Designation: D 2786 – 91 (Reapproved 2001)ε1

An American National Standard

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 D 2786; 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.

ε[1] NOTE—Footnote 5 was editorially corrected in November 2001.

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:*

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

D 3239 Test Method for Aromatic Types Analysis of Gas-Oil Aromatic 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 Groupings*:

3.1.1.1

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

3.1.1.2

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

3.1.1.3

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

3.1.1.4

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

3.1.1.5

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

3.1.1.6

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

3.1.1.7

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

3.1.1.8

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

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 using a summation of mass fragment groups most characteristic of each molecular type. Calculations are carried out by the

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

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

[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.

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 D 2549.

5. Significance and Use

5.1 A knowledge of the hydrocarbon composition of process streams and petroleum products boiling within the range of 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.

5.2 This test method, when used together with Test Method D 3239, 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 Recommended 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*.

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

	Σ71	Σ 69	Σ 109	Σ 149	Σ 189	Σ 229	Σ 269	Σ91
				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

TABLE 1 *Continued*

	Σ71	Σ 69	Σ 109	Σ 149	Σ 189	Σ 229	Σ 269	Σ91
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
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*

	Σ71	Σ 69	Σ 109	Σ 149	Σ 189	Σ 229	Σ 269	Σ91
				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