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## Standard Test Method for Determination of Individual Components in Spark Ignition Engine Fuels by 50-Metre Capillary High Resolution Gas Chromatography<sup>1</sup>

This standard is issued under the fixed designation D6733; 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 ( $\epsilon$ ) 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 with boiling ranges up to ~~225°C~~ 225 °C. Other light liquid hydrocarbon mixtures typically encountered in petroleum refining operations, such as, blending stocks (naphthas, reformates, alkylates, and so forth) may also be analyzed; however, statistical data was obtained only with blended spark-ignition engine fuels. The tables in [Annex A1](#) enumerate the components reported. Component concentrations are determined in the range from ~~0.10 to 15 mass %~~ 0.10 % to 15 % by mass. The procedure may be applicable to higher and lower concentrations for the individual components; however, the user must verify the accuracy if the procedures are used for components with concentrations outside the specified ranges.

1.2 This test method is applicable also to spark-ignition engine fuel blends containing oxygenated components. However, in this case, the oxygenate content must be determined by Test Methods [D5599](#) or [D4815](#).

1.3 Benzene co-elutes with 1-methylcyclopentene. Benzene content must be determined by Test Method [D3606](#) or [D5580](#).

1.4 Toluene co-elutes with 2,3,3-trimethylpentane. Toluene content must be determined by Test Method [D3606](#) or [D5580](#).

1.5 Although a majority of the individual hydrocarbons present are determined, some co-elution of compounds is encountered. If this procedure is utilized to estimate bulk hydrocarbon group-type composition (PONA) the user of such data should be cautioned that error may 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 interlaboratory cooperative study, this procedure is applicable to samples having concentrations of olefins less than ~~20 mass %~~ 20 % by mass. However, significant interfering coelution with the olefins above C<sub>7</sub> 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. Many of the olefins in spark ignition fuels are at a concentration below 0.10 %; they are not reported by this test method and may bias the total olefin results low.

1.5.1 Total olefins in the samples may be obtained or confirmed, or both, by Test Method [D1319](#) (volume %) or other test methods, such as those based on multidimensional PONA type of instruments.

1.6 If water is or is suspected of being present, its concentration may be determined, if desired, by the use of Test Method [D1744](#). Other compounds containing sulfur, nitrogen, and so forth, may also be present, and may co-elute with the hydrocarbons. If determination of these specific compounds is required, it is recommended that test methods for these specific materials be used, such as Test Method [D5623](#) for sulfur compounds.

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

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

<sup>1</sup> This test method is under the jurisdiction of ASTM Committee [D02](#) on Petroleum ~~Products~~ Products, Liquid Fuels, and Lubricants and is the direct responsibility of Subcommittee [D02.04.0L](#) on Gas Chromatography Methods.

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## 2. Referenced Documents

### 2.1 ASTM Standards:<sup>2</sup>

- 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)<sup>3</sup>
- D3606 Test Method for Determination of Benzene and Toluene in Finished Motor and Aviation Gasoline by Gas Chromatography
- D4057 Practice for Manual Sampling of Petroleum and Petroleum Products
- D4420 Test Method for Determination of Aromatics in Finished Gasoline by Gas Chromatography (Withdrawn 2004)<sup>3</sup>
- D4815 Test Method for Determination of MTBE, ETBE, TAME, DIPE, tertiary-Amyl Alcohol and C<sub>1</sub> to C<sub>4</sub> Alcohols in Gasoline by Gas Chromatography
- D5580 Test Method for Determination of Benzene, Toluene, Ethylbenzene, *p/m*-Xylene, *o*-Xylene, C<sub>9</sub> 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

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

## 5. Significance and Use

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

## 6. Apparatus

6.1 *Instrumentation*—A gas chromatograph capable of operating under the conditions outlined in Table 1, equipped with a split

<sup>2</sup> 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.

<sup>3</sup> The last approved version of this historical standard is referenced on www.astm.org.

**TABLE 1 Operating Conditions**

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

injector, a carrier gas pressure control, and a flame ionization detector which are required.

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

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

6.3.1 Sampling rate of ~~10 Hz~~ 10 Hz or more with a storage of sampling data for later processing.

6.3.2 Capacity for at least 400 peaks/analysis.

6.3.3 Identification of individual components from retention time; software can be used to automatically identify the peaks with the index system determined from [Table A1.1](#) or [Table A1.2](#).

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

6.5 *Capillary Column*—A ~~50 m~~ 50 m fused silica capillary column with an internal diameter of ~~0.2 mm~~, 0.2 mm, containing a ~~0.5 μm~~ 0.5 μm film thickness of bonded dimethylpolysiloxane phase is used. The features must be respected to reproduce the separation of the reference chromatogram. The column must meet the criteria of efficiency, resolution, and polarity defined in Section 10.

## 7. Reagents and Materials

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

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

7.3 *Oxidizing Gas*, air, 99 mol %. (~~Warning—Compressed gas under high pressure.~~Warning)—Compressed gas under high pressure.)

7.4 *n-Pentane*, 99+ mol % pure. (~~Warning—Extremely flammable. Harmful if inhaled.~~Warning)—Extremely flammable. Harmful if inhaled.)

7.5 *n-Hexane*, 99+ mol % pure. (~~Warning—Extremely flammable. Harmful if inhaled.~~Warning)—Extremely flammable. Harmful if inhaled.)

7.6 *n-Heptane*, 99+ mol % pure. (~~Warning—Extremely flammable. Harmful if inhaled.~~Warning)—Extremely flammable. Harmful if inhaled.)

7.7 *2-Methylheptane*, 99+ mol % pure. (~~Warning—Extremely flammable. Harmful if inhaled.~~Warning)—Extremely flammable. Harmful if inhaled.)

7.8 *4-Methylheptane*, 99+ mol % pure. (~~Warning—Extremely flammable. Harmful if inhaled.~~Warning)—Extremely flammable. Harmful if inhaled.)

7.9 *n-Octane*, 99+ mol % pure. (~~Warning—Extremely flammable. Harmful if inhaled.~~Warning)—Extremely flammable. Harmful if inhaled.)

7.10 *n-Dodecane*, 99+ mol % pure. (~~Warning—Extremely flammable. Harmful if inhaled.~~Warning)—Extremely flammable. Harmful if inhaled.)

7.11 *Toluene*, 99+ mol % pure. (~~Warning—Extremely flammable. Harmful if inhaled.~~Warning)—Extremely flammable. Harmful if inhaled.)

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

## 8. Sampling

8.1 *Container Sampling*—Samples shall be taken as described in Practice [D4057](#) for instructions on manual sampling into open container.

8.2 The sample and a ~~2 mL~~ 2 mL vial must be cooled at ~~4°C~~ 4 °C. Part of the sample is transferred to *the vial up to 80 %* of its volume, and aluminum cap with septum is crimped.

## 9. Preparation of Apparatus

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

9.2 *Operating Conditions*—Two sets of operating conditions are proposed in [Table 1](#), the first with an initial column temperature above the ambient temperature, the second with a sub-ambient column temperature profile. Adjust the operating conditions of the gas chromatograph to conform to the first or second method.

9.3 *Carrier Gas Pressure*—Set a correct carrier gas pressure using the system performance mixture such that the retention time of *n*-Heptane, *n*-Octane and *n*-Dodecane are between the values given in **Table 2**.

## 10. System Performance Evaluation

10.1 Evaluation of the column and linearity of the split injection are carried out with a system performance mixture defined in **7.12** and with the column temperature conditions defined in the following table.

Initial temperature	35°C
Hold time	50 min.
Final temperature	220°C
Hold time	20 min.
Rate	3°C/min.
Initial temperature	35 °C
Hold time	50 min
Final temperature	220 °C
Hold time	20 min
Rate	3 °C/min.

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

10.2.1 *Efficiency*—The number of theoretical plates is calculated with the normal octane peak using **Eq 1**:

$$n = 5.545(Rt/W_{0.5})^2 \quad (1)$$

where:

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

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

10.2.2 *Resolution*—Resolution is determined between the peaks of 2-methylheptane and 4-methylheptane using **Eq 2**:

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

where:

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

10.2.2.1 The resolution must be equal to 4 or 4 or greater than 1.20.

10.2.3 *Polarity*—Polarity is defined by the McReynolds constant of toluene, using **Eq 3**:

$$Rn_{tol} = Ki_{ana} - Ki_{squalane} \quad (3)$$

where:

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

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

10.2.3.1 Toluene Kovats index is calculated using **Eq 4**:

$$Ki_{ana} = 700 + 100 \left( \frac{\log T'_{R(t)} - \log T'_{R(h)}}{\log T'_{R(o)} - \log T'_{R(h)}} \right) \quad (4)$$

**TABLE 2 Reference Retention Times of Normal Paraffins**

NOTE 1—Minutes and tenths of a minute.

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

where:

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

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

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

10.2.4.1 *Measurement of the Stability*—Carry out one temperature programming defined in 10.1 without injecting any sample. Subtract the area slices at the start of the analysis with those corresponding to ~~±20 min~~ 120 min (average of three slices).

10.2.4.2 *Stability Standardization*—Standardization is carried out using the system performance mixture defined in 7.12 with the column temperature conditions defined in 10.1. The value obtained in 10.2.4.1 is divided by the maximum area slice of *N*-octane and multiplied by 100. The value obtained must be less than 2 %. If this is not the case, check for possible leaks, or recondition the column according to the manufacturer's recommendations.

10.3 *Evaluation of the Linearity of the Split Injector*—Evaluation is carried out using the system performance mixture defined in 7.12 with the column temperature conditions defined in 10.1. The % (m/m) of each compound is determined from the corrected area % using the response factors for each compound given in Table A1.1 or Table A1.2. The relative percent error is determined from the known mixture concentrations according to Eq 5:

$$\text{Relative \% error} = \frac{100 (\text{calculated concentration} - \text{known concentration})}{\text{known concentration}} \quad (5)$$

10.3.1 The relative error must not exceed 3 %.

## 11. Response Factor

11.1 Theoretical response factors are used for correction of the detector response of hydrocarbons. The response factor for each compound is relative to that of benzene taken equal to unity and is listed in Tables 1 and 2. For peaks corresponding to the co-elution of compounds with benzene, toluene, and oxygenates, the response factor is the one of the co-eluted compound of % (m/m). Co-eluted compounds are footnoted in Tables A1.1 and A1.2.

## 12. Procedure

12.1 *Preparation of Apparatus*—After optimization of the carrier gas pressure (9.3) and evaluation of apparatus (Section 10), set the temperature program corresponding to the selected method (Table 1).

12.2 *Injection of Sample*—Inject with a ~~55 µL~~ or ~~10 µL~~ 10 µL syringe, manually or by autosampler, the size corresponding to the method (Table 1).

12.3 *Integration of Chromatogram*—Integration codes must be selected to obtain a horizontal baseline with a perpendicular drop to the baseline for partially resolved peaks. An example of correct baseline is given in Figs. A1.1 and A1.2.

12.4 *Identification*—Each peak is identified by matching the retention time with that of compounds listed in Table 1 or Table 2 and standard chromatogram given in Fig. A1.1 or Fig. A1.2. A specific software program using the data of Table 1 or Table 2 can be employed.

12.4.1 If an oxygenate has been determined by Test Methods D4815 or D5599 and is not in the table, it is necessary to prepare a mixture of a weighed amount of this oxygenate in a known spark-ignition engine fuel to determine its retention time and response factor and then add it to the table.

## 13. Calculation

13.1 *Calculation of % (m/m) of Each Compound Without Co-elution and Not Corrected for Co-elutions*—% (m/m) of each component without co-elution and no corrections of co-elutions is calculated according to Eq 6:

$$C_i = \frac{A_i B_i}{\sum_{i=0} (A_i B_i + A_{im} B_{im})} 100 \quad (6)$$

where:

- $C_i$  = % (m/m) of compound *i* without co-elution and no correction of coelutions,  
 $A_i$  = peak area of compound *i* without co-elution (benzene, toluene, and oxygenates),  
 $A_{im}$  = peak area of compounds co-eluting (benzene, toluene, and oxygenates),  
 $B_i$  = response factor for component *i* (given in Table A1.1 or Table A1.2), and  
 $B_{im}$  = response factor for components co-eluted with benzene, toluene, and oxygenates.

13.2 *Calculation of Components Coeluted with Benzene, Toluene, and Oxygenates*—Benzene and toluene contents are determined by Test Methods **D3606** or **D4420** or **D5580**; oxygenates content is determined by Test Methods **D4815** or **D5599**. The % (m/m) of components coeluted with benzene, toluene, and oxygenates is calculated according **Eq 7**:

$$C_{\text{coeluted}} = C_{\text{int}} \cdot 0.01 \left[ 100 - \sum \left( C_{\text{ext}} - C_{\text{ext}} \times \frac{B_{\text{int}}}{B_{\text{ext}}} \right) \right] - C_{\text{ext}} \times \frac{B_{\text{int}}}{B_{\text{ext}}} \quad (7)$$

where:

- $C_{\text{coeluted}}$  = % (m/m) of component eluted with benzene, toluene, or oxygenates,
- $C_{\text{int}}$  = % (m/m) calculated with **Eq 6** for the peak with co-elution,
- $C_{\text{ext}}$  = % (m/m) of benzene, toluene, or oxygenates determined by other method, and
- $B_{\text{ext}}$  = response factor of benzene, toluene, or oxygenates.

13.3 *Calculation of Other Components*—% (m/m) of other components is calculated using **Eq 8**:

$$C_i = C_i' \frac{100 - \sum C_{\text{coeluted}} - \sum C_{\text{ext}}}{\sum C_i'} \quad (8)$$

## 14. Report

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

## 15. Precision<sup>4</sup>

15.1 *Individual Components*—The precision of this test method was determined by a statistical analysis of interlaboratory test results. It applies only to a range from 0.1 to 15 % (m/m), for all components with a resolution greater than 1.0 and without co-elution with oxygenate components. When two components of the same hydrocarbon type have a resolution less than 1.0, the precision can be applied by adding the concentration of two components. The precision is the same for all: (a) light components (saturates and olefins) with a carbon number of 4 and 5, (b) saturates and olefins with a range of carbon number from 6 to 12, and to (c) aromatics. This precision is as follows:

15.1.1 *Repeatability*—The difference between successive test results, obtained by the same operator with the same apparatus under constant operating conditions on identical test material, in the normal and correct operation of the test method, would exceed the value given in the **Table 3** in only one case in twenty.

15.1.2 *Reproducibility*—The difference between two single and independent results, obtained by different operators in different laboratories on nominally identical test material, in the normal and correct operation of the test method, would exceed the values given in the **Table 3** in only one case in twenty.

## 16. Keywords

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

## ANNEX

### (Mandatory Information)

#### A1. METHOD 1, PEAK NUMBER, RETENTION TIME, RESPONSE FACTOR, HYDROCARBON TYPE, AND CARBON NUMBER

<sup>4</sup> Supporting data of interlaboratory cooperative study program, statistical analysis, and precision determination are available from ASTM International Headquarters. Request RR: D02:1520.

**TABLE 3 Repeatability and Reproducibility for Individual Components**

	Range of Carbon	Range, % (m/m)	Repeatability, X (%(m/m))	Reproducibility, X (% (m/m))
Light Components	C4–C5	0.1–14	0.04 · X	0.16 · X
Paraffins	C6–C12	0.1–11.5	0.01 + 0.03 · X	0.04 + 0.07 · X
Naphthenes	C6–C8	0.1–3		
Olefins	C6–C8	0.1–1		
Aromatics	C6–C12	0.1–14	0.05 + 0.02 · X	0.1 + 0.06 · X

A1.1 **Table A1.1** and **Table A1.2** include Method 1/Method 2 peak numbers, retention time, response factor, hydrocarbon type, and carbon number for each component. **Fig. A1.1** and **Fig. A1.2** include Method 1/Method 2 reference chromatograms.

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**TABLE A1.1 Method 1—Peak Numbers, Retention Time, Response Factor, Hydrocarbon Type and Carbon Number for Each Component**

NOTE 1—Legend—Hydrocarbon types—NP = normal paraffins, IP = isoparaffins, NA = naphthenes, OL = olefins, AR = aromatics, Ox = oxygenates.

Nb	Compounds	Retention, min.	Response Factor	Hydrocarbon Type	Carbon No.
1	Propane	4.14	1.125	Ip	3
2	Isobutane <sup>A</sup>	4.47	1.112	Ip	4
2	Methanol <sup>A</sup>	4.47	2.850	Ox	1
3	Isobutene+1-butene	4.66	1.075	OI	4
4	N-butane	4.74	1.112	NP	4
5	Trans-2-butene	4.84	1.075	OI	4
6	C <sub>4</sub> -diolefin	4.88	1.045	OL	4
7	CIS-2-butene	5.00	1.075	OL	4
8	Ethanol	5.17	2.300	OX	2
9	3-Methyl-1-butene	5.45	1.075	OL	5
10	Isopentane	5.76	1.105	IP	5
11	1-pentene	6.05	1.075	OL	5
12	2-Methyl-1-butene	6.20	1.075	OL	5
13	N-Pentane	6.31	1.105	NP	5
14	Isoprene	6.43	1.075	OL	5
15	Trans-2-pentene	6.49	1.075	OL	5
16	Tertiobutylalcohol	6.60	1.490	OX	5
17	CIS-2-pentene	6.70	1.075	OL	5
18	2-Methyl-2-butene	6.84	1.075	OL	5
19	1,Trans-3-pentadiene	6.91	1.075	OL	5
20	1,CIS-3-pentadiene	7.28	1.075	OL	5
21	2,2-Dimethylbutane	7.36	1.100	IP	6
22	1-Cyclopentene	7.99	1.075	OL	5
23	4-Methyl-1-pentene	8.12	1.075	OL	6
24	3-Methyl-1-pentene	8.19	1.075	OL	6
25	Cyclopentane <sup>A</sup>	8.46	1.075	NA	5
25	MTBE <sup>A</sup>	8.46	1.520	OX	5
26	2,3-Dimethylbutane	8.52	1.100	IP	6
27	4-Methyl-CIS-2-pentene	8.61	1.075	OL	6
28	2-Methylpentane	8.70	1.100	IP	6
29	4-Methyl-trans-2-pentene	9.04	1.075	OL	6
30	3-Methylpentane	9.41	1.100	IP	6
31	2-Methyl-1-pentene	9.66	1.075	OL	6
32	1-Hexene	9.70	1.075	OL	6
33	2-Ethyl-1-butene	10.32	1.075	OL	6
34	N-Hexane	10.40	1.110	NP	6
35	Trans-3-hexene	10.51	1.075	OL	6
36	CIS-3-hexene	10.59	1.075	OL	6
37	Trans-2-hexene	10.69	1.075	OL	6
38	2-Methyl-2-pentene	10.84	1.075	OL	6
39	4-Methyl-1-cyclopentene	10.99	1.075	OL	6
40	3-Methyl-trans-2-pentene	11.06	1.075	OL	6
41	3-Methyl-1-cyclopentene	11.19	1.075	OL	6
42	CIS-2-Hexene	11.31	1.075	OL	6
43	C <sub>6</sub> -olefin	11.46	1.075	OL	6
44	ETBE	11.62	1.520	OX	6
45	3-Methyl-CIS-2-pentene	11.74	1.075	OL	6
46	2,2-Dimethylpentane	12.06	1.099	IP	7
47	1-Methylcyclopentane	12.23	1.075	NA	6
48	2,4-Dimethylpentane	12.53	1.099	IP	7
49	C <sub>6</sub> -olefin	12.78	1.075	OL	6
50	2,2,3-Trimethylbutane	13.93	1.099	IP	7
51	C <sub>6</sub> -olefin	13.08	1.075	OL	6
52	C <sub>7</sub> -olefin	13.45	1.075	OL	7
53	C <sub>7</sub> -olefin	13.56	1.075	OL	7
54	C <sub>7</sub> -olefin	13.84	1.075	OL	7
55	C <sub>7</sub> -olefin	13.93	1.075	OL	7
56	Benzene <sup>A</sup>	14.08	1.000	AR	6
56	1-Methyl-1-cyclopentene <sup>A</sup>	14.08	1.075	OL	6
57	C <sub>7</sub> -olefin	14.23	1.075	OL	7
58	C <sub>7</sub> -olefin	14.36	1.075	OL	7
59	3,3-Dimethylpentane	14.61	1.099	IP	7
60	C <sub>7</sub> -olefin	14.77	1.075	OL	7
61	Cyclohexane	14.93	1.075	NA	6
62	C <sub>7</sub> -olefin	15.13	1.075	OL	7
63	C <sub>7</sub> -olefin	15.24	1.075	OL	7
64	C <sub>7</sub> -olefin	15.44	1.075	OL	7
65	C <sub>7</sub> -olefin	15.68	1.075	OL	7
66	2-Methylhexane	15.84	1.099	IP	7
67	2,3-Dimethylpentane	15.99	1.099	IP	7
68	1,1-Dimethylcyclopentane	16.24	1.075	NA	7
69	Cyclohexene	16.44	1.075	OL	6
70	3-Methylhexane	16.70	1.099	IP	7



**TABLE A1.1** *Continued*

Nb	Compounds	Retention, min.	Response Factor	Hydrocarbon Type	Carbon No.
71	C <sub>7</sub> -olefin	17.04	1.075	OP	7
72	CIS-1,3-dimethylcyclopentane	17.32	1.075	NA	7
73	Trans-1,3-dimethylcyclopentane	17.61	1.075	NA	7
74	3-ethylpentane	17.76	1.099	IP	7
75	Trans-1,2-dimethylcyclopentane	17.92	1.075	NA	7
76	2,2,4-Trimethylpentane	18.16	1.096	IP	8
76	C <sub>7</sub> -olefin	18.16	1.075	OL	7
77	C <sub>7</sub> -olefin	18.74	1.075	OL	7
78	C <sub>7</sub> -olefin	19.13	1.075	OL	7
79	N-heptane	19.36	1.099	NP	7
80	C <sub>7</sub> -olefin	19.57	1.075	OL	7
81	C <sub>7</sub> -olefin	19.69	1.075	OL	7
82	C <sub>7</sub> -olefin	19.90	1.075	OL	7
83	C <sub>7</sub> -olefin	20.08	1.075	OL	7
84	C <sub>7</sub> -olefin	20.47	1.075	OL	7
85	C <sub>7</sub> -olefin	20.87	1.075	OL	7
86	C <sub>7</sub> -olefin	21.30	1.075	OL	7
87	C <sub>7</sub> -olefin	21.53	1.075	OL	7
88	1-Methylcyclohexane	21.61	1.075	NA	7
88	CIS-1,2-dimethylcyclopentane	21.61	1.075	NA	7
89	1,1,3-Trimethylcyclopentane	22.02	1.075	NA	8
89	2,2-Dimethylhexane	22.02	1.096	IP	8
90	C <sub>8</sub> -olefin	22.49	1.075	OL	8
91	C <sub>8</sub> -olefin	22.70	1.075	OL	8
92	1-ethylcyclopentane	23.09	1.075	NA	7
93	2,2,3-Trimethylpentane	23.33	1.096	IP	8
93	2,5-Dimethylhexane	23.33	1.096	IP	8
94	2,4-Dimethylhexane	23.57	1.096	IP	8
95	1,trans2,CIS4-trimethylcyclopentane	24.24	1.075	NA	8
96	3,3-Dimethylhexane	24.44	1.096	IP	8
97	C <sub>8</sub> -olefin	24.94	1.075	OL	8
98	1,Trans2,CIS3-trimethylcyclopentane	25.21	1.075	NA	8
99	2,3,4-Trimethylpentane	25.64	1.096	IP	8
100	2,3,3-Trimethylpentane	26.17	1.096	IP	8
100	Toluene	26.17	1.008	AR	7
101	C <sub>8</sub> -olefin	26.38	1.075	OL	8
102	C <sub>8</sub> -olefin	26.67	1.075	OL	8
103	C <sub>8</sub> -olefin	26.79	1.075	OL	8
104	2,3-Dimethylhexane	27.16	1.096	IP	8
105	2-Methyl-3-ethylpentane	27.30	1.096	IP	8
106	C <sub>8</sub> -olefin	27.54	1.075	OL	8
107	2-Methylheptane	28.02	1.096	IP	8
108	4-Methylheptane	28.23	1.096	IP	8
109	3,4-Dimethylhexane	28.36	1.096	IP	8
110	1,CIS2,Trans4-trimethylcyclopentane	28.41	1.075	NA	8
111	C <sub>8</sub> -olefin	28.76	1.075	OL	8
112	3-Methylheptane	29.08	1.096	IP	8
113	3-Ethylhexane	29.22	1.096	IP	8
114	1,CIS-3-dimethylcyclohexane	29.46	1.075	NA	8
114	1,Trans-4-dimethylcyclohexane	29.46	1.075	NA	8
114	1,CIS2,Trans3-trimethylcyclopentane	29.46	1.075	NA	8
115	C <sub>8</sub> -olefin	29.81	1.075	OL	8
116	1,1-Dimethylcyclohexane	30.01	1.075	NA	8
117	C <sub>8</sub> -olefin	30.24	1.075	OL	8
118	2,2,5-Trimethylhexane	30.67	1.093	IP	8
119	1-ME-T3-ethylcyclopentane	30.81	1.075	NA	8
119	C <sub>8</sub> -olefin	30.81	1.075	OL	8
120	1-Methyl-CIS-3-ethylcyclopentane	31.11	1.075	NA	8
120	C <sub>8</sub> -olefin	31.11	1.075	OL	8
121	1-Methyl-trans-2-ethylcyclopentane	31.29	1.075	NA	8
121	C <sub>8</sub> -olefin	31.29	1.075	OL	8

**TABLE A1.1** *Continued*

Nb	Compounds	Retention, min.	Response Factor	Hydrocarbon Type	Carbon No.
122	1-Methyl-1-ethylcyclopentane	31.43	1.075	NA	8
122	C <sub>8</sub> -olefin	31.43	1.075	OL	8
123	1,Trans-2-dimethylcyclopentane	31.68	1.075	OL	7
124	C <sub>8</sub> -olefin	31.97	1.075	OL	8
125	C <sub>8</sub> -olefin	32.17	1.075	OL	8
126	C <sub>8</sub> -olefin	32.58	1.075	OL	8
127	C <sub>8</sub> -olefin	32.81	1.075	OL	8
128	C <sub>8</sub> -naphthene	33.01	1.075	NA	8
128	N-octane	33.01	1.096	NP	8
129	C <sub>8</sub> -olefin	33.56	1.075	OL	8
130	C <sub>8</sub> -olefin	33.81	1.075	OL	8
131	2,2,4-Trimethylhexane	34.04	1.093	IP	9
132	C <sub>8</sub> -olefin	34.76	1.075	OL	8
133	C <sub>8</sub> -olefin	34.93	1.075	OL	8
134	C <sub>8</sub> -olefin	35.15	1.075	OL	8
135	2,3,5-Trimethylhexane	35.46	1.093	IP	9
136	2,2-Dimethylheptane	35.67	1.093	IP	9
137	1,CIS-2-Dimethylcyclohexane	36.02	1.075	NA	8
138	C <sub>9</sub> -olefin	36.25	1.075	OL	9
139	2,4-Dimethylheptane	36.65	1.093	IP	9
140	4,4-Dimethylheptane	36.91	1.093	IP	9
141	C <sub>9</sub> -olefin	37.17	1.075	OL	9
142	1-Ethylcyclohexane	37.35	1.075	NA	8
143	C <sub>9</sub> -olefin	37.52	1.075	OL	9
144	2,6-Dimethylheptane	37.66	1.093	IP	8
145	C <sub>9</sub> -naphthene	37.93	1.075	NA	9
146	C <sub>9</sub> -naphthene	38.05	1.075	NA	9
147	C <sub>9</sub> -naphthene	38.21	1.075	NA	9
148	2,5-Dimethylheptane	38.68	1.093	IP	9
149	C <sub>8</sub> -olefin	38.87	1.075	OL	8
150	C <sub>8</sub> -olefin	39.05	1.075	OL	8
151	C <sub>8</sub> -olefin	39.23	1.075	OL	8
152	C <sub>8</sub> -olefin	39.46	1.075	OL	8
153	C <sub>8</sub> -olefin	39.80	1.075	OL	8
154	ethylbenzene	40.19	1.018	AR	8
155	C <sub>8</sub> -olefin	40.41	1.075	OL	8
156	C <sub>9</sub> -naphthene	40.60	1.075	NA	9
157	C <sub>9</sub> -naphthene	40.89	1.075	NA	9
158	C <sub>8</sub> -olefin	41.09	1.075	OL	8
159	C <sub>8</sub> -olefin	41.24	1.075	OL	8
160	Metaxylene	41.69	1.018	AR	8
161	Paraxylene	41.83	1.018	AR	8
162	C <sub>9</sub> -naphthene	42.20	1.075	NA	9
163	3,4-Dimethylheptane	42.32	1.093	IP	9
164	4-Ethylheptane	42.68	1.093	IP	9
165	C <sub>9</sub> -olefin	42.91	1.075	OL	8
166	4-Methyloctane	43.16	1.093	IP	9
167	2-Methyloctane	43.33	1.093	IP	9
168	C <sub>9</sub> -naphthene	43.51	1.075	NA	9
169	C <sub>9</sub> -naphthene	43.71	1.075	NA	9
170	3-Ethylheptane	44.21	1.093	IP	9
171	3-Methyloctane	44.43	1.093	IP	9
172	Orthoxylene	45.12	1.018	AR	8
173	C <sub>9</sub> -naphthene	45.33	1.075	NA	9
174	C <sub>9</sub> -naphthene	45.66	1.075	NA	9
175	C <sub>9</sub> -naphthene	46.08	1.075	NA	9
176	C <sub>10</sub> -isoparaffin	46.26	1.086	IP	10
177	C <sub>10</sub> -isoparaffin	46.58	1.086	IP	10
178	C <sub>10</sub> -isoparaffin	46.72	1.086	IP	10
179	C <sub>10</sub> -isoparaffin	46.98	1.086	IP	10
180	C <sub>10</sub> -isoparaffin	47.29	1.086	IP	10
181	C <sub>9</sub> -naphthene	47.80	1.075	NA	9
182	C <sub>9</sub> -naphthene	48.10	1.075	NA	9
183	C <sub>9</sub> -naphthene	48.40	1.075	NA	9
184	C <sub>9</sub> -naphthene	48.68	1.075	NA	9
185	N-nonane	48.85	1.093	NP	9
186	C <sub>9</sub> -olefin	49.25	1.075	OL	9
187	C <sub>9</sub> -olefin	49.50	1.075	OL	9
188	C <sub>9</sub> -olefin	49.70	1.075	OL	9
189	isopropylbenzene	50.34	1.025	AR	9
190	C <sub>9</sub> -olefin	50.59	1.075	OL	9
191	C <sub>9</sub> -naphthene	50.81	1.025	NA	9