Designation: D2786 – 91 (Reapproved 2016)

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

This standard is issued under the fixed designation D2786; 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 mass spectrometry of seven saturated hydrocarbon types and one aromatic type in saturate petroleum fractions having average carbon numbers 16 through 32. The saturate types include alkanes (0-rings), single-ring naphthenes, and five fused naphthene types with 2, 3, 4, 5, and 6 rings. The nonsaturate type is monoaromatic. Noncondensed naphthenes are analyzed as single rings. Samples must be nonolefinic and must contain less than 5 volume % monoaromatic. Composition data are in volume percent.

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:*[3]

D2549 Test Method for Separation of Representative Aromatics and Nonaromatics Fractions of High-Boiling Oils by Elution Chromatography

D3239 Test Method for Aromatic Types Analysis of Gas-Oil Aromatic Fractions by High Ionizing Voltage Mass Spectrometry

E137 Practice for Evaluation of Mass Spectrometers for Quantitative Analysis from a Batch Inlet (Withdrawn 1992)[4]

3. Terminology

3.1 *Definitions of Terms Specific to This Standard:*

3.1.1 *Characteristic Mass Groupings:*

3.1.1.1

$$\sum 71 = 71+85+99+113\ (\text{alkanes}). \quad (1)$$

3.1.1.2

$$\sum 69 = 69+83+97+111+125+139\ (1-\text{ring}). \quad (2)$$

3.1.1.3

$$\sum 109 = 109+123+137+151+165+179+193\ (2-\text{ring}). \quad (3)$$

3.1.1.4

$$\sum 149 = 149+163+177+191+205+219+233+247\ (3-\text{ring}). \quad (4)$$

3.1.1.5

$$\sum 189 = 189+203+217+231+245+259+273+287+301\ (4-\text{ring}). \quad (5)$$

3.1.1.6

$$\sum 229 = 229+243+257+271+285+299+313+327+341+355\ (5-\text{ring}). \quad (6)$$

3.1.1.7

$$\sum 269 = 269+283+297+311+325+339+353+367+381+395+409\ (6-\text{ring}). \quad (7)$$

3.1.1.8

$$\sum 91 = 91+105+117+119+129+131+133+143+145+147+157+159+171\ (\text{monoaromatic}). \quad (8)$$

4. Summary of Test Method

4.1 The relative abundance of alkanes (0-ring), 1-ring, 2-ring, 3-ring, 4-ring, 5-ring, and 6-ring naphthenes in petroleum saturate fractions is determined by mass spectrometry

[1] This test method is under the jurisdiction of ASTM Committee D02 on Petroleum Products, Liquid Fuels, and Lubricants and is the direct responsibility of Subcommittee D02.04.0M on Mass Spectroscopy.

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[2] Hood, A., and O'Neal, M. J., *Advances in Mass Spectrometry,* AMSPA, Waldron, 1959, p. 175.

[3] For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

[4] The last approved version of this historical standard is referenced on www.astm.org.

using a summation of mass fragment groups most characteristic of each molecular type. Calculations are carried out by the use of inverted matrices (derived from ion intensity calibration sensitivities) that are specific for any average carbon number. The saturate fraction is obtained by liquid elution chromatography, see Test Method D2549.

5. Significance and Use

5.1 A knowledge of the hydrocarbon composition of process streams and petroleum products boiling within the range of 205 °C to 540 °C (400 °F 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.

5.2 This test method, when used together with Test Method D3239, 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 E137.

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 °C to 350 °C to provide an appropriate sampling device.

6.3 *Microburet or Constant-Volume Pipet.*

7. Reagents

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

8. Calibration

8.1 Calibration matrix inverses are attached in Table 1 which may be used directly provided the following procedures are followed.

TABLE 1 Calibration Matrix Inverses

	∑71	∑ 69	∑ 109	∑ 149	∑ 189	∑ 229	∑ 269	∑91
				C_{16} Inverse				
n-Alkanes								
0 Ring	0.5344	−0.0292	−0.0066	0.0215	0.0299	...	...	−0.0151
1 Ring	−0.0610	0.3403	−0.2146	−0.1162	−0.0362	...	...	−0.0112
2 Ring	−0.0039	0.0170	0.8491	−0.6968	−0.3420	...	...	−0.0048
3 Ring	0.0000	−0.0004	+ 0.0115	1.7220	−1.3545	...	...	0.0152
4 Ring	0.0001	0.0004	0.0039	−0.0138	3.2594	...	...	−0.0485
MA	−0.0007	−0.0029	−0.0237	−0.1566	−0.3494	...	...	0.3521
Isoalkanes								
0 Ring	0.6543	−0.0358	−0.0081	0.0264	0.0366	...	...	−0.0185
1 Ring	−0.0866	0.3416	−0.2143	−0.1171	−0.0377	...	...	−0.0101
2 Ring	−0.0053	0.0172	0.8492	−0.6968	−0.3420	...	...	−0.0046
3 Ring	0.0001	−0.0004	0.0115	1.7220	−1.3545	...	...	0.0152
4 Ring	0.0000	0.0004	0.0039	−0.0138	3.2594	...	...	−0.0485
MA	0.0001	−0.0029	−0.0237	−0.1565	−0.3493	...	...	0.3521
				C_{17} Inverse				
n-Alkanes								
0 Ring	0.5243	−0.0311	−0.0075	0.0227	0.0322	...	...	−0.0163
1 Ring	−0.0660	0.3403	−0.2130	−0.1164	−0.0385	...	...	−0.0121
2 Ring	−0.0038	0.0154	0.8375	−0.6826	−0.3318	...	...	−0.0052
3 Ring	0.0000	−0.0004	0.0095	1.6824	−1.3111	...	...	0.0166
4 Ring	0.0001	0.0004	0.0039	−0.0147	3.1247	...	...	−0.0527
MA	−0.0007	−0.0027	−0.0220	−0.1514	−0.3331	...	...	0.3612
Isoalkanes								
0 Ring	0.6435	−0.0382	−0.0092	0.0279	0.0395	...	...	−0.0200
1 Ring	−0.0942	0.3418	−0.2125	−0.1176	−0.0403	...	...	−0.0112
2 Ring	−0.0054	0.0155	0.8375	−0.6826	−0.3319	...	...	−0.0052
3 Ring	0.0000	−0.0002	0.0090	1.6825	−1.3111	...	...	0.0166
4 Ring	0.0000	0.0004	0.0040	−0.0147	3.1247	...	...	−0.0527
MA	0.0000	−0.0027	−0.0220	−0.1514	−0.3331	...	...	0.3612
				C_{18} Inverse				
n-Alkanes								
0 Ring	0.5175	−0.0338	−0.0085	0.0234	0.0344	...	...	−0.0178
1 Ring	−0.0720	0.3404	−0.2091	−0.1183	−0.0404	...	...	−0.0136
2 Ring	−0.0039	0.0138	0.8183	−0.6626	−0.3213	...	...	−0.0057
3 Ring	0.0000	−0.0003	0.0062	1.6426	−1.2784	...	...	0.0179
4 Ring	0.0001	0.0004	0.0040	−0.0158	3.0158	...	...	−0.0567
MA	−0.0007	−0.0025	−0.0206	−0.1445	−0.3010	...	...	0.3677
Isoalkanes								
0 Ring	0.6335	−0.0414	−0.0103	0.0286	0.0422	...	...	−0.0215
1 Ring	−0.1016	0.3424	−0.2086	−0.1197	−0.0424	...	...	−0.0126
2 Ring	−0.0054	0.0140	0.8184	−0.6626	−0.3214	...	...	−0.0056
3 Ring	0.0000	−0.0003	0.0062	1.6426	−1.2784	...	...	0.0179
4 Ring	0.0000	0.0004	0.0040	−0.0158	3.0158	...	...	−0.0566

TABLE 1 *Continued*

	∑71	∑ 69	∑ 109	∑ 149	∑ 189	∑ 229	∑ 269	∑91
MA	−0.0002	−0.0025	−0.0206	−0.1445	−0.3200	...	...	0.3677
				C_{19} Inverse				
n-Alkanes								
0 Ring	0.5109	−0.0363	−0.0094	0.0202	0.0404	...	...	−0.0190
1 Ring	−0.0773	0.3396	−0.2080	−0.1161	−0.0413	...	...	−0.0154
2 Ring	−0.0038	0.0118	0.8076	−0.6491	−0.3184	...	...	−0.0061
3 Ring	0.0000	−0.0003	0.0032	1.6068	−1.2432	...	...	0.0193
4 Ring	0.0001	0.0004	0.0041	−0.0179	2.9192	...	...	−0.0614
MA	−0.0008	−0.0023	−0.0192	−0.1369	−0.2980	...	...	0.3764
Isoalkanes								
0 Ring	0.6239	−0.0443	−0.0115	0.0246	0.0494	...	...	−0.0232
1 Ring	−0.1079	0.3418	−0.2073	−0.1173	−0.0438	...	...	−0.0142
2 Ring	−0.0053	0.0120	0.8077	−0.6493	−0.3184	...	...	−0.0061
3 Ring	0.0000	−0.0002	0.0030	1.6068	−1.2432	...	...	0.0193
4 Ring	0.0001	0.0004	0.0041	−0.0179	2.9192	...	...	−0.0614
MA	−0.0004	−0.0023	−0.0192	−0.1369	−0.2980	...	...	0.3764
				C_{20} Inverse				
n-Alkanes								
0 Ring	0.5099	−0.0397	0.0105	0.0183	0.0458	0.0412	...	−0.0223
1 Ring	−0.0835	0.3403	−0.2066	−0.1137	−0.0418	0.0375	...	−0.0190
2 Ring	−0.0036	0.0097	0.7972	−0.6412	−0.3106	−0.1542	...	0.0000
3 Ring	0.0000	−0.0003	−0.0014	1.5634	−1.2179	−0.5944	...	0.0468
4 Ring	0.0000	0.0000	0.0012	−0.0409	2.7690	−1.4656	...	−0.0029
5 Ring	0.0004	0.001	0.0085	0.0630	0.0996	4.2055	...	−0.1831
MA	−0.0008	−0.0022	−0.0188	−0.1382	−0.2910	−0.4521	...	0.4049
Isoalkanes								
0 Ring	0.6188	−0.0481	−0.0127	0.0222	0.0555	0.0499	...	−0.0270
1 Ring	−0.1151	0.3427	−0.2059	−0.1149	−0.0446	0.0350	...	−0.0176
2 Ring	−0.0051	0.0098	0.7972	−0.6412	−0.3107	−0.1544	...	0.0001
3 Ring	0.0001	−0.0003	−0.0014	1.5634	−1.2179	−0.5944	...	0.0468
4 Ring	0.0000	0.0000	0.0012	−0.0409	2.7690	−1.4656	...	−0.0029
5 Ring	0.0003	0.0010	0.0085	0.0630	0.0996	4.2054	...	−0.1831
MA	−0.0007	−0.0022	−0.0188	−0.1382	−0.2910	−0.4521	...	0.4049
				C_{21} Inverse				
n-Alkanes								
0 Ring	0.5077	−0.0431	−0.0119	0.0195	0.0454	0.0441	...	−0.0242
1 Ring	−0.0888	0.3393	−0.2025	−0.1147	−0.0429	0.0334	...	−0.0212
2 Ring	−0.0033	0.0074	0.7808	−0.6176	−0.3082	−0.1470	...	−0.0003
3 Ring	−0.0001	−0.0002	−0.0037	1.5192	−1.1698	−0.5596	...	0.0483
4 Ring	0.0000	0.0000	0.0014	−0.0416	2.6715	−1.4243	...	−0.0056
5 Ring	0.0004	0.0009	0.0078	0.0592	0.0898	3.9781	...	−0.1851
MA	−0.0009	−0.0020	−0.0173	−0.1308	−0.2717	−0.4172	...	−0.4123
Isoalkanes								
0 Ring	0.6140	−0.0522	−0.0144	0.0235	0.0550	0.0533	...	−0.0292
1 Ring	−0.1216	0.3421	−0.2016	−0.1158	−0.0458	0.0305	...	−0.0196
2 Ring	−0.0048	0.0076	0.7811	−0.6176	−0.3082	−0.1472	...	−0.0001
3 Ring	−0.0001	−0.0002	−0.0037	1.5192	−1.1698	−0.5596	...	0.0483
4 Ring	0.0000	0.0000	0.0014	−0.0416	2.6715	−1.4232	...	−0.0056
5 Ring	0.0005	0.0009	0.0078	0.0592	0.0893	3.9781	...	−0.1851
MA	−0.0010	−0.0020	−0.0173	−0.1308	−0.2717	−0.4172	...	0.4123
				C_{22} Inverse				
n-Alkanes								
0 Ring	0.5084	−0.0474	−0.0133	0.0210	0.0435	0.0484	...	−0.0263
1 Ring	−0.0946	0.3397	−0.1995	−0.1145	−0.0440	0.0307	...	−0.0240
2 Ring	−0.0030	0.0050	0.7661	−0.6016	−0.3016	−0.1444	...	−0.0005
3 Ring	−0.0002	0.0000	−0.0072	1.4778	−1.1214	−0.5559	...	0.0517
4 Ring	0.0000	0.0000	0.0018	−0.0411	2.5629	−1.3179	...	−0.0117
5 Ring	0.0004	0.0008	0.0072	0.0564	0.0829	3.7619	...	−0.1890
MA	−0.0010	−0.0018	−0.0161	−0.1252	−0.2574	−0.3897	...	0.4237
Isoalkanes								
0 Ring	0.6096	0.0568	−0.0160	0.0252	0.0521	0.0580	...	−0.0316
1 Ring	−0.1267	0.3427	−0.1986	−0.1158	−0.0468	0.0277	...	−0.0223
2 Ring	−0.0044	0.0053	0.7662	−0.6016	−0.3018	−0.1445	...	−0.0004
3 Ring	−0.0003	0.0000	−0.0072	1.4778	−1.1213	−0.5559	...	0.0517
4 Ring	0.0001	0.0000	0.0018	−0.0411	2.5629	−1.3179	...	−0.0177
5 Ring	0.0007	0.0008	0.0072	0.0564	0.0829	3.7619	...	−0.1890
MA	−0.0015	−0.0018	−0.0161	−0.1253	−0.2574	−0.3897	...	0.4238

TABLE 1 *Continued*

	∑71	∑ 69	∑ 109	∑ 149	∑ 189	∑ 229	∑ 269	∑91
				C_{23} Inverse				
n-Alkanes								
0 Ring	0.5093	−0.0518	−0.0153	0.0226	0.0407	0.0521	...	−0.0285
1 Ring	−0.1003	0.3404	−0.1976	−0.1142	−0.0446	0.0282	...	−0.0269
2 Ring	−0.0024	0.0021	0.7580	−0.5880	−0.3011	−0.1405	...	−0.0008
3 Ring	−0.0002	0.0001	−0.0103	1.4393	−1.0839	−0.5414	...	0.0542
4 Ring	0.0001	0.0000	0.0020	−0.0425	2.4806	−1.2840	...	−0.0149
5 Ring	0.0005	0.0007	0.0066	0.0539	0.0750	3.6015	...	−0.1927
MA	−0.0011	−0.0017	−0.0148	−0.1189	−0.2409	−0.3560	...	0.4300
Isoalkanes								
0 Ring	0.6093	−0.0619	−0.0183	0.0270	0.0487	0.0624	...	−0.0341
1 Ring	−0.1338	0.3439	−0.1965	−0.1156	−0.0473	0.0248	...	−0.0250
2 Ring	−0.0038	0.0023	0.7580	−0.5882	−0.3013	−0.1406	...	−0.0008
3 Ring	−0.0004	0.0001	−0.0103	1.4393	−1.0839	−0.5415	...	0.0542
4 Ring	0.0001	0.0000	0.0020	−0.0426	2.4806	−1.2840	...	−0.0149
5 Ring	0.0009	0.0007	0.0066	0.0539	0.0750	3.6016	...	−0.1927
MA	−0.0190	−0.0016	−0.0148	−0.1189	−0.2410	−0.3561	...	0.4300
				C_{24} Inverse				
n-Alkanes								
0 Ring	0.5105	−0.0566	−0.0174	0.0249	0.0434	0.0528	0.0372	−0.0324
1 Ring	−0.1061	0.3414	−0.1960	−0.1128	−0.0420	0.0288	0.0761	−0.0337
2 Ring	−0.0016	−0.0011	0.7505	−0.5807	−0.2908	−0.1418	0.0047	−0.0011
3 Ring	−0.0003	0.0004	−0.0146	1.4098	−1.0564	−0.5371	−0.2987	0.0706
4 Ring	0.0000	−0.0001	0.0014	−0.0506	2.3673	−1.2328	−0.6560	0.0085
5 Ring	0.0004	0.0005	0.0048	0.0407	0.0457	3.3827	−0.9376	−0.1544
6 Ring	0.0005	0.0006	0.0055	0.0457	0.0911	0.1138	3.9809	−0.1763
MA	−0.0012	−0.0015	−0.0143	−0.1190	−0.2369	−0.3388	−0.4136	0.4594
Isoalkanes								
0 Ring	0.6094	−0.0675	−0.0208	0.0297	0.0518	0.0631	0.0444	−0.0397
1 Ring	−0.1403	0.3451	−0.1948	−0.1145	−0.0449	0.0253	0.0736	−0.0315
2 Ring	−0.0032	−0.0009	0.7506	−0.5808	−0.2910	−0.1420	0.0045	−0.0010
3 Ring	−0.0006	0.0004	−0.0145	1.4098	−1.0564	−0.5352	−0.2986	0.0706
4 Ring	0.0000	−0.0001	0.0014	−0.0506	2.3673	−1.2328	−0.6560	0.0085
5 Ring	0.0009	0.0005	0.0048	0.0407	0.0457	3.3828	−0.9376	−0.1544
6 Ring	0.0010	0.0005	0.0055	0.0457	0.0911	0.1139	3.9809	−0.1764
MA	−0.0026	−0.0014	−0.0142	−0.1190	−0.2370	−0.3389	−0.4137	0.4595
				C_{25} Inverse				
n-Alkanes								
0 Ring	0.5132	−0.0621	−0.0196	0.0262	0.0471	0.0493	0.0383	−0.0344
1 Ring	−0.1115	0.3425	−0.1930	−0.1133	−0.0435	0.0302	0.0753	−0.0380
2 Ring	−0.0009	−0.0040	0.7378	−0.5623	−0.2821	−0.1450	−0.0032	−0.0005
3 Ring	−0.0005	0.0006	−0.0185	1.3763	−1.0229	−0.5229	−0.2858	0.0741
4 Ring	0.0000	−0.0001	0.0019	−0.0520	2.2834	−1.1777	−0.6213	0.0034
5 Ring	0.0005	0.0005	0.0043	0.0389	0.0409	3.2347	−0.8915	−0.1577
6 Ring	0.0005	0.0005	0.0048	0.0424	0.0836	0.1304	3.7174	−0.1753
MA	−0.0013	−0.0014	−0.0128	−0.1125	−0.2213	−0.3157	−0.3738	0.4652
Isoalkanes								
0 Ring	0.6096	−0.0738	−0.0233	0.0311	0.0559	0.0586	0.0455	−0.0409
1 Ring	−0.1449	0.3465	−0.1918	−0.1150	−0.0461	0.0256	0.0727	−0.0358
2 Ring	−0.0023	−0.0039	0.7378	−0.5624	−0.2821	−0.1452	−0.0032	−0.0005
3 Ring	−0.0008	0.0007	−0.0185	1.3762	−1.0229	−0.5229	−0.2857	0.0741
4 Ring	0.0000	−0.0001	0.0019	−0.0520	2.2834	−1.1777	−0.6213	0.0034
5 Ring	0.0011	0.0004	0.0043	0.0389	0.0410	3.2347	−0.8914	−0.1578
6 Ring	0.0012	0.0004	0.0048	0.0424	0.0836	0.1034	3.7175	−0.1754
MA	−0.0032	−0.0012	−0.0127	−0.1126	−0.2215	−0.3159	−0.3740	0.4653
				C_{26} Inverse				
n-Alkanes								
0 Ring	0.5161	−0.0679	−0.0225	0.0282	0.0500	0.0496	0.0388	−0.0369
1 Ring	−0.1166	0.3429	−0.1912	−0.1146	−0.0445	0.0291	0.0764	−0.0425
2 Ring	0.0003	−0.0080	0.7313	−0.5486	−0.2776	−0.1391	−0.0096	−0.0006
3 Ring	−0.0005	0.0010	−0.0225	1.3441	−0.9981	−0.4986	−0.2786	0.0779
4 Ring	0.0000	−0.0001	0.0023	−0.0526	2.2145	−1.1323	−0.5916	−0.0014
5 Ring	0.0005	0.0004	0.0039	0.0372	0.0355	3.0605	−0.8433	−0.1603
6 Ring	0.0005	0.0005	0.0044	0.0402	0.0776	0.0914	3.4893	−0.1773
MA	−0.0014	−0.0012	−0.0118	−0.1079	−0.2080	−0.2883	−0.3450	0.4762
Isoalkanes								
0 Ring	0.6106	−0.0804	−0.0267	0.0334	0.0592	0.0586	0.0459	−0.0436
1 Ring	−0.1513	0.3475	−0.1897	−0.1165	−0.0479	0.0254	0.0700	−0.0401
2 Ring	−0.0012	−0.0078	0.7315	−0.5487	−0.2778	−0.1393	−0.0100	−0.0002
3 Ring	−0.0011	0.0011	−0.0225	1.3441	−0.9981	−0.4986	−0.2786	0.0779
4 Ring	0.0001	−0.0001	0.0023	−0.0526	2.2145	−1.1323	−0.5916	−0.0014
5 Ring	0.0013	0.0003	0.0039	0.0372	0.0356	3.0606	−0.8433	−0.1604
6 Ring	0.0015	0.0003	0.0044	0.0402	0.0777	0.0915	3.4894	−0.1774
MA	−0.0040	−0.0009	−0.0117	−0.1081	−0.2083	−0.2885	−0.3452	0.4763
				C_{27} Inverse				

TABLE 1 *Continued*

	∑71	∑ 69	∑ 109	∑ 149	∑ 189	∑ 229	∑ 269	∑91
n-Alkanes								
0 Ring	0.5207	−0.0742	−0.0259	0.0301	0.0543	0.0504	0.0374	−0.0393
1 Ring	−0.2119	0.3430	−0.1872	−0.1135	−0.0461	0.0276	0.0696	−0.0477
2 Ring	0.0014	−0.0118	0.7203	−0.5347	−0.2754	−0.1418	−0.0158	0.0000
3 Ring	−0.0008	0.0014	−0.0270	1.3144	−0.9676	−0.4789	−0.2650	0.0810
4 Ring	0.0001	−0.0001	0.0027	−0.0532	2.1375	−1.0763	−0.5666	−0.0083
5 Ring	0.0005	0.0004	0.0035	0.0355	0.0310	2.9059	−0.7842	−0.1629
6 Ring	0.0006	0.0004	0.0039	0.0373	0.0704	0.0814	3.2533	−0.1756
MA	−0.0015	−0.0011	−0.0106	−0.1027	−0.1933	−0.2678	−0.3125	0.4834
Isoalkanes								
0 Ring	0.6117	−0.0872	−0.0305	0.0354	0.0637	0.0592	0.0439	−0.0462
1 Ring	−0.1562	0.3479	−0.1855	−0.1155	−0.0497	0.0238	0.0672	−0.0450
2 Ring	0.0000	−0.0116	0.7204	−0.5348	−0.2756	−0.1420	−0.0160	0.0001
3 Ring	−0.0014	0.0015	−0.0270	1.3144	−0.9677	−0.4789	−0.2650	0.0811
4 Ring	0.0001	−0.0002	0.0027	−0.0532	2.1375	−1.0763	−0.5666	−0.0083
5 Ring	0.0016	0.0002	0.0035	0.0356	0.0300	2.9060	−0.7842	−0.1630
6 Ring	0.0017	0.0002	0.0038	0.0374	0.0706	0.0815	3.2534	−0.1757
MA	−0.0048	−0.0006	−0.0105	−0.1028	−0.1937	−0.2681	−0.3127	0.4836
				C_{28} Inverse				
n-Alkanes								
0 Ring	0.5245	−0.0815	−0.0296	0.0332	0.0579	0.0525	0.0346	−0.0419
1 Ring	−0.1275	0.3448	−0.1848	−0.1140	−0.0466	0.0253	0.0698	−0.0545
2 Ring	0.0032	−0.0165	0.7148	−0.5230	−0.2670	−0.1396	−0.0208	0.0003
3 Ring	−0.0010	0.0019	−0.0304	1.2771	−0.9282	−0.4724	−0.2582	0.0855
4 Ring	0.0001	−0.0002	0.0031	−0.0538	2.0568	−1.0243	−0.5430	−0.0142
5 Ring	0.0006	0.0003	0.0032	0.0340	0.0263	2.7716	−0.7622	−0.1666
6 Ring	0.0006	0.0003	0.0035	0.0355	0.0667	0.0725	3.0949	−0.1791
MA	−0.0017	−0.0009	−0.0097	−0.0981	−0.1837	−0.2444	−0.2892	0.4945
Isoalkanes								
0 Ring	0.6174	−0.0959	−0.0349	0.0390	0.0682	0.0618	0.0408	−0.0493
1 Ring	−0.1625	0.3502	−0.1827	−0.1163	−0.0504	0.0217	0.0676	−0.5016
2 Ring	0.0016	−0.0162	0.7149	−0.5232	−0.2671	−0.1396	−0.0209	0.0004
3 Ring	−0.0018	0.0021	−0.0304	1.2771	−0.0283	−0.4725	−0.2583	0.0855
4 Ring	0.0002	−0.0002	0.0031	−0.0538	2.0568	−1.0243	−0.5430	−0.0142
5 Ring	0.0020	0.0001	0.0031	0.0341	0.0264	2.7717	−0.7621	−0.1667
6 Ring	0.0021	0.0001	0.0034	0.0356	0.0669	0.0726	3.0950	−0.1792
MA	−0.0058	−0.0003	0.0094	−0.0983	−0.1841	−0.2448	−0.2895	0.4948
				C_{29} Inverse				
n-Alkanes								
0 Ring	0.5305	−0.0902	−0.0337	0.0353	0.0639	0.0565	0.0347	−0.0441
1 Ring	−0.1342	0.3482	−0.1825	−0.1143	−0.0495	0.0225	0.0668	−0.0613
2 Ring	0.0049	−0.0214	0.7054	−0.5089	−0.2628	−0.1371	−0.0261	0.0007
3 Ring	−0.0013	0.0025	−0.0356	1.2520	−0.8991	−0.4619	−0.2492	0.0900
4 Ring	0.0002	−0.0002	0.0037	−0.0558	1.9849	−0.9773	−0.5067	−0.0237
5 Ring	0.0006	0.0003	0.0027	0.0322	0.0216	2.6445	−0.7174	−0.1685
6 Ring	0.0006	0.0003	0.0029	0.0327	0.0612	0.0656	2.8747	−0.1773
MA	−0.0018	−0.0008	−0.0086	−0.0925	−0.1724	−0.2300	−0.2603	0.5016
Isoalkanes								
0 Ring	0.6202	−0.1055	−0.0394	0.0413	0.0747	0.0661	0.0406	−0.0515
1 Ring	−0.1684	0.3540	−0.1803	−0.1166	−0.0536	0.0189	0.0644	−0.0584
2 Ring	0.0033	−0.0211	0.7054	−0.5091	−0.2631	−0.1372	−0.0263	0.0008
3 Ring	−0.0023	0.0027	−0.0356	1.2520	−0.8992	−0.4620	−0.2494	0.0901
4 Ring	0.0004	−0.0003	0.0036	−0.0557	1.9850	−0.9773	−0.5067	−0.0237
5 Ring	0.0023	0.0000	0.0027	0.0323	0.0218	2.6447	−0.7172	−0.1686
6 Ring	0.0024	0.0000	0.0030	0.0328	0.0614	0.0658	2.8748	−0.1775
MA	−0.0068	0.0001	−0.0079	−0.0928	−0.1730	−0.2305	−0.2606	0.5020
				C_{30} Inverse				
n-Alkanes								
0 Ring	0.5352	−0.0989	−0.0388	0.0385	0.0707	0.0600	0.0359	−0.0468
1 Ring	−0.1397	0.3508	−0.1801	−0.1125	−0.0526	0.0196	0.0647	−0.0687
2 Ring	0.0071	−0.0272	0.7014	−0.5010	−0.2562	−0.1355	−0.0317	0.0012
3 Ring	−0.0015	0.0033	−0.0408	1.2276	−0.8689	−0.4464	−0.2343	0.0942
4 Ring	0.0002	−0.0003	0.0042	−0.0560	1.9167	−0.9357	−0.4859	−0.0327
5 Ring	0.0007	0.0002	0.0024	0.0301	0.0176	2.5139	−0.6842	−0.1712
6 Ring	0.0007	0.0002	0.0027	0.0300	0.0570	0.0563	2.6980	−0.1781
MA	−0.0020	−0.0006	−0.0079	−0.0864	−0.1632	−0.2080	−0.2359	0.5121
Isoalkanes								
0 Ring	0.6232	−0.1151	−0.0452	0.0445	0.0823	0.0699	0.0417	−0.0545
1 Ring	−0.1735	0.3570	−0.1776	−0.1148	−0.0570	0.0158	0.0624	−0.0657
2 Ring	0.0055	−0.0268	0.7016	−0.5010	−0.2565	−0.1356	−0.0318	0.0021
3 Ring	−0.0027	0.0036	−0.0407	1.2275	−0.8691	−0.4466	−0.2344	0.0944
4 Ring	0.0006	−0.0004	0.0041	−0.0560	1.9168	−0.9456	−0.4859	−0.0327
5 Ring	0.0027	−0.0002	0.0023	0.0302	0.0178	2.5142	−0.6841	−0.1714
6 Ring	0.0028	−0.0002	0.0026	0.0302	0.0573	0.0566	2.6981	−0.1782
MA	−0.0079	0.0005	−0.0070	−0.0868	−0.1640	−0.2086	−0.2363	0.5127

TABLE 1 *Continued*

	∑71	∑ 69	∑ 109	∑ 149	∑ 189	∑ 229	∑ 269	∑91
				C_{31} Inverse				
n-Alkanes								
0 Ring	0.5434	−0.1086	−0.0446	0.0411	0.0749	0.0637	0.0375	−0.0488
1 Ring	−0.1461	0.3529	−0.1757	−0.1134	−0.0529	0.0178	0.0601	−0.0784
2 Ring	0.0097	−0.0334	0.6937	−0.4895	−0.2463	−0.1371	−0.0348	0.0030
3 Ring	−0.0020	0.0044	−0.0471	1.2055	−0.8440	−0.4316	−0.2258	0.0990
4 Ring	0.0003	−0.0004	0.0048	−0.0583	1.8512	−0.8912	−0.4645	−0.0413
5 Ring	0.0007	0.0002	0.0022	0.0292	0.0144	2.3848	−0.6467	−0.1741
6 Ring	0.0007	0.0002	0.0023	0.0287	0.0535	0.0496	2.5297	−0.1794
MA	−0.0021	−0.0005	−0.0068	−0.0837	−0.1550	−0.1893	−0.2155	0.5223
Isoalkanes								
0 Ring	0.6286	−0.1256	−0.0515	0.0475	0.0867	0.0737	0.0434	−0.0564
1 Ring	−0.1788	0.3594	−0.1731	−0.1160	−0.0573	0.0138	0.0579	−0.0755
2 Ring	0.0081	−0.0331	0.6938	−0.4896	−0.2464	−0.1374	−0.0370	0.0033
3 Ring	−0.0035	0.0047	−0.0471	1.2054	−0.8442	−0.4318	−0.2260	0.0990
4 Ring	0.0009	−0.0005	0.0047	−0.0582	1.8512	−0.8912	−0.4645	−0.0413
5 Ring	0.0031	−0.0003	0.0020	0.0294	0.0147	2.3851	−0.6465	−0.1743
6 Ring	0.0031	−0.0003	0.0021	0.0289	0.0538	0.0499	2.5299	−0.1796
MA	−0.0092	0.0010	−0.0062	−0.0843	−0.1559	−0.1901	−0.2160	0.5230
				C_{32} Inverse				
n-Alkanes								
0 Ring	0.5524	−0.1199	−0.0522	0.0451	0.0830	0.0690	0.0393	−0.0513
1 Ring	−0.1527	0.3568	−0.1724	−0.1132	−0.0567	0.0145	0.0576	−0.0886
2 Ring	0.0130	−0.0409	0.6907	−0.4755	−0.2442	−0.1333	−0.0390	0.0050
3 Ring	−0.0026	0.0056	−0.0523	1.1703	−0.8144	−0.4180	−0.2142	0.1027
4 Ring	0.0004	−0.0005	0.0053	−0.0594	1.7832	−0.8458	−0.4427	−0.0494
5 Ring	0.0008	0.0001	0.0019	0.0282	0.0106	2.2659	−0.6013	−0.1790
6 Ring	0.0008	0.0001	0.0020	0.0267	0.0487	0.0443	2.3575	−0.1786
MA	−0.0023	−0.0003	−0.0058	−0.0797	−0.1444	−0.1774	−0.1926	0.5328
Isoalkanes								
0 Ring	0.6349	−0.1378	−0.0600	0.0519	0.0954	0.0793	0.0451	−0.0590
1 Ring	−0.1841	0.3636	−0.1694	−0.1158	−0.0615	0.0106	0.0553	−0.0856
2 Ring	0.0119	−0.0405	0.6908	−0.4756	−0.2444	−0.1335	−0.0414	0.0051
3 Ring	−0.0042	0.0060	−0.0521	1.1702	−0.8114	−0.4183	−0.2144	0.1029
4 Ring	0.0012	−0.0007	0.0053	−0.0594	1.7833	−0.8457	−0.4426	−0.0495
5 Ring	0.0035	−0.0005	0.0016	0.0284	0.0110	2.2663	−0.6011	−0.1792
6 Ring	0.0035	−0.0005	0.0018	0.0269	0.0491	0.0447	2.3577	−0.1789
MA	−0.0105	0.0015	−0.0050	−0.0803	−0.1457	−0.1785	−0.1932	0.5336

8.2 *Instrumental Conditions*—Repeller settings are adjusted to optimum based on *m/e* 226 ion of *n*-hexadecane. A magnetic field is used that will permit a scan over the mass range 65 *m/e* to 410 *m/e*. An ionization voltage of 70 eV and an ionizing current in the range 10 µA to 70 µA is used.

NOTE 1—The instrument conditions and calibration matrix inverses described in this method are based on the use of a 180° magnetic-deflection type mass spectrometer (CEC Model 21–103). It is not known if the calibration matrix inverses, included in this method, are suitable for use on other mass spectrometer types.

8.3 *Calibration Standard*—The calibration coefficients in this method were obtained for ion source conditions such that the ∑ 69/∑ 71 ratio was 0.20/1.0 for *n*-hexadecane. The cooperative study of this method indicated an acceptable range for the ∑ ratio was between 0.18 to 0.22.

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 67 to 409.

10. Calculation

10.1 *Recording Mass Spectra*—Read peak heights from the mass spectrum of the sample corresponding to the m/e^+ itemized under 3.1.1.1 to 3.1.1.8, inclusive, and correct all peaks for heavy isotopes by the use of the two peaks immediately preceding the peak to be corrected.

10.2 Form the peak summations described under 3.1.1.1 to 3.1.1.8, inclusive.

10.3 *Selection of Proper Inverse from* Table 2*:*

NOTE 2—Sample history and physical property data provide the best criteria for inverse selection and are preferred, if available, over the described procedure.

10.3.1 The carbon number of the largest deisotoped C_nH_{2n+2} peak is assumed to be the average carbon number.

TABLE 2 Precision Summary Based on Cooperative Data

	Volume Percent	σ_r	σ_R	r	R
0 Ring	10.5	0.5	1.6	1.5	5.4
1 Ring	17.3	0.5	1.5	1.8	5.0
2 Ring	15.8	0.2	1.5	0.5	4.9
3 Ring	16.7	0.2	1.0	0.8	3.2
4 Ring	30.1	0.6	3.4	2.0	11.0
5 Ring	6.8	0.3	1.3	0.9	4.3
6 Ring	2.8	0.2	1.1	0.7	3.5

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

10.3.2 The following equation will determine whether the iso or normal inverse coefficients should be used.

$$\text{Set} = (ab)/[(ab)+(cd)] = r \quad (9)$$

where:

a = respective normal paraffin sensitivity factor from the table below,
b = deisotoped average C_nH_{2n+2} peak (corresponds to molecular weight of n-paraffin),
c = respective isoparaffin sensitivity factor from the table below,
d = deisotoped $C_nH_{2\ n+1}$ peak at two carbon numbers less than the average C_nH_{2n+2} peak (n-paraffin peak – 29 mass units), and
r = ratio.

If r is 0.50 or higher, use the respective n-paraffin inverse coefficients; otherwise use the isoparaffin inverse coefficients. Interpolate where necessary.

	Sensitivity Factors	
Average Carbon No.	n-Paraffins	Isoparaffins
16	0.347	0.0364
20	0.606	0.0505
24	1.250	0.0735
28	2.439	0.1061
32	4.000	0.1380

NOTE 3—The sensitivity factors in the above table are valid when the mass spectrometer is operated in such a mode as to give a 127/226 ratio for n-hexadecane of 1.4, approximately. If this ratio cannot be attained, an individual laboratory should replace the above factors with sensitivity data representative of actual instrument operation.

10.4 After the proper inverse has been selected, carry out the following calculations:

$$a = (b_1c_1) \pm (b_2c_2) \pm (b_3c_3) \pm \ldots \pm (b_{\ 8}c_8) \quad (10)$$

where:

a = partial ion intensity of alkanes,
b_1 = $\sum$ 71, $b_2 = \sum$ 69, etc., and
c_1 = $\sum$ 71 inverse, $c_2 = \sum$ 69 inverse, etc.

Repeat the corresponding calculation to obtain a solution for 1-ring, 2-ring, 3-ring, etc.

10.5 Normalize all partial ion intensities to 100.0 and report as volume percent.

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 1, is as follows:

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 2 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 2 only in one case in twenty.

NOTE 4—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 gas oil; mass spectrometry; petroleum; saturates