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

## 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[3]

E 137 Practice for Evaluation of Mass Spectrometers for Quantitative Analysis from a Batch Inlet[4]

## 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

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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] 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 |

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 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
```

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      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
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  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
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 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
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       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
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                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
```

8

```
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
```

```
      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
```

```
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 | 69 | 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 | |
| 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 | |

(Note: "90." appears in the left margin beside Chrysenes row.)

**TABLE 5   Precision Summary Based on Cooperative Data**

| | Vol % | $\sigma_r$ | $\sigma_R$ | 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 |

$\sigma_r$ = repeatability standard deviation
$\sigma_R$ = 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