Designation: D 3239 – 91 (Reapproved 2001)

An American National Standard

Standard Test Method for
Aromatic Types Analysis of Gas-Oil Aromatic Fractions by High Ionizing Voltage Mass Spectrometry[1]

This standard is issued under the fixed designation D 3239; 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[2] 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 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.

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 2549 Test Method for Separation of Representative Aromatics and Nonaromatics Fractions of High-Boiling Oils by Elution Chromatography[3]

D 2786 Test Method for Hydrocarbon Types Analysis of Gas-Oil Saturate Fractions by High Ionizing Voltage Mass Spectrometry[4]

E 137 Practice for Evaluation of Mass Spectrometers for Quantitative Analysis from a Batch Inlet[5]

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*:

$$\begin{aligned}\Sigma 78 = {} & 78 + 92 + 106 + 120 + \text{..to end, polyisotopic} \\ & + 91 + 105 + 119 + \text{..to end, monoisotopic}\end{aligned} \tag{1}$$

3.1.3 *Class II*:

$$\begin{aligned}\Sigma 104 = {} & 104 + 118 + 132 + 146 + \text{..to end, polyisotopic} \\ & + 117 + 131 + 145 + \text{..to end, monoisotopic}\end{aligned} \tag{2}$$

3.1.4 *Class III*:

$$\begin{aligned}\Sigma 129 = {} & 130 + 144 + 158 + 172 + \text{..to end, polyisotopic} \\ & + 129 + 143 + 157 + 171 + \text{..to end, monoisotopic}\end{aligned} \tag{3}$$

3.1.5 *Class IV*:

$$\begin{aligned}\Sigma 128 = {} & 128 + 142 + 156 + 170 + \text{..to end, polyisotopic} \\ & + 141 + 155 + 169 + \text{..to end, monoisotopic}\end{aligned} \tag{4}$$

3.1.6 *Class V*:

$$\begin{aligned}\Sigma 154 = {} & 154 + 168 + 182 + 196 + \text{..to end, polyisotopic} \\ & + 167 + 181 + 195 + \text{..to end, monoisotopic}\end{aligned} \tag{5}$$

3.1.7 *Class VI*:

$$\begin{aligned}\Sigma 166 = {} & 166 + 180 + 194 + 208 + \text{..to end, polyisotopic} \\ & + 179 + 193 + 207 + \text{..to end, monoisotopic}\end{aligned} \tag{6}$$

3.1.8 *Class VII*:

$$\begin{aligned}\Sigma 178 = {} & 178 + 192 + 206 + 220 + \text{..to end, polyisotopic} \\ & + 191 + 205 + 219 + \text{..to end, monoisotopic}\end{aligned} \tag{7}$$

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

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

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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.

TABLE 1 Classes, Compound Types, and Empirical Formulae

Class	Type	Formula
I	0	alkylbenzenes, C_nH_{2n-6}
I	1	benzothiophenes, $C_nH_{2n-10}S$
I	2	naphthenephenanthrenes, C_nH_{2n-20}
II	0	naphthenebenzenes, C_nH_{2n-8}
II	1	pyrenes, C_nH_{2n-22}
II	2	unidentified
III	0	dinaphthenebenzenes, C_nH_{2n-10}
III	1	chrysenes, C_nH_{2n-24}
III	2	unidentified
IV	0	naphthalenes, C_nH_{2n-12}
IV	1	dibenzothiophenes, $C_nH_{2n-16}S$
IV	2	unidentified
V	0	acenaphthenes + dibenzofurans, C_nH_{2n-14} and $C_nH_{2n-16}O$
V	1	perylenes, C_nH_{2n-28}
V	2	unidentified
VI	0	fluorenes, C_nH_{2n-16}
VI	1	dibenzanthracenes, C_nH_{2n-30}
VI	2	unidentified
VII	0	phenanthrenes, C_nH_{2n-18}
VII	1	naphthobenzothiophenes, $C_nH_{2n-22}S$
VII	2	unidentified

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 obtained by liquid elution chromatography (see Test Method D 2549).

NOTE 2—Monoisotopic peaks heights are obtained by correcting the polyisotopic heights for naturally occurring heavy isotopes, assuming that only ions of C_nH_{2n+2} to C_nH_{2-11} are present. This is not strictly accurate for aromatics, but the errors introduced by such assumption are trivial.

5. Significance and Use

5.1 A knowledge of the hydrocarbon composition of process streams and petroleum products boiling within the range 205 to 540°C (400 to 1000°F) is useful in following the effect of changes in process variables, diagnosing the source of plant upsets, and in evaluating the effect of changes in composition on product performance properties. This method, when used together with Test Method D 2786, provides a detailed analysis of the hydrocarbon composition of such materials.

6. Apparatus

6.1 *Mass Spectrometer*—The suitability of the mass spectrometer to be used with this method shall be proven by performance tests described both herein and in Practice E 137.

6.2 *Sample Inlet System*—Any inlet system may be used that permits the introduction of the sample without loss, contamination, or change in composition. The system must function in the range from 125 to 350°C to provide an appropriate sampling device.

6.3 *Microburet or Constant-Volume Pipet.*

6.4 *Mass Spectrum Digitizer*—It is recommended that a mass spectrum digitizer be used in obtaining the analysis, because it is necessary to use the heights of most of the peaks in the spectrum. Any digitizing system capable of supplying accurate mass numbers and peak heights is suitable.

6.5 *Electronic Digital Computer*—The computations for this analysis are not practical without the use of a computer. Any computer capable of providing approximately 60 K bytes in core and capable of compiling programs written in FORTRAN IV should be suitable.

7. Reagent

7.1 *n-Hexadecane*. (**Warning**—Combustible-Very harmful.)

8. Calibration

8.1 Calibration equations in the computer program given in Table 2 may be used directly provided the following procedures are followed:

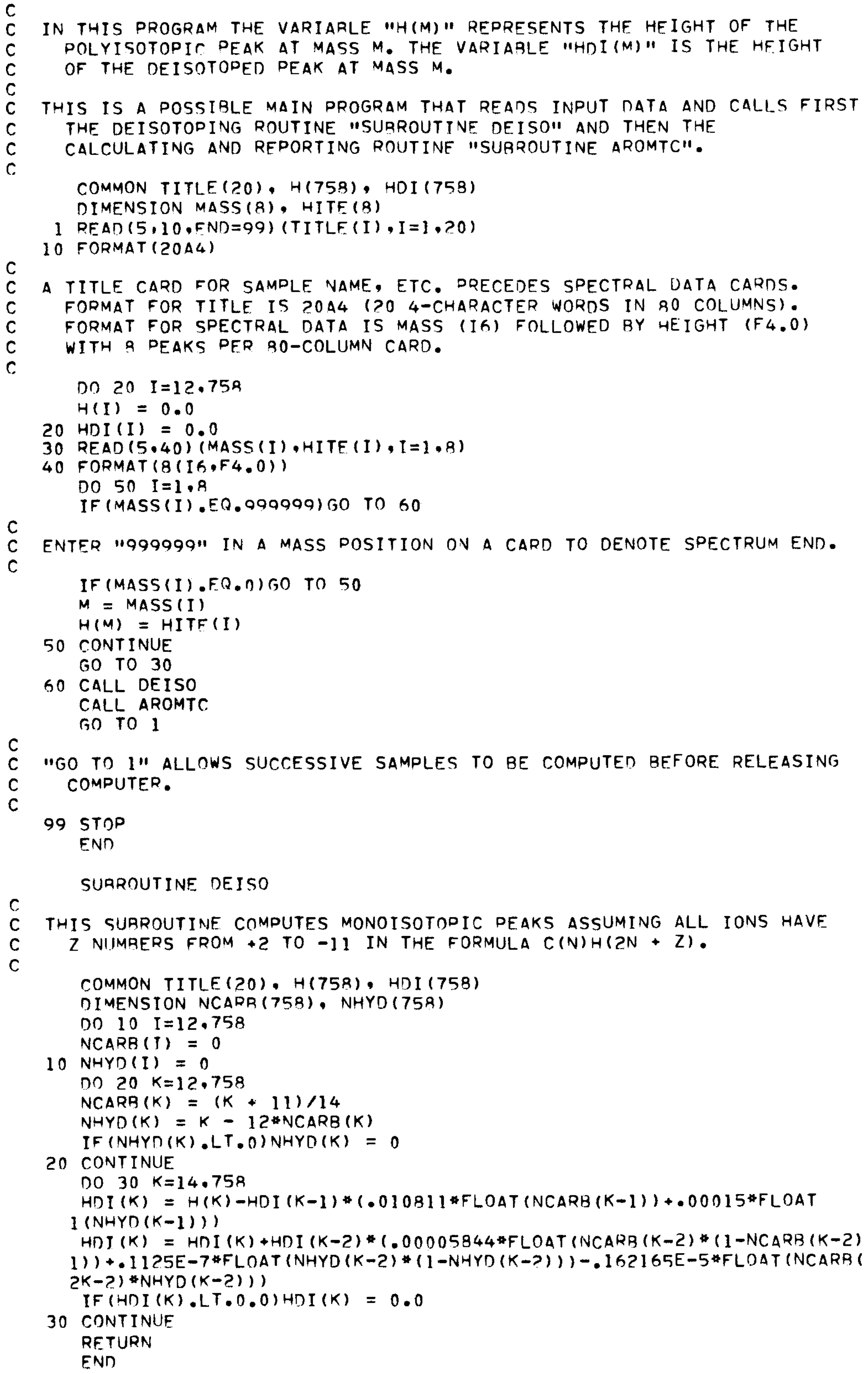
8.1.1 *Instrumental Conditions*—Repeller settings are adjusted to maximize the *m/e* 226 ion of *n*-hexadecane. A magnetic field is used that will permit a scan over the mass range from 78 to 700. An ionizing voltage of 70 eV and an ionizing current in the range from 10 to 70 µA is used.

NOTE 3—The instrument conditions and calibration equations described in this method are based on the use of a 180° magnetic-deflection type mass spectrometer (CEC Model 21-103). Satisfactory results have been obtained with some other magnetic deflection instruments. It is not known if the equations are suitable for use on all other mass spectrometer types.

8.1.2 *Computer Program*—The FORTRAN program given in Table 2 contains all the equations for calculating the analysis, including those for calculating monoisotopic peak heights. The program is compiled and linked to create a computer load module that is available whenever needed. When the spectrum shown in Table 3 is processed, thee results should agree with those shown in Table 4.

TABLE 2 High Ionizing Voltage, Low Resolution Mass Spectrometric Analysis of Gas Oil Aromatic Fractions

* The "end statement" designated is specific for IBM computers. The user may modify the FORTRAN program to suit his individual needs.



```
C
C  IN THIS PROGRAM THE VARIABLE "H(M)" REPRESENTS THE HEIGHT OF THE
C    POLYISOTOPIC PEAK AT MASS M. THE VARIABLE "HDI(M)" IS THE HEIGHT
C    OF THE DEISOTOPED PEAK AT MASS M.
C
C  THIS IS A POSSIBLE MAIN PROGRAM THAT READS INPUT DATA AND CALLS FIRST
C    THE DEISOTOPING ROUTINE "SUBROUTINE DEISO" AND THEN THE
C    CALCULATING AND REPORTING ROUTINE "SUBROUTINE AROMTC".
C
      COMMON TITLE(20), H(758), HDI(758)
      DIMENSION MASS(8), HITE(8)
    1 READ(5,10,END=99)(TITLE(I),I=1,20)
   10 FORMAT(20A4)
C
C  A TITLE CARD FOR SAMPLE NAME, ETC. PRECEDES SPECTRAL DATA CARDS.
C    FORMAT FOR TITLE IS 20A4 (20 4-CHARACTER WORDS IN 80 COLUMNS).
C    FORMAT FOR SPECTRAL DATA IS MASS (I6) FOLLOWED BY HEIGHT (F4.0)
C    WITH 8 PEAKS PER 80-COLUMN CARD.
C
      DO 20 I=12,758
      H(I) = 0.0
   20 HDI(I) = 0.0
   30 READ(5,40)(MASS(I),HITE(I),I=1,8)
   40 FORMAT(8(I6,F4.0))
      DO 50 I=1,8
      IF(MASS(I).EQ.999999)GO TO 60
C
C  ENTER "999999" IN A MASS POSITION ON A CARD TO DENOTE SPECTRUM END.
C
      IF(MASS(I).EQ.0)GO TO 50
      M = MASS(I)
      H(M) = HITE(I)
   50 CONTINUE
      GO TO 30
   60 CALL DEISO
      CALL AROMTC
      GO TO 1
C
C  "GO TO 1" ALLOWS SUCCESSIVE SAMPLES TO BE COMPUTED BEFORE RELEASING
C    COMPUTER.
C
   99 STOP
      END

      SUBROUTINE DEISO
C
C  THIS SUBROUTINE COMPUTES MONOISOTOPIC PEAKS ASSUMING ALL IONS HAVE
C    Z NUMBERS FROM +2 TO -11 IN THE FORMULA C(N)H(2N + Z).
C
      COMMON TITLE(20), H(758), HDI(758)
      DIMENSION NCARB(758), NHYD(758)
      DO 10 I=12,758
      NCARB(I) = 0
   10 NHYD(I) = 0
      DO 20 K=12,758
      NCARB(K) = (K + 11)/14
      NHYD(K) = K - 12*NCARB(K)
      IF(NHYD(K).LT.0)NHYD(K) = 0
   20 CONTINUE
      DO 30 K=14,758
      HDI(K) = H(K)-HDI(K-1)*(.010811*FLOAT(NCARB(K-1))+.00015*FLOAT
     1(NHYD(K-1)))
      HDI(K) = HDI(K)+HDI(K-2)*(.00005844*FLOAT(NCARB(K-2)*(1-NCARB(K-2)
     1))+.1125E-7*FLOAT(NHYD(K-2)*(1-NHYD(K-2)))-.162165E-5*FLOAT(NCARB(
     2K-2)*NHYD(K-2)))
      IF(HDI(K).LT.0.0)HDI(K) = 0.0
   30 CONTINUE
      RETURN
      END
```

TABLE 2 *Continued*

```
      SUBROUTINE AROMTC
C
C THIS ROUTINE GIVES THE ANALYSIS OF AROMATICS FRACTIONS FROM PETROLEUM
C   USING THE PROCEDURE DESCRIBED IN ANAL CHEM 41, 1548-54 (1969)
C
      COMMON TITLE(20), H(758), HDI(758)
      DIMENSION AIN(7,7), BA(7), BB(7), SR(758)
      DATA AIN /+1.8094,-.1952,+.0124,-.0027,-.0015,-.0011,-.0028,
     2          -.1601,+2.0479,-.2806,-.0401,+.0082,+.0012,+.0000,
     3          -.0943,-.2287,+2.3024,-.4936,-.0601,-.0155,-.0089,
     4          -.0292,+.0033,-.0580,+1.9404,-.1337,-.0117,-.0043,
     5          -.0022,-.0003,-.0026,-.0195,+1.9773,-.1823,+.0123,
     6          -.0420,+.0026,-.0018,-.0151,-.0584,+2.0616,-.4193,
     7          -.2346,-.1069,-.0267,-.0019,-.0057,-.0904,+1.9904/
C
C     INITIALIZE SQUARE ROOT ARRAY
C
      DO 2132 I=12,750
 2132 SR(I) = 0.0
C
C     ASSEMBLE APPROPRIATE PEAKS IN MASS SPECTRUM OF AROMATIC FRACTION
C      FOR PROCESSING IN A 7 X 7 MATRIX. QUANTITIES A6,A7,A8,ETC. REFER
C      INITIALLY TO SUMS OF PEAKS AT Z NUMBERS 6,7,8,ETC. A6,A8,ETC. ARE
C      LATER REDEFINED TO INCLUDE THE ODD Z-NUMBER SUM CORRESPONDING TO
C      THE PARENT-1 SERIES (A6 = A6 + A7, A8 = A8 + A9, ETC.)
C
      A6 = 0.0
      DO 2106 M=78,750,14
 2106 A6 = A6 + H(M)
      A7 = 0.0
      DO 2107 M=91,750,14
 2107 A7 = A7 + HDI(M)
      A6 = A6 + A7
      A8 = 0.0
      DO 2108 M=104,750,14
 2108 A8 = A8 + H(M)
      A9 = 0.0
      DO 2109 M=117,750,14
 2109 A9 = A9 + HDI(M)
      A8 = A8 + A9
      A10 = 0.0
      DO 2110 M=130,750,14
 2110 A10 = A10 + H(M)
      A11 = 0.0
      DO 2111 M=129,750,14
 2111 A11 = A11 + HDI(M)
      A10 = A10 + A11
      A12 = 0.0
      DO 2112 M=128,750,14
 2112 A12 = A12 + H(M)
      A13 = 0.0
      DO 2113 M=141,750,14
 2113 A13 = A13 + HDI(M)
      A12 = A12 + A13
      A14 = 0.0
      DO 2114 M=154,750,14
 2114 A14 = A14 + H(M)
      A15 = 0.0
      DO 2115 M=167,750,14
 2115 A15 = A15 + HDI(M)
      A14 = A14 + A15
      A16 = 0.0
      DO 2116 M=166,750,14
 2116 A16 = A16 + H(M)
      A17 = 0.0
      DO 2117 M=179,750,14
 2117 A17 = A17 + HDI(M)
      A16 = A16 + A17
      A18 = 0.0
      DO 2118 M=178,750,14
 2118 A18 = A18 + H(M)
      A19 = 0.0
      DO 2119 M=191,750,14
```

TABLE 2 *Continued*

```
 2119 A19 = A19 + HDI(M)
      A18 = A18+ A19
C
C     CORRECT THE PEAK SUMS FOR THE PRESENCE OF IRRELEVANT IONS AT
C       MASSES 175,176,189,190,200,213
C
      CDI175 =HDI(161)-(HDI(161)-HDI(203))/3.0
      IF(HDI(175).GE.CDI175) GO TO 1046
      CDI175 = HDI(175)
C
C     ABOVE STATEMENTS CORRECT HDI(175)
C     NEXT STATEMENTS CORRECT H(176)
C
 1046 CH176 = H(162)-(H(162)-H(204))/3.0
      IF(H(176).GE.CH176)GO TO 1048
      CH176 = H(176)
C
C     NEXT STATEMENTS CORRECT HDI(189)
C
 1048 CDI189 = CDI175 - (CDI175-HDI(203))/2.0
      IF(HDI(189).GE.CDI189)GO TO 1049
      CDI189 = HDI(189)
C
C     NEXT STATEMENTS CORRECT H(190)
C
 1049 CH190 = CH176-(CH176-H(204))/2.0
      IF(H(190).GE.CH190) GO TO 2101
      CH190 = H(190)
C
C     NEXT STATEMENTS CORRECT H(200)
C
 2101 CH200 =(H(186)+H(214))/2.0
      IF(H(200).GE.CH200) GO TO 2102
      CH200 = H(200)
C
C     NEXT STATEMENTS CORRECT HDI(213)
C
 2102 CDI213 =(HDI(199)+HDI(227))/2.0
      IF(HDI(213).GE.CDI213) GO TO 2103
      CDI213 = HDI(213)
C
C     NEXT STATEMENTS CORRECT THE A6,A8,ETC. SUMS
C
 2103 A6 =A6-(HDI(175)+HDI(189) +H(176)+H(190))
     1 +CDI175 +CDI189+ CH176+ CH190
      A10 = A10-(H(200)+HDI(213))+CH200+CDI213
C
C     REDEFINE A6,A8,ETC. AS SUBSCRIPTED VARIABLE AND MULTIPLY BY THE
C     AROMATICS INVERSE AIN(I,J)
C
      BA(1) = A6
      BA(2) = A8
      BA(3) = A10
      BA(4) = A12
      BA(5) = A14
      BA(6) = A16
      BA(7) = A18
      DO 2125 J=1,7
      BB(J)=0.0
      DO 2124 I=1,7
 2124 BB(J)=BB(J)+BA(I)*AIN(J,I)
 2125 CONTINUE
      DO 2127 J=1,7
      IF(BB(J))2126,2127,2127
 2126 BB(J)=0.0
 2127 CONTINUE
      AA6 = BB(1)
      AA8 = BB(2)
      AA10 = BB(3)
      AA12 = BB(4)
      AA14 = BB(5)
      AA16 = BB(6)
      AA18 = BB(7)
      SUMAA = 0.0
      DO 2128 J=1,7
```

TABLE 2 *Continued*

```
 2128 SUMAA = SUMAA+BB(J)
C
C     VALUES OF AA6,AA8,ETC. ARE DIVISIONS CALCULATED FOR NOMINAL Z=-6,
C      -8,ETC. SUMAA IS SUM OF THE AA VALUES AND REPRESENTS THE TOTAL
C      DIVISIONS OF AROMATICS CALCULATED.
C     THE FOLLOWING STATEMENTS RESOLVE OVERLAPPING TYPES IN Z = -6,
C
      A7 = A7-HDI(175)-HDI(189)+CDI175+CDI189
      HDI(175)=CDI175
      HDI(189)=CDI189
      DO 2130 M=105.750.14
      IF(HDI(M))2130,2131,2130
 2130 CONTINUE
 2131 MM = M-14
      SLOPE =(((0.72*HDI(105))**0.5)-(HDI(MM))**0.5)/
     1 (90.71-(1000.0/FLOAT(MM))**2)
      B = (0.72*HDI(105))**0.5-90.71*SLOPE
      DO 2133 M=147.MM,14
      REALM = M
 2133 SR(M) = SLOPE*(1000.0/REALM)**2 +B
C
C     ABOVE IS FOR Z = -6 AND STORES SQUARE ROOTS OF ALKYL BENZENE PEAK
C      HEIGHTS IN ARRAY SR(I).BELOW IS FOR Z = -8
C
      DO 2134 M=215.750,14
      IF(HDI(M))2134.2135,2134
 2134 CONTINUE
 2135 MN = M-14
      SLOPE = (((0.66*HDI(173))**0.5)-(HDI(MN))**0.5)/
     1 (34.12 -(1000.0/FLOAT(MN))**2)
      B = (0.66*HDI(173))**0.5-34.12*SLOPE
      DO 2136 M=215,MN,14
      REALM = M
 2136 SR(M) = SLOPE*(1000.0/REALM)**2 +B
C
C     BELOW IS FOR Z = -10
C
      A11 = A11 - HDI(213)+CDI213
      HDI(213) = CDI213
      DO 2137 M=241,750.14
      IF(HDI(M))2137.2138,2137
 2137 CONTINUE
 2138 MO = M-14
      SLOPE =((HDI(185))**0.5-(HDI(MO))**0.5)/
     1 (29.22-(1000.0/FLOAT(MO))**2)
      B= HDI(185)**0.5 - 29.22*SLOPE
      DO 2139 M=241,MO,14
      REALM = M
 2139 SR(M) = SLOPE*(1000.0/REALM)**2+B
C
C     BELOW IS FOR Z = -12
C
      DO 2140 M=197,750,14
      IF(HDI(M))2140,2141,2140
 2140 CONTINUE
 2141 MP = M-14
      SLOPE =(((0.25*HDI(183))**0.5)-(HDI(MP))**0.5)/
     1 (29.86-(1000.0/FLOAT(MP))**2)
      B = (0.25*HDI(183))**0.5 - 29.86*SLOPE
      DO 2142 M=197.MP,14
      REALM = M
 2142 SR(M) = SLOPE*(1000.0/REALM)**2+B
C
C     BELOW IS FOR Z = -14
C
      DO 2143 M=265,750,14
      IF(HDI(M))2143.2144,2143
 2143 CONTINUE
 2144 MQ = M-14
      SLOPE = (((0.64*HDI(251))**0.5)-(HDI(MQ))**0.5)/
     1 (15.87-(1000.0/FLOAT(MQ))**2)
      B = (0.64*HDI(251))**0.5 - 15.87*SLOPE
```

TABLE 2 *Continued*

```
      DO 2145 M=265,MQ,14
      REALM = M
 2145 SR(M) = SLOPE*(1000.0/REALM)**2+B
C
C     BELOW IS FOR Z = -16
C
      DO 2146 M=291,750,14
      IF(HDI(M))2146,2147,2146
 2146 CONTINUE
 2147 MR = M-14
      SLOPE = (((0.7*HDI(277))**0.5)-(HDI(MR))**0.5)/
     1 (13.03-(1000.0/FLOAT(MR))**2)
      B = (0.7*HDI(277))**0.5-13.03*SLOPE
      DO 2148 M=291,MR,14
      REALM = M
 2148 SR(M) = SLOPE*(1000.0/REALM)**2+B
C
C     BELOW IS FOR Z = -18
C
      DO 2149 M=247,750,14
      IF(HDI(M) )2149,2150,2149
 2149 CONTINUE
 2150 MS = M-14
      SLOPE = (((0.58*HDI(233))**0.5)-(HDI(MS))**0.5)/
     1 (18.42-(1000.0/FLOAT(MS))**2)
      B = (0.58*HDI(233))**0.5-18.42*SLOPE
      DO 2151 M=247,MS,14
      REALM = M
 2151 SR(M) = SLOPE*(1000.0/REALM)**2+B
C
C     THE SQUARE ROOT ARRAY HAS BEEN CALCULATED. FOR CERTAIN SPECTRA IT
C      MAY BE POSSIBLE TO GET SLOPE AND INTERCEPT VALUES IN REGIONS OF
C      ZERO PEAK HEIGHT. IF THIS OCCURS, ERRORS MIGHT BE ENTERED IN THE
C      SR ARRAY. THE FOLLOWING SETS SR TO ZERO AT MASSES WHERE HDI=0.0
C
      DO 2153 I=12,750
      IF(HDI(I)) 2152,2152,2153
 2152 SR(I) = 0.0
 2153 CONTINUE
C
C     THE SR ARRAY IS SQUARED TO GIVE UNCORRECTED PEAK HEIGHTS OF THE
C      NOMINAL Z TYPES
C
      DO 2154 I=12,750
 2154 SR(I) =(SR(I)**2)
C
C     CORRECT CERTAIN VALUES IN SR(I) FOR NONLINEARITY OF SQ RT RELATION
C
      SR(147) = SR(147)*1.44
      SR(197) = SR(197)*3.10
      SR(211) = SR(211)*2.52
      SR(225) = SR(225)*2.07
      SR(239) = SR(239)*1.83
      SR(253) = SR(253)*1.59
      SR(267) = SR(267)*1.39
      SR(281) = SR(281)*1.28
      SR(295) = SR(295)*1.26
      SR(309) = SR(309)*1.14
      SR(323) = SR(323)*1.06
      SR(265) = SR(265)*1.42
      SR(279) = SR(279)*1.24
      SR(293) = SR(293)*1.12
      SR(307) = SR(307)*1.06
      SR(291) = SR(291)*1.24
      SR(305) = SR(305)*1.15
      SR(319) = SR(319)*1.07
      SR(333) = SR(333)*1.06
      SR(347) = SR(347)*1.05
      SR(361) = SR(361)*1.03
      SR(247) = SR(247)*1.61
      SR(261) = SR(261)*1.50
      SR(275) = SR(275)*1.44
      SR(289) = SR(289)*1.37
      SR(303) = SR(303)*1.28
```

TABLE 2 *Continued*

```
      SR(317) = SR(317)*1.28
      SR(331) = SR(331)*1.21
      SR(345) = SR(345)*1.10
      SR(359) = SR(359)*1.09
      SR(373) = SR(373)*1.07
      SR(387) = SR(387)*1.05
C
C     IT IS NECESSARY THAT NO VALUE SR(M) EXCEEDS THE CORRESPONDING
C      VALUE HDI(M)
      DO 2156 M=12,750
      IF(SR(M)-HDI(M))2156,2156,2155
 2155 SR(M) = HDI(M)
 2156 CONTINUE
C
C     CALCULATE PORTIONS OF A7 DUE TO A6A,A10S,A20A AND OTHER TYPES
C
      A6A = 0.0
      DO 2157 M=91,133,14
 2157 A6A = A6A+HDI(M)
      DO 2158 M=147,MM,14
 2158 A6A = A6A+SR(M)
      A10S = 0.0
      DO 2159 M=147,189,14
 2159 A10S = A10S + HDI(M) - SR(M)
      A10S = A10S/.75
      A20A = A7-A6A-A10S
      IF(A20A)2160,2161,2161
 2160 A20A = 0.0
      A10S = A7-A6A
 2161 CONTINUE
C
C     CALCULATE DIVISIONS OF A6A,A10S,AND A20A
C
      TRASH = (A6-AA6*.5579)*(A7/A6)
      IF(TRASH.LT.0.0)TRASH = 0.0
      A7 = A7 - TRASH
      IF(A7.LE.0.0)A7 = 1.0
      A6A = A6A - TRASH
      IF(A6A.LT.0.0)A6A = 0.0
      IF(A6A.EQ.0.0)A7=A10S+A20A
      A6A =(A6A/A7)*AA6
      A10S = (A10S/A7)*AA6
      A20A = (A20A/A7)*AA6
C
C     CALCULATE PORTIONS OF A9 DUE TO A8A,A22A,AND OTHER TYPES
C
      A8A = 0.0
      DO 2162 M=117,201,14
 2162 A8A = A8A+HDI(M)
      DO 2163 M=215,MN,14
 2163 A8A = A8A+SR(M)
      A22A = 0.0
      DO 2164 M=215,257,14
 2164 A22A = A22A + HDI(M) - SR(M)
      A22A = A22A/.75
      A36A = A9-A8A-A22A
      IF(A36A)2165,2166,2166
 2165 A36A = 0.0
      A22A = A9-A8A
 2166 CONTINUE
C
C     CALCULATE DIVISIONS OF A8A,A22A,AND OTHER TYPES
C
      TRASH = (A8-AA8*.4997)*(A9/A8)
      IF(TRASH.LT.0.0)TRASH = 0.0
      A9 = A9 - TRASH
      IF(A9.LE.0.0)A9 = 1.0
      A8A = A8A - TRASH
      IF(A8A.LT.0.0)A8A = 0.0
      IF(A8A.EQ.0.0)A9=A22A+A36A
      A8A =(A8A/A9)*AA8
      A22A = (A22A/A9)*AA8
      A36A = (A36A/A9)*AA8
```

TABLE 2 *Continued*

```
C
C      CALCULATE PORTIONS OF A11 DUE TO A10A,A24A,AND OTHER TYPES
C
       A10A = 0.0
       DO 2167 M=129,227,14
 2167  A10A = A10A+HDI(M)
       DO 2168 M=241,MO,14
 2168  A10A = A10A+SR(M)
       A24A = 0.0
       DO 2169 M=241,283,14
 2169  A24A = A24A + HDI(M) - SR(M)
       A24A = A24A/.75
       A38A = A11-A10A-A24A
       IF(A38A)2170,2171,2171
 2170  A38A = 0.0
       A24A = A11-A10A
 2171  CONTINUE
C
C      CALCULATE DIVISIONS OF A10A,A24A,AND OTHER TYPES
C
       TRASH = (A10-AA10*.4435)*(A11/A10)
       IF(TRASH.LT.0.0)TRASH = 0.0
       A11 = A11 - TRASH
       IF(A11.LE.0.0)A11 = 1.0
       A10A = A10A - TRASH
       IF(A10A.LT.0.0)A10A = 0.0
       IF(A10A.EQ.0.0)A11=A24A+A38A
       A10A =(A10A/A11)*AA10
       A24A =(A24A/A11)*AA10
       A38A =(A38A/A11)*AA10
C
C      CALCULATE PORTIONS OF A13 DUE TO A12A,A16S,AND OTHER TYPES
C
       A12A = 0.0
       DO 2172 M=141,183,14
 2172  A12A = A12A+HDI(M)
       DO 2173 M=197,MP,14
 2173  A12A = A12A+SR(M)
       A16S = 0.0
       DO 2174 M=197,225,14
 2174  A16S = A16S + HDI(M) - SR(M)
       A16S = A16S/.625
       A26A = A13-A12A-A16S
       IF(A26A)2175,2176,2176
 2175  A26A = 0.0
       A16S = A13-A12A
 2176  CONTINUE
C
C      CALCULATE DIVISIONS OF A12A,A16S,A26A
C
       TRASH = (A12-AA12*.5192)*(A13/A12)
       IF(TRASH.LT.0.0)TRASH = 0.0
       A13 = A13 - TRASH
       IF(A13.LE.0.0)A13 = 1.0
       A12A = A12A - TRASH
       IF(A12A.LT.0.0)A12A = 0.0
       IF(A12A.EQ.0.0)A13=A16S+A26A
       A12A = (A12A/A13)*AA12
       A16S = (A16S/A13)*AA12
       A26A = (A26A/A13)*AA12
C
C      CALCULATE PORTION OF A15 DUE TO A14A,A28A,AND OTHER TYPES
C
       A14A = 0.0
       DO 2177 M=167,251,14
 2177  A14A = A14A+HDI(M)
       DO 2178 M=265,MQ,14
 2178  A14A = A14A+SR(M)
       A28A = 0.0
       DO 2179 M=265,307,14
 2179  A28A = A28A + HDI(M) - SR(M)
       A28A = A28A/.75
       A42A = A15-A14A-A28A
```

TABLE 2 *Continued*

```
      IF(A42A)2180,2181,2181
 2180 A42A = 0.0
      A28A = A15-A14A
 2181 CONTINUE
C
C     CALCULATE DIVISIONS OF A14A,A28A,AND OTHER TYPES
C
      TRASH = (A14-AA14*.5075)*(A15/A14)
      IF(TRASH.LT.0.0)TRASH = 0.0
      A15 = A15 - TRASH
      IF(A15.LE.0.0)A15 = 1.0
      A14A = A14A - TRASH
      IF(A14A.LT.0.0)A14A = 0.0
      IF(A14A.EQ.0.0)A15=A28A+A42A
      A14A = (A14A/A15)*AA14
      A28A = (A28A/A15)*AA14
      A42A = (A42A/A15)*AA14
C
C     CALCULATE PORTIONS OF A17 DUE TO A16A,A30A,AND OTHER TYPES
C
      A16A = 0.0
      DO 2182 M=179,277,14
 2182 A16A = A16A+HDI(M)
      DO 2183 M=291,MR,14
 2183 A16A = A16A+SR(M)
      A30A = 0.0
      DO 2184 M=291,333,14
 2184 A30A = A30A + HDI(M) - SR(M)
      A30A = A30A/.75
      A44A = A17-A16A-A30A
      IF(A44A)2185,2186,2186
 2185 A44A = 0.0
      A30A = A17-A16A
 2186 CONTINUE
C
C     CALCULATE DIVISIONS OF A16A,A30A,AND OTHER TYPES
C
      TRASH = (A16-AA16*.4910)*(A17/A16)
      IF(TRASH.LT.0.0)TRASH = 0.0
      A17 = A17 - TRASH
      IF(A17.LE.0.0)A17 = 1.0
      A16A = A16A - TRASH
      IF(A16A.LT.0.0)A16A = 0.0
      IF(A16A.EQ.0.0)A17=A30A+A44A
      A16A = (A16A/A17)*AA16
      A30A = (A30A/A17)*AA16
      A44A = (A44A/A17)*AA16
C
C     CALCULATE PORTIONS OF A19 DUE TO A18A,A22S,A32A
C
      A18A = 0.0
      DO 2187 M=191,233,14
 2187 A18A = A18A+HDI(M)
      DO 2188 M=247,MS,14
 2188 A18A = A18A+SR(M)
      A22S = 0.0
      DO 2189 M=247,289,14
 2189 A22S = A22S + HDI(M) - SR(M)
      A22S = A22S/.75
      A32A = A19-A18A-A22S
      IF(A32A)2190,2191,2191
 2190 A32A = 0.0
      A22S = A19-A18A
 2191 CONTINUE
C
C     CALCULATE DIVISIONS OF A18A,A22S,AND OTHER TYPES
C
      TRASH = (A18-AA18*.5073)*(A19/A18)
      IF(TRASH.LT.0.0)TRASH = 0.0
      A19 = A19 - TRASH
      IF(A19.LE.0.0)A19 = 1.0
      A18A = A18A - TRASH
      IF(A18A.LT.0.0)A18A = 0.0
      IF(A18A.EQ.0.0)A19=A22S+A32A
      A18A = (A18A/A19)*AA18
      A22S = (A22S/A19)*AA18
      A32A = (A32A/A19)*AA18
```

TABLE 2 *Continued*

```
C
C      THIS COMPLETES CALCULATION OF AROMATICS BREAKDOWN
C      VOLUME PERCENTS ARE NEXT CALCULATED
C
       V6A = 100.0*A6A/SUMAA
       V10S = 100.0*A10S/SUMAA
       V20A = 100.0*A20A/SUMAA
       V8A = 100.0*A8A/SUMAA
       V22A = 100.0*A22A/SUMAA
       V36A = 100.0*A36A/SUMAA
       V10A = 100.0*A10A/SUMAA
       V24A = 100.0*A24A/SUMAA
       V38A = 100.0*A38A/SUMAA
       V12A = 100.0*A12A/SUMAA
       V16S = 100.0*A16S/SUMAA
       V26A = 100.0*A26A/SUMAA
       V14A = 100.0*A14A/SUMAA
       V28A = 100.0*A28A/SUMAA
       V42A = 100.0*A42A/SUMAA
       V16A = 100.0*A16A/SUMAA
       V30A = 100.0*A30A/SUMAA
       V44A = 100.0*A44A/SUMAA
       V18A = 100.0*A18A/SUMAA
       V22S = 100.0*A22S/SUMAA
       V32A = 100.0*A32A/SUMAA
C
       AMONO = A6A+A8A+A10A
       VMONO = V6A+V8A+V10A
       ADI = A12A+A14A+A16A
       VDI = V12A+V14A+V16A
       ATRI = A18A+A20A
       VTRI = V18A+V20A
       ATETRA = A22A+A24A
       VTETRA = V22A+V24A
       APENTA = A28A+A30A
       VPENTA = V28A+V30A
       ATHIO = A10S+A16S+A22S
       VTHIO = V10S+V16S+V22S
       AUNID = A36A+A38A+A26A+A42A+A44A+A32A
       VUNID = V36A+V38A+V26A+V42A+V44A+V32A
C
       WRITE (6,2500)
       WRITE (6,2501)(TITLE(I),I=1,20)
       WRITE (6,2502)AMONO.VMONO,A6A,V6A,A8A,V8A,A10A,V10A
       WRITE (6,2503)ADI,VDI.A12A.V12A.A14A,V14A,A16A,V16A
       WRITE (6,2504)ATRI,VTRI.A18A,V18A,A20A.V20A
       WRITE (6,2505)ATETRA.VTETRA,A22A,V22A,A24A,V24A
       WRITE (6,2506)APENTA.VPENTA,A28A,V28A,A30A,V30A
       WRITE (6,2507)ATHIO,VTHIO,A10S,V10S,A16S,V16S,A22S,V22S
       WRITE (6,2508)AUNID,VUNID,A36A,V36A,A38A.V38A,A26A,V26A,A42A,V42A,
      1 A44A,V44A,A32A,V32A
 2500 FORMAT (1H1 9X,44HMASS SPECTRAL ANALYSIS OF AROMATIC FRACTIONS)
 2501 FORMAT (1H0.20A4//38X,27HCALC. ION SUMS   VOLUME PCT)
 2502 FORMAT (1H0,8X.13HMONOAROMATICS,24X,F7.0,6X,F7.1/10X,13HALKYLBENZE
      1NES,15X,F7.0,6X,F7.1/10X,17HNAPHTHENEBENZENES,11X,F7.0,6X,F7.1/
      210X,19HDINAPHTHENEBENZENES,9X,F7.0,6X,F7.1)
 2503 FORMAT (1H0,8X,11HDIAROMATICS,26X,F7.0,6X,F7.1/10X,12HNAPHTHALENES
      1,16X,F7.0,6X,F7.1/10X,28HACENAPHTHENES, DIBENZOFURANS,F7.0.6X,F7.1
      2/10X,9HFLUORENES,19X,F7.0,6X,F7.1)
 2504 FORMAT (1H0,8X,12HTRIAROMATICS,25X,F7.0,6X,F7.1/10X,13HPHENANTHREN
      1ES,15X,F7.0,6X,F7.1/10X,22HNAPHTHENEPHENANTHRENES.6X,F7.0,6X,F7.1)
 2505 FORMAT (1H0,8X,14HTETRAAROMATICS,23X,F7.0,6X,F7.1/10X,7HPYRENES,21
      1X,F7.0,6X,F7.1/10X,9HCHRYSENES,19X,F7.0,6X,F7.1)
 2506 FORMAT (1H0,8X.14HPENTAAROMATICS,23X,F7.0,6X,F7.1/10X,9HPERYLENES,
      119X,F7.0,6X,F7.1/10X,17HDIBENZANTHRACENES,11X,F7.0,6X,F7.1)
 2507 FORMAT (1H0,8X,19HTHIOPHENO AROMATICS,18X,F7.0,6X,F7.1/10X,15HBENZ
      1OTHIOPHENES,13X,F7.0,6X,F7.1/10X,17HDIBENZOTHIOPHENES,11X,F7.0,6X,
      2F7.1/10X,22HNAPHTHOBENZOTHIOPHENES,6X,F7.0,6X,F7.1)
 2508 FORMAT (1H0.8X,22HUNIDENTIFIED AROMATICS,15X,F7.0,6X,F7.1/10X,37HC
      1LASS I  INCL WITH NAPH PHENANTHRENES/10X,8HCLASS II,20X,F7.0,6X,F7
      2.1/10X,9HCLASS III,19XF7.0,6X,F7.1/10X,8HCLASS IV,20X,F7.0,6X,F7.1
      3/10X,7HCLASS V.21X,F7.0,6X,F7.1/10X,8HCLASS VI.20X,F7.0,6X,F7.1/10
      4X,9HCLASS VII,19X,F7.0,6X,F7.1)
       RETURN
       END
```

8.1.2.1 *Data Input Format*—The input format suggested in the main program may be changed to suit the needs of individual laboratories provided that true masses and peak heights are stored in the *H(M)* array.

8.1.2.2 *FORTRAN IV Language*—Changes in the program may be required for compatibility with the particular computing system to be used. These are permitted provided that the altered program gives the results shown in Table 4 with the input data of Table 3.

NOTE 4—The program, as shown in Table 2, has run satisfactorily on IBM System 360 computers.

9. Procedure

9.1 If the mass spectrometer has been in continuous operation, no additional preparation is necessary before analyzing samples. However, if the spectrometer has been turned on only recently, check its operation according to the manufacturer's instructions to ensure stability before proceeding.

9.2 Obtain the mass spectrum of the sample, scanning from mass 76 to the high-mass end of the spectrum.

10. Calculations

10.1 *Recording Mass Spectrum*—Read peak heights and the corresponding masses for all peaks in the spectrum of the sample. Use the data, along with sample identification, as input to the computer.

11. Precision and Bias

11.1 The precision of this test method as obtained by statistical examination of interlaboratory test results on a sample having the composition given in Table 5, is as follows:

TABLE 3 PC-69-378 Test Spectrum for Gas Oil Aromatics Analysis

MASS	HT	MASS	HT	MASS	HT	MASS	HT	MASS	HT	MASS	HT	MASS	HT	MASS	HT
78	126	79	332	80	98	81	610	82	128	83	532	84	76	85	181
86	46	87	77	88	72	89	140	90	35	91	694	92	210	93	216
94	93	95	480	96	108	97	301	98	62	99	53	100	54	101	158
102	92	103	127	104	174	105	984	106	387	107	187	108	107	109	264
110	68	111	143	112	55	113	132	114	117	115	402	116	194	117	400
118	270	119	1045	120	389	121	164	122	70	123	152	124	48	125	104
126	134	127	175	128	407	129	482	130	287	131	655	132	272	133	662
134	225	135	112	136	47	137	98	138	78	139	146	140	72	141	406
142	297	143	496	144	289	145	739	146	212	147	289	148	102	149	94
150	83	151	140	152	247	153	229	154	163	155	486	156	264	157	438
158	226	159	533	160	144	161	161	162	70	163	119	164	76	165	477
166	204	167	268	168	180	169	434	170	209	171	318	172	140	173	316
174	106	175	125	176	129	177	104	178	334	179	414	180	204	181	312
182	160	183	280	184	134	185	226	186	98	187	218	188	96	189	306
190	143	191	297	192	262	193	380	194	200	195	318	196	132	197	191
198	98	199	179	200	112	201	158	202	300	203	253	204	144	205	307
206	255	207	316	208	171	209	240	210	117	211	168	212	90	213	198
214	93	215	374	216	213	217	225	218	156	219	269	220	216	221	238
222	133	223	169	224	124	225	154	226	184	227	181	228	200	229	320
230	206	231	244	232	171	233	197	234	162	235	172	236	112	237	150
238	113	239	257	240	136	241	189	242	174	243	251	244	196	245	214
246	167	247	153	248	130	249	134	250	132	251	118	252	192	253	200
254	124	255	178	256	172	257	190	258	173	259	156	260	152	261	131
262	121	263	145	264	124	265	162	266	156	267	153	268	128	269	156
270	155	271	144	272	144	273	114	274	142	275	105	276	149	277	115
278	130	279	136	280	143	281	133	282	132	283	127	284	133	285	114
286	127	287	97	288	124	289	114	290	123	291	94	292	125	293	112
294	134	295	115	296	127	297	108	298	122	299	95	300	130	301	82
302	127	303	93	304	111	305	85	306	122	307	93	308	123	309	95
310	120	311	92	312	116	313	91	314	120	315	78	316	116	317	77
318	106	319	78	320	116	321	81	322	115	323	80	324	118	325	82
326	118	327	78	328	115	329	69	330	112	331	68	332	101	333	68
334	109	335	75	336	108	337	73	338	108	339	75	340	108	341	67
342	110	343	62	344	107	345	61	346	98	347	61	348	102	349	75
350	108	351	69	352	104	353	67	354	100	355	57	356	104	357	56
358	102	359	54	360	92	361	54	362	96	363	69	364	102	365	73
366	104	367	63	368	96	369	56	370	98	371	50	372	95	373	49
374	84	375	47	376	88	377	54	378	90	379	55	380	90	381	54
382	88	383	49	384	91	385	46	386	87	387	44	388	76	389	43
390	80	391	47	392	84	393	48	394	84	395	48	396	80	397	45
398	84	399	42	400	81	401	41	402	67	403	38	404	70	405	41
406	76	407	42	408	75	409	42	410	72	411	40	412	77	413	38
414	76	415	38	416	60	417	34	418	63	419	34	420	66	421	38
422	66	423	38	424	64	425	36	426	68	427	34	428	66	429	33
430	54	431	30	432	56	433	33	434	59	435	33	436	59	437	34
438	57	439	32	440	61	441	30	442	58	443	30	444	47	445	27
446	49	447	28	448	53	449	30	450	54	451	30	452	52	453	28
454	54	455	27	456	50	457	26	458	41	459	23	460	44	461	25
462	46	463	26	464	47	465	26	466	45	467	25	468	48	469	24
470	44	471	23	472	36	473	21	474	38	475	22	476	40	477	22
478	41	479	23	480	40	481	22	482	40	483	21	484	38	485	20
486	31	487	17	488	33	489	19	490	35	491	19	492	35	493	20
494	34	495	18	496	35	497	18	498	33	499	17	500	26	501	15
502	28	503	15	504	30	505	17	506	30	507	18	508	29	509	17
510	30	511	16	512	28	513	18	514	22	515	13	516	24	517	14
518	25	519	14	520	26	521	14	522	24	523	14	524	24	525	14
526	24	527	13	528	18	529	11	530	20	531	12	532	20	533	12
534	21	535	12	536	20	537	11	538	20	539	11	540	18	541	11
542	15	543	9	544	16	545	11	546	18	547	10	548	18	549	10
550	16	551	9	552	16	553	9	554	14	555	8	556	11	557	7
558	11	559	8	560	13	561	8	562	14	563	8	564	12	565	8
566	12	567	9	568	11	569	8	570	9	571	6	572	10	573	8
574	10	575	6	576	10	577	6	578	9	579	6	580	9	581	6
582	8	583	5	584	7	585	5	586	7	587	5	588	7	589	5
590	8	591	6	592	8	593	4	594	7	595	4	596	6	597	4
598	5	599	4	600	6	601	4	602	6	603	4	604	6	605	4
606	5	607	3	608	5	609	3	610	4	611	3	612	4	613	3
614	4	615	4	616	4	617	3	618	4	619	3	620	4	621	3
622	4	624	3	626	3	628	3	630	3	632	3999999				

TABLE 4 Mass Spectral Analysis of Aromatic Fractions
PC-69-378 Test Spectrum for Gas Oil Aromatics Analysis

	Calc. Ion	Sums	Volume	%
Monoaromatics:		28498.		38.9
Alkylbenzenes	9703.		13.3	
Naphthenebenzenes	9017.		12.3	
Dinaphthenebenzenes	9778.		13.4	
Diaromatics:		19158.		26.2
Naphthalenes	4774.		6.5	
Acenaphthenes, dibenzofurans	6576.		9.0	
Fluorenes	7809.		10.7	
Triaromatics:		9625.		13.1
Phenanthrenes	6156.		8.4	
Naphthenephenanthrenes	3470.		4.7	
Tetraaromatics:		6070.		8.3
Pyrenes	3980.		5.4	
90. Chrysenes	2090.		2.9	
Pentaaromatics:		1658.		2.3
Perylenes	1293.		1.8	
Dibenzanthracenes	366.		0.5	
Thiopheno Aromatics:		1872.		2.6
Benzothiophenes	565.		0.8	
Dibenzothiophenes	968.		1.3	
Naphthobenzothiophenes	339.		0.5	
Unidentified Aromatics:		6322.		8.6
Class I incl with Naphthenephenanthrenes				
Class II	614.		0.8	
Class III	838.		1.1	
Class IV	3431.		4.7	
Class V	546.		0.7	
Class VI	281.		0.4	
Class VII	612.		0.8	

TABLE 5 Precision Summary Based on Cooperative Data

	Vol %	σ_r	σ_R	*r*	R
Alkylbenzenes	13.7	0.3	1.0	1.2	3.0
Naphthenebenzenes	13.3	0.1	1.1	0.5	3.3
Dinaphthenebenzenes	13.7	0.2	0.4	0.9	1.1
Naphthalenes	6.7	0.2	0.8	0.9	2.3
Acenaphthenes/dibenzofurans	9.0	0.1	0.2	0.5	0.5
Fluorens	10.7	0.1	0.2	0.3	0.6
Phenanthrenes	8.6	0.1	0.3	0.2	1.0
Naphthenephenanthrenes	4.5	0.2	0.4	0.7	1.2
Pyrenes	5.7	0.1	0.5	0.3	1.6
Chrysenes	2.8	0.2	0.4	0.5	1.1
Perylenes	1.7	0.1	0.2	0.3	0.6
Dibenzanthracenes	0.4	0.1	0.1	0.2	0.4
Benzothiophenes	1.0	0.2	0.4	0.8	1.1
Dibenzothiophenes	1.5	0.1	0.3	0.3	0.8
Naphthabenzothiophenes	0.5	0.1	0.3	0.3	1.0
Class II Unidentified	0.4	0.1	0.4	0.3	1.1
Class III Unidentified	0.6	0.1	0.4	0.4	1.2
Class IV Unidentified	4.1	0.2	0.5	0.6	1.6
Class V Unidentified	0.5	0.1	0.3	0.5	0.8
Class VI Unidentified	0.2	0.1	0.1	0.3	0.4
Class VII Unidentified	0.4	0.2	0.2	0.5	0.7

σ_r = repeatability standard deviation
σ_R = reproducibility standard deviation
r = repeatability
R = reproducibility

11.1.1 *Repeatability*—The difference between successive test results obtained by the same operator with the same apparatus under constant operating conditions on identical test material, would in the long run, in the normal and correct operation of the test method, exceed the values shown in Table 5 only in one case in twenty.

11.1.2 *Reproducibility*—The difference between two single and independent results, obtained by different operators working in different laboratories on identical test material, would in the long run, in the normal and correct operation of the test method, exceed the values shown in Table 5 only in one case in twenty.

NOTE 5—If samples are analyzed that differ appreciably in composition from the sample used for the interlaboratory study, this precision statement may not apply.

11.2 *Bias*—The quantities determined are defined by the conditions employed in this empirical method, and a statement of bias is therefore not appropriate.

12. Keywords

12.1 aromatic; gas oil; mass spectrometry; petroleum

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