081							100.93	986.0	0.445	100.96	986.2	0.026

TABLE A1.2 *Continued*

		PONA-Va			Alkylate			Reformate			Naphtha			Indolene		
Component	Ave. RI	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%
I21	987.40	101.12	987.3	0.082	101.06	986.9	0.029				101.18	987.2	0.113	101.18	987.2	0.050
I22	988.60	101.38	988.5	0.059	101.19	987.5	0.038									
I23	989.12										101.54	988.8	0.181			
N37	990.53	101.80	990.4	0.035							101.86	990.2	0.091			
	991.24	102.02	991.4	0.019							102.13	991.4	0.022			
decane-1	992.81															
1t-methyl-2-n-propylcyclohexane	993.55	102.53	993.6	0.078							102.51	993.1	0.122			
2,3-dimethyloctene-2	993.56															
I24	994.53	102.70	994.3	0.052	102.60	993.7	0.051				102.75	994.2	0.173	102.72	994.1	0.096
i-butylbenzene	995.95	103.00	995.7	0.027				103.00	995.3	0.127	103.05	995.5	0.065	103.07	995.6	0.049
	996.20				103.17	996.2	0.023									
I25	996.84	103.10	996.1	0.030	103.31	996.9	0.017							103.30	996.6	0.030
		103.29	997.0	0.056												
sec-butylbenzene	997.79	103.44	997.6	0.051				103.46	997.3	0.129	103.49	997.4	0.327	103.52	997.6	0.086
	998.70				103.80	999.0	0.008									
n-decane	1000.20	103.99	1000.0	0.739				104.00	999.6	0.048	104.08	1000.0	3.484	104.06	1000.0	0.211
I26	1001.71				104.18	1001.1	0.028				104.34	1001.9	0.051	104.29	1001.7	0.020
N38	1003.39	104.46	1003.4	0.049							104.56	1003.5	0.056			
1,2,3-trimethylbenzene	1006.88	104.87	1006.4	0.311				104.90	1005.9	1.075	104.94	1006.2	0.561	104.96	1006.5	0.751
	1008.70	105.16	1008.5	0.018	105.16	1008.2	0.007				105.25	1008.4	0.087			
1,3-methyl-i-propylbenzene	1009.84	105.33	1009.7	0.057				105.34	1009.1	0.132	105.38	1009.4	0.170	105.40	1009.6	0.078
N39	1011.33															
1,4-methyl-i-propylbenzene	1013.24	105.81	1013.1	0.050				105.83	1012.6	0.039	105.86	1012.8	0.137	105.89	1013.1	0.026
I27	1014.33	105.97	1014.2	0.013	105.94	1013.7	0.006				106.02	1014.0	0.038			
I28	1015.86	106.19	1015.8	0.013	106.33	1016.5	0.013							106.43	1017.0	0.052
I29	1017.87	106.45	1017.7	0.028							106.52	1017.5	0.102			
2-3-dihydroindene	1019.44	106.62	1018.9	0.257	106.73	1019.4	0.011	106.64	1018.4	0.463	106.68	1018.7	0.146	106.71	1018.9	0.208
	1022.40				107.15	1022.3	0.008				106.96	1020.6	0.101			
sec-butylcyclohexane	1023.07	107.23	1023.1	0.056							107.29	1023.0	0.230	107.28	1022.9	0.016
	1024.50	107.45	1024.7	0.051	107.35	1023.7	0.009				107.50	1024.4	0.095	107.48	1024.4	0.018
											107.63	1025.4	0.055			
I30	1024.82	107.68	1026.3	0.034				107.68	1025.7	0.029	107.77	1026.3	0.044			
	1025.70															
	1026.50															
1,2-methyl-i-propylbenzene	1027.73	107.90	1027.8	0.109				107.91	1027.4	0.013	107.96	1027.7	0.747	107.98	1027.8	0.035
3-ethylnonane	1029.40	108.48	1031.8	0.063							108.55	1031.7	0.376	108.49	1031.4	0.217
	1031.13				108.38	1030.9	0.044									
N40	1032.29															
	1032.60										108.71	1032.9	0.105			
I31	1033.20	108.67	1033.2	0.089							108.85	1033.8	0.115	108.82	1033.7	0.012
	1035.50															
I32	1036.92	109.17	1036.6	0.053							109.24	1036.5	0.242	109.27	1036.8	0.017
	1038.53	109.45	1038.5	0.020	109.37	1037.7	0.014				109.50	1038.3	0.060	109.48	1038.2	0.101
1,3-diethylbenzene	1039.97	109.63	1039.7	0.173				109.64	1039.4	0.477	109.73	1039.9	0.215	109.70	1039.7	0.143
	1040.50				109.92	1041.5	0.030									
1,3-methyl-n-propylbenzene	1042.60	110.01	1042.4	0.257				110.04	1042.1	0.942	110.06	1042.2	0.260	110.06	1042.2	0.737
I33	1044.35	110.31	1044.4	0.064							110.36	1044.2	0.329			
1,4-diethylbenzene	1045.25															
1,4-methyl-n-propylbenzene	1046.40	110.57	1046.2	0.152	110.60	1046.1	0.008	110.59	1045.9	0.596	110.62	1046.0	0.110	110.65	1046.2	0.264
n-butylbenzene	1047.48	110.72	1047.2	0.097				110.74	1046.9	0.224	110.77	1047.0	0.147	110.79	1047.2	0.080
1,3-dimethyl-5-ethylbenzene	1049.78	111.07	1049.6	0.249				111.10	1049.4	0.934	111.12	1049.4	0.184	111.15	1049.6	0.402
											111.27	1050.4	0.042			
1,2-diethylbenzene	1051.72	111.32	1051.2	0.038				111.36	1051.1	0.070				111.42	1051.4	0.027
I34	1051.80	111.49	1052.4	0.040							111.55	1052.3	0.246			
t-decahydronaphthalene	1053.12													111.68	1053.1	0.023
N41	1054.60	111.83	1054.7	0.032							111.88	1054.6	0.093			
	1055.80	111.95	1055.5	0.013							112.05	1055.7	0.062			
1,2-methyl-n-propylbenzene	1057.87	112.26	1057.5	0.123				112.28	1057.3	0.277	112.31	1057.4	0.176	112.34	1057.6	0.139
I35	1058.87	112.46	1058.9	0.018							112.50	1058.7	0.047			
					112.83	1061.1	0.038									
I36	1060.15	112.59	1059.8	0.014							112.66	1059.8	0.036			
I37	1062.62	113.03	1062.7	0.091	113.10	1062.9	0.007	113.05	1062.5	0.009	113.08	1062.6	0.199	112.93	1061.5	0.400
	1063.96													113.20	1063.3	0.059
I38	1065.53	113.47	1065.6	0.090	113.47	1065.4	0.006	113.49	1065.4	0.009	113.52	1065.5	0.231	113.57	1065.8	0.037
											113.67	1066.5	0.052			
1,4,dimethyl-2-ethylbenzene	1068.05	113.80	1067.7	0.185				113.82	1067.6	0.502	113.85	1067.7	0.108	113.87	1067.8	0.229
A3	1068.90															
1,3-dimethyl-4-ethylbenzene	1069.53	114.01	1069.2	0.316				114.05	1069.2	0.530	114.05	1069.0	0.380	114.11	1069.3	0.230
I39	1071.12	114.32	1071.2	0.033							114.36	1071.0	0.061	114.27	1070.4	0.202
	1072.49				114.17	1070.0	0.025									
I40	1074.39	114.72	1073.8	0.147				114.74	1073.7	0.050				114.80	1073.8	0.022
1,2-dimethyl-4-ethylbenzene	1075.25	114.89	1074.9	0.360				114.92	1074.9	0.886	114.93	1074.8	0.388	114.98	1075.0	0.419
	1076.00				115.06	1075.8	0.005									

TABLE A1.2 *Continued*

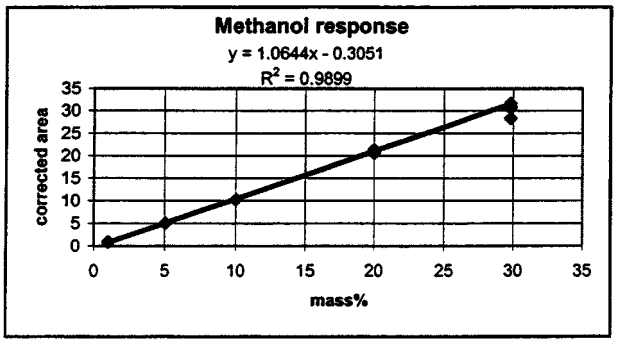
		PONA-Va			Alkylate			Reformate			Naphtha			Indolene		
Component	Ave. RI	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%
	1077.91	115.28	1077.5	0.017							115.30	1077.2	0.080			
I41	1079.65										115.65	1079.4	0.064			
1,3-dimethyl-2-ethylbenzene	1080.68	115.72	1080.3	0.053				115.74	1080.2	0.045	115.77	1080.2	0.036	115.82	1080.5	0.040
I42	1081.60	115.94	1081.7	0.012	115.90	1081.3	0.015				116.07	1082.2	0.035	116.00	1081.7	0.168
I43	1084.18	116.32	1084.1	0.017							116.35	1084.0	0.044			
	1085.30	116.44	1084.9	0.016							116.49	1084.9	0.055			
	1086.54										116.71	1086.3	0.072	116.70	1086.2	0.013
	1088.20										117.08	1088.7	0.059	117.00	1088.1	0.024
	1088.88	117.04	1088.8	0.027												
											117.28	1090.0	0.041			
undecene-1	1090.45	117.30	1090.4	0.035										117.40	1090.7	0.029
1,4-methyl-t-butylbenzene	1092.00	117.51	1091.8	0.032				117.50	1091.5	0.051	117.55	1091.7	0.063			
1,2-dimethyl-3-ethylbenzene	1093.12	117.66	1092.7	0.115				117.68	1092.7	0.226	117.71	1092.7	0.118	117.74	1092.8	0.147
	1094.89	118.05	1095.2	0.016												
	1095.78	118.15	1095.6	0.020							118.17	1095.6	0.052			
1,2-ethyl-i-propylbenzene	1097.22	118.34	1097.0	0.014				118.34	1097.0	0.015	118.37	1096.9	0.021	118.42	1097.1	0.025
	1098.54	118.53	1098.3	0.018				118.61	1098.7	0.013	118.61	1098.4	0.034			
n-undecane	1100.00	118.81	1100.0	0.381				118.82	1100.0	0.009	118.86	1100.0	0.753	118.86	1099.9	0.058
	1101.00													119.07	1101.6	0.021
1,4-ethyl-i-propylbenzene	1102.50	119.13	1102.7	0.018												
1,2,4,5-tetramethylbenzene	1104.83	119.32	1104.4	0.147				119.33	1104.4	0.473	119.36	1104.3	0.073	119.39	1104.4	0.283
1,2-methyl-n-butylbenzene	1107.30															
1,2,3,5-tetramethylbenzene	1108.79	119.77	1108.3	0.200				119.79	1108.3	0.621	119.82	1108.3	0.073	119.85	1108.3	0.393
	1110.82													120.14	1110.8	0.013
	1112.39	120.16	1111.5	0.028												
	1115.92	120.65	1115.8	0.023				120.75	1116.4	0.007				120.62	1114.9	0.017
	1120.13	121.18	1120.2	0.023										121.25	1120.2	0.012
	1121.30	121.30	1121.2	0.025							121.36	1121.4	0.015			
1,2-methyl-t-butylbenzene	1122.80															
	1124.62													121.83	1125.1	0.013
5-methylindan	1127.35	121.95	1126.7	0.283				121.97	1126.7	0.372	122.09	1127.5	0.019	122.02	1126.7	0.083
	1129.83				122.42	1130.4	0.008									
I43	1131.42	122.52	1131.5	0.026							122.57	1131.5	0.012	122.52	1130.9	0.041
4-methylindan	1133.70	122.75	1133.4	0.072				122.76	1133.4	0.124	122.79	1133.4	0.011	122.82	1133.4	0.022
	1134.90	122.90	1134.6	0.031										123.01	1135.0	0.011
1,2-ethyl-n-propylbenzene	1136.52	123.09	1136.2	0.078				123.11	1136.2	0.161	123.13	1136.2	0.022	123.16	1136.3	0.021
2-methylindan	1138.11	123.23	1137.4	0.266				123.25	1137.4	0.353				123.31	1137.5	0.084
1,3-methyl-n-butylbenzene	1140.67	123.60	1140.4	0.036				123.56	1140.0	0.009						
1,3-di-i-propylbenzene	1142.70	123.81	1142.1	0.071				123.82	1142.2	0.172	123.85	1142.2	0.019	123.88	1142.2	0.113
s-pentylbenzene	1144.27	124.03	1144.0	0.094										124.10	1144.0	0.013
	1148.00	124.52	1148.0	0.047				124.54	1148.0	0.053				124.59	1148.0	0.017
n-pentylbenzene	1149.04	124.62	1148.8	0.049												
	1149.83	124.71	1149.5	0.047				124.73	1149.6	0.034						
1t-M-2-(4-MP)cyclopentane	1151.80															
1,2-di-i-propylbenzene	1153.16	125.11	1152.8	0.042				125.13	1152.8	0.071				125.18	1152.9	0.015
	1154.09	125.23	1153.8	0.056				125.24	1153.8	0.066				125.29	1153.7	0.012
	1157.64	125.65	1157.2	0.045				125.67	1157.3	0.068				125.72	1157.3	0.021
1,4-di-i-propylbenzene	1159.52	125.91	1159.4	0.110				125.90	1159.2	0.085				125.95	1159.1	0.017
	1161.30													126.29	1161.8	0.013
tetrahydronaphthalene	1163.30	126.41	1163.3	0.051				126.37	1162.9	0.007						
	1165.13													126.61	1164.5	0.021
	1166.34	126.73	1166.0	0.060				126.74	1165.9	0.117				126.80	1166.0	0.021
naphthalene	1168.01	126.89	1167.3	0.285				126.91	1167.3	0.891				126.96	1167.3	0.148
1-t-butyl-3,5-dimethylbenzene	1169.25	127.15	1169.3	0.015												
1,4-ethyl-t-butylbenzene	1173.72	127.68	1173.6	0.099				127.66	1173.3	0.010				127.81	1174.1	0.057
I45	1177.88	128.15	1177.3	0.114				128.18	1177.4	0.036				128.15	1176.8	0.043
I46	1179.46	128.34	1178.8	0.063				128.29	1178.3	0.010						
	1181.20							128.35	1178.8	0.010						
I47	1183.44	128.85	1182.9	0.081				128.87	1182.9	0.031						
I48	1187.14	129.31	1186.5	0.068				129.33	1186.6	0.011						
1,3-di-n-propylbenzene	1188.64	129.53	1188.2	0.075				129.55	1188.3	0.077				129.60	1188.3	0.026
A5	1190.24	129.73	1189.8	0.058				129.75	1189.8	0.050				129.80	1189.9	0.022
dodecene-1	1192.19															
A6	1198.52	130.79	1198.1	0.037				130.80	1198.1	0.045				130.86	1198.1	0.017
n-dodecane	1200.00	131.03	1200.0	0.332										131.10	1200.0	0.014
	1202.51	131.30	1202.6	0.025												
	1208.41	131.86	1208.0	0.027				131.84	1207.7	0.009						
1,3,5-triethylbenzene	1211.79															
	1216.27	132.68	1215.9	0.030				132.68	1215.8	0.009						
	1217.50	132.83	1217.3	0.061				132.86	1217.4	0.024				132.91	1217.6	0.009
	1222.36	133.32	1222.0	0.060				133.33	1221.9	0.023						
	1223.70	133.52	1223.9	0.055				133.53	1223.9	0.022						
	1225.08	133.66	1225.2	0.025				133.65	1225.0	0.014				133.72	1225.3	0.006

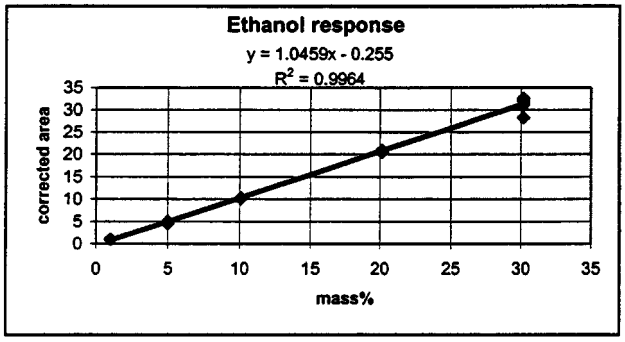
TABLE A1.2 *Continued*

		PONA-Va			Alkylate			Reformate			Naphtha			Indolene		
Component	Ave. RI	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%	Min.	INDEX	Mass%
	1228.64	133.97	1228.2	0.040				134.03	1228.6	0.010						
	1230.00													134.15	1229.3	0.004
1,2,4-triethylbenzene	1230.83															
	1232.23	134.40	1232.2	0.052												
	1236.42	134.84	1236.4	0.058				134.87	1236.5	0.002						
	1237.42	134.98	1237.7	0.012												
1,4-methyl-n-pentylbenzene	1241.71	135.34	1241.1	0.110				135.35	1241.0	0.083				135.39	1241.1	0.015
	1244.15	135.63	1243.8	0.068												
	1246.48	135.86	1246.0	0.013				135.89	1246.1	0.007						
	1248.73	136.12	1248.4	0.013				136.12	1248.3	0.007						
	1251.16	136.38	1250.8	0.029												
n-hexylbenzene	1252.85	136.57	1252.5	0.052												
	1255.61	136.84	1255.1	0.101				136.84	1254.9	0.055						
	1257.39	137.11	1257.6	0.029												
	1259.54	137.25	1258.9	0.050				137.25	1258.7	0.021						
	1262.15	137.61	1262.2	0.041												
	1266.71	138.08	1266.5	0.062												
	1269.02	138.31	1268.6	0.030										138.30	1268.3	0.015
I49	1270.79	138.43	1269.8	0.015										138.59	1270.9	0.007
1,2,3,4,5-pentamethylbenzene	1274.04	138.82	1273.3	0.107				138.85	1273.5	0.067				138.92	1273.9	0.027
	1277.23													139.25	1277.0	0.010
	1279.96	139.49	1279.4	0.022												
2-methylnaphthalene	1282.57	139.75	1281.7	0.353				139.77	1281.8	0.786				139.82	1282.1	0.059
	1286.59	140.11	1285.1	0.010												
	1287.50	140.22	1286.0	0.034										140.40	1287.4	0.019
	1288.77	140.46	1288.2	0.029												
tridecene-1	1290.10															
	1292.41													140.84	1291.5	0.011
	1295.08	141.16	1294.6	0.042												
1-methylnaphthalene	1297.72	141.42	1296.9	0.152				141.44	1296.8	0.377				141.49	1297.3	0.035
n-tridecane	1300.00	141.77	1300.0	0.234										141.85	1300.6	0.007
C14+	1300.50															

A2. HYDROCARBON DATA

A2.1 The tables and Fig. A2.1 in this annex relate to Procedure B. Table A2.1 presents hydrocarbon data.





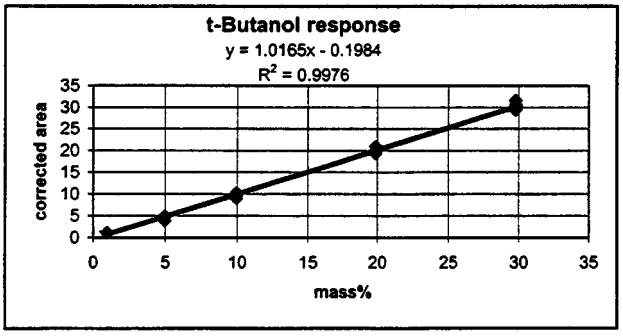
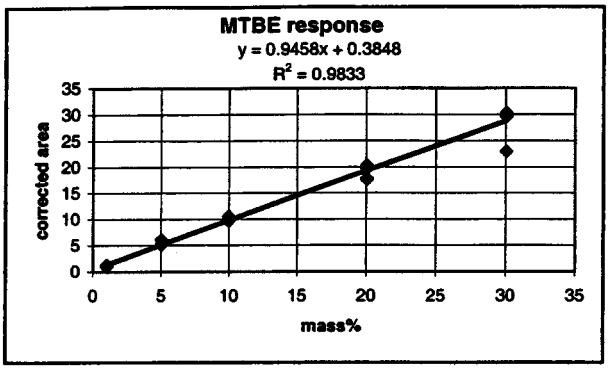
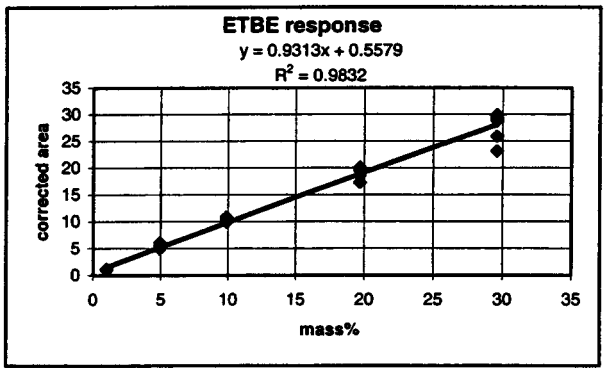


FIG. A2.1 Determination of Calculated Oxygenate Response from IHA Method





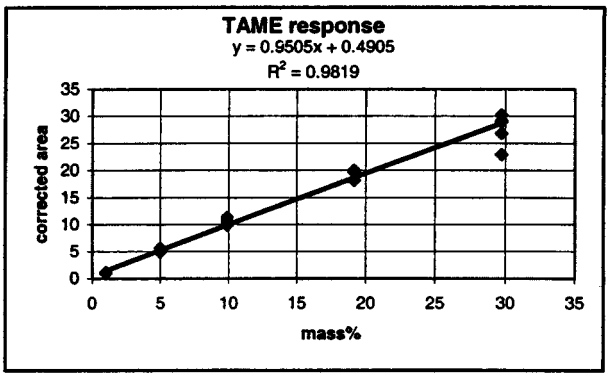


FIG. A2.1 Determination of Calculated Oxygenate Response from IHA Method *(continued)*

TABLE A2.1 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 23D*N*-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-c_5=.

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 analysing 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, (C_1)
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
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	27.09	84.16	0.874
86	Methylethylketone (MEK)	28.00	72.06	1.570
88	3-methylpentane	29.15	86.18	0.895
90	C6-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	Methy-sec-butylether (MSBE)	30.66	88.09	1.550
98	C6-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

TABLE A2.1 *Continued*

Peak No.	New Name	Retention Time	Molecular Mass, MWt	Theoretical Mass Rf, (C_1)
104	*N*-hexane	32.75	86.18	0.895
106	Cis-3-hexene	33.41	84.16	0.874
108	Di-isopropylether (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-tertbutylether (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	.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	C7-olefin	40.30	98.19	0.874
148	C7-olefin	40.68	98.19	0.874
150	C7-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	C7-olefin	43.06	98.19	0.874
162	C2-methyl-3-hexene	43.37	98.19	0.874
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	C7-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+C7-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-amylmethylether (TAME)	48.10	102.18	1.210
194	C7-olefin	48.46	98.19	0.874
196	C7-olefin	48.64	98.19	0.874
198	3-methylhexane	49.05	100.21	0.892
200	C7-olefin	49.47	98.19	0.874
202	C7-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	C7-olefin	51.43	98.19	0.874
214	2,2,4-trimethylpentane	51.61	114.23	0.890
216	C7-olefin	51.75	98.19	.874
218	1-heptene	52.05	98.19	0.874
220	C7-olefin	52.18	98.19	0.874
222	2,3-dimethyl-1,3-pentadiene	52.69	96.18	0.874
224	C7-diolefin	53.00	96.18	0.856
226	C7-olefin	53.36	98.19	0.874
228	C7-diolefin	53.81	96.18	0.856
230	C7-diolefin	54.13	96.18	0.856
232	C7-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

TABLE A2.1 *Continued*

Peak No.	New Name	Retention Time	Molecular Mass, MWt	Theoretical Mass Rf, (C_1)
250	C7-diolefin+C7-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	C7-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	C8-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+C8-olefin	61.59	114.23	0.890
280	2,4-dimethylhexane	61.91	114.23	0.890
282	C7-triolefin+C8-olefin	62.28	96.18	0.856
284	Trans,cis-1,2,4-trimethylcyclopentane	62.68	112.22	0.874
286	3,3-dimethylhexane+C8-olefin	63.13	114.23	0.890
288	C7-triolefin+C8-olefin	63.39	96.18	0.856
290	C8-olefin	63.69	112.22	0.874
292	Trans,cis-1,2,3-trimethylcyclopentane	64.27	112.22	0.874
294	C8-olefin	64.52	112.22	0.874
296	C8-olefin	64.73	112.22	0.874
298	C8-olefin	64.82	112.22	0.874
300	2,3,4-trimethylpentane	64.94	114.23	0.890
302	C7-diolefin	65.25	96.18	0.856
304	Toluene	65.50	92.06	0.821
306	2,3,3-trimethylpentane	65.76	114.23	0.890
308	C8-olefin	65.90	112.22	0.874
310	C8-diolefin	66.12	110.21	0.859
312	C8-olefin	66.48	112.22	0.874
314	C8-olefin	66.65	112.22	0.874
316	C8-olefin	67.08	112.22	0.874
318	C8-diolefin+C8-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+C7-triolefin	68.04	112.22	0.874
326	C8-diolefin+C8-paraffin	68.31	110.21	0.859
328	C8-olefin	68.41	112.22	0.874
330	C8-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	C8-diolefin+C7-olefin	69.41	112.22	0.874
338	C8-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	C8-diolefin	70.51	110.21	0.874
350	C8-olefin	70.72	112.22	0.874
352	C8-olefin	70.92	112.22	0.874
354	1,1-dimethylcyclohexane	71.18	112.22	0.874
356	C8-olefin	71.43	112.22	0.874
358	C8-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	C8-olefin	73.26	112.22	0.874
374	Trans-1,2-dimethylcyclohexane	73.36	112.22	0.874
376	C8-olefin	73.48	112.22	0.874
378	C8-olefin	73.68	112.22	0.874
380	Trans-3-C8-Olefin	74.08	112.11	0.874
382	C8-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	C8-olefin	75.33	112.22	0.874
392	C8-olefin	75.49	112.22	0.874
394	Trans-2-octene	75.62	112.22	0.874

TABLE A2.1 *Continued*

Peak No.	New Name	Retention Time	Molecular Mass, MWt	Theoretical Mass Rf, (C_1)
396	Isopropylcyclopentane	75.72	112.22	0.874
398	C9-olefin	75.85	126.24	0.874
400	C9-olefin	75.89	126.24	0.874
402	C9-olefin	75.90	126.24	0.874
404	C9-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	C9-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	C9-olefin	78.90	126.24	0.874
426	C9-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	C9-olefin	79.85	126.24	0.874
438	1,1,4-trimethylcyclohexane	80.05	126.24	0.874
440	C9-olefin	80.28	126.24	0.874
442	C9-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
448	C9-olefin	80.88	126.24	0.874
450	3,3-DMheptane	81.00	128.26	0.888
452	C9-paraffin	81.13	128.26	0.888
454	C9-olefin	81.34	126.24	0.874
456	2,3,3-trimethylhexane	81.56	128.26	0.888
458	C9-olefin	81.68	126.24	0.874
460	Ethylbenzene	81.96	106.08	0.827
462	C9-olefin	82.00	126.24	0.874
464	Trans-1,2,4-trimethylcyclohexane	82.31	126.24	0.874
466	C9-olefin	82.33	126.24	0.874
468	2,3,4-trimethylhexane	82.63	128.26	0.888
470	C9-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	C9-olefin	84.08	126.24	0.874
486	3-methyl-3-ethylhexane	84.26	128.26	0.888
488	C9-olefin	84.41	126.24	0.874
490	4-ethylheptane	84.52	128.26	0.888
492	4-methyloctane+C9-olefin	84.70	128.26	0.888
494	2-methyloctane	84.84	128.26	0.888
496	C9-olefin	85.01	126.24	0.874
498	C9-paraffin	85.18	128.26	0.888
500	C9-olefin	85.36	126.24	0.874
502	3-ethylbentane	85.51	128.26	0.888
504	3-methyloctane	85.69	128.26	0.888
506	C9-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	C9-olefin	86.47	126.24	0.874
516	C9-paraffin	86.57	128.26	0.888
518	C9-paraffin	86.75	128.26	0.888
520	C9-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	C9-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	C9-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	C9-paraffin	89.09	128.26	0.888
540	*N*-nonane	89.24	128.26	0.888

TABLE A2.1 *Continued*

Peak No.	New Name	Retention Time	Molecular Mass, MWt	Theoretical Mass Rf, (C_1)
542	C10-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	C10-olefin	90.09	140.27	0.874
552	C10-paraffin	90.18	142.28	0.887
554	C10-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	C9-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	C10-olefin	93.79	140.27	0.874
592	Propylbenzene	93.96	120.20	0.832
594	3,3-dimethyloctane	94.27	142.28	0.887
596	3-methyl-5-ethylheptane	94.54	142.28	0.887
598	C10-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	C10-olefin	97.69	140.27	0.874
626	C10-paraffin	97.83	142.28	0.887
628	C10-paraffin	98.16	142.28	0.887
630	1,2,4-trimethylbenzene	98.49	120.20	0.832
632	C10-paraffin	98.74	142.28	0.887
634	C10-paraffin	98.90	142.28	0.887
636	Isobutylcyclohexane	99.10	140.27	0.874
638	C10-paraffin	99.09	142.28	0.887
640	C10-paraffin	99.22	142.37	0.887
642	1-decene	99.52	140.27	0.874
644	C10-paraffin	99.66	142.28	0.887
646	C10-paraffin	99.70	142.28	0.887
648	C10-aromatic	99.75	134.22	0.837
650	C10-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	C10-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	C11-paraffin	100.67	156.32	0.886
666	C11-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	C11-paraffin	101.55	156.32	0.886
674	1-methyl-4-isopropylbenzene	101.73	134.22	0.837
676	C11-paraffin	102.06	156.32	0.886
678	C11-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	C11-paraffin	102.87	156.32	0.886
686	1-methyl-2-isopropylbenzene	103.03	134.22	0.837

TABLE A2.1 *Continued*

Peak No.	New Name	Retention Time	Molecular Mass, MWt	Theoretical Mass Rf, (C_1)
688	3-ethylnonane	103.26	156.32	0.886
690	C11-paraffin	103.37	156.32	0.886
692	Naphthene	103.55	140.27	0.874
694	C11-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	C11-paraffin	105.39	156.32	0.886
712	C10-aromatic	105.49	134.22	0.837
714	C10-aromatic	105.64	134.22	0.837
716	C10-aromatic	105.75	134.22	0.837
718	1-methy-2-propylbenzenes	105.85	134.22	0.837
720	C10-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	C11-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	C11-paraffin	107.06	156.32	0.886
736	3-methyldecane	107.27	156.32	0.886
738	C1-indane	107.35	132.00	0.837
740	1,2-dimethyl-4-ethylbenzene	107.46	134.22	0.837
742	C11-paraffin	107.76	156.32	0.886
744	1,3-dimethyl-2-ethylbenzene	108.01	134.22	0.837
746	C11-paraffin	108.58	156.32	0.886
748	C11-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	C12-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	C11-aromatic	110.74	148.25	0.840
772	C12-paraffin	110.84	170.34	0.885
774	C11-aromatic	110.94	148.25	0.840
776	C11-aromatic	111.05	148.25	0.840
778	C11-aromatic	111.12	148.25	0.840
780	1-tert-butyl-2-methylbenzene	111.56	148.25	0.840
782	C11-aromatic	111.65	148.25	0.840
784	1-ethyl-2-propylbenzene	111.76	148.25	0.840
786	C11-aromatic	112.00	148.25	0.840
788	C11-aromatic	112.22	148.25	0.840
790	C11-aromatic	112.34	148.25	0.840
792	1-methyl-3-butylbenzene	112.52	148.25	0.840
794	C11-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	C11-aromatic	113.74	148.25	0.840
804	C11-aromatic	113.85	148.25	0.840
806	C11-aromatic	114.02	148.25	0.840
808	C12-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	148.25	0.840
818	1,2-dimethylindane	115.19	148.25	0.840
820	1,6-dimethylindane	115.33	148.25	0.840
822	C11-aromatic	115.55	170.34	0.885
824	1-ethylindane	115.65	148.25	0.885
826	2-ethylindane	115.88	148.25	0.840
828	Ethyl-1,3,5-trimythylbenzene	116.00	162.34	0.885
830	1,3-dipropylbenzene	116.21	162.34	0.843
832	*N*-dodecane	116.55	170.34	0.885

TABLE A2.1 *Continued*

Peak No.	New Name	Retention Time	Molecular Mass, MWt	Theoretical Mass Rf, (C_1)
834	Ethyl-1,2,4-trimythylbenzene	116.69	162.34	0.885
836	C11-aromatic	117.07	148.25	0.840
838	C11-aromatic	117.19	148.25	0.840
840	C12-aromatic+C2-indane	117.55	162.30	0.843
842	2,4-dimethylindane	117.99	148.25	0.840
844	4-ethylindane	118.13	148.25	0.840
846	1-tert-butyl-4-ethylbenzene	118.59	162.30	0.843
848	1,3-dimethylindane	119.07	148.25	0.843
850	1-methyl-4-pentylbenzene	119.60	162.30	0.843
852	4,7-dimethylindane	119.65	148.25	0.843
854	5,6-dimethylindane	119.70	148.25	0.843
856	C12-aromatic	119.77	162.30	0.843
858	Hexylbenzene	119.87	162.30	0.843
860	C6-benzene	119.93	162.30	0.843
862	C6-benzene	119.98	162.30	0.843
864	C6-benzene	120.20	162.30	0.843
866	4,5-dimethylindane	120.30	148.25	0.843
868	C6-benzene	120.80	163.30	0.843
870	2-methylnaphthalene	121.42	142.08	0.806
872	C6-benzene	121.65	162.30	0.843
874	C6-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	C6-benzene	122.40	162.30	0.843
882	C2-tetralin	122.80	162.30	0.843
884	C6-benzene	123.20	162.30	0.843
886	C6-benzene	124.00	162.30	0.843
888	C13-paraffin	125.60	198.34	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

A2.2 Table A2.2 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 below:

A2.2.1 For each analyte to qualify for a precision statement, it must be present in at least 6 samples, and detected by at least 6 labs, at least once, as per D2-1007 requirements.

A2.2.2 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.

TABLE A2.2 Repeatability and Reproducibility of IHA Determinations

NOTE 1—Short analyte names were used. By using the number beside this name it will correspond to a full name in Table A2.1.

NOTE 2—C_2 Benzene refer to grouping ethylbenzene, M, P, and O-xylene as a group.

NOTE 3—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.

NOTE 4—The summaries for the paraffins, isoparaffins, C_2 benzene and oxygenates follow the same procedure that was used for the analytes. The statistics for the grouping are shown here 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 and/or naphthenic constituents 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 referred to in Section 2.

NOTE 5—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.
C_{max} – upper concentration limit that r_{est}, R_{est} is applicable.

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	13.4	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	22DMC4	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	methylenecyC5	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

TABLE A2.2 *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	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
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
	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
	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
	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
	372	378	C8='S	3.4	5.3	7.9	109.3	124.4	141	0.02	0.26
	374	380	t-3-C8=	0	1.5	9.4	50.8	67.2	86.9	0.02	0.12
	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
	406	394	t2C8=	3	6.5	12.2	45.6	72.5	108.4	0.02	0.28
	408	396	iPrcyC5	5.8	7.4	9.3	31.7	50.8	76.5	0.03	0.36
	416	404	C9=	0.3	2.9	9.9	46.9	63.8	84.4	0.02	0.14
	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
	436	424	C9=	1.9	6	13.7	34.7	47.5	63.1	0.01	0.07
	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
	460	448	C9='S	3.3	8.4	17.1	40.1	56.4	76.6	0.01	0.07
	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

TABLE A2.2 *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	503	478	23DMC7	5.1	7.6	10.9	45.3	73.5	111.5	0.03	0.16
	504	480	35DMC7	7.2	9.8	13	44.1	82.8	139.2	0.02	0.07
	506	482	34DMC7	6.5	10.1	15	42.5	67.7	101.4	0.02	0.07
	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
	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
	572	526	C9P	4.5	7.2	10.7	28.7	55.7	95.9	0.03	0.6
	582	532	C9P	7.5	11.1	15.6	16.9	23.1	30.8	0.02	0.24
	586	534	t3C9=	4.6	9.1	16	27.3	38.8	53.2	0.01	0.16
	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
	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
	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
	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
	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
	674	632	C10-P	7.1	12.9	21.4	35.6	81.2	155.1	0.01	0.32
	675	634	C10P	2.6	6.2	12.3	25.2	55.1	102.4	0.01	0.34
	684	648	C10A	5.2	9.3	15.1	22.8	38.2	59.4	0.01	0.3
	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
	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
	714	682	sBucyC6	8.7	12.7	17.6	46.7	70.2	100.5	0.01	0.06
	718	686	1M2iPrbenz	4.6	8.4	13.7	48	88.1	146	0.02	0.33
	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
	768	744	13DM2Ebenz	6.2	9.6	14	37.9	68.9	113.3	0.03	0.35
	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
	824	782	C11A	8.7	11.3	14.2	32.9	55.6	86.9	0.02	0.07
	826	784	1E2Prbenz?	5	7.5	10.7	14.2	25.2	40.8	0.09	0.44
	828	786	C11A	8.5	11.8	15.7	23.4	35.1	50.3	0.02	0.1
	830	788	C11A	8.8	12.3	16.7	35.7	49.9	67.5	0.02	0.1
	832	790	C11A	9.7	13.4	17.8	22.9	39.6	63	0.02	0.1

TABLE A2.2 *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]	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
	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
	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
	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
	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]Represents 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

A2.3 *Caution for the Summary of Oxygenates (Table A2.3)*—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 %

A2.4 Precision statement for the olefins and cycloparaffins is determined by taking the square root of the value determined in the summary multiply; by the coeffiencent (r_{coef}) for repeatability and the coeffiencent (R_{coef}) for the reproducibility.

Name	rmin	r_{coef}	rmax	R_{min}	R_{coef}	R_{max}	C_{min}	C_{max}
cycloparaf	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

A2.4.1 Precision for the aromatics does not depend on level and is stated below in wt. %.

Name	rmin	r %	rmax	R_{min}	R %	R_{max}	C_{min}	C_{max}
aromatics	0.8549	0.98	1.155	2.151	2.706	3.651	15	50

A2.5 Tables A2.4-A2.11 present data from the oxygenate linearity study.

TABLE A2.3 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

TABLE A2.4 Oxygenates Relative Response Factors

NOTE 1—All RRF relative to N-C7=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 Range	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 A2.5 IHA Method Oxygenates linearity Cooperative Study Laboratory 1

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

TABLE A2.6 IHA Method Oxygenates Linearity Cooperative Study Laboratory #2

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

TABLE A2.7 IHA Method Oxygenates Linearity Cooperative Study Laboratory #3

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

TABLE A2.8 IHA Method Oxygenate Linearity Cooperative Study Laboratory #4

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

TABLE A2.9 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	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							

TABLE A2.10 IHA Method Oxygenate Linearity Cooperative Study Laboratory #6

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							

TABLE A2.11 IHA Method Oxygenate Linearity Cooperative Study Laboratory #7

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

A3. MANDATORY INFORMATION FOR PROCEDURE C

A3.1 Table A3.1 presents the retention time, response factor hydrocarbon type and carbon number for each component for Procedure C, Method 1. Table A3.2 presents identical data for Procedure C, Method 2.

A3.2 Fig. A3.1 and Fig. A3.2 present reference chromatograms for Procedure C, Methods 1 and 2.

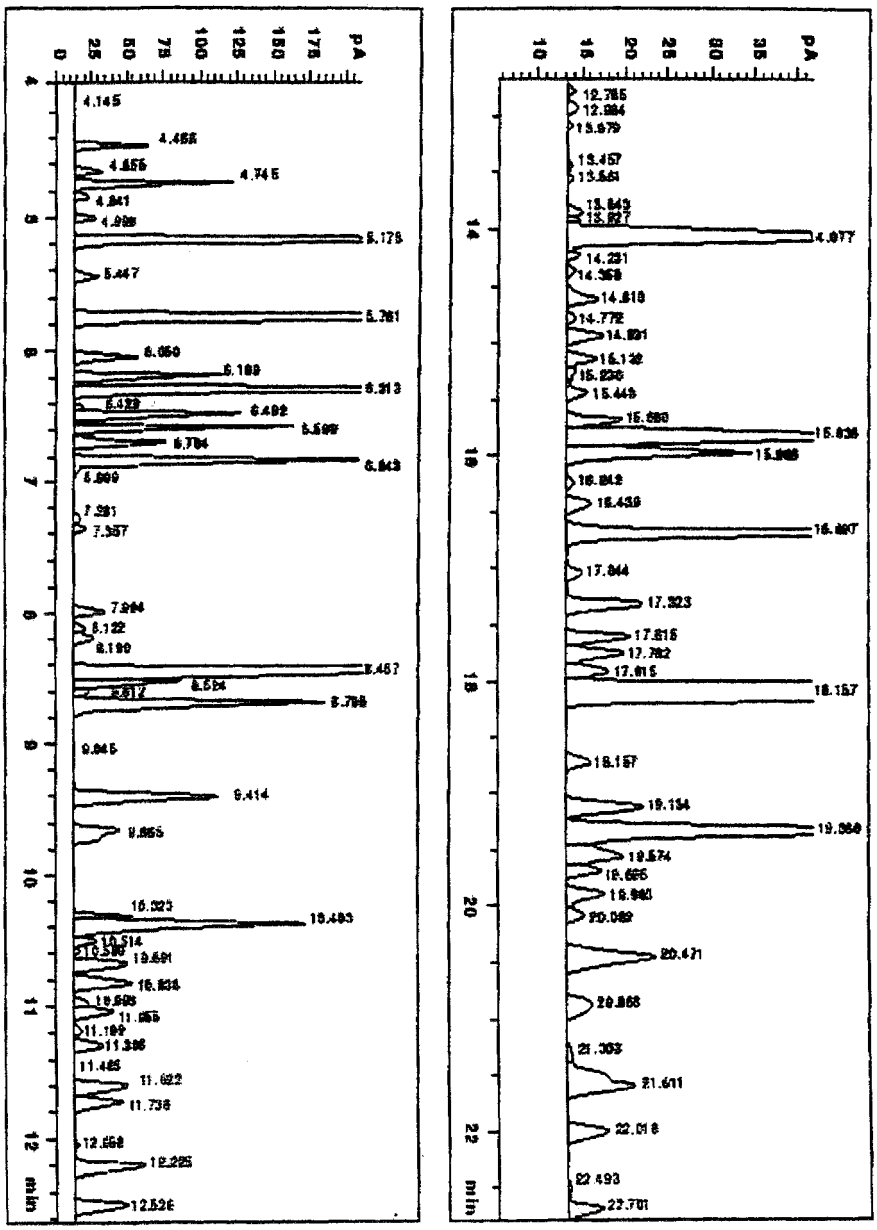


FIG. A3.1 Reference Chromatogram (a and b) Method 1

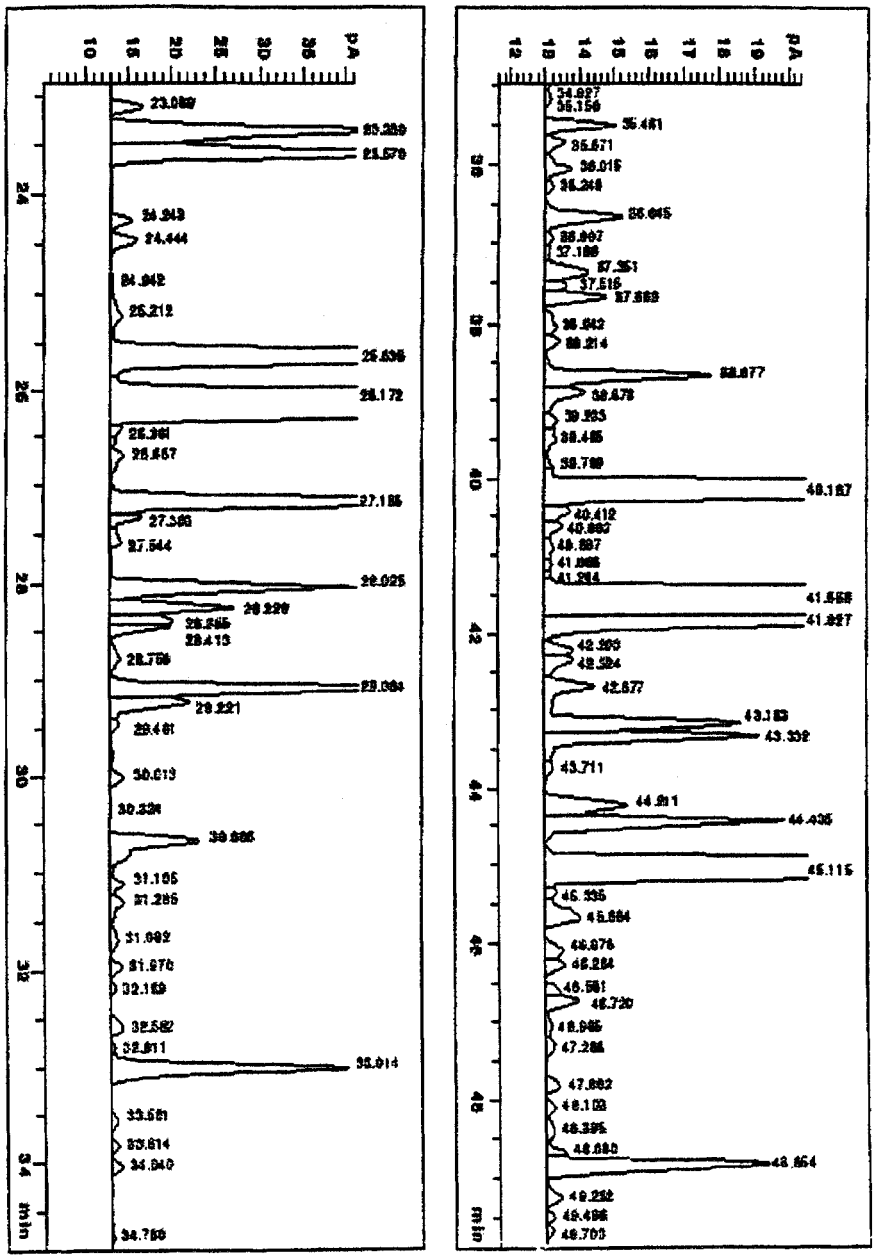


FIG. A3.1 Reference Chromatogram (c and d) Method 1 *(continued)*

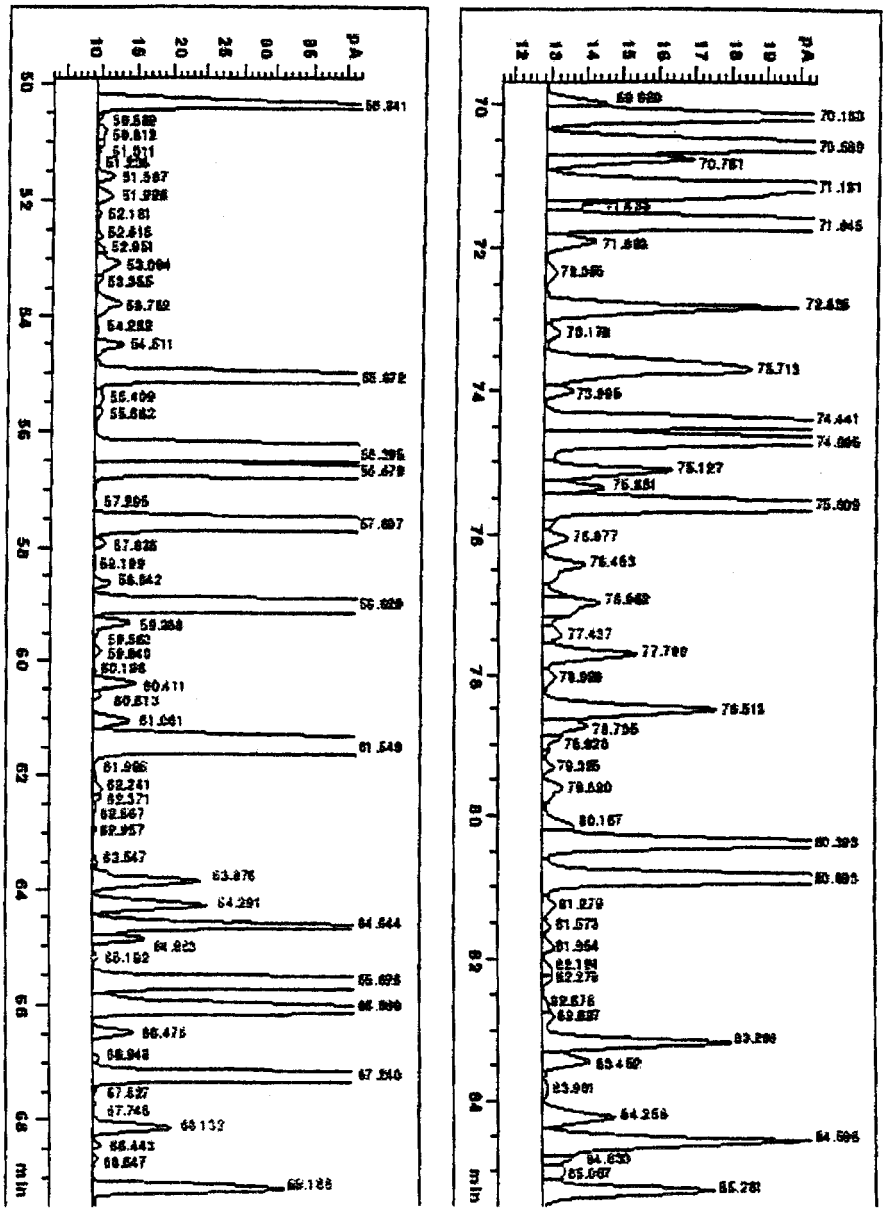


FIG. A3.1 Reference Chromatogram (e and f) Method 1 *(continued)*

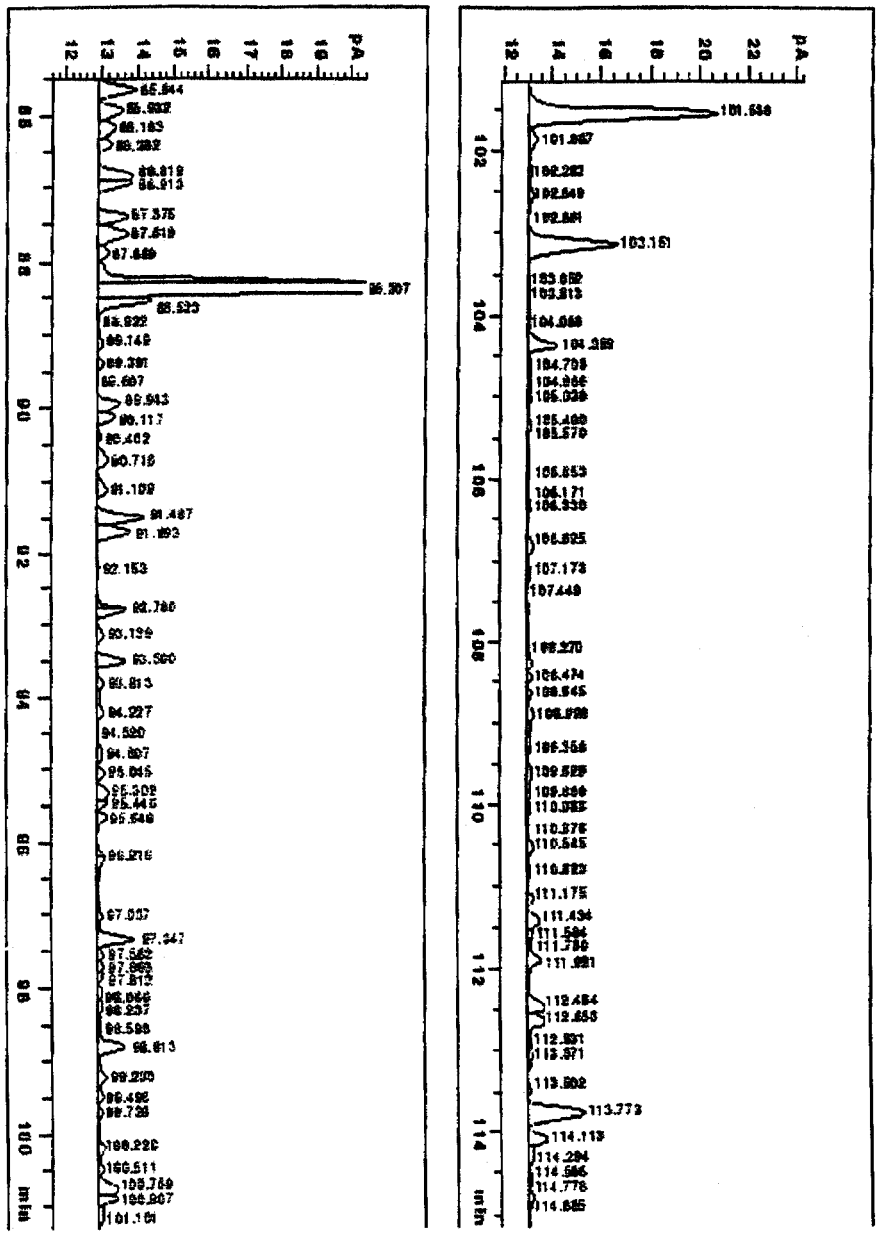


FIG. A3.1 Reference Chromatogram (g and h) Method 1 *(continued)*

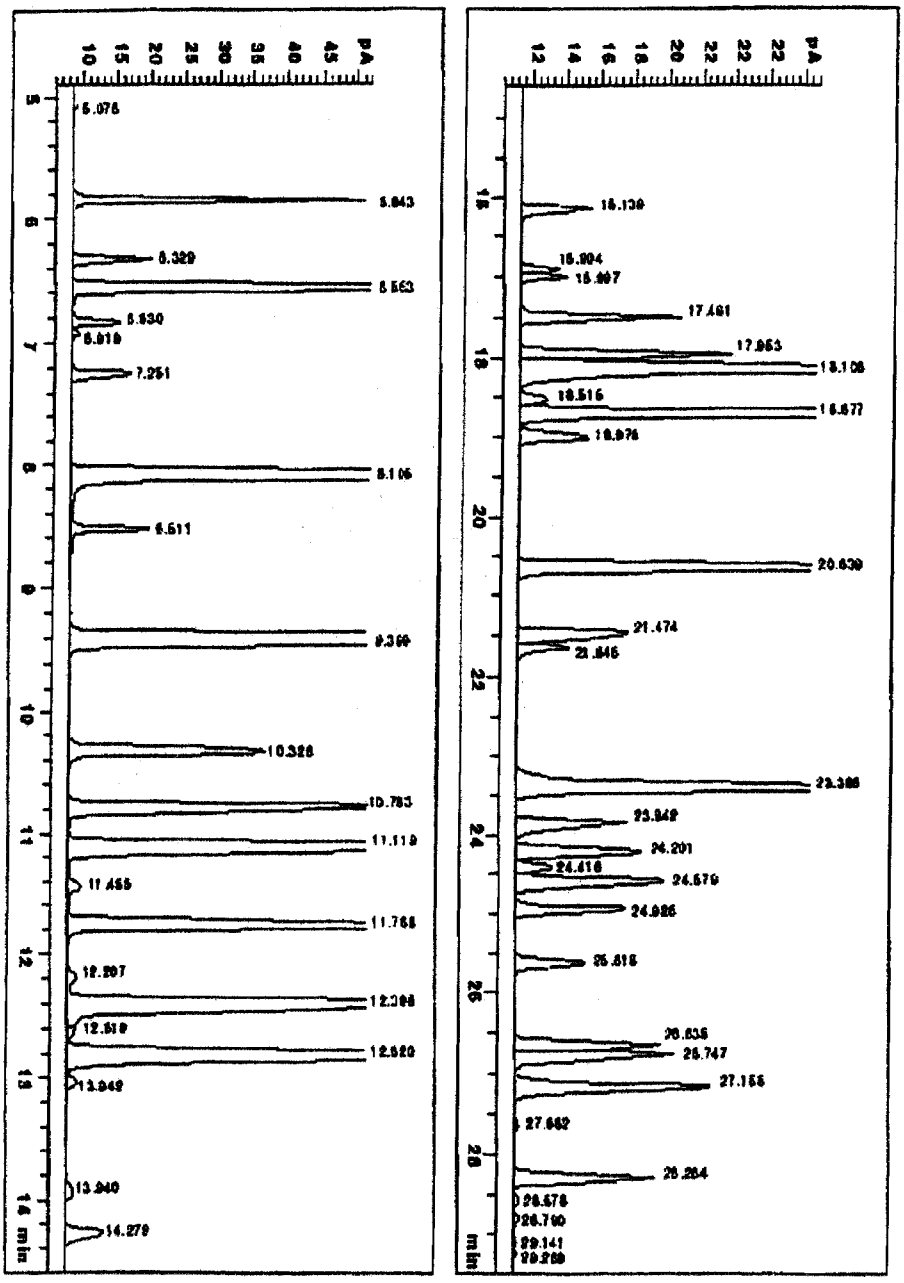


FIG. A3.2 Reference Chromatogram (a and b) Method 2

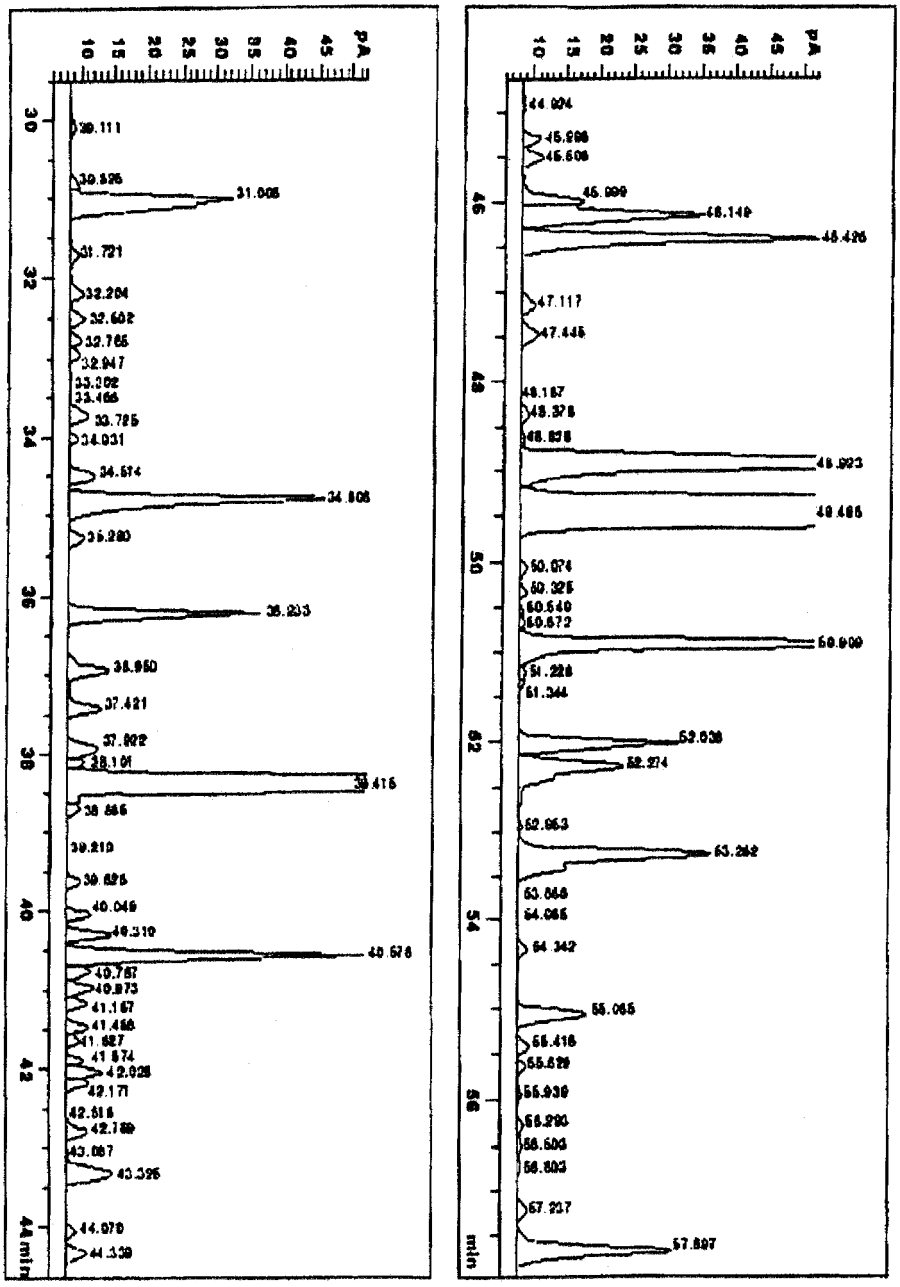


FIG. A3.2 Reference Chromatogram (c and d) Method 2 *(continued)*

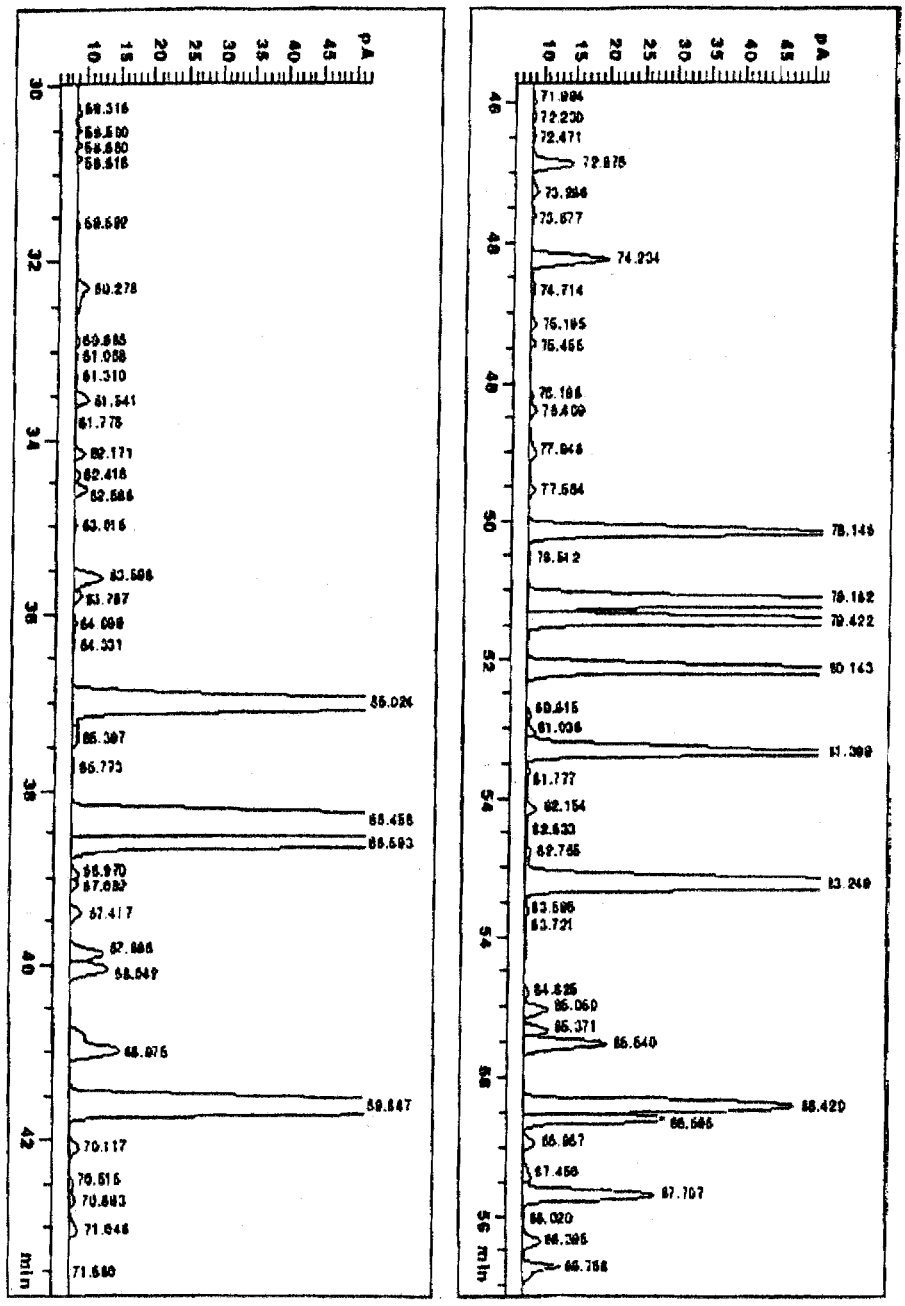


FIG. A3.2 Reference Chromatogram (e and f) Method 2 *(continued)*

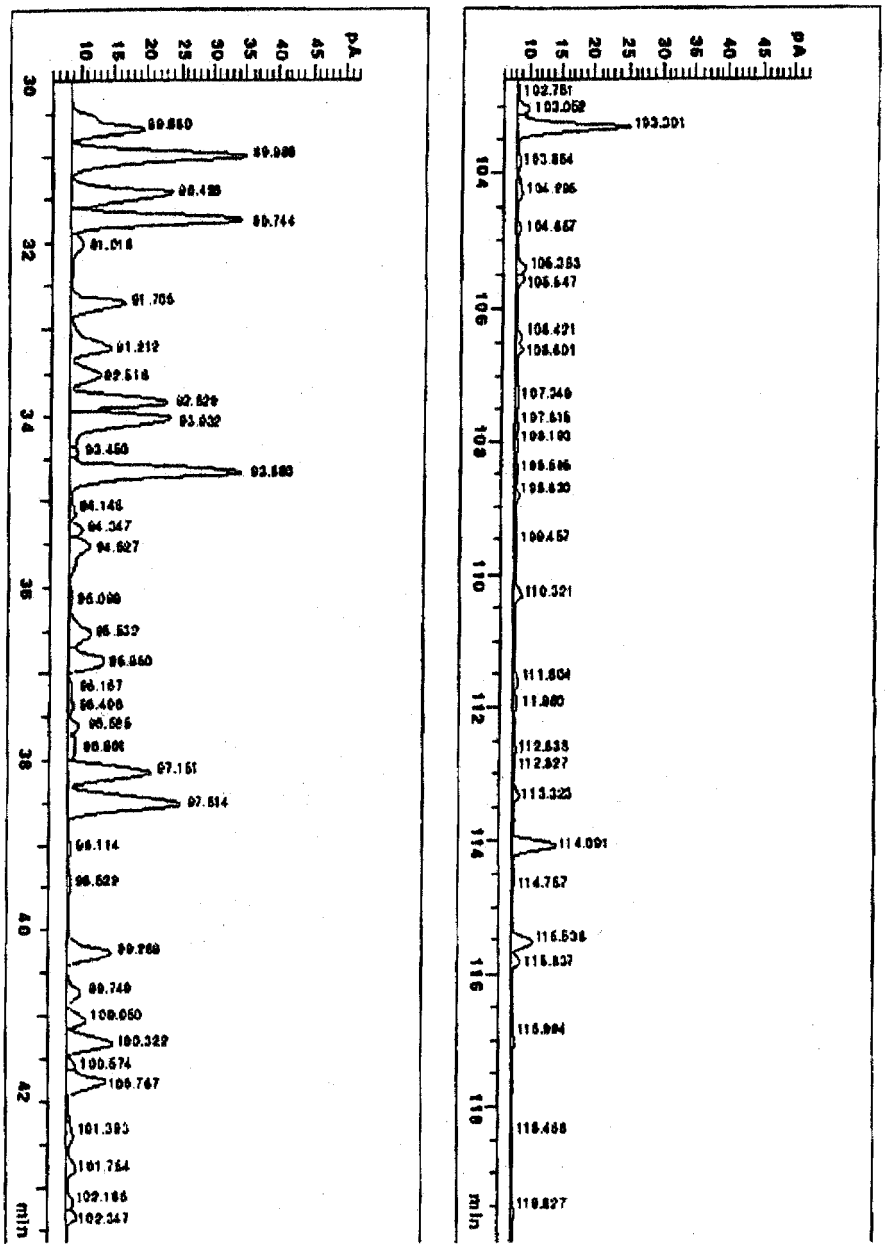


FIG. A3.2 Reference Chromatogram (g and h) Method 2 *(continued)*

TABLE A3.1 Retention Time, Response Factor, Hydrocarbon Type and Carbon Number for Each Component for Procedure C-1

NOTE 1—Legend for Hydrocarbon types: NP–normal paraffins; IP–iso paraffins; NA–naphthenes; OL–olefins; AR–aromatics; Ox–oxygenates.

Compounds	Retention Time, min.	Response Factor	Hydrocarbon Type	Carbon No.
Propane	4.14	1.125	IP	3
Isobutane[A]	4.47	1.112	IP	4
Methanol[A]	4.47	2.850	OX	1
Isobutene+1-butene	4.66	1.075	OL	4
N-butane	4.74	1.112	NP	4
Trans-2-butene	4.84	1.075	OL	4
C_4-diolefin	4.88	1.045	OL	4
CIS-2-butene	5.00	1.075	OL	4
Ethanol	5.17	2.300	OX	2
3-Methyl-1-butene	5.45	1.075	OL	5
Isopentane	5.76	1.105	IP	5
1-pentene	6.05	1.075	OL	5
2-methyl-1-butene	6.20	1.075	OL	5
N-pentane	6.31	1.105	NP	5
Isoprene	6.43	1.045	OL	5
Trans-2-pentene	6.49	1.075	OL	5
Tertiobutyl alcohol	6.60	1.490	OX	5
CIS-2-pentene	6.70	1.075	OL	5
2-methyl-2-butene	6.84	1.075	OL	5
1,trans-3-pentadiene	6.91	1.045	OL	5
1,CIS-3-pentadiene	7.28	1.045	OL	5
2,2-dimethylbutane	7.36	1.100	IP	6
1-cyclopentene	7.99	1.075	OL	5
4-methyl-1-pentene	8.12	1.075	OL	6
3-methyl-1-pentene	8.19	1.075	OL	6
Cyclopentane[A]	8.46	1.075	NA	5
MTBE[A]	8.46	1.520	OX	5
2,3-dimethylbutane	8.52	1.100	IP	6
4-methyl-cis-2-pentene	8.61	1.075	OL	6
2-methylpentane	8.70	1.100	IP	6
4-methyl-trans-2-pentene	9.04	1.075	OL	6
3-methylpentane	9.41	1.100	IP	6
2-methyl-1-pentene	9.66	1.075	OL	6
1-hexene	9.70	1.075	OL	6
2-ethyl-1-butene	10.32	1.075	OL	6
N-hexane	10.40	1.110	NP	6
Trans-3-hexene	10.51	1.075	OL	6
CIS-3-hexene	10.59	1.075	OL	6
Trans-2-hexene	10.69	1.075	OL	6
2-methyl-2-pentene	10.84	1.075	OL	6
4-methyl-1-cyclopentene	10.99	1.075	OL	6
3-methyl-trans-2-pentene	11.06	1.075	OL	6
3-methyl-1-cyclopentene	11.19	1.075	OL	6
CIS-2-hexene	11.31	1.075	OL	6
C_6-olefin	11.46	1.075	OL	6
ETBE	11.62	1.520	OX	6
3-methyl-CIS-2-pentene	11.74	1.075	OL	6
2,2-dimethylpentane	12.06	1.099	IP	7
1-methylcyclopentane	12.23	1.075	NA	6
2,4-dimethylpentane	12.53	1.099	IP	7
C_6-olefin	12.78	1.075	OL	6
2,2,3-trimethylbutane	13.93	1.099	IP	7
C_6-olefin	13.08	1.075	OL	6
C_7-olefin	13.45	1.075	OL	7
C_7-olefin	13.56	1.075	OL	7
C_7-olefin	13.84	1.075	OL	7
C_7-olefin	13.93	1.075	OL	7
Benzene[A]	14.08	1.000	AR	6
1-methyl-1-cyclopentene[A]	14.08	1.075	OL	6
C_7-olefin	14.23	1.075	OL	7
C_7-olefin	14.36	1.075	OL	7
3,3-dimethylpentane	14.61	1.099	IP	7
C_7-olefin	14.77	1.075	OL	7
Cyclohexane	14.93	1.075	NA	6
C_7-olefin	15.13	1.075	OL	7
C_7-olefin	15.24	1.075	OL	7
C_7-olefin	15.44	1.075	OL	7
C_7-olefin	15.68	1.075	OL	7
2-methylhexane	15.84	1.099	IP	7
2,3-dimethylpentane	15.99	1.099	IP	7
1,1-dimethylcyclopentane	16.24	1.075	NA	7

TABLE A3.1 *Continued*

Compounds	Retention Time, min.	Response Factor	Hydrocarbon Type	Carbon No.
Cyclohexene	16.44	1.075	OL	6
3-methylhexane	16.70	1.099	IP	7
C_7-olefin	17.04	1.075	OP	7
CIS-1,3-dimethylcyclopentane	17.32	1.075	NA	7
Trans-1,3-dimethylcyclopentane	17.61	1.075	NA	7
3-ethylpentane	17.76	1.099	IP	7
Trans-1,2-dimethylcyclopentane	17.92	1.075	NA	7
2,2,4-trimethylpentane	18.16	1.096	IP	8
C_7-olefin	18.16	1.075	OL	7
C_7-olefin	18.74	1.075	OL	7
C_7-olefin	19.13	1.075	OL	7
N-heptane	19.36	1.099	NP	7
C_7-olefin	19.57	1.075	OL	7
C_7-olefin	19.69	1.075	OL	7
C_7-olefin	19.90	1.075	OL	7
C_7-olefin	20.08	1.075	OL	7
C_7-olefin	20.47	1.075	OL	7
C_7-olefin	20.87	1.075	OL	7
C_7-olefin	21.30	1.075	OL	7
C_7-olefin	21.53	1.075	OL	7
1-methylcyclohexane	21.61	1.075	NA	7
CIS-1,2-dimethylcyclopentane	21.61	1.075	NA	7
1,1,3-trimethylcyclopentane	22.02	1.075	NA	8
2,2-dimethylhexane	22.02	1.096	IP	8
C_8-olefin	22.49	1.075	OL	8
C_8-olefin	22.70	1.075	OL	8
1-ethylcyclopentane	23.09	1.075	NA	7
2,2,3-trimethylpentane	23.33	1.096	IP	8
2,5-dimethylhexane	23.33	1.096	IP	8
2,4-dimethylhexane	23.57	1.096	IP	8
1,trans2,CIS4-trimethylcyclopentane	24.24	1.075	NA	8
3,3-dimethylhexane	24.44	1.096	IP	8
C_8-olefin	24.94	1.075	OL	8
1,trans2,CIS3-trimethylcyclopentane	25.21	1.075	NA	8
2,3,4-trimethylpentane	25.64	1.096	IP	8
2,3,3-trimethylpentane[A]	26.17	1.096	IP	8
Toluene[A]	26.17	1.008	AR	7
C_8-olefin	26.38	1.075	OL	8
C_8-olefin	26.67	1.075	OL	8
C_8-olefin	26.79	1.075	OL	8
2,3-dimethylhexane	27.16	1.096	IP	8
2-methyl-3-ethylpentane	27.30	1.096	IP	8
C_8-olefin	27.54	1.075	OL	8
2-methylheptane	28.02	1.096	IP	8
4-methylheptane	28.23	1.096	IP	8
3,4-dimethylhexane	28.36	1.096	IP	8
1,CIS2,trans4-trimethylcyclopentane	28.41	1.075	NA	8
C_8-olefin	28.76	1.075	OL	8
3-methylheptane	29.08	1.096	IP	8
3-ethylhexane	29.22	1.096	IP	8
1,CIS-3-dimethylcyclohexane	29.46	1.075	NA	8
1,trans-4-dimethylcyclohexane	29.46	1.075	NA	8
1,CIS2,trans3-trimethylcyclopentane	29.46	1.075	NA	8
C_8-olefin	29.81	1.075	OL	8
1,1-dimethylcyclohexane	30.01	1.075	NA	8
C_8-olefin	30.24	1.075	OL	8
2,2,5-trimethylhexane	30.67	1.093	IP	8
1-ME-T3-ethylcyclopentane	30.81	1.075	NA	8
C_8-olefin	30.81	1.075	OL	8
1-methyl-CIS-3-ethylcyclopentane	31.11	1.075	NA	8
C_8-olefin	31.11	1.075	OL	8
1-methyl-trans-2-ethylcyclopentane	31.29	1.075	NA	8
C_8-olefin	31.29	1.075	OL	8
1-methyl-1-ethylcyclopentane	31.43	1.075	NA	8
C_8-olefin	31.43	1.075	OL	8
1,trans-2-dimethylcyclopentane	31.68	1.075	OL	7
C_8-olefin	31.97	1.075	OL	8
C_8-olefin	32.17	1.075	OL	8
C_8-olefin	32.58	1.075	OL	8
C_8-olefin	32.81	1.075	OL	8
C_8-naphthene	33.01	1.075	NA	8
N-octane	33.01	1.096	NP	8
C_8-olefin	33.56	1.075	OL	8

TABLE A3.1 *Continued*

Compounds	Retention Time, min.	Response Factor	Hydrocarbon Type	Carbon No.
C_8-olefin	33.81	1.075	OL	8
2,2,4-trimethylhexane	34.04	1.093	IP	
C_8-olefin	34.76	1.075	OL	8
C_8-olefin	34.93	1.075	OL	8
C_8-olefin	35.15	1.075	OL	8
2,3,5-trimethylhexane	35.46	1.093	IP	9
2,2-dimethylheptane	35.67	1.093	IP	9
1,CIS-2-dimethylcyclohexane	36.02	1.075	NA	8
C_9-olefin	36.25	1.075	OL	9
2,4-dimethylheptane	36.65	1.093	IP	9
4,4-dimethylheptane	36.91	1.093	IP	9
C_9-olefin	37.17	1.075	OL	9
1-ethylcyclohexane	37.35	1.075	NA	8
C_9-olefin	37.52	1.075	OL	9
2,6-dimethylheptane	37.66	1.093	IP	8
C_9-naphthene	37.93	1.075	NA	9
C_9-naphthene	38.05	1.075	NA	9
C_9-naphthene	38.21	1.075	NA	9
2,5-dimethylheptane	38.68	1.093	IP	9
C_8-olefin	38.87	1.075	OL	8
C_8-olefin	39.05	1.075	OL	8
C_8-olefin	39.23	1.075	OL	8
C_8-olefin	39.46	1.075	OL	8
C_8-olefin	39.80	1.075	OL	8
Ethylbenzene	40.19	1.018	AR	8
C_8-olefin	40.41	1.075	OL	8
C_9-naphthene	40.60	1.075	NA	9
C_9-naphthene	40.89	1.075	NA	9
C_8-olefin	41.09	1.075	OL	8
C_8-olefin	41.24	1.075	OL	8
Metaxylene	41.69	1.018	AR	8
Paraxylene	41.83	1.018	AR	8
C_9-naphthene	42.20	1.075	NA	9
3,4-dimethylheptane	42.32	1.093	IP	9
4-ethylheptane	42.68	1.093	IP	9
C_9-olefin	42.91	1.075	OL	8
4-methyloctane	43.16	1.093	IP	9
2-methyloctane	43.33	1.093	IP	9
C_9-naphthene	43.51	1.075	NA	9
C_9-naphthene	43.71	1.075	NA	9
3-ethylheptane	44.21	1.093	IP	9
3-methyloctane	44.43	1.093	IP	9
Orthoxylene	45.12	1.018	AR	8
C_9-naphthene	45.33	1.075	NA	9
C_9-naphthene	45.66	1.075	NA	9
C_9-naphthene	46.08	1.075	NA	9
C_{10}-isoparaffin	46.26	1.086	IP	10
C_{10}-isoparaffin	46.58	1.086	IP	10
C_{10}-isoparaffin	46.72	1.086	IP	10
C_{10}-isoparaffin	46.98	1.086	IP	10
C_{10}-isoparaffin	47.29	1.086	IP	10
C_9-naphthene	47.80	1.075	NA	9
C_9-naphthene	48.10	1.075	NA	9
C_9-naphthene	48.40	1.075	NA	9
C_9-naphthene	48.68	1.075	NA	9
N-nonane	48.85	1.093	NP	9
C_9-olefin	49.25	1.075	OL	9
C_9-olefin	49.50	1.075	OL	9
C_9-olefin	49.70	1.075	OL	9
Isopropylbenzene	50.34	1.025	AR	9
C_9-olefin	50.59	1.075	OL	9
C_9-naphthene	50.81	1.025	NA	9
C_9-olefin	51.01	1.075	OL	9
C_9-olefin	51.24	1.075	OL	9
C_{10}-isoparaffin	51.59	1.086	IP	10
C_{10}-isoparaffin	51.93	1.086	IP	10
C_{10}-isoparaffin	52.18	1.086	IP	10
C_9-naphthene	52.62	1.075	NA	9
C_{10}-isoparaffin	52.85	1.086	IP	10
C_{10}-isoparaffin	53.08	1.086	IP	10
C_{10}-naphthene	53.35	1.025	NA	10
2,7-dimethyloctane	53.78	1.086	IP	9
C_{10}-isoparaffin	54.23	1.086	IP	10

TABLE A3.1 *Continued*

Compounds		Retention Time, min.	Response Factor	Hydrocarbon Type	Carbon No.
2,6-dimethyloctane		54.51	1.086	IP	9
3,3-dimethyloctane		54.80	1.086	IP	9
N-propylbenzene		55.07	1.025	AR	9
3,6-dimethyloctane		55.34	1.086	IP	9
C_{10}-isoparaffin		55.41	1.086	IP	10
C_{10}-isoparaffin		55.66	1.086	IP	10
1-methyl,3-ethylbenzene		56.40	1.025	AR	9
1-methyl,4-ethylbenzene		56.68	1.025	AR	9
C_{10}-isoparaffin		57.30	1.086	IP	10
1,3,5-trimethylbenzene		57.61	1.025	AR	9
4-ethyloctane		57.94	1.086	IP	10
C_{10}-isoparaffin		58.20	1.086	IP	10
C_{10}-isoparaffin		58.28	1.086	IP	10
5-methylnonane		58.64	1.086	IP	10
1-methyl,2-ethylbenzene		59.03	1.025	AR	9
4-methylnonane		59.03	1.086	IP	10
2-methylnonane		59.34	1.086	IP	10
C_{10}-naphthene		59.56	1.075	NA	10
3-ethyloctane		59.84	1.086	IP	10
C_{10}-isoparaffin		60.19	1.086	IP	10
3-methylnonane		60.41	1.086	IP	10
C_{10}-naphthene		60.61	1.075	NA	10
C_{10}-naphthene		61.06	1.075	NA	10
1,2,4-trimethylbenzene		61.55	1.025	AR	9
C_{11}-isoparaffin	from	62.00	1.086	IP	11
	to	64.10			
C_{10}-aromatic		64.29	1.025	AR	10
C_{10}-aromatic		64.64	1.025	AR	10
N-decane		64.86	1.086	NP	10
C_{11}-isoparaffin		65.22	1.086	IP	11
1,2,3-trimethylbenzene		65.63	1.025	AR	9
1-methy,4-isopropylbenzene		66.08	1.025	AR	10
1-methyl,3-isopropylbenzene		66.47	1.025	AR	10
C_{11}-isoparaffin		66.95	1.086	IP	11
Indan		67.24	1.025	AR	9
C_{11}-isoparaffin		67.53	1.086	IP	11
C_{11}-isoparaffin		67.74	1.086	IP	11
1-methyl,2-isopropylbenzene		68.13	1.025	AR	10
2,6-dimethylnonane		68.43	1.025	IP	10
C_{11}-isoparaffin		68.65	1.086	IP	11
C_{11}-isoparaffin		69.19	1.086	IP	11
C_{11}-isoparaffin		69.98	1.086	IP	11
1,3-diethylbenzene		70.16	1.030	AR	10
1-methyl,3*N*-propylbenzene		70.58	1.030	AR	10
C_{10}-aromatic		70.76	1.025	AR	10
1-methyl,4*N*-propylbenzene		71.13	1.030	AR	10
C_{10}-aromatic		71.43	1.025	AR	10
1,3-dimethyl,5-ethylbenzene		71.64	1.030	AR	10
1,4-diethylbenzene		71.89	1.030	AR	10
C_{12}-isoparaffine		72.36	1.086	IP	12
1-methyl,2*N*-propylbenzene		72.84	1.030	AR	10
C_{12}-isoparaffin		73.18	1.086	IP	12
C_{12}-isoparaffin		73.71	1.086	IP	12
C_{12}-isoparaffin		73.99	1.086	IP	12
1,4-dimethyl,2-ethylbenzene		74.44	1.030	AR	10
1,3-dimethyl,4-ethylbenzene		74.69	1.030	AR	10
C_{12}-isoparaffin		75.13	1.086	IP	12
1-methylindan		75.35	1.030	AR	10
1,2-dimethyl,4-ethylbenzene		75.61	1.030	AR	10
1,3-dimethyl-2-ethylbenzene		76.08	1.030	AR	10
C_{11}-isoparaffin		76.45	1.086	IP	11
C_{12}-isoparaffin	from	76.64	1.086	IP	12
	to	78.20			
1,2-dimethyl-3-ethylbenzene		78.51	1.030	AR	10
C_{10}-naphthene		78.73	1.075	NA	10
C_{12}-isoparaffin		78.92	1.086	IP	12
C_{12}-isoparaffin		79.32	1.086	IP	12
C_{12}-isoparaffin		79.62	1.086	IP	12
N-undecane		80.17	1.086	NP	11
1,2,4,5-tetramethylbenzene		80.39	1.030	AR	10
1,2,3,5-tetramethylbenzene		80.89	1.030	AR	10
C_{12}-isoparaffin		81.28	1.086	IP	12
C_{11}-naphthene	from	81.53	1.075	NA	11

TABLE A3.1 *Continued*

Compounds		Retention Time, min.	Response Factor	Hydrocarbon Type	Carbon No.
	to	83.00			
5-methylindan		83.21	1.030	AR	10
C_{11}-aromatic		83.45	1.030	AR	11
C_{11}-aromatic		83.90	1.033	AR	11
C_{11}-aromatic		84.26	1.033	AR	11
4-methylindan		84.60	1.030	AR	10
C_{11}-aromatic		84.83	1.033	AR	11
C_{11}-aromatic		85.07	1.033	AR	11
1,2,3,4-tetramethylbenzene		85.28	1.030	AR	10
C_{11}-aromatic	from	85.64	1.033	AR	11
	to	87.70			
C_{12}-isoparaffin		87.86	1.086	IP	12
C_{12}-isoparaffin		88.09	1.086	IP	12
Naphthalene		88.33	1.030	AR	10
C_{12}-isoparafin		88.52	1.086	IP	12
C_{12}-isoparafin		88.92	1.086	IP	12
C_{11}-aromatic		89.15	1.033	AR	11
C_{12}-isoparafin		89.39	1.086	IP	12
C_{12}-isoparafin		89.61	1.086	IP	12
C_{11}-aromatic		89.94	1.033	AR	11
C_{12}-isoparaffin		90.12	1.086	IP	12
C_{11}-aromatic	from	90.40	1.033	AR	11
	to	93.30			
N-dodecane		93.50	1.086	NP	12
C_{13}-isoparaffin		93.81	1.033	IP	13
C_{11}-aromatic	from	94.23	1.033	AR	11
	to	98.06			
C_{11}+-aromatic	from	98.30	1.033	AR	11+
	to	99.30			
C_{13}-isoparaffin	from	99.46	1.033	AR	11+
	to	101.30			
2-methylnaphthalene		101.54	1.033	AR	11
C_{11}+-aromatic	from	101.70	1.033	AR	11+
	to	103.00			
1-methylnaphthalene		103.15	1.033	AR	11
Hydrocarbon C_{12}+	>	103.20	1.035		

[A]Co-eluted compounds.

TABLE A3.2 Method C2, Retention Time, Response Factor, Hydrocarbon Type and Carbon Number for Each Component

Compounds	Retention Time, min.	Response Factor	Hydrocarbon Type	Carbon No.
Propane	5.08	1.125	IP	3
Isobutane	5.84	1.112	IP	4
Methanol	6.06	2.850	OX	1
isobutene+1-butene	6.33	1.075	OL	4
N-butane	6.55	1.112	NP	4
Trans-2-butene	6.83	1.075	OL	4
C_4-diolefin	6.92	1.045	OL	4
CIS-2-butene	7.25	1.075	OL	4
Ethanol	8.10	2.300	OX	2
3-methyl-1-butene	8.51	1.075	OL	5
isopentane	9.40	1.105	IP	5
1-pentene	10.33	1.075	OL	5
2-methyl-1-butene	10.78	1.075	OL	5
N-pentane	11.12	1.105	NP	5
isoprene	11.45	1.045	OL	5
trans-2-pentene	11.77	1.075	OL	5
C_5-diene	12.20	1.045	OL	5
CIS-2-pentene[A]	12.40	1.075	OL	5
Tertiobutylalcohol[A]	12.40	1.490	OX	5
2-methyl-2-butene	12.82	1.075	OL	5
1,trans-3-pentadiene	13.04	1.075	OL	5
1,CIS-3-pentadiene	13.94	1.075	OL	5
2,2-dimethylbutane	14.28	1.100	IP	6
1-cyclopentene	16.14	1.075	OL	5
4-methyl-1-pentene	16.90	1.075	OL	6
3-methyl-1-pentene	17.00	1.075	OL	6
Cyclopentane	17.49	1.075	NA	5
2,3-dimethylbutane	17.95	1.100	IP	6
MTBE	18.11	1.520	OX	5
4-methyl-CIS-2-pentene	18.52	1.075	OL	6
2-methylpentane	18.68	1.100	IP	6
4-methyl-trans-2-pentene	18.98	1.075	OL	6
3-methylpentane	20.64	1.100	IP	6
2-methyl-1-pentene	21.47	1.075	OL	6
1-hexene	21.64	1.075	OL	6
2-ethyl-1-butene	23.30	1.075	OL	6
N-hexane	23.39	1.110	NP	6
Trans-3-hexene	23.84	1.075	OL	6
CIS-3-hexene	23.84	1.075	OL	6
Trans-2-hexene	24.20	1.075	OL	6
4-methyl-1-cyclopentene	24.42	1.075	OL	6
2-methyl-2-pentene	24.58	1.075	OL	6
3-methyl-trans-2-pentene	24.92	1.075	OL	6
3-methyl-1-cyclopentene	24.92	1.075	OL	6
CIS-2-hexene	25.62	1.075	OL	6
C_6-olefin	25.93	1.075	OL	6
3-methyl-CIS-2-pentene	26.64	1.075	OL	6
ETBE	26.75	1.520	OX	6
2,2-dimethylpentane	27.15	1.099	IP	6
1-methylcyclopentane	27.15	1.075	NA	6
C_6-olefin	27.66	1.075	OL	6
2,4-dimethylpentane	28.28	1.099	IP	7
C_6-olefin	28.28	1.075	OL	6
C_6-olefin	28.58	1.075	OL	6
2,2,3-trimethylbutane	28.79	1.099	IP	7
C_6-olefin	29.14	1.075	OL	6
C_7-olefin	29.27	1.075	OL	7
C_7-olefin	30.11	1.075	OL	7
C_7-olefin	30.82	1.075	OL	7
Benzene[A]	31.01	1.000	AR	6
1-methyl-1-cyclopentene[A]	31.01	1.075	OL	6
C_7-olefin	31.72	1.075	OL	7
3,3-dimethylpentane	32.20	1.075	IP	7
Cyclohexane	32.50	1.075	NA	6
C_7-olefin	32.76	1.075	OL	7
C_7-olefin	32.95	1.075	OL	7
C_7-olefin	33.30	1.075	OL	7
C_7-olefin	33.46	1.075	OL	7
C_7-olefin	33.72	1.075	OL	7
C_7-olefin	34.03	1.075	OL	7
C_7-olefin	34.51	1.075	OL	7
2-methylhexane	34.81	1.099	IP	7
2,3-dimethylpentane	34.81	1.099	IP	7

TABLE A3.2 *Continued*

Compounds	Retention Time, min.	Response Factor	Hydrocarbon Type	Carbon No.
1,1-dimethylcyclopentane	34.81	1.075	NA	7
Cyclohexene	35.28	1.075	OL	7
3-methylhexane	36.23	1.099	IP	7
C_7-olefin	36.95	1.075	OL	7
CIS-1,3-dimethylcyclopentane	36.95	1.075	NA	7
Trans-1,3-dimethylcyclopentane	37.42	1.075	NA	7
3-ethylpentane	37.92	1.099	IP	7
Trans-1,2-dimethylcyclopentane	38.10	1.075	NA	7
2,2,4-trimethylpentane	38.42	1.096	IP	8
C_7-olefin	38.58	1.075	OL	7
C_7-naphthene	38.68	1.075	NA	7
C_7-olefin	39.21	1.075	OL	7
C_7-olefin	39.63	1.075	OL	7
C_7-olefin	40.05	1.075	OL	7
C_7-olefin	40.31	1.075	OL	7
N-heptane	40.58	1.099	NP	7
C_7-olefin	40.77	1.075	OL	7
C_7-olefin	40.97	1.075	OL	7
C_7-olefin	41.17	1.075	OL	7
C_7-olefin	41.46	1.075	OL	7
C_7-olefin	41.63	1.075	OL	7
C_7-olefin	41.87	1.075	OL	7
C_7-olefin	42.03	1.075	OL	7
C_7-olefin	42.17	1.075	OL	7
C_7-olefin	42.62	1.075	OL	7
C_7-olefin	42.79	1.075	OL	7
C_7-olefin	43.09	1.075	OL	7
1-methylcyclohexane	43.32	1.075	NA	7
CIS-1,2-dimethylcyclopentane	43.32	1.075	NA	7
1,1,3-trimethylcyclopentane	44.07	1.075	NA	8
2,2-dimethylhexane	44.34	1.096	IP	8
C_8-olefin	44.92	1.075	OL	8
C_8-olefin	45.30	1.075	OL	8
1-ethylcyclopentane	45.51	1.075	NA	7
2,2,3-trimetylpentane	46.00	1.096	IP	8
2,5-dimethylhexane	46.15	1.096	IP	8
2,4-dimethylhexane	46.43	1.096	IP	8
1,trans2,CIS4-trimethylcyclopentane	47.12	1.075	NA	8
3,3-dimethylhexane	47.44	1.096	IP	8
C_8-olefin	47.64	1.075	OL	8
C_8-olefin	48.19	1.075	OL	8
1,trans2,CIS3-trimethylcyclopentane	48.38	1.075	NA	8
C_8-olefin	48.63	1.075	OL	8
2,3,4-trimetylpentane	48.92	1.096	IP	8
2,3,3-trimetylpentane[A]	49.50	1.096	IP	8
Toluene[A]	49.50	1.008	AR	7
C_8-olefin	50.07	1.075	OL	8
C_8-olefin	50.32	1.075	OL	8
C_8-olefin	50.54	1.075	OL	8
C_8-olefin	50.67	1.075	OL	8
2,3-dimethylhexane	50.91	1.096	IP	8
2-methyl-3-ethylpentane	51.23	1.096	IP	8
C_8-naphthene	51.34	1.075	NA	8
2-methylheptane	52.04	1.096	IP	8
4-methylheptane	52.27	1.096	IP	8
3,4-dimethylhexane	52.34	1.096	IP	8
C_8-olefin	52.60	1.075	OL	8
C_8-olefin	52.95	1.075	OL	8
3-methylheptane	53.26	1.096	IP	8
1,CIS-3-dimethylcyclohexane	53.40	1.075	NA	8
1,trans-4-dimethylcyclohexane	53.40	1.075	NA	8
1,CIS2,trans3-trimethylcyclopentane	53.40	1.075	NA	8
C_8-olefin	53.87	1.075	OL	8
C_8-olefin	54.08	1.075	OL	8
C_8-olefin	54.34	1.075	OL	8
C_8-olefin	54.73	1.075	OL	8
2,2,5-trimethylhexane	55.06	1.093	IP	9
1-me-T3-ethylcyclopentane	55.42	1.075	NA	8
C_8-olefin	55.42	1.075	OL	8
1-methyl-CIS-3-ethylcyclopentane	55.63	1.075	NA	8
C_8-olefin	55.63	1.075	OL	8
1-methyl-trans-2-ethylcyclopentane	55.84	1.075	NA	8
C_8-olefin	55.84	1.075	OL	8

TABLE A3.2 *Continued*

Compounds	Retention Time, min.	Response Factor	Hydrocarbon Type	Carbon No.
1-methyl-1-ethylcyclopentane	55.94	1.075	NA	8
C_8-olefin	55.94	1.075	OL	8
1,trans-2-dimethylcyclopentane	56.29	1.075	NA	8
C_8-olefin	56.50	1.075	OL	8
C_8-olefin	56.80	1.075	OL	8
C_8-olefin	57.24	1.075	OL	8
C_8-naphthene	57.70	1.075	NA	8
N-octane	57.70	1.096	NP	8
C_8-olefin	58.32	1.075	OL	8
C_8-olefin	58.50	1.075	OL	8
C_8-olefin	58.66	1.075	OL	8
2,2,4-trimethylhexane	58.82	1.093	IP	9
C_8-olefin	59.59	1.075	OL	8
2,3,5-trimethylhexane	60.28	1.093	IP	9
C_8-olefin	60.40	1.075	OL	8
2,2-dimethylheptane	60.89	1.093	IP	9
C_8-olefin	61.07	1.075	OL	8
1,CIS-2-dimethylcyclohexane	61.31	1.075	NA	8
2,4-dimethylheptane	61.54	1.093	IP	9
C_8-olefin	60.40	1.075	OL	8
1-ethylcyclohexane	62.17	1.075	NA	8
C_9-naphthene	62.42	1.075	NA	9
2,6-dimethylheptane	62.59	1.093	IP	9
C_9-naphthene	63.02	1.075	NA	9
2,5-dimethylheptane	63.60	1.093	IP	9
C_8-olefin	63.79	1.075	IP	9
C_8-olefin	64.10	1.075	OL	8
C_8-olefin	64.33	1.075	OL	8
Ethylbenzene	65.02	1.018	OL	8
C_9-naphthene	65.40	1.075	AR	8
C_8-olefin	65.77	1.075	OL	8
Metaxylene	66.46	1.018	AR	8
Paraxylene	66.60	1.018	AR	8
C_9-naphthene	66.97	1.075	NA	9
3,4-dimethylheptane	67.08	1.093	IP	9
4-ethylheptane	67.42	1.093	IP	9
4-methyloctane	67.89	1.093	IP	9
2-methyloctane	68.04	1.093	IP	9
C_9-isoparaffin	68.78	1.075	IP	9
3-ethylheptane	68.97	1.093	IP	9
3-methyloctane	68.97	1.093	IP	9
Orthoxylene	69.65	1.018	AR	8
C_9-naphthene	70.12	1.075	NA	9
C_9-naphthene	70.52	1.075	NA	9
C_{10}-isoparaffin	70.68	1.086	IP	10
C_{10}-isoparaffin	71.05	1.086	IP	10
C_{10}-isoparaffin	71.58	1.086	IP	10
C_9-olefin	71.99	1.075	OL	9
C_9-olefin	72.23	1.075	OL	9
C_9-naphthene	72.47	1.075	NA	9
C_9-naphthene	72.88	1.075	NA	9
N-nonane	72.88	1.093	NP	9
C_9-naphthene	73.29	1.075	NA	9
C_9-olefin	73.68	1.075	OL	9
isopropylbenzene	74.23	1.025	AR	9
C_{10}-isoparaffin	74.71	1.025	IP	10
C_{10}-isoparaffin	75.19	1.086	IP	10
C_{10}-isoparaffin	75.46	1.086	IP	10
C_{10}-isoparaffin	76.20	1.086	IP	10
C_{10}-isoparaffin	76.41	1.086	IP	10
2,7-dimethyloctane	77.05	1.086	IP	10
2,6-dimethyloctane	77.56	1.086	IP	10
N-propylbenzene	78.15	1.025	AR	9
C_{10}-isoparaffin	78.51	1.086	IP	10
1-methyl,3-ethylbenzene	79.18	1.025	AR	9
1-methyl,4-ethylbenzene	79.42	1.025	AR	9
1,3,5-trimethylbenzene	80.14	1.025	AR	9
C_{10}-isoparaffin	80.81	1.086	IP	10
C_{10}-isoparaffin	81.04	1.086	IP	10
1-methyl,2-ethylbenzene	81.31	1.025	AR	9
C_{10}-isoparaffin	81.78	1.086	IP	10
C_{10}-isoparaffin	82.15	1.086	IP	10
C_{10}-naphthene	82.53	1.075	NA	9

TABLE A3.2 *Continued*

Compounds		Retention Time, min.	Response Factor	Hydrocarbon Type	Carbon No.
C_{10}-isoparaffin		82.76	1.086	IP	10
1,2,4-trimethylbenzene		83.25	1.025	AR	9
C_{10}-naphthene		83.60	1.086	NA	10
C_{10}-isoparaffin		83.72	1.086	IP	10
C_{10}-aromatic		84.82	1.025	AR	10
C_{10}-aromatic		85.05	1.025	AR	10
C_{10}-aromatic		85.37	1.025	AR	10
N-decane		85.54	1.086	NP	10
C_{10}-aromatic		85.87	1.025	AR	10
1,2,3-trimethylbenzene		86.42	1.025	AR	9
1-methyl,4-isopropylbenzene		86.59	1.025	AR	10
1-methyl,3-isopropylbenzene		86.97	1.025	AR	10
C_{11}-isoparaffin		87.45	1.025	IP	10
Indan		87.71	1.025	AR	9
C_{11}-isoparaffin		88.02	1.025	IP	10
1-methyl,2-isopropylbenzene		88.40	1.025	AR	10
C_{11}-isoparaffin		88.77	1.025	IP	10
1,3-diethylbenzene		89.68	1.030	AR	10
1-methyl,3*N*-propylbenzene		89.99	1.030	AR	10
1-methyl,4*N*-propylbenzene		90.43	1.030	AR	10
1,3-dimethyl,5-ethylbenzene		90.74	1.030	AR	10
C_{10}-aromatic		91.02	1.030	AR	10
1-methyl,2*N*-propylbenzene		91.71	1.030	AR	10
C_{12}-isoparaffin		92.21	1.086	IP	12
C_{12}-isoparaffin		92.51	1.086	IP	12
1,4-dimethyl,2-ethylbenzene		92.83	1.030	AR	10
1,3-dimethyl,4-ethylbenzene		93.02	1.030	AR	10
C_{12}-isoparaffin		93.45	1.086	IP	12
1-methylindan		93.68	1.030	AR	10
1,2-dimethyl,4-ethylbenzene		93.68	1.030	AR	10
C_{12}-isoparaffin		94.15	1.086	IP	12
C_{12}-isoparaffin		94.35	1.086	IP	12
1,3-dimethyl-2-ethylbenzene		94.53	1.030	AR	10
C_{11}-isoparaffin		95.09	1.086	IP	11
C_{12}-isoparaffin		95.53	1.086	IP	12
1,2-dimethyl-3-ethylbenzene		95.85	1.030	AR	10
C_{10}-naphthene		96.17	1.075	NA	10
C_{12}-isoparaffin		96.41	1.086	IP	12
N-undecane		96.59	1.086	NP	11
C_{12}-isoparaffin		96.80	1.086	IP	12
1,2,4,5-tetramethylbenzene		97.15	1.030	AR	10
1,2,3,5-tetramethylbenzene		97.51	1.030	AR	10
C_{11}-naphthene		98.11	1.075	NA	11
C_{11}-isoparaffin		98.53	1.025	IP	10
5-methylindan		99.27	1.030	AR	10
C_{11}-aromatic		99.75	1.033	AR	11
C_{11}-aromatic		100.05	1.033	AR	11
4-methylindan		100.32	1.030	AR	10
C_{11}-aromatic		100.57	1.033	AR	11
1,2,3,4-tetramethylbenzene		100.77	1.030	AR	10
C_{11}-aromatic	from	101.25	1.033	AR	11
	to	103.20			
Naphthalene		103.30	1.030	AR	10
C_{12}-isoparaffin		103.85	1.086	IP	12
C_{11}-aromatic	from	104.10	1.030	AR	11
	to	107.50			
N-dodecane		107.81	1.086	NP	12
C_{11}+-aromatic	from	107.90	1.033	AR	11+
	to	114.00			
2-methylnaphthalene		114.09	1.033	AR	11
1-methylnaphthalene		115.54	1.033	AR	11
Hydrocarbon C_{12}+	>	115.70	1.035		

[A]Co-eluted compounds.

APPENDIXES

(Nonmandatory Information)

X1. COMPARISON TABLES

X1.1 The following tables (see Tables X1.1-X1.6) show comparisons between Procedures A and B and other test 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 test methods are well within the reproducibilities of the test methods. The sample numbers refer to the interlaboratory 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 X1.1 Comparison of Benzene Results Between Procedure A and B, and Test Method D 5580

Benzene (wt %)			
Sample	Test Method D 5580	Procedure A	Procedure B
2	1.52	1.58	1.61
6	1.05	1.12	1.12
8	1.10	1.15	1.16
10	1.13	1.19	1.18
13	0.14	0.17	0.16
14	0.62	0.69	0.70
Average	0.93	0.98	0.99

TABLE X1.2 Comparison of Toluene Results Between Procedure A and B, and Test Method D 5580

Toluene (wt %)			
Sample	Test Method D 5580	Procedure A	Procedure B
2	4.3	4.5	4.6
6	2.1	2.0	1.9
8	10.1	10.3	11.4
10	5.0	5.2	6.1
13	3.3	3.3	2.9
14	4.4	4.7	5.3
Average	4.9	5.0	5.4

TABLE X1.3 Comparison of Total Aromatic Results Between Procedure A and B, Test Method D 5580, and PIONA Method

Total Aromatics (wt %)				
Sample	Test Method D 5580	PIONA[A]	Procedure A	Procedure B
2	30.3	28.2	30.2	32.6
6	18.9	18.7	18.3	20.0
8	49.1	49.0	47.6	51.0
10	23.9	24.5	23.1	25.4
13	19.7	19.8	19.3	22.4
14	23.8	24.6	24.2	27.5
Average	27.6	27.5	27.1	29.8

[A] Multidimentional PIONA

TABLE X1.4 Comparison of Total Olefin Results Between Procedure A and B, and PIONA Method

Total Olefins (wt %)			
Sample	PIONA[A]	Procedure A	Procedure B
2	7.1	4.5	4.4
6	9.8	8.7	9.4
8	6.6	6.1	6.2
10	15.1	12.9	13.7
13	11.1	10.6	11.1
14	24.6	19.5	22.2
Average	12.4	10.9	11.2

[A] Multidimentional PIONA

TABLE X1.5 Comparison of Total Oxygenate Results Between Procedure A and B, and PIONA Method

Total Oxygenates (wt %)			
Sample	PIONA[A]	Procedure A	Procedure B
2[B]	15.3	15.1	16.1
6[B]	7.0	7.8	8.1
8[B]	4.2	4.3	4.5
10[C]	>8	10.5	10.0
13[B]	20.5	20.2	19.9
14[B]	2.8	2.9	3.2
Average	N/A	10.1	10.3

[A] Multidimentional PIONA
[B] Major oxygenates=MTBE
[C] Major oxygenate=Ethanol

TABLE X1.6 Comparison of Total Paraffins and Total Naphthalene Results Between Procedure A and B, and PIONA Method

	Total Paraffins (wt %)			Total Naphthenes (wt %)		
Sample	PIONA[A]	Procedure A	Procedure B	PIONA[A]	Procedure A	Procedure B
8	35.6	38.0	35.0	2.2	2.7	2.8
10	41.1	45.5	42.3	5.6	6.5	6.7
13	42.6	46.0	43.0	1.3	2.1	3.5
14	34.1	41.3	37.9	5.9	9.3	7.6
Average	38.4	42.7	39.6	3.8	5.2	5.2

[A] Multidimentional PIONA

X2. BIBLIOGRAPHY

X2.1 The following publications in DHA analyses may be useful as background and are recommended to the user of these test procedures.

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