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Standard Test Method for Hydrocarbon Types in Low Olefinic Gasoline by Mass Spectrometry[1]

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1. Scope

1.1 This test method covers the determination by mass spectrometry of the total paraffins, monocycloparaffins, dicycloparaffins, alkylbenzenes, indans or tetralins or both, and naphthalenes in gasoline having an olefin content of less than 3 volume % and a 95 % distillation point of less than 210°C (411°F) as determined in accordance with Test Method D 86. Olefins are determined by Test Method D 1319, or by Test Method D 875.

1.2 It has not beeen determined whether this test method is applicable to gasolines containing oxygenated compounds (for example, alcohols and ethers).

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

2. Referenced Documents

2.1 *ASTM Standards:*

D 86 Test Method for Distillation of Petroleum Products[2]
D 875 Test Method for Calculation of Olefins and Aromatics in Petroleum Distillates from Bromine Number and Acid Absorption[3]
D 1319 Test Method for Hydrocarbon Types in Liquid Petroleum Products by Fluorescent Indicator Adsorption[2]
D 2001 Test Method for Depentanization of Gasoline and Naphthas[2]
D 2002 Test Methods for Isolation of Representative Saturates Fraction from Low-Olefinic Petroleum Naphthas[2]

3. Terminology

3.1 *Definitions of Terms Specific to This Standard:* [4]

3.1.1 The summations of characteristic mass fragments are defined as follows:

3.1.1.1

$$\Sigma 43 \text{ (paraffins)} = \text{total peak height of } m/e^{+}\ 43 + 57 + 71 + 85 + 99. \tag{1}$$

3.1.1.2

$$\Sigma 41 \text{ (monocycloparaffins)} = \text{total peak height of } m/e^{+}\ 41 + 55 + 69 + 83 + 97. \tag{2}$$

3.1.1.3

$$\Sigma 67 \text{ (dicycloparaffins)} = \text{total peak height of } m/e^{+}\ 67 + 68 + 81 + 82 + 95 + 96 \tag{3}$$

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3.1.1.4

$$\Sigma 77 \text{ (alkylbenzenes)} = \text{total peak height of } m/e^{+}\ 77 + 78 + 79 + 91 + 92 + 105 + 106 + 119 + 120 + 133 + 134 + 147 + 148 + 161 + 162. \tag{4}$$

3.1.1.5

$$\Sigma 103 \text{ (indans and tetralins)} = \text{total peak height of } m/e^{+}\ 103 + 104 + 117 + 118 + 131 + 132 + 145 + 146 + 159 + 160. \tag{5}$$

3.1.1.6

$$\Sigma 128 \text{ (naphthalenes)} = \text{total peak height of } m/e^{+}\ 128 + 141 \pm 142 + 155 + 156. \tag{6}$$

3.1.1.7

$$T = \text{total ion intensity} = \Sigma 41 + \Sigma 43 + \Sigma 67 + \Sigma 77 + \Sigma 103 + \Sigma 128. \tag{7}$$

3.2 *carbon number*, by definition, is the average number of carbon atoms in the sample.

3.3 A mass number with a plus sign as superscript is defined as the peak height associated with the same mass number.

4. Summary of Test Method

4.1 Samples are analyzed by mass spectrometry, based on the summation of characteristic mass fragments, to determine the concentration of the hydrocarbon types. The average number of carbon atoms of the sample is estimated from spectral data. Calculations are made from calibration data which are dependent upon the average number of carbon atoms of the sample. Results are expressed in liquid volume percent.

5. Significance and Use

5.1 A knowledge of the hydrocarbon composition of gasoline process streams, blending stocks and finished motor

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[1] This test method is under the jurisdiction of ASTM Committee D-2 on Petroleum Products and Lubricants and is the direct responsibility of Subcommittee D02.04on Hydrocarbon Analysis.

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

[3] Discontinued; see *1984 Annual Book of ASTM Standards*, Vol 05.01.

[4] Equations in 3.1.1 are identical to those in 11.1.

fuels is useful in following the effect of changes in plant operating conditions, diagnosing process upsets, blending finished products and in evaluating the relationship between composition and performance properties.

6. Apparatus

6.1 *Mass Spectrometer*—Any mass spectrometer that passes the performance test described in Section 8.

NOTE 1—Calibration and precision data for this method were obtained on Consolidated Electrodynamics Corp. Type 21-101, 21-102, and 21-103 mass spectrometers. These instruments operated with an ion source temperature at or near 250°C and at a constant magnetic field of about 3100 to 3500 gauss. Laboratories using either Consolidated Electrodynamics Corp. mass spectrometers that operate with different parameters or instruments other than this design should check the applicability of the calibration data in Table 1. If necessary, individual laboratories should develop their own calibration data using the blends described in Table 2.

6.2 *Sample Inlet System*—Any sample inlet system that allows the introduction of the text mixture (8.2) without loss, contamination, or change of composition.

NOTE 2—Laboratory testing has shown that, unless a special sampling technique or a heated inlet system is used, relatively large errors will occur in the determination of small quantities of indans, tetralins, and naphthalenes.

6.3 *Manometer*—A manometer suitable for direct reading in the 0 to 100-mtorr (0 to 13-Pa) range is optional.

NOTE 3—The expression mtorr as used in this procedure replaces the older μ (micron) unit of pressure.

6.4 *Microburet or Constant-Volume Pipet*.

7. Reference Standards

7.1 Samples of the following hydrocarbons will be required: 2-methylpentane, 2,4-dimethylpentane, *n*-octane, methylcyclopentane, methylcyclohexane, *cis*-1,2-dimethylcyclohexane, benzene, toluene, and *p*-xylene (**Warning**—see Note 4). Only reagent grade chemicals conforming to the specifications of the Committee on Analytical Reagents of the American Chemical Society,[5] National Institute of Standards and Technology (NIST) standard hydrocarbon samples, or other hydrocarbons of equal purity should be used.

NOTE 4—**Warning:** Extremely flammable liquids. Benzene is a poison, carcinogen, and is harmful or fatal if swallowed.

8. Performance Test

8.1 *Calibration for Test Mixture*—Calibrate the instrument in accordance with the manufacturer's instructions for the compounds listed in 7.1, using the same manipulative technique as described in 10.2. Express the calibration data in units of peak height per unit of liquid volume (V) at constant sensitivity. Determine $\Sigma 41/V$, $\Sigma 43/V$, and $\Sigma 77/V$ for each of the reference standards and calculate a weighted average value for each hydrocarbon group type in accordance with the composition of the test mixture as described in 8.2. Construct an inverse from the averaged coefficients.

NOTE 5—The volume, V, ordinarily is expressed as microlitres.

NOTE 6—A desk calculator frequently is used for the calculation of 8.1 and in such cases small inverse terms can be undesirable. If necessary, it is permissible to divide all averaged coefficients by some suitable constant prior to inversion in order to obtain larger values in the inverse.

8.2 *Test Mixture*—Prepare the synthetic mixture by weight from reference standards[5] to obtain a final composition approximating the following but accurately known within ± 0.07 %:

TABLE 1 Calibration Data

	$\Sigma 43/T$	$\Sigma 41/T$	$\Sigma 67/T$	$\Sigma 77/T$	$\Sigma 103/T$	$\Sigma 128/T$	Reference[A]
Paraffins:							
C_6	0.6949	0.3025	0.0019	0.0006	...	...	(1)
C_7	0.7379	0.2583	0.0027	0.0010	...	...	(3)
C_8	0.7592	0.2362	0.0032	0.0014	...	...	(3)
C_9	0.7462	0.2350	0.0052	0.0021	...	0.0113	(12)
C_{10}	0.7772	0.2007	0.0056	0.0014	...	0.0151	(13)
Monocycloparaffins:							
C_6	0.1234	0.8218	0.0460	0.0086	...	...	(1)
C_7	0.0731	0.8213	0.0952	0.0104	...	...	(3)
C_8	0.0737	0.8279	0.0866	0.0117	...	...	(3)
C_9	0.0884	0.8029	0.0942	0.0140	0.0003	0.0003	(12)
C_{10}	0.1471	0.6272	0.2176	0.0080	...	...	(13)
Dicycloparaffins:							
C_8	0.0057	0.1848	0.7843	0.0246	0.0004	...	(4)
C_9	0.0171	0.2270	0.7070	0.0483	0.0005	...	(5)
C_{10}	0.0114	0.2973	0.6582	0.0324	0.0006	...	(6)
Alkylbenzenes:							
C_6	0.0004	0.0004	...	0.9992	...	...	(2)
C_7	0.0146	0.0120	0.0007	0.9726	...	...	(3)
C_8	0.0033	0.0112	0.0007	0.9488	0.0359	...	(3)
C_9	0.0061	0.0218	0.0020	0.9103	0.0598	...	(12)
C_{10}	0.0095	0.0350	0.0025	0.8656	0.0839	0.0034	(13)
Indans and tetralins:							
C_9	0.0144	0.0101	0.0002	0.1600	0.8154	...	(7)
C_{10}	0.0062	0.0123	0.0044	0.2314	0.7236	0.0222	(8)
C_{11}	0.0231	0.0199	0.0017	0.1619	0.7456	0.0477	(9)
Naphthalenes:							
C_{10}	0.0121	0.0037	0.0008	0.0581	0.0065	0.9188	(10)
C_{11}	0.0702	0.0140	0.0011	0.0172	0.0018	0.8957	(11)

[A] References to source of calibration data:

(1) National cooperative by letter of Nov. 22, 1965.
(2) Local task group cooperative by meeting of March 1966.
(3) National cooperative by letter of Aug. 6, 1962.
(4) API No. 448, 100 %, bicyclo-(3.3.0)-octane.
(5) Shell data, 100 %, for 1-methyl-cis-(3.3.0)-bicyclooctane.
(6) API No. 412, 100 %, trans-decalin.
(7) Unweighted API No. 413 and No. 1214 spectra of indan.
(8) API No. 1103, 13 %; API No. 1104, 13 %; API No. 941, 37 %; API No. 539, 37 %.
(9) Unweighted averages of API Nos. 1216, 1106, 1107, 1108, 1109.
(10) Unweighted average of local task group (3 laboratories) data.
(11) Unweighted average of API No. 990 and No. 991.
(12) National cooperative by letter of Oct. 11, 1967.
(13) Proposed Method of Test for Hydrocarbon Types in Low Olefinic Gasoline by Mass Spectrometry; Appendix VII D2-1958.

Reference Standard	Liquid Volume Percent in Mixture	Approximate Weight in Grams to Give 5 mL of Mixture
2-Methylpentane	7.2	0.237
2,4-Dimethylpentane	9.4	0.318
n-Octane	16.6	0.587
Methylcyclopentane	7.1	0.267
Methylcyclohexane	10.0	0.387
cis-1,2-Dimethylcyclohexane	15.5	0.620
Benzene	7.7	0.341
Toluene	10.0	0.436
p-Xylene	16.5	0.714
	100.0	3.907

Record the mass spectrum of the test mixture from m/e^+ 32 to 120 using the manipulative technique as described in 10.2. Compute $\Sigma 41/V$, $\Sigma 43/V$, and $\Sigma 77/V$ from the spectrum of the test mixture and calculate the composition using these values and the inverse of 8.1. The calculated composition should agree with known concentrations within the following limits:

	Percent
Total paraffins	±0.8
Total cycloparaffins	±1.3
Total aromatics	±0.7

If the test mixture cannot be analyzed successfully, consideration should be given to interference, stability, sensitivity, resolution, sample handling, or ability of the analyst.

8.3 *Background*—After pumping out the test mixture specified in 10.2, scan the mass spectrum from m/e^+40 to 100. Background peaks at 43 and 91 should be less than 0.1 % of the corresponding peaks in the mixture spectrum. If both tests of performance are met, it may be presumed that the instrument is satisfactory for sample analysis.

9. Sample Preparation

9.1 Depentanize the sample in accordance with Test Method D 2001.

9.2 Determine the olefin content of the depentanized sample

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