This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.

Designation: D6730 – 22

Standard Test Method for Determination of Individual Components in Spark Ignition Engine Fuels by 100-Metre Capillary (with Precolumn) High-Resolution Gas Chromatography[1]

This standard is issued under the fixed designation D6730; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope*

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

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

1.3 This test method also determines methanol, ethanol, *t*-butanol, methyl *t*-butyl ether (MTBE), ethyl *t*-butyl ether (ETBE), and *t*-amyl methyl ether (TAME) in spark ignition engine fuels in the concentration range from 1 % to 30 % by mass. However, the cooperative study data provided insufficient statistical data for obtaining a precision statement for these compounds.

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 naphthenic (for example, virgin naphthas) constituents above *n*-octane may reflect significant errors in PONA-type groupings. Based on the gasoline samples in the interlaboratory cooperative study, this test method is applicable to samples containing less than 25 % by mass of olefins. However, some interfering co-elution with the olefins above C_7 is possible, particularly if blending components or their higher boiling cuts such as those derived from fluid catalytic cracking (FCC) are analyzed, and the total olefin content may not be accurate. Annex A1 of this test method compares results of the test method with other test methods for selected components, including olefins, and several group types for several interlaboratory cooperative study samples. Although benzene, toulene, and several oxygenates are determined, when doubtful as to the analytical results of these components, confirmatory analyses can be obtained by using the specific test methods listed in the reference section.

1.4.1 Total olefins in the samples may be obtained or confirmed, or both, if necessary, by Test Method D1319 (percent by volume) or other test methods, such as those based on multidimentional PONA-type of instruments.

1.5 If water is or is suspected of being present, its concentration may be determined, if desired, by the use of Test Method D1744 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 D4815 and D5599 for oxygenates, and Test Method D5623 for sulfur compounds, or equivalent.

1.6 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

1.7 *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, health, and environmental practices and determine the applicability of regulatory limitations prior to use.*

1.8 *This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the*

[1] This test method is under the jurisdiction of ASTM Committee D02 on Petroleum Products, Liquid Fuels, and Lubricants and is the direct responsibility of Subcommittee D02.04.0L on Gas Chromatography Methods.

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*A Summary of Changes section appears at the end of this standard

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Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.

2. Referenced Documents

2.1 *ASTM Standards:*[2]

D1319 Test Method for Hydrocarbon Types in Liquid Petroleum Products by Fluorescent Indicator Adsorption

D1744 Test Method for Determination of Water in Liquid Petroleum Products by Karl Fischer Reagent (Withdrawn 2016)[3]

D3700 Practice for Obtaining LPG Samples Using a Floating Piston Cylinder

D4057 Practice for Manual Sampling of Petroleum and Petroleum Products

D4177 Practice for Automatic Sampling of Petroleum and Petroleum Products

D4307 Practice for Preparation of Liquid Blends for Use as Analytical Standards

D4626 Practice for Calculation of Gas Chromatographic Response Factors

D4815 Test Method for Determination of MTBE, ETBE, TAME, DIPE, tertiary-Amyl Alcohol and C_1 to C_4 Alcohols in Gasoline by Gas Chromatography

D5580 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

D5599 Test Method for Determination of Oxygenates in Gasoline by Gas Chromatography and Oxygen Selective Flame Ionization Detection

D5623 Test Method for Sulfur Compounds in Light Petroleum Liquids by Gas Chromatography and Sulfur Selective Detection

E355 Practice for Gas Chromatography Terms and Relationships

E594 Practice for Testing Flame Ionization Detectors Used in Gas or Supercritical Fluid Chromatography

E1510 Practice for Installing Fused Silica Open Tubular Capillary Columns in Gas Chromatographs

3. Terminology

3.1 *Definitions*—This test method makes reference to many common gas chromatographic procedures, terms, and relationships. Detailed definitions can be found in Practice E355.

4. Summary of Test Method

4.1 A representative sample of the petroleum liquid is introduced into a gas chromatograph equipped with an open tubular (capillary) column coated with a methyl silicone liquid phase, modified with a capillary precolumn. 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 presented on a strip chart recorder or digitally, or both, by way of an integrator or integrating computer. Each eluting component is identified by comparing its retention time to that established by analyzing reference standards or samples under identical conditions. The concentration of each component in percent by mass is determined by normalization of the peak areas after correction with detector response factors. Unknown components are reported as a total unknown percent by mass.

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 can be determined through the use of this test method.

5.2 This test method is adopted from earlier development and enhancement.[4,5,6,7] The chromatographic operating conditions and column tuning process, included in this test method, were developed to provide and enhance the separation and subsequent determination of many individual components not obtained with previous single-column analyses. The column temperature program profile is selected to afford the maximum resolution of possible co-eluting components, especially where these are of two different compound types (for example, a paraffin and a naphthene).

5.3 Although a majority of the individual hydrocarbons present in petroleum distillates are determined, some co-elution of compounds is encountered. If this test method is utilized to determine 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, constituents above octane may reflect significant errors in PONA-type groupings.

5.4 If water is or is suspected of being present, its concentration is determined by the use of Test Method D1744. Other compounds containing oxygen, sulfur, nitrogen, and so forth may also be present, and may co-elute with the hydrocarbons. When known co-elution exists, these are noted in the test method data tables. If determination of these specific compounds is required, it is recommended that test methods for

[2] For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

[3] The last approved version of this historical standard is referenced on www.astm.org.

[4] Johansen, N.G., and Ettre, L.S., "Retention Index Values of Hydrocarbons on Open Tubular Columns Coated with Methyl Silicone Liquid Phases," *Chromatographia*, Vol 5, No. 10, October 1982.

[5] Johansen, N.G., Ettre, L.S., and Miller, R.L., "Quantitative Analysis of Hydrocarbons by Structural Group Type in Gasolines and Distillates. Part 1," *Journal of Chromatography*, Vol 256, 1983, pp. 393–417.

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

[7] Schubert, A.J. and Johansen, N.J., "Cooperative Study to Evaluate a Standard Test Method for the Speciation of Gasolines by Capillary Gas Chromatography," SAE Paper No. 930144, March 1993.

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these specific materials be used, such as Test Method D4815 and D5599 for oxygenates, Test Method D5580 for aromatics, and Test Method D5623 for sulfur compounds.

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 E594, 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. Automated injections are highly recommended. Microsyringes, auto-syringe samplers, or valves capable of 0.1 µL 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 per 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 s 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 polarity. Until adequate columns are commercially available, the currently used methyl silicone columns can be modified or *tuned* to meet the method column specifications. See Section 11 for a description of the column performance 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.

Material	fused silica
Length	100 m
Internal diameter	0.25 mm
Liquid phase	methyl silicone
Film thickness	0.50 µm
Theoretical plates, n, pentane at 35 °C	~ 400 000 to 500 000
Retention factor, k, pentane at 35 °C	0.45 to 0.50
Resolution, R, *t*-butanol and 2-methylbutene-2 at 35 °C	3.25 to 5.25
Peak symmetry, *t*-butanol at 35 °C	> 1.0 to < 5.0

6.4.2 *Precolumn*—A variable length (1 m to 4 m) of 5 % phenyl/95 % dimethylpolysiloxane 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 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 percent 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 D4307, of individual hydrocarbons and oxygenates of interest is used for system and column evaluation (see Table 1). (**Warning—**see 7.5.2.) Fig. 1 is a chromatogram of the recommended mixture in Table 1.

[8] *ACS Reagent Chemicals, Specifications and Procedures for Reagents and Standard-Grade Reference Materials*, 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. Pharmacopeial Convention, Inc. (USPC), Rockville, MD.

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TABLE 1 System and Column Evaluation Mixture

	%
Ethanol	8.00
n-pentane	2.00
t-butanol	0.50
2-methylbutene-2	2.50
2,3-dimethylbutane	0.50
Methyl-*t*-butyl ether	10.00
n-hexane	2.00
1-methylcyclopentene	0.50
Benzene	1.00
Cyclohexane	28.90
3-ethylpentane	0.20
1,2*t*-dimethylcyclopentane	0.50
n-heptane	2.00
2,3,3-trimethylpentane	0.50
Toluene	7.00
n-octane	2.00
Ethylbenzene	25.00
p-xylene	1.00
2,3-dimethylheptane	0.20
n-nonane	2.00
5-methylnonane	0.20
1-methyl-2-ethylbenzene	0.50
n-decane	1.00
n-undecane	0.50
1,2,3,5-tetramethylbenzene	0.25
Naphthalene	0.50
n-dodecane	0.25
1-methylnaphthalene	0.25
n-tridecane	0.25

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 (Practices D4057 and D4177). If the sample as received does not meet the upper boiling range requirements of 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 D3700 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 D4057 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 precooled 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 100 m column and, if required, a precolumn according to the manufacturer's or supplier's instructions and Annex A1. See Practice E1510/8 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 min ± 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 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):*

9.5.1.1 P = (head pressure (psig) + ambient pressure)/ambient pressure.

9.5.1.2 j = compressibility factor = $3/2((P^2-1)/(P^3-1))$.

9.5.1.3 $u_o = u_{ave}/j$ = column outlet velocity.

9.5.1.4 $A_c = \text{pi}(r)^2$ = column cross-sectional area (cm^2). where r = column internal radius (cm).

9.5.1.5 Flow rate (cm^3/min) = $u_0 \times A_c \times 60$.

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

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

9.5.3.1 $U_{ave} = 100 \times 100/6.98 \times 60 = 23.88$ cm/s.

9.5.3.2 P = 40 psig + 12.0/12.0 = 4.33.

9.5.3.3 $j = 3/2((18.778\text{-}1)/(81.370\text{-}1)) = 0.33$

9.5.3.4 $u_o = 23.88/0.33 = 71.96$ cm/s.

9.5.3.5 $A_c = \text{pi}(0.025/2)^2 = 4.9 \times 10^{-4}$ cm^2.

9.5.3.6 Flow rate = $71.96 \times 4.9 \times 10^{-4} \times 60 = 2.12$ cm^3/min.

9.5.3.7 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.

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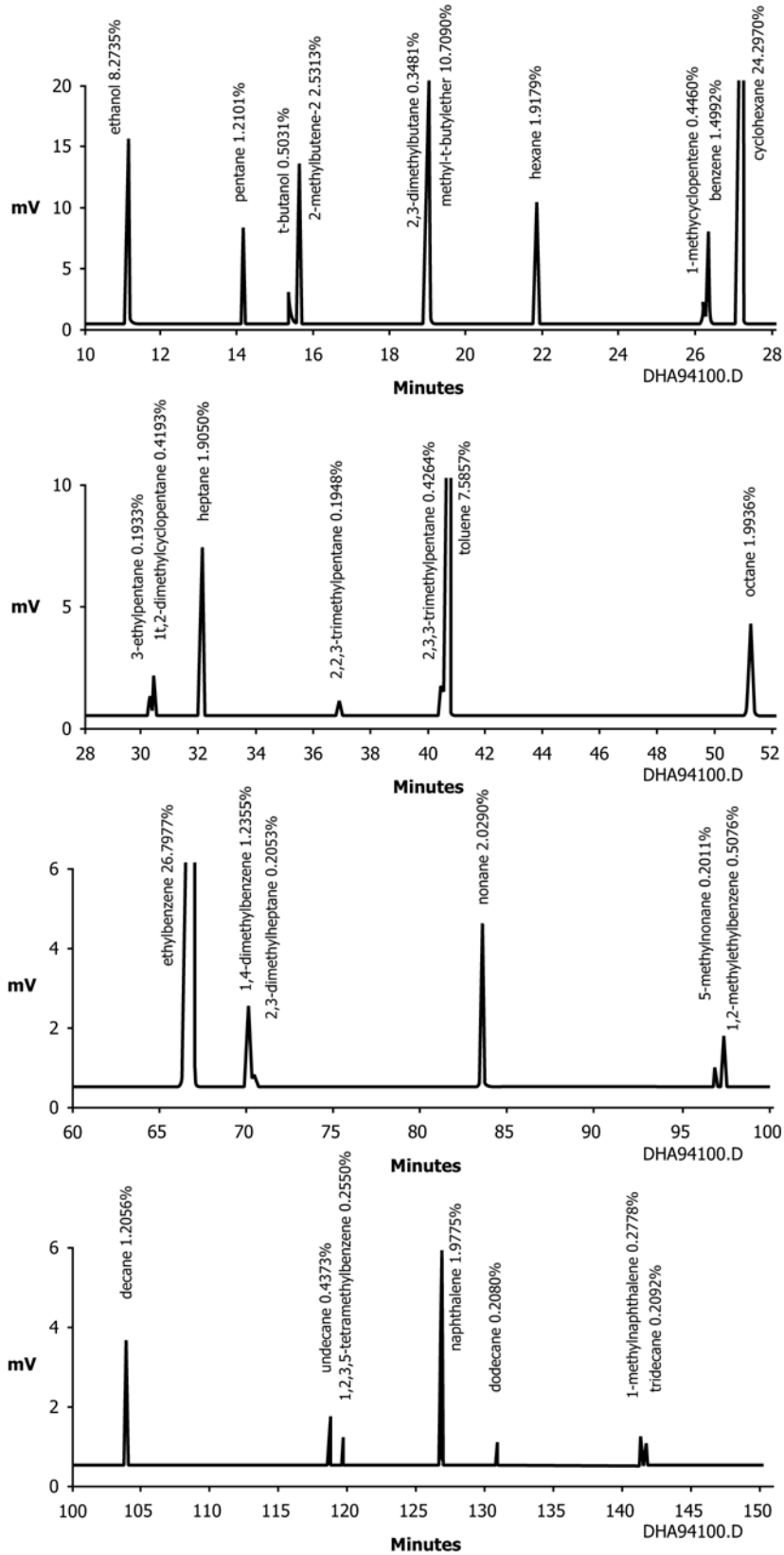

FIG. 1 DHA Speciation Analysis—System and Column Evaluation Mixture (7.5.5)

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TABLE 2 GC 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 µL – 0.2 µL
Detector	
Type	flame Ionization
Temperature	250 °C
Use manufacturers recommended detector gas flows or:	
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

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 following values and, for each set of conditions inject the listed quantities of the system and column evaluation mixture (7.5.5), using the operating conditions listed in Table 2 or as determined in Section 12.

injector temperature: 250 °C< split: 100:1, split: 200:1 > sample: 0.2 µL, 0.5 µL, 1.0 µL

injector temperature: 300 °C< split: 100:1, split: 200:1 > sample: 0.2 µL, 0.5 µL, 1.0 µL

10.3 Compare the calculated concentrations to the known standard concentrations after calculating the corrected area normalization using the response factors from 13.2 and Table A1.1.

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

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 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, Fig. 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.

11.2.1 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:

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

where:

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

11.3.1 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:

$$R = 2(t_{R2-M-Butene-2} - t_{RTBA})/1.699(w_{1/2h2-M-Butene-2} + w_{1/2hTBA}) \quad (5)$$

11.4.1 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. Increase

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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.

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

11.5.1 This test method 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-methylbutene-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 (Fig. 2).

12.3.2 *i-propanol/2-methylbutene-1* and *t-butanol/2-methylbutene-2*—*i*-propanol will appear resolved between

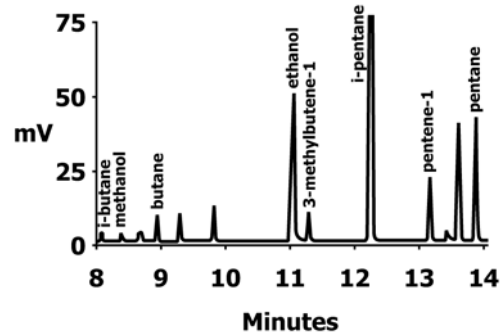

FIG. 2 *i*-butane/methanol and ethanol/3-methyl-butene-1

pentene-1 and 2-methyl-butene-1, *t*-butanol will appear resolved between *c*-pentene-2 and 2-methylbutene-2.

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 (Fig. 3).

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 (Fig. 4).

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 (Fig. 5).

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 (Fig. 6).

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 (Fig. 7).

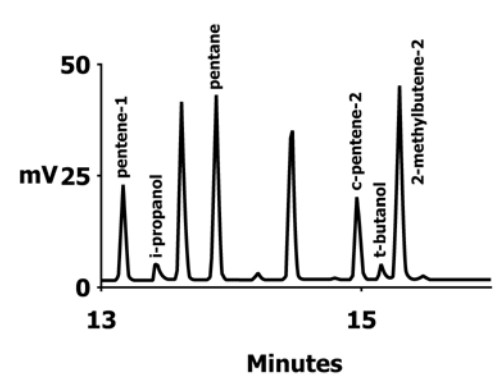

FIG. 3 *i* propanol/2-methyl/butene-1 and *t* butanol/2-methylbutene-2

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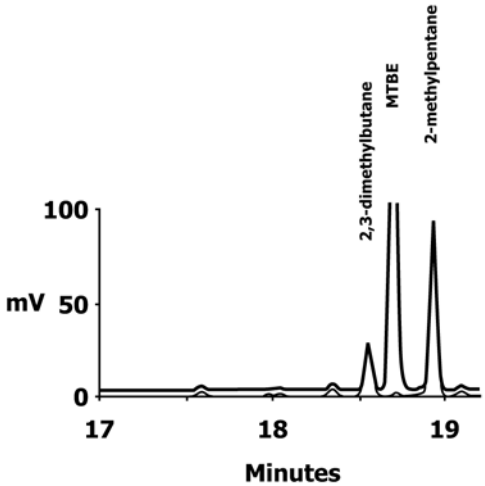

FIG. 4 2,3-dimethylbutane/methyl-*t* butylether

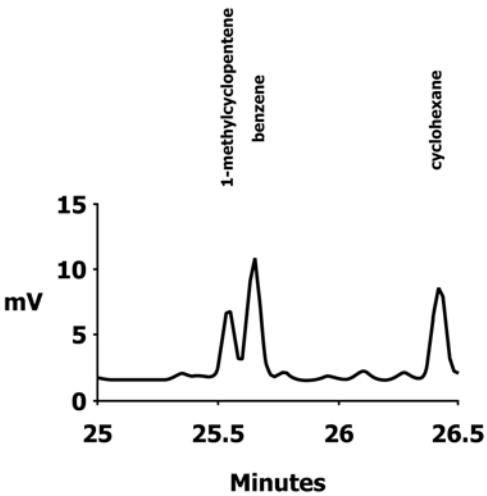

FIG. 5 1-methylcyclopentene/benzene

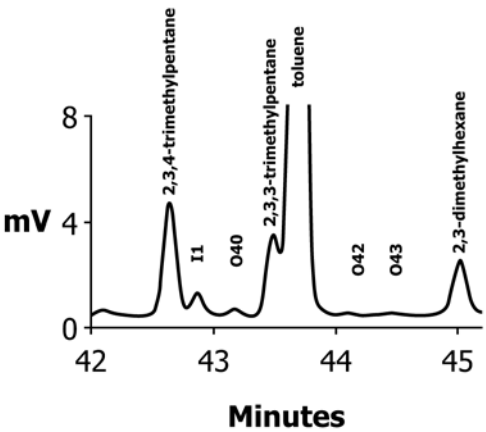

FIG. 6 2,3,3-trimethylpentane/toluene

12.3.7 *l17 (Unknown)/1,2-methylethylbenzene* —The unknown isoparaffin (l17) 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

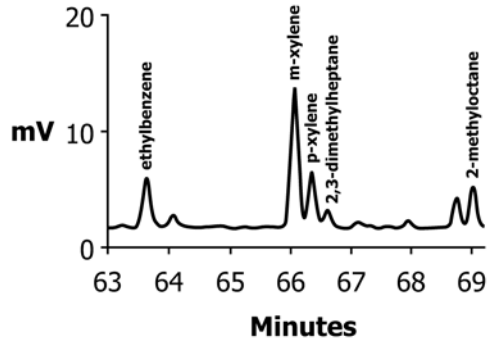

FIG. 7 *p*-xylene/2,3-dimethylheptane

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 (Fig. 8).

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 (Fig. 9).

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.

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 D4626. The response factors, as listed in Table 3, are relative to that calculated for heptane. Calculations are based on the following equation:

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

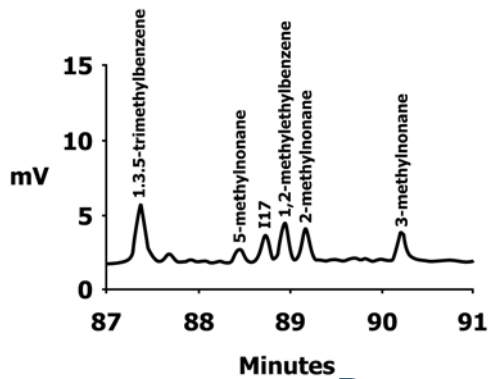

FIG. 8 I17 (unknown)/1,2-methylethylbenzene

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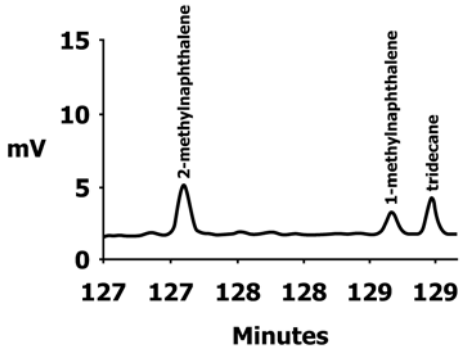

FIG. 9 1-methylnaphthalene/tridecane

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 is the correction factor with heptane as unity (1.0000), and
0.7487 is used with methane as unity.

13.3 *Quantitative, Oxygenates*—Determine response factors for methanol, ethanol, and other oxygenated compounds experimentally. The principles in Practice D4626 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 Figs. 10 and 11). Each individual apparatus must be calibrated using gravimetrically prepared standards, covering the sample concentration ranges expected and the scope of this test method. Standards used must comply with the requirements in Section 7. Figs. 10 and 11 present 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 specified in Table 1 or as determined in Section 12.

14.2 Set the recorder or integration device, or both, 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

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 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 2 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 D1744, 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.

$$\text{component \% (m/m)} = \text{corrected peak area} \times (100 - \text{\% undetected})/\text{total corrected peak area} \quad (9)$$

16. Report

16.1 Report the concentration of each component as mass %, % (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 caution 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 A1.3 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 A1.3 for the gasoline components.

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

[9] Supporting data is available from ASTM International Headquarters in the form of a research report. Request RR:D02-1518. Contact ASTM Customer Service at service@astm.org.

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TABLE 3 Theoretical FID Relative Response Factors

Carbon No.	Saturated Paraffins	Unsaturated Paraffins	Saturated Naphthenes	Unsaturated Naphthenes	Aromatics
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

18. Keywords

18.1 detailed hydrocarbon analysis; DHA; gas chromotography; hydrocarbons; open tubular column; oxygenates; PIONA; PONA

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Oxygenates Relative Response Factors

	Lab 1	Lab 2	Lab 3	Lab 4	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	980.1566		
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	967.7888	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	1332.2069	2041.1591		
	0.5890	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	1488.8626	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	869.6032		
	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	862.7846	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. 10 Determination of Oxygenate Response—DHA Speciation Analysis

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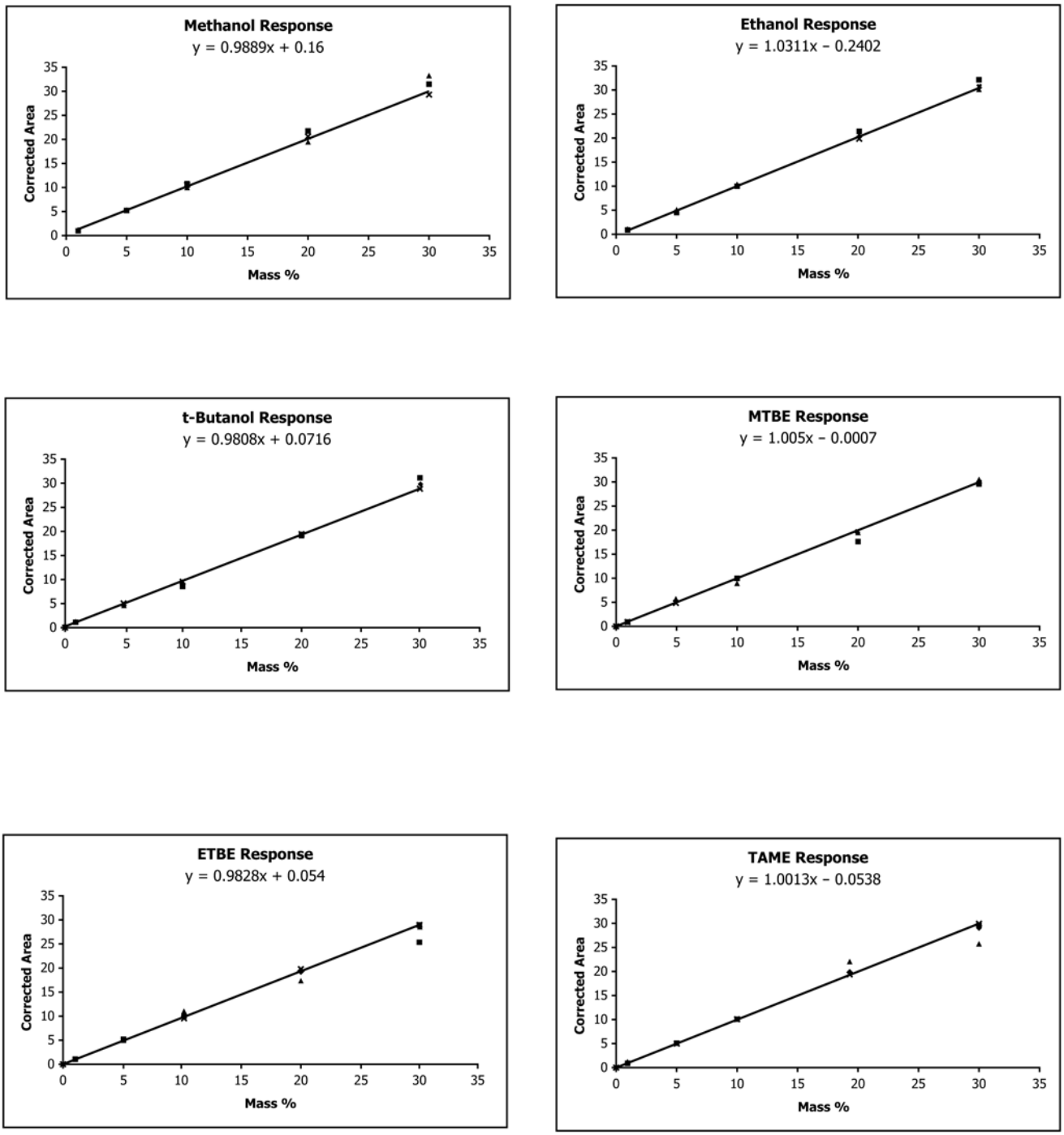

FIG. 11 Graphical Representation Determination of Oxygenate Response—DHA Speciation Analysis

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TABLE 4 Repeatability and Reproducibility of DHA Determinations

NOTE 1—The following is a partial list of precision data that has been prepared by statisticians of CS94 in accordance with RR:D2-1007, 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 laboratories, at least once. The (repeatability standard deviation)/mean value for each analyte/sample combination must be less than or equal to 0.1, as per LOQ requirements which, while not a standard, is what CS94 is recommending.

NOTE 3—

Legend:

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, and
C_{max} = upper concentration limit that r_{est}, R_{est} is applicable.

Component	Average 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

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ANNEX

(Mandatory Information)

A1. PROCEDURE FOR ADJUSTING THE SELECTIVITY OF A DHA METHYL SILICONE 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 methyl silicone 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 methyl silicone 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 methyl silicone capillary column, using a 35 °C 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 oxygenates cannot be corrected by the addition of the precolumn. Tailing peaks may also be the result of an active injector liner or packing material, or both, 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 methyl silicone. The film thickness is likely not critical, only the total amount of phase. Lengths ranging from 1 mto more than 3 m have been necessary to provide sufficient selectivity, depending on the initial selectivity of the methyl silicone column used. One metre 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 one, two, and three metres 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 m 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 key component separations are shown. These analyses were made using the conditions given in Table 2. 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 DHA analyses.

A1.10 Tables A1.4-A1.9 show comparisons between this test method and other methods for several compound types. Multidimensional PIONA is included since it tends to give reasonable peak compound type groupings for total olefins, total paraffins, and total naphthenes. The differences for benzene and toluene among the indicated methods are well within the reproducibilities of the methods. The sample numbers refer to the 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.

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TABLE A1.1 DHA Component Data

NOTE 1—These data consist of the current physical constants used in the cooperative study. The average RI 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).

					RFA Gasoline			CCF Gasoline		
Component	Average RI	RRF	MW	Relative Density	Min.	Index	Mass %	Min.	Index	Mass %
Methane	100.00	1.121	16.043	0.2600						
Ethylene	178.10	1.050	28.054	0.3000						
Ethane	200.00	1.051	30.070	0.3399						
Propylene	284.00	1.030	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	0.980	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
O_1	469.00	0.980	70.135	0.6300	12.030	470.03	0.005			
O_2	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[A]	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	1.050	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						
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			
O_5	547.70	1.020	70.135	0.6500						
O_6	549.70	1.020	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
O_8	578.00	0.980	84.162	0.6736	20.042		0.002	19.893		0.002
2-Methyl-1,4-pentadiene	579.00	0.980	82.146	0.6940	20.078		0.002			
?	581.00							20.002		0.002
1,5-Hexadiene	581.90	0.980	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
O_{11}	592.00	0.980	84.162	0.6780						
2-Butanol[B]	593.50	1.563	74.120	0.8080						
?	596.00				21.474	596.35	0.007			
1c/t,4-Hexadiene	597.14	0.980	84.146	0.7000	21.571	597.22	0.004			
2-Ethylbutene-1	598.95	0.980	84.162	0.6944						

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TABLE A1.1 *Continued*

Component	Average RI	RRF	MW	Relative Density	RFA Gasoline Min.	RFA Gasoline Index	RFA Gasoline Mass %	CCF Gasoline Min.	CCF Gasoline Index	CCF Gasoline Mass %
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	0.980	82.146	0.7622	22.920	611.74	0.055	22.921	611.77	0.025
O_{13}	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
O_{14}	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
i-Butanol[B]	622.40	1.334	74.120	0.8030						
4-4-Dimethyl-t-pentene-2	623.10	0.980	98.189	0.6936						
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-Tirmethylbutene-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	639.26	0.008	25.378	638.27	0.005
O_{17}	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[A]	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	0.980	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	0.980	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			
1,5-Heptadiene	691.60	0.980	93.168	0.7500						
O_{25}	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

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TABLE A1.1 *Continued*

Component	Average RI	RRF	MW	Relative Density	RFA Gasoline Min.	RFA Gasoline Index	RFA Gasoline Mass %	CCF Gasoline Min.	CCF Gasoline Index	CCF Gasoline Mass %
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						
O_{28}	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
O_{29}	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
O_{30}	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[A]	720.72	0.980	112.216	0.7482						
O_{32}	721.00	0.980	98.189	0.7322						
O_{33}	722.00	0.980	112.216	0.7322						
O_{34}	723.00	0.980	112.216	0.7322						
O_{35}	724.35	0.980	98.189	0.7322	36.531	724.50	0.013	36.398	724.50	0.005
O_{36}	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
O_{37}	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
O_{38}	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
O_{39}	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
O_{40}	749.37	0.980	98.189	0.7322	41.157	749.56	0.058	41.160	749.54	0.032
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
O_{41}	752.20	0.980	112.220	0.7322						
O_{42}	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
O_{43}	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
O_{44}	761.73	0.980	112.220	0.7322	43.709	761.99	0.076	43.712	761.97	0.041
O_{45}	762.20	0.980	112.220	0.7322						
O_{46}	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[A]	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	0.980	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	56.135	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	0.980	110.200	0.7650	47.117	777.33	0.011	46.298	777.29	0.006
O_{48}	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[A]	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

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TABLE A1.1 *Continued*

Component	Average RI	RRF	MW	Relative Density	RFA Gasoline Min.	RFA Gasoline Index	RFA Gasoline Mass %	CCF Gasoline Min.	CCF Gasoline Index	CCF Gasoline Mass %
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
O_{50}	805.50	0.980	112.216	0.7196						
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						
O_{52}	810.62	0.980	126.240	0.7196	55.508	810.81	0.011	55.545	810.84	0.006
O_{53}	813.47	0.980	126.240	0.7196	56.268	813.67	0.035	56.295	813.72	0.016
N_1	815.02	0.980	112.216	0.7800	56.655	815.09	0.012	55.395	814.95	0.007
?	815.60				56.673		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
N_2	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
N_3	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			
1,3,5-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
N_4	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[A]	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
N_7	850.89	0.980	112.216	0.7800	66.993	850.52	0.008	65.931	851.33	0.005
N_8	852.36	0.980	112.216	0.7800	68.017	852.57	0.017	67.247	852.64	0.010
N_{10}	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
N_{11}	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
?	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
N_{12}	863.00	0.980	126.243	0.7800	72.374	863.22	0.017	70.111		0.005
N_{13}	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
N_{14}	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

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TABLE A1.1 *Continued*

Component	Average RI	RRF	MW	Relative Density	RFA Gasoline Min.	RFA Gasoline Index	RFA Gasoline Mass %	CCF Gasoline Min.	CCF Gasoline Index	CCF Gasoline Mass %
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
N_{15}	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
N_{18}	887.87	0.980	126.243	0.7800	81.060	888.07	0.038	81.621	888.18	0.017
N_{19}	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
N_{20}	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
N_{21}	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						
N_{22}	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
N_{23}/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						
?	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
N_{25}	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
N_{26}	913.43	0.980	126.243	0.7900						
N_{27}	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
N_{28}	926.32	0.980	126.243	0.7900	89.078	926.37	0.005	90.227		0.003
N_{29}	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
N_{30}	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
N_{31}	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

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TABLE A1.1 *Continued*

Component	Average RI	RRF	MW	Relative Density	RFA Gasoline Min.	RFA Gasoline Index	RFA Gasoline Mass %	CCF Gasoline Min.	CCF Gasoline Index	CCF Gasoline Mass %
N_{32}	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
N_{33}	958.16	0.980	140.270	0.800						
?	958.90				95.762	958.89	0.008	96.900		0.003
?	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[A]	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
N_{37}	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	0.990	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	0.990	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
N_{38}	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
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
N_{39}	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
N_{40}	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

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TABLE A1.1 *Continued*

Component	Average RI	RRF	MW	Relative Density	RFA Gasoline Min.	RFA Gasoline Index	RFA Gasoline Mass %	CCF Gasoline Min.	CCF Gasoline Index	CCF Gasoline Mass %
?	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
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	125.048	1134.95	0.013

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TABLE A1.1 *Continued*

Component	Average RI	RRF	MW	Relative Density	RFA Gasoline Min.	RFA Gasoline Index	RFA Gasoline Mass %	CCF Gasoline Min.	CCF Gasoline Index	CCF Gasoline Mass %
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
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-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
?	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

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