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E137 Practice for Evaluation of Mass Spectrometers for Quantitative Analysis from a Batch Inlet (Withdrawn 1992)[4]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