



Standard Test Method for Aromatic Types Analysis of Gas-Oil Aromatic Fractions by High Ionizing Voltage Mass Spectrometry¹

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1. Scope

1.1 This test method² covers the determination by high ionizing voltage, low resolution mass spectrometry of 18 aromatic hydrocarbon types and 3 aromatic thiophenotypes in straight run aromatic petroleum fractions boiling within the range from 205 to 540°C (400 to 1000°F) (corrected to atmospheric pressure). Samples must be nonolefinic, must contain not more than 1 mass % of total sulfur, and must contain not more than 5 % nonaromatic hydrocarbons. Composition data are in volume percent.

NOTE 1—Although names are given to 15 of the compound types determined, the presence of other compound types of the same empirical formulae is not excluded. All other compound types in the sample, unidentified by name or empirical formula, are lumped into six groups in accordance with their respective homologous series.

1.2 *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.*

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

2. Referenced Documents

2.1 ASTM Standards:

D 2549 Test Method for Separation of Representative Aromatics and Nonaromatics Fractions of High-Boiling Oils by Elution Chromatography³

D 2786 Test Method for Hydrocarbon Types Analysis of Gas-Oil Saturate Fractions by High Ionizing Voltage Mass Spectrometry⁴

E 137 Practice for Evaluation of Mass Spectrometers for Quantitative Analysis from a Batch Inlet⁵

3. Terminology

3.1 Definitions of Terms Specific to This Standard:

3.1.1 Characteristic Mass Summations— Classes I–VII:

3.1.2 Class I:

$$\Sigma 78 = 78 + 92 + 106 + 120 + \text{..to end, polyisotopic} \\ + 91 + 105 + 119 + \text{..to end, monoisotopic} \quad (1)$$

3.1.3 Class II:

$$\Sigma 104 = 104 + 118 + 132 + 146 + \text{..to end, polyisotopic} \\ + 117 + 131 + 145 + \text{..to end, monoisotopic} \quad (2)$$

3.1.4 Class III:

$$\Sigma 129 = 130 + 144 + 158 + 172 + \text{..to end, polyisotopic} \\ + 129 + 143 + 157 + 171 + \text{..to end, monoisotopic} \quad (3)$$

3.1.5 Class IV:

$$\Sigma 128 = 128 + 142 + 156 + 170 + \text{..to end, polyisotopic} \\ + 141 + 155 + 169 + \text{..to end, monoisotopic} \quad (4)$$

3.1.6 Class V:

$$\Sigma 154 = 154 + 168 + 182 + 196 + \text{..to end, polyisotopic} \\ + 167 + 181 + 195 + \text{..to end, monoisotopic} \quad (5)$$

3.1.7 Class VI:

$$\Sigma 166 = 166 + 180 + 194 + 208 + \text{..to end, polyisotopic} \\ + 179 + 193 + 207 + \text{..to end, monoisotopic} \quad (6)$$

3.1.8 Class VII:

$$\Sigma 178 = 178 + 192 + 206 + 220 + \text{..to end, polyisotopic} \\ + 191 + 205 + 219 + \text{..to end, monoisotopic} \quad (7)$$

3.1.9 *Classes, Compound Types, Empirical Formulae*— See Table 1.

4. Summary of Test Method

4.1 The relative abundance of seven classes (I–VII) of aromatics in petroleum aromatic fractions is determined by mass spectrometry using a summation of peaks most characteristic of each class. Calculations are carried out by the use of a 7 by 7 inverted matrix derived from published spectra of pure aromatic compounds. Each summation of peaks includes the polyisotopic homologous series that contains molecular ions and the monoisotopic homologous series one mass unit less than the molecular ion series. Using characteristic summations found in the monoisotopic molecular ion—1 series of peaks, each class is further resolved to provide relative abundances of three compound types: nominal (Type 0), first overlap (Type 1), and second overlap (Type 2). The aromatic fraction is

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² Robinson, C. J., and Cook, G. L., *Analytical Chemistry* (ANCHA), Vol 41, 1969, p. 1548.

³ *Annual Book of ASTM Standards*, Vol 05.01.

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

⁵ Discontinued—See 1992 *Annual Book of ASTM Standards*, Vol 05.03.