# MOLECULAR WEIGHT PREDICTS NORMAL BOILING POINTS–AN EXTENSION TO BRANCHED CHAIN COMPOUNDS

*By* B. C. MATHUR AND N. R. KULOOR*

*(Department of Chemical Engineering, Indian Institute of Science, Bangalore-12, India)*

[Received: June 3, 1970]

ABSTRACT

*Boiling points of Branched Chain Compounds have been predicted using molecular weight as the simple correlation property by the equation,*

$T_b = n_1 (M) + c_1$, $T_b$ – *Boiling point* °C, $M$ – *Molecular weight*, $n_1$, $c_1$ – *constants.*

Das *et. al*[1]. proposed a simple correlation to predict normal boiling point of hydrocarbons and organic liquids using molecular weight as the correlation property with an average error of 2.5%. The same approach used for critical properties,[2,3,4] has been extended for the prediction of normal boiling points of isomeric compounds of aliphatic and aromatic hydrocarbons, cyclohexanes, cyclohexenes, cyclopentanes, cyclopentenes and group of alkyl naphthalenic and styrene compounds.

The present method is based on a simple correlation using molecular weight as the input property. A linear relationship is obtained when normal boiling points are plotted on ordinary co-ordinates against molecular weights for different isomeric groups of 384 compounds, whose molecular weight ranged from 56.10 to 296.47 and whose boiling points varied between 20.06 to 41.5 degree centigrade.

Figures 1 and 2 show the linear relationships for alkanes and alkyl naphthalenes. Similar relationships are obtained for other groups considered. Since each group contains a number of compounds of the same molecular weight and approximately same boiling points, only one or two compounds of a given molecular weight in each group are considered.

Table I groups all the 384 isomeric compounds into different series and gives normal boiling points obtained from literature[5]. These are compared with normal boiling points calculated by the present correlation and gives the percentage error. The compounds, marked with asterisk for which the per cent deviation is more than 10 are not considered in the calculation of the average percentage error.

* Deceased.

The general equation for the prediction of normal boiling point is

$$T_b = n_1 (M) + c_1 \qquad [1]$$

The values of the constants $n_1$ & $c_1$ for different groups are given in Table 2. The overall average absolute error is found to be 3.35%.

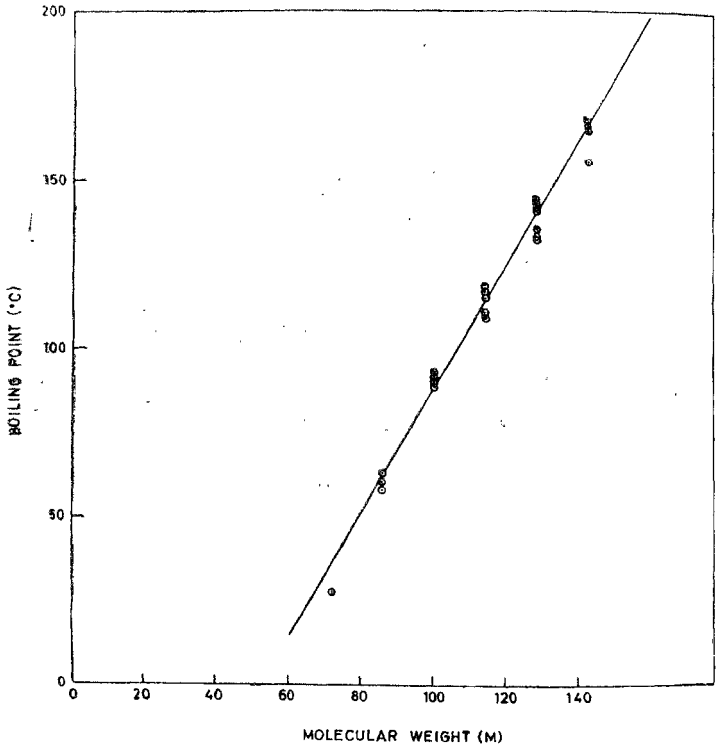


FIG. 1

Relation between Boiling point ($T_b$) vs. Molecular weight ($M$) of Alkanes

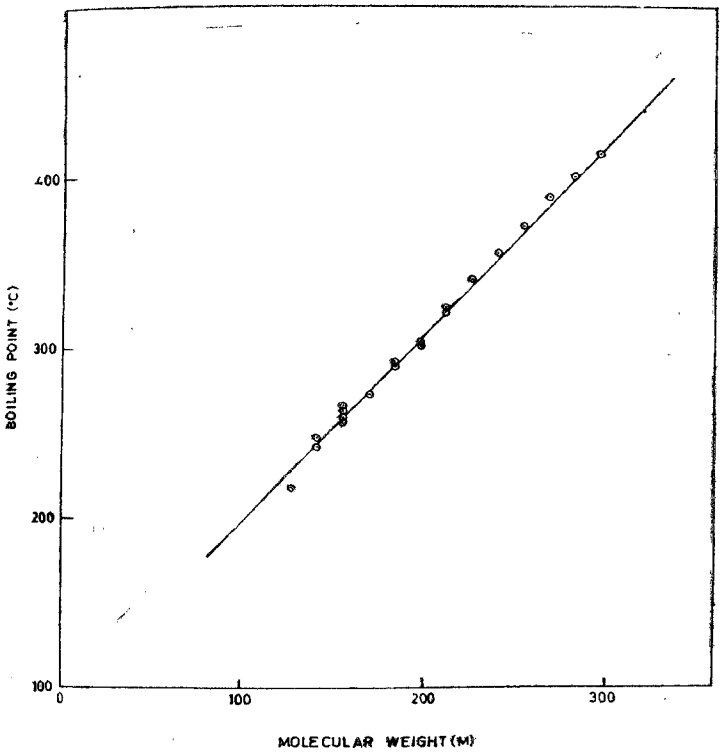


FIG. 2

Relation between Boiling point ($T_b$) vs. Molecular weight ($M$) of Alkyl Naphthalenes.

TABLE I

Experimental and Calculated values of Boiling Points

| | | | $T_b$ | | |
|---|---|---|---|---|---|
| | | M. | Lit. | Calc. | % Error |
| *I. Alkanes*: | | | | | |
| 1. | Isobutane | 58.12 | ---- | ..... | ..... |
| 2. | Isopentane | 72.14 | 27.85 | 37.70 | 35.40* |
| 3. | 3-Methyl pentane | 86.17 | 63.28 | 63.20 | −1.26 |
| 4. | Isohexane | ,, | 60.27 | ,, | 4.86 |
| 5. | 2,2-Dimethyl butane | ,, | 49.74 | ,, | 27.10* |
| 6. | 2,3-Dimethyl butane | ,, | 57.98 | ,, | 9.05 |
| 7. | 2-Methyl hexane | 100.19 | 90.05 | 92.10 | 2 16 |
| 8. | 3-Methyl hexane | ,, | 91.85 | ,, | 1.37 |
| 9. | 3-Ethyl pentane | ,, | 93.47 | ,, | −1.47 |
| 10. | 2,2-Dimethyl pentane | ,, | 79.19 | ,, | 16.30* |
| 11. | 2.3-Dimethyl pentane | ,, | 89.79 | ,, | 2.58 |
| 12. | 2,4-Dimethyl pentane | ,, | 80.50 | ,, | 14.40* |
| 13. | 3,3-Dimethyl pentane | ,, | 86.06 | ,, | 7.00 |
| 14. | 2,2,3-Trimethyl butane | ,, | 80.88 | ,, | 13.90* |
| 15. | 2-Methyl heptane | 114.22 | 117.64 | 116.00 | −1.41 |
| 16. | 3-Methyl heptane | ,, | 118.92 | ,, | −2.46 |
| 17. | 4-Methyl heptane | ,, | 117.70 | ,, | −1.45 |
| 18. | 3-Ethyl hexane | ,, | 118.53 | ,, | −2.14 |
| 19. | 2,2-Dimethyl hexane | ,, | 106.84 | ,, | 8.60 |
| 20. | 2,3-Dimethyl hexane | ,, | 115.60 | ,, | 0 35 |
| 21. | 2,4-Dimethyl hexane | ,, | 109 42 | ,, | 6.02 |
| 22. | 2,5-Dimethyl hexane | ,, | 109.10 | ,, | 6.32 |
| 23. | 3,3-Dimethyl hexane | ,, | 111.96 | ,, | 4.55 |
| 24. | 3,4-Dimethyl hexane | ,, | 117.72 | ,, | −1.46 |
| 25. | 3-Ethyl-2-methyl pentane | ,, | 115.65 | ,, | 0.35 |
| 26. | 3-Ethyl-3-methyl pentane | ,, | 118.25 | ,, | −2.19 |
| 27. | 2,2,3-Trimethyl pentane | ,, | 109.84 | ,, | 5.65 |
| 28. | 2,2,4-Trimethyl pentane | ,, | 99.23 | ,, | 17.15* |
| 29. | 2,3,3-Trimethyl pentane | ,, | 114.76 | ,, | 1.08 |
| 30. | 2,3,4-Trimethyl pentane | ,, | 113.46 | ,, | 2.24 |
| 31. | 2,2,3,3-Tetramethyl butane | ,, | 106.47 | ,, | 8.95 |

TABLE I—(*contd.*)

| | | | $T_b$ | | |
|---|---|---|---|---|---|
| | | M | Lit. | Calc. | % Error |
| 32. | 2-Methyl octane | 128.25 | 143.26 | 142.00 | −0.89 |
| 33. | 3-Methyl octane | ,, | 144.18 | ,, | −1.51 |
| 34. | 4-Methyl octane | ,, | 142 48 | ,, | −0.34 |
| 35. | 3-Ethyl heptane | ,, | 143.00 | ,, | −0.70 |
| 36. | 4-Ethyl heptane | ,, | 141.20 | ,, | 0.57 |
| 37. | 2,2-Dimethyl heptane | ,, | 132 69 | ,, | 7.02 |
| 38. | 2,3-Dimethyl heptane | ,, | 140.50 | ,, | 1.07 |
| 39. | 2,4-Dimethyl heptane | ,, | 133.50 | ,, | 6.77 |
| 40. | 2,5-Dimethyl heptane | ,, | 136.00 | ,, | 4.41 |
| 41. | 2,6-Dimethyl heptane | ,, | 135.21 | ,, | 5.01 |
| 42. | 3,3-Dimethyl heptane | ,, | 137.30 | ,, | 3.41 |
| 43. | 3,4-Dimethyl heptane | ,, | 140.60 | ,, | 0.99 |
| 44. | 3,5-Dimethyl heptane | ,, | 136.00 | ,, | 4.41 |
| 45. | 4,4-Dimethyl heptane | ,, | 135.20 | ,, | 5.01 |
| 46. | 3-Ethyl-2-2-methyl hexane | ,, | 138.00 | ,, | 2.90 |
| 47. | 4-Ethyl-2-methyl hexane | ,, | 133.80 | ,, | 6.88 |
| 48. | 3-Ethyl-3-methyl hexane | ,, | 140.60 | ,, | 0.99 |
| 49. | 4-Ethyl-3-methyl hexane | ,, | 140.40 | ,, | 1.14 |
| 50. | 2,2,3-Trimethyl hexane | ,, | 133.60 | ,, | 7.05 |
| 51. | 2,2,4-Trimethyl hexane | ,, | 126.54 | ,, | 12.30* |
| 52. | 2,2,5-Trimethyl hexane | ,, | 124.08 | ,, | 14.45* |
| 53. | 2,3,3-Trimethyl hexane | ,, | 137.68 | ,, | 3.15 |
| 54. | 2,3,4-Trimethyl hexane | ,, | 139.00 | ,, | 1.16 |
| 55. | 2,3,5-Trimethyl hexane | ,, | 131.34 | ,, | 8.10 |
| 56. | 2,4,4-Trimethyl hexane | ,, | 130 64 | ,, | 8.70 |
| 57. | 3,3,4-Trimethyl hexane | ,, | 140.46 | ,, | 1.10 |
| 58. | 3,3-Diethyl pentane | ,, | 146.16 | ,, | −2.84 |
| 59. | 3-Ethyl-2-dimethyl pentane | ,, | 133.83 | ,, | 6.11 |
| 60. | 3-Ethyl-2,3-dimethyl pentane | ,, | 142.00 | ,, | 0.00 |
| 61. | 3-Ethyl-2,4-dimethyl pentane | ,, | 136.73 | ,, | 3.86 |
| 62. | 2,2,3,3-Tetramethyl pentane | ,, | 140 27 | ,, | 1.22 |
| 63. | 2,2,3,4-Tetramethyl pentane | ,, | 133.01 | ,, | 6.75 |
| 64. | 2,2,4,4-Tetramethyl pentane | ,, | 122.28 | ,, | 16.20* |

TABLE I—(*contd.*)

| | | $T_b$ | | | |
|---|---|---|---|---|---|
| | | M. | Lit. | Calc. | % Error |
| 65. | 2,3,3,4-Tetramethyl pentane | 142.28 | 141.55 | 142.00 | 0.39 |
| 66. | 2-Methyl nonane | ,, | 166.80 | 167.50 | 0.91 |
| 67. | 3-Methyl nonane | ,, | 167.80 | ,, | −0.81 |
| 68. | 4-Methyl nonane | ,, | 165.70 | ,, | 1.27 |
| 69. | 5-Methyl nonane | ,, | 165.10 | ,, | 1.64 |
| 70. | 3-Ethyl octane | ,, | 168.00 | ,, | −0 30 |
| 71. | 4-Ethyl octane | ,, | 168.00 | ,, | −0 30 |
| 72. | 2,2-Dimethyl octane | ,, | 155.00 | ,, | 8.70 |
| 73. | 2,3-Dimethyl octane | ,, | 163.80 | ,, | 1.65 |
| 74. | 2,4-Dimethyl octane | ,, | 153.00 | ,, | 9.48 |
| 75. | 2,5-Dimethyl octane | ,, | 158.00 | ,, | 6 00 |
| 76. | 2,6-Dimethyl octane | ,, | 158.54 | ,, | 5 66 |
| 77. | 2,7-Dimethyl octane | ,, | 159.87 | ,, | 4.79 |
| 78. | 3,3-Dimethyl octane | ,, | 161.20 | ,, | 3.90 |
| 79. | 3,4-Dimethyl octane | ,, | 166.00 | ,, | 0.91 |
| 80. | 3,5-Dimethyl octane | ,, | 160.00 | ,, | 4.68 |
| 81. | 3,6-Dimethyl octane | ,, | 160.00 | ,, | 4.68 |
| 82. | 4,4-Dimethyl octane | ,, | 161.00 | ,, | 4.04 |
| 83. | 4,5-Dimethyl octane | ,, | 162.13 | ,, | 3.30 |
| 84. | Propyl heptane | ,, | 162.00 | ,, | 3.39 |
| 85. | 4-Isopropyl heptane | ,, | 160.00 | ,, | 4 68 |
| 86. | 3-Ethyl-2-methyl heptane | ,, | 166.00 | ,, | 0 91 |
| 87. | 4-Ethyl-2-methyl heptane | ,, | 160.00 | ,, | 4 68 |
| 88. | 5-Ethyl-2-methyl heptane | ,, | 159.70 | ,, | 4.89 |
| 89. | 3-Ethyl-3-methyl heptane | ,, | 163.80 | ,, | 2.26 |
| 90. | 4-Ethyl-3-methyl heptane | ,, | 167.00 | ,, | 0.30 |
| 91. | 5-Ethyl-3-methyl heptane | ,, | 161.00 | ,, | 4 04 |
| 92. | 3-Ethyl-4-methyl heptane | ,, | 167.00 | ,, | 0.30 |
| 93. | 4-Ethyl-4-methyl heptane | ,, | 167.00 | ,, | 0 30 |
| 94. | 2,2,3-Trimethyl heptane | ,, | 158.00 | ,, | 6.00 |
| 95. | 2,2,4-Trimethyl heptane | ,, | 147.70 | ,, | 13.40* |
| 96. | 2,2,5-Trimethyl heptane | ,, | 148.00 | ,, | 13.20* |
| 97. | 2,2,6-Trimethyl heptane | ,, | 148.20 | ,, | 13.00* |

TABLE 1—(*contd.*)

| | | $T_b$ | | | |
|---|---|---|---|---|---|
| | | M | Lit. | Calc. | % Error |
| 98. | 2,3,3-Trimethyl heptane | 142.28 | 160.00 | 167.50 | 4.68 |
| 99. | 2,3,4-Trimethyl heptane | ,, | 163.00 | ,, | 2.76 |
| 100. | 2,3,5-Trimethyl heptane | ,, | 157.00 | ,, | 6.70 |
| 101. | 2,3,6-Trimethyl heptane | ,, | 155.00 | ,, | 8.07 |
| 102. | 2,4,4-Trimethyl heptane | ,, | 153.00 | ,, | 9.50 |
| 103. | 2,4,5-Trimethyl heptane | ,, | 157.00 | ,, | 6.70 |
| 104. | 2,4,6-Trimethyl heptane | ,, | 144.80 | ,, | 15.70* |
| 105. | 2,5,5-Trimethyl heptane | ,, | 152.80 | ,, | 9.64 |
| 106. | 3,3,4-Trimethyl heptane | ,, | 164.00 | ,, | 2.13 |
| 107. | 3,3,5-Trimethyl heptane | ,, | 155.68 | ,, | 7.60 |
| 108. | 3,4,4-Trimethyl heptane | ,, | 164.00 | ,, | 2.13 |
| 109. | 3,4,5-Trimethyl heptane | ,, | 164.00 | ,, | 2.13 |
| 110. | 3-Isopropyl-2-methyl hexane | ,, | 163.00 | ,, | 2.76 |
| 111. | 3,3-Diethyl hexane | ,, | 166.30 | ,, | 7.21 |
| 112. | 3,4-Diethyl hexane | ,, | 162.00 | ,, | 3.39 |
| 113. | 3-Ethyl-2,2-dimethyl hexane | ,, | 159.00 | ,, | 5.35 |
| 114. | 4-Ethyl-2,2-dimethyl hexane | ,, | 147.00 | ,, | 13.90* |
| 115. | 3-Ethyl-2,3-dimethyl hexane | ,, | 169.00 | ,, | 9.89 |
| 116. | 4-Ethyl-2,3-dimethyl hexane | ,, | 164.00 | ,, | 2.13 |
| 117. | 3-Ethyl-2,4-dimethyl hexane | ,, | 164.00 | ,, | 2.13 |
| 118. | 4-Ethyl-2,4-dimethyl hexane | ,, | 158.00 | ,, | 6.00 |
| 119. | 3-Ethyl-2,5-dimethyl hexane | ,, | 157.00 | ,, | 6.70 |
| 120. | 4-Ethyl-2,5-dimethyl hexane | ,, | 165.00 | ,, | 1.52 |
| 121. | 3-Ethyl-3,4-dimethyl hexane | ,, | 170.00 | ,, | −1.47 |
| 122. | 2,2,3,3-Tetramethyl hexane | ,, | 160.31 | ,, | 3.79 |
| 123. | 2,2,3,4-Tetramethyl hexane | ,, | 154.90 | ,, | 8.15 |
| 124. | 2,2,3,5-Tetramethyl hexane | ,, | 148.40 | ,, | 12.81* |
| 125. | 2,2,4,4-Tetramethyl hexane | ,, | 153.30 | ,, | 9.25 |
| 126 | 2,2,4,5-Tetramethyl hexane | ,, | 147 88 | ,, | 13.22* |
| 127. | 2,3,5,5-Tetramethyl hexane | ,, | 137.46 | ,, | 21 90* |
| 128. | 2,3,3,4-Tetramethyl hexane | ,, | 164 59 | ,, | 1 77 |
| 129. | 2,3,3,5-Tetramethyl hexane | ,, | 153 00 | ,, | 9.50 |
| 130. | 2,3,4,4-Tetramethyl hexane | ,, | 162 20 | ,, | 3.27 |

TABLE I—(*contd*)

| | | $T_b$ | | | |
|---|---|---|---|---|---|
| | | M | Lit. | Calc. | % Error |
| 131. | 2,3,4,5-Tetramethyl hexane | 142.28 | 161.00 | 167.50 | 4.03 |
| 132. | 3,3,4,4-Tetramethyl hexane | ,, | 170.00 | ,, | −1.47 |
| 133. | 3-Isopropyl-2,4-dimethyl pentane | ,, | 157.04 | ,, | 6.64 |
| 134. | 3,3-Diethyl-2-methyl pentane | ,, | 174.00 | ,, | −3.73 |
| 135. | 3-Ethyl-2,2,3-trimethyl pentane | ,, | 168.00 | ,, | −0 30 |
| 136. | 3-Ethyl-2,2,4-trimethyl pentane | ,, | 155.00 | ,, | 8.07 |
| 137. | 3-Ethyl-2,3,4-trimethyl pentane | ,, | 169.00 | ,, | −0.89 |
| 138. | 2,2,3,3,4-Pentamethyl pentane | ,, | 166.05 | ,, | 0 87 |
| 139. | 2,2,3,4,4-Pentamethyl pentane | ,, | 159 29 | ,, | 5.12 |
| | Average Error ... | | | | 3.70 |
| *II.* | *Alkenes*: | | | | |
| 1. | cis-2-butene | 56.11 | ..... | ..... | ..... |
| 2. | trans-2-butene | ,, | ..... | ..... | ..... |
| 3. | Isobutene | ,, | ..... | ..... | ..... |
| 4. | cis-2-pentene | 70.13 | 36.94 | 36.90 | −0 11 |
| 5. | trans-2-pentene | ,, | 36.35 | ,, | 1.49 |
| 6. | 2-Methyl-1-butene | ,, | 31.16 | ,, | 18.43* |
| 7. | 3-Methyl-1-butene | ,, | 20.16 | ,, | 80.40* |
| 8. | 2-Methyl-2-butene | ,, | 38.56 | ,, | −4.31 |
| 9. | cis-2-hexene | 84.16 | 63.48 | 64.70 | 1.93 |
| 10. | trans-2-hexene | ,, | 67.87 | ,, | −4.18 |
| 11. | cis-3-hexene | ,, | 66.44 | ,, | −2.62 |
| 12. | trans-3-hexene | ,, | 67 08 | ,, | −3.55 |
| 13. | 2-Methyl-1-pentene | ,, | 60.70 | ,, | 6.57 |
| 14. | 3-Methyl-1-pentene | ,, | 54.14 | ,, | 27 70* |
| 15. | 4-Methyl-1-pentene | ,, | 53.88 | ,, | 20.20* |
| 16. | 2-Methyl-2-pentene | ,, | 67.29 | ,, | −3.85 |
| 17. | 3-Methyl-cis-2-pentene | ,, | 70.45 | ,, | −8.17 |
| 18. | 3-Methyl-trans-2-pentene | ,, | 67 63 | ,, | −4.34 |
| 19. | 3-Methyl-cis-2-pentene | ,, | 56.30 | ,, | 14.90* |
| 20. | 4-Methyl-trans-2-pentene | ,, | 58.55 | ,, | 10.50* |

TABLE 1—(*contd.*)

| | | $T_b$ | | |
|---|---|---|---|---|
| | M | Lit. | Calc. | % Error |
| 21. 2-Ethyl-1-butene | 84.16 | 64.66 | 64.70 | 0.67 |
| 22. 2,3-Dimethyl-1-butene | ,, | 55.67 | ,, | 16.20* |
| 23. 3,3-Dimethyl-1-butene | ,, | 41.24 | ,, | 57.00* |
| 24. 2,3-Dimethyl-2-butene | ,, | 73.21 | ,, | −11.60* |
| 25. cis-2-heptene | 98.18 | 98.50 | 92.00 | −6.70 |
| 26. trans-2-heptene | ,, | 97.95 | ,, | −6.08 |
| 27. cis-3-heptene | ,, | 95.75 | ,, | −3.92 |
| 28. trans-3-heptene | ,, | 97.67 | ,, | −5.81 |
| 29. 2-Methyl-1-hexene | ,, | 92.00 | ,, | Zero |
| 30. 3-Methyl-1-hexene | ,, | 84.00 | ,, | 9.55 |
| 31. 4-Methyl-1-hexene | ,, | 86.73 | ,, | 6.10 |
| 32. 5-Methyl-1-hexene | ,, | 85.31 | ,, | 7.44 |
| 33. 2-Methyl-2-hexene | ,, | 95.41 | ,, | −3.58 |
| 34. 3-Methyl-cis-2-hexene | ,, | 94.00 | ,, | −2.13 |
| 35. 3-Methyl-trans-2-hexene | ,, | 94.00 | ,, | −2.13 |
| 36. 4-Methyl-cis-2-hexene | ,, | 87.37 | ,, | 5.31 |
| 37. 4-Methyl-trans-2-hexene | ,, | 87.60 | ,, | 5.02 |
| 38. 5-Methyl-cis-2-hexene | ,, | 91.00 | ,, | 1.10 |
| 39. 5-Methyl-trans-2-hexene | ,, | 86.00 | ,, | 7.00 |
| 40. 2-Methyl-cis-3-hexene | ,, | 86.00 | ,, | 7.00 |
| 41. 2-Methyl-trans-3-hexene | ,, | 86.00 | ,, | 7.00 |
| 42. 3-Methyl-cis-3-hexene | ,, | 95.35 | ,, | −3.52 |
| 43. 3-Methyl-trans-3-hexene | ,, | 93.55 | ,, | −1.67 |
| 44. 2-Ethyl-1-pentene | ,, | 94.00 | ,, | −2.13 |
| 45. 3-Ethyl-1-pentene | ,, | 85.13 | ,, | 8.06 |
| 46. 2,3-Dimethyl-1-pentene | ,, | 84.26 | ,, | 9.16 |
| 47. 2,4-Dimethyl-1-pentene | ,, | 81.64 | ,, | 12.30* |
| 48. 3,3-Dimethyl-1-pentene | ,, | 77.54 | ,, | 18.60* |
| 49. 3,4-Dimethyl-1-pentene | ,, | 81.00 | ,, | 13.60* |
| 50. 4,4-Dimethyl-1-pentene | ,, | 72.49 | ,, | 27.00* |
| 51. 3-Ethyl-2-pentene | ,, | 96.01 | ,, | −4.18 |
| 52. 2,3-Dimethyl-2-pentene | ,, | 97.46 | ,, | −5.61 |
| 53. 2,4-Dimethyl-2-pentene | ,, | 83.44 | ,, | 10.30* |

TABLE I.—(*contd.*)

| | | $T_b$ | | | |
|---|---|---|---|---|---|
| | | M. | Lit. | Calc. | % Error |
| 54. | 3,4-Dimethyl-cis-2-pentene | 98.18 | 87.00 | 92.00 | 5.75 |
| 55. | 3,4-Dimethyl-trans-2-pentene | ,, | 87.00 | ,, | 5.75 |
| 56. | 4,4-Dimethyl-cis-2-pentene | ,, | 80.42 | ,, | 14.40* |
| 57. | 4,4-Dimethyl-trans-2-pentene | ,, | 76.75 | ,, | 19.80* |
| 58. | 2-Ethyl-3-methyl-1-butene | ,, | 89.00 | ,, | 3.37 |
| 59. | 2,3,3-Trimethyl-1-butene | ,, | 77.87 | ,, | 18.20* |
| 60. | cis-2-octene | 112.21 | 125.64 | 119.64 | −5.05 |
| 61. | trans-2-octene | ,, | 125.00 | 119.30 | −4.56 |
| 62. | cis-3-octene | ,, | 122.90 | ,, | −2.93 |
| 63. | trans-3-octene | ,, | 123.30 | ,, | −3.24 |
| 64. | cis-4-octene | ,, | 122.54 | ,, | −2.64 |
| 65. | trans-4-octene | ,, | 122.25 | ,, | −2.41 |
| 66. | 2-Methyl-1-heptene | ,, | 119.30 | ,, | Zero |
| 67. | 3-Methyl-1-heptene | ,, | 111.00 | ,, | 7.45 |
| 68. | 4-Methyl-1-heptene | ,, | 112.80 | ,, | 5.76 |
| 69. | 5-Methyl-1-heptene | ,, | 113.30 | ,, | 5.28 |
| 70. | 6-Methy-1-heptene | ,, | 113.20 | ,, | 5.37 |
| 71. | 2-Methy-2-heptene | ,, | 122.60 | ,, | −2.69 |
| 72. | 3-Methyl-cis-2-heptene | ,, | 122.00 | ,, | −2.21 |
| 73. | 3-Methyl-trans-2-heptene | ,, | 122.00 | ,, | −2.21 |
| 74. | 4-Methyl-cis-2-heptene | ,, | 114.00 | ,, | 4.65 |
| 75. | 4-Methyl-trans-2-heptene | ,, | 114.00 | ,, | 4.65 |
| 76. | 5-Methyl-cis-2-heptene | ,, | 118.00 | ,, | 1.10 |
| 77. | 5-Methyl-trans-2-heptene | ,, | 118.00 | ,, | 1.10 |
| 78. | 6-Methyl-cis-2-heptene | ,, | 117.00 | ,, | 1.97 |
| 79. | 6-Methyl-trans-2-heptene | ,, | 117.00 | ,, | 1.97 |
| 80. | 2-Methyl-cis-3-heptene | ,, | 112.00 | ,, | 6.51 |
| 81. | 2-Methyl-trans-3-heptene | ,, | 112.00 | ,, | 6.51 |
| 82. | 3-Methyl-cis-3-heptene | ,, | 121.00 | ,, | −1.41 |
| 83. | 3-Methyl-trans-3-heptene | ,, | 121.00 | ,, | −1.41 |
| 84. | 4-Methyl cis-3-heptene | ,, | 122.00 | ,, | −2.21 |
| 85. | 4-Methyl-trans-3-heptene | ,, | 122.00 | ,, | −2.21 |
| 86. | 5-Methyl-cis-3-heptene | ,, | 112.00 | ,, | 6.51 |

TABLE I—(*contd.*)

| | | | $T_b$ | | |
|---|---|---|---|---|---|
| | | M | Lit. | Calc. | % Error |
| 87. | 5-Methyl-trans-3-heptene | 112.21 | 112.00 | 119.30 | 6.51 |
| 88. | 6-Methyl-trans-3-heptene | ,, | 115.08 | ,, | 3.74 |
| 89. | 6-Methyl-trans-3-heptene | ,, | 115.00 | ,, | 3.74 |
| 90. | 2-Ethyl-1-hexene | ,, | 120.00 | ,, | −0.58 |
| 91. | 3-Ethyl-1-hexene | ,, | 110.38 | ,, | 7 97 |
| 92. | 4-Ethyl-1-hexene | ,, | 113 00 | ,, | 4.70 |
| 93. | 2, 3-Dimethyl-1-hexene | ,, | 110.50 | ,, | 7.50 |
| 94. | 2, 4-Dimethyl-1-hexene | ,, | 111.20 | ,, | 7 27 |
| 95. | 2, 5-Dimethyl-1-hexene | ,, | 111.60 | ,, | 6.30 |
| 96. | 3, 3-Dimethyl-1-hexene | ,, | 104.00 | ,, | 14.70* |
| 97. | 3, 4-Dimethyl-1-hexene | ,, | 112.00 | ,, | 6.51 |
| 98. | 3, 5-Dimethyl-1-hexene | ,, | 104.00 | ,, | 14.70* |
| 99. | 4, 4-Dimethyl-1-hexene | ,, | 107.00 | ,, | 11.50* |
| 100. | 4, 5-Dimethyl-1-hexene | ,, | 109 00 | ,, | 9.45 |
| 101. | 5, 5-Dimethyl-1-hexene | ,, | 102 50 | ,, | 16.40* |
| 102. | 3-Ethyl-cis-2-hexene | ,, | 121.00 | ,, | 1.41 |
| 103. | 3-Ethyl-trans-2-hexene | ,, | 101.00 | ,, | 1.41 |
| 104. | 4-Ethyl-cis-2-hexene | ,, | 113.00 | ,, | 5.57 |
| 105. | 4-Ethyl-trans-2-hexene | ,, | 113.00 | ,, | 5.57 |
| 106. | 2, 3-Dimethyl-2-hexene | ,, | 121.77 | ,, | −2.03 |
| 107. | 2, 4-Dimethyl-2-hexene | ,, | 110.60 | ,, | 14.70* |
| 108. | 2, 5-Dimethyl-2-hexene | ,, | 112.20 | ,, | 6.51 |
| 109. | 3, 4-Dimethyl-cis-2-hexene | ,, | 116.00 | ,, | 2.85 |
| 110. | 3, 4-Dimethyl-trans-2-hexene | ,, | 116.00 | ,, | 2.85 |
| 111. | 3, 5-Dimethyl-cis-2-hexene | ,, | 112.00 | ,, | 6.51 |
| 112. | 3, 5-Dimethyl-trans-2-hexene | ,, | 112.00 | ,, | 6.51 |
| 113. | 4, 4-Dimethyl-cis-2-hexene | ,, | 106.00 | ,, | 12.60* |
| 114. | 4, 4-Dimethyl-trans-2-hexene | ,, | 106 00 | ,, | 12.60* |
| 115. | 4, 5-Dimethyl-cis-2-hexeme | ,, | 110.00 | ,, | 8.45 |
| 116. | 4, 5-Dimethyl-trans-2-hexene | ,, | 110 00 | ,, | 8.45 |
| 117. | 5,5-Dimethyl-cis-2-hexene | ,, | 106.90 | ,, | 11.60* |
| 118. | 5,5-Dimethyl-trans-2-hexene | ,, | 104.10 | ,, | 14.60* |
| 119. | 3-Ethyl-3-hexene | ,, | 116 00 | ,, | 2.85 |

TABLE I—(*contd*)

| | | $T_b$ | | | |
|---|---|---|---|---|---|
| | | M | Lit. | Calc. | % Error |
| 120. | 2,2-Dimethyl-cis-3-hexene | 112.21 | 105.43 | 119.30 | 13.15* |
| 121. | 2,2-Dimethyl-trans-3-hexene | ,, | 100.85 | ,, | 17.00* |
| 122. | 2,3-Dimethyl-cis-3-hexene | ,, | 114.00 | ,, | 4.65 |
| 123. | 2,3-Dimethyl-trans-3-hexene | ,, | ,, | ,, | 4.65 |
| 124. | 1,4-Dimethyl-cis-3-hexene | ,, | 109.00 | ,, | 9.45 |
| | | | | Average Error | 4.43 |
| *III.* | *Alkyl Benzenes* | | | | |
| 1. | Isopropyl benzene | 120.19 | 152.39 | 161.00 | 5.65 |
| 2. | 1,2,3-Trimethyl benzene | ,, | 176.08 | ,, | −8.56 |
| 3. | 1,2,4-Trimethyl benzene | ,, | 169.35 | ,, | −4.94 |
| 4. | 1,3,5-Trimethyl benzene | ,, | 164.71 | ,, | −2.25 |
| 5. | o-Ethyltoluene | ,, | 165.15 | ,, | −2.51 |
| 6. | m-Ethyltoluene | ,, | 161.30 | ,, | −0.19 |
| 7. | p-Ethyltoluene | ,, | 161.98 | ,, | −0.61 |
| 8. | Isobutyl benzene | 134.21 | 172.75 | 181.00 | 4.77 |
| 9. | sec-Butyl benzene | ,, | 173.30 | ,, | 4.44 |
| 10. | tert-Butyl benzene | ,, | 169.11 | ,, | 7.01 |
| 11. | o-Propyl toluene | ,, | 184.80 | ,, | −2.06 |
| 12. | m-Propyl toluene | ,, | 181.80 | ,, | −0.44 |
| 13. | p-Propyl toluene | ,, | 183.80 | ,, | −1.25 |
| 14. | o-Isopropyl toluene | ,, | 178.15 | ,, | 1.59 |
| 15. | m-Isopropyl toluene | ,, | 175.14 | ,, | 3.34 |
| 16. | p-Isopropyl toluene | ,, | 177.10 | ,, | 2.20 |
| 17. | 1,2-Diethyl benzene | ,, | 183.42 | ,, | −1.32 |
| 18. | 1,3-Diethyl benzene | ,, | 181.10 | ,, | −0.06 |
| 19. | 1,4-Diethyl benzene | ,, | 183.75 | ,, | −1.50 |
| 20. | 2-Ethyl-1,3-dimethyl benzene | ,, | 190.01 | ,, | −4.74 |
| 21. | 2-Ethyl-1,4-dimethyl benzene | ,, | 186.91 | ,, | −3.17 |
| 22. | 3-Ethyl-1,2-dimethyl benzene | ,, | 193.91 | ,, | −6.67 |
| 23. | 4-Ethyl-1,2-dimethyl benzene | ,, | 189.75 | ,, | −4.61 |
| 24. | 4-Ethyl-1,3-dimethyl benzene | ,, | 188.41 | ,, | −3.93 |
| 25. | 5-Ethyl-1,3-dimethyl benzene | ,, | 183.75 | ,, | −1.75 |

TABLE I—(*contd*)

| | | $T_b$ | | | |
|---|---|---|---|---|---|
| | | M | Lit. | Calc. | % Error |
| 26. | 1,2,3,4-Tetramethyl benzene | 134.21 | 205.04 | 181.00 | −11.71* |
| 27. | 1,2,3,5-Tetramethyl benzene | ,, | 198.00 | ,, | −8 60 |
| 28. | 1,2,4,5-Tetramethyl benzeue | ,, | 196.80 | ,, | −8.02 |
| 29. | (1-Methyl butyl) benzene | 148.24 | 193.00 | 202.00 | 4.66 |
| 30. | (1-Ethyl propyl) benzene | ,, | 191.00 | ,, | 5.76 |
| 31. | (2-Methyl butyl) benzene | ,, | 197.00 | ,, | 2.56 |
| 32. | Isopentyl benzene | ,, | 198.38 | ,, | 1.56 |
| 33. | (1,1-Dimethyl propyl) benzene | ,, | 192.38 | ,, | 5.00 |
| 34. | (1,2-Dimethyl propyl) benzene | ,, | 188.00 | ,, | 7.45 |
| 35. | (2,2-Dimethyl propyl) benzene | ,, | 186.00 | ,, | 8 60 |
| 36. | 1-n-Butyl-2-methyl benzene | ,, | 208.00 | ,, | −2.88 |
| 37. | 1-n-Butyl-3-methyl benzene | ,, | 205 00 | ,, | −1.46 |
| 38. | 1-n-Butyl-4-methyl benzene | ,, | 207.00 | ,, | −2.42 |
| 39. | 1-sec-butyl-2-methyl benzene | ,, | 196 00 | ,, | 3.06 |
| 40. | 1-sec-butyl-3-methyl benzene | ,, | 194.00 | ,, | 4.12 |
| 41. | 1-sec-butyl-4-methyl benzene | ,, | 197.00 | ,, | 2.54 |
| 42. | o-Isobutyl toluene | ,, | 196.00 | ,, | 3.06 |
| 43. | 1-Isobutyl-3-methyl benzene | ,, | 194.00 | ,, | 4.12 |
| 44. | 1-Isobutyl-4-methyl benzene | ,, | 196.00 | ,, | 3 06 |
| 45. | 1-tert-Isobutyl-3-methyl benzene | ,, | 200 45 | ,, | 0.76 |
| 46. | 1-tert-3-methyl benzene | ,, | 189.26 | ,, | 6.75 |
| 47. | 1-tert-butyl-4-methyl benzene | ,, | 192.76 | ,, | 4.79 |
| 48. | 1-Ethyl-2-n-propyl benzene | ,, | 200.00 | ,, | −0.44 |
| 49. | 1-Ethyl-3-n-propyl benzene | ,, | 201.00 | ,, | 0 48 |
| 50. | 1-Ethyl-4-n-propyl benzene | ,, | 205.00 | ,, | −1.46 |
| 51. | 1-Ethyl-2-isopropyl benzene | ,, | 193.00 | ,, | 4 66 |
| 52. | 1-Ethyl-3-isopropyl | ,, | 192.00 | ,, | 5.21 |
| 53. | 1-Ethyl-4-isopropyl benzene | ,, | 196.00 | ,, | 3.06 |
| 54. | 1,2-Dimethyl-3-n-propyl benzene | ,, | 210.70 | ,, | 4 01 |
| 55. | 1,2-Dimethyl-4-n-propyl benzene | ,, | 208.90 | ,, | −3 30 |
| 56. | 1,3-Dimethyl-2-n-propyl benzene | ,, | 207 60 | ,, | −2.70 |
| 57. | 1,3-Dimethyl-4-n-prcpyl benzene | ,, | 206 60 | ,, | −2 22 |
| 58. | 1,3-Dimethyl-5-n-propyl benzene | ,, | 202.40 | ,, | −0.12 |

TABLE I – (*contd.*)

| | | $T_b$ | | | |
|---|---|---|---|---|---|
| | | M. | Lit. | Calc. | % Error |
| 59. | 1,4-Dimethyl-3-n-propyl benzene | 148.24 | 204.30 | 202 00 | −0.12 |
| 60. | 1,2-Dimethyl-3-isopropyl benzene | ,, | 202.60 | ,, | −0.29 |
| 61. | 1,2-Dimethyl-4-isopropyl benzene | ,, | 201.80 | ,, | 0.09 |
| 62. | 1,3-Dimethyl-3-isopropyl benzene | ,, | 199 00 | ,, | 1.51 |
| 63. | 1,3-Dimethyl-4-isopropyl benzene | ,, | 199 10 | ,, | 1.51 |
| 64. | 1,3-Dimethyl-5-isopropyl benzene | ,, | 194 50 | ,, | 3.86 |
| 65. | 1,4-Dimethyl-5-isopropyl benzene | ,, | 196.20 | ,, | 2 95 |
| 66. | 2,3-Diethyl-1-methyl benzene | ,, | 206.60 | ,, | −2 22 |
| 67. | 2,4-Diethyl 1-methyl benzene | ,, | 205 00 | ,, | −1.47 |
| 68. | 2,5-Diethyl-1-methyl benzene | ,, | 207.10 | ,, | −2 46 |
| 69. | 2,6-Diethyl-1-methyl benzene | ,, | 208 80 | ,, | −3.25 |
| 70. | 3,3-Diethyl-1-methyl benzene | ,, | 203.60 | ,, | −0.78 |
| 71. | 3,5-Diethyl-1-methyl benzene | ,, | 200.70 | ,, | 0.63 |
| 72. | 2-Ethyl-1,3,5-trimethyl benzene | ,, | 212.40 | ,, | −4.88 |
| 73. | 3-Ethyl-1,2,4-trimethyl benzene | ,, | 216.60 | ,, | −6.76 |
| 74. | 4-Ethyl-1,2,3-trimithyl benzene | ,, | 214.40 | ,, | −8.21 |
| 75. | 5 Ethyl-1,2,3-trimethyl benzene | ,, | 215.80 | ,, | −6.41 |
| 76. | 5-Ethyl-1,2,4-trimethyl benzene | ,, | 213.00 | ,, | −5 17 |
| 77. | 6-Ethyl-1,2,4-trimethyl benzene | ,, | ,, | ,, | −5 17 |
| 78. | Pentamethyl benzene | ,, | 231.80 | ,, | −12.40* |
| | | | | Average Error | 3.37 |
| *IV.* | *Alkyl Naphthalenes* : | | | | |
| 1. | Naphthalene | 128.17 | 217.95 | 230.00 | 5.55 |
| 2. | 1-Methyl naphthalene | 142.19 | 244.64 | 245.00 | 0.35 |
| 3. | 2-Methyl naphthalene | ,, | 241.05 | ,, | 1.84 |
| 4. | 1-Ethyl naphthalene | 156.22 | 258.67 | 261.00 | 0.90 |
| 5. | 2-Ethyl naphthalene | ,, | 257.90 | ,, | 1 20 |
| 6. | 1,2-Dimethyl naphthalene | ,, | 266 00 | ,, | −1.88 |
| 7. | 1,3-Dimethyl naphthalene | ,, | 263.00 | ,, | −0.76 |
| 8. | 1,4-Dimethyl naphthalene | ,, | 268.00 | ,, | −2.62 |
| 9. | 1,5-Dimethyl naphthalene | ,, | 265.00 | ,, | −1 51 |

TABLE I – (*contd.*)

| | | $T_b$ | | |
|---|---|---|---|---|
| | M | Lit. | Calc. | % Error |
| 10. 1,6-Dimethyl naphthalene | 156 22 | 263.00 | 261.00 | −0 76 |
| 11. 1,7-Dimethyl naphthalene | ,, | 263 00 | ,, | −0.76 |
| 12. 1,8-Dimethyl naphtalene | ,, | 270.00 | ,, | −2.33 |
| 13. 2,3-Dimethyl naphthalene | ,, | 268.00 | ,, | −2.62 |
| 14. 2,6-Dimethyl naphthalene | ,, | 262.00 | ,, | −0.38 |
| 15. 2,7-Dimethyl naphthalene | ,, | 263.00 | ,, | −0.76 |
| 16. 1-n-Propyl naphthalene | 170 24 | 272.50 | 276.50 | 1.47 |
| 17. 2-n-Propyl naphthalene | ,, | 273.50 | ,, | 1.10 |
| 18. 8-n-Butyl naphthalene | 184 27 | 289.30 | 291.20 | 0.66 |
| 19. 2-n-Butyl naphthalene | ,, | 292.00 | ,, | −0.28 |
| 20. 1-n-Pentyl naphthalene | 198.30 | 307.00 | 307.1 | 0.04 |
| 21. 2-n-Pentyl naphtalene | ,, | 310.00 | ,, | −0.94 |
| 22. 1-n-Hexyl naphthalene | 212 32 | 322.00 | 323.00 | 0.32 |
| 23. 2-n-Hexyl naphthalene | ,, | 324.00 | ,, | −0.62 |
| 24. 1-n-Hepthyl naphthalene | 226.35 | 340.00 | 339.00 | −0.30 |
| 25. 2-n-Heptyl naphthalene | 226.35 | 241.00 | ,, | −0.59 |
| 26. 1-n-Octyl naphthalene | 240 37 | 356.00 | 357.00 | 0.28 |
| 27. 2-n-Octyl naphthalene | ,, | 357.00 | ,, | ... |
| 28. 1-n-Nonyl naphthalene | 254.40 | 372.00 | 370.00 | −0.54 |
| 29. 2-n-Nonyl naphthalene | ,, | ,, | ,, | −0.54 |
| 30. 1-n-Decyl naphthalene | 268.43 | 387.00 | ,, | −0.52 |
| 31. 2-n-Nonyl naphthalene | ,, | 401.00 | 400.00 | −0 24 |
| 32. 1-n-Undecyl naphthalene | 282.45 | ,, | ,, | −0.24 |
| 33. 2-n-Undecyl naphthalene | ,, | ,, | ,, | −0.24 |
| 34. 1-n-Dodecyl naphthalene | 296.48 | 415.00 | ,, | −0.48 |
| 35. 2-n-Dodecyl naphthalene | ,, | 414.00 | ,, | −0.29 |
| | | Average Error | | 0.975 |
| *V. Styrenes*: | | | | |
| 1. Styrene | 104.15 | 145.2 | 147.0 | 0.13 |
| 2. α-Methyl styrene | 118.17 | 165.38 | 167.00 | 0.98 |
| 3. β-Metyl styrene | ,, | 170 00 | ,, | −1.76 |

TABLE 1—(*contd.*)

| | | $T_b$ | | | |
|---|---|---|---|---|---|
| | | M | Lit. | Calc. | % Error |
| 4. | o-Methyl styrene | 118.17 | 169.00 | 167.00 | −1.19 |
| 5. | m-Methyl styrene | ,, | 171.00 | ,, | −2.68 |
| 6. | p-Methyl styrene | ,, | 172.78 | ,, | −3.35 |
| 7. | m and p-Vinyl toluene | ,, | 167.00 | ,, | ... |
| 8. | m-Ethyl styrene | 132.20 | 190.12 | 184.50 | 2.96 |
| 9. | p-Ethyl styrene | ,, | 192.78 | ,, | 4 30 |
| 10. | p-Isopropyl styrene | 146.22 | 204.15 | 203.00 | 0.57 |
| 11. | p-Isopropyl-α-methyl styrene | 160.25 | 220 00 | 214.00 | 3.09 |
| | | | Average Error | | 1 94 |
| *VI.* | *Cyclopentanes*: | | | | |
| 1. | 1,1-Dimethyl cyclopentane | 98.18 | 87.84 | 96 00 | 10 45* |
| 2. | cis-1,2-Dimethyl cyc opentane | ,, | 99.53 | 96.20 | −3.34 |
| 3. | trans-1,2-Dimethyl cyclopentane | ,, | 91.86 | ,, | 4.72 |
| 4. | cis-1,3-Dimethyl cyclopentane | ,, | 91.72 | ,, | 4.88 |
| 5. | trans-1,3-dimethyl cyclopentane | ,, | 90.77 | ,, | 6.00 |
| 6. | Isopropyl cyclopentane | 112.21 | 126.41 | 120.60 | −4.60 |
| 7. | 1-Ethyl-1-methyl cyclopentane | ,, | 121.52 | ,, | −0.76 |
| 8. | cis-1-Ethyl-2-methyl cyclopentane | ,, | 128.05 | ,, | −5.81 |
| 9. | trans-1-Ethyl-2-methyl cyclopentane | ,, | 121.20 | ,, | −0.50 |
| 10. | cis-1-Ethyl-3-methyl cyclopentane | ,, | 121.40 | ,, | −0.66 |
| 11. | trans-1-Ethyl-3-methyl cyclopentane | ,, | 120.80 | ,, | −0.16 |
| 12. | 1,1,2-Trimethyl cyclopentane | ,, | 113.60 | ,, | 5.00 |
| 13. | 1,1,3-Trimethyl cyclopentane | ,, | 104.89 | ,, | 15.00* |
| 14. | 1,cis-2,cis-3-trimethyl cyclopentane | ,, | 123.00 | ,, | −1.96 |
| 15. | 1,cis-2, trans-3-trimethyl ,, | ,, | 117.50 | ,, | 2.64 |
| 16. | 1,trans-2,cis-3-trimethyl ,, | ,, | 110 20 | ,, | 9 45 |
| 17. | 1,cis-2, cis-4-trimethyl ,, | ,, | 118 00 | ,, | 2 20 |
| 18. | 1,cis-2, trans-4-trimethyl ,, | ,, | 116 73 | ,, | 3 32 |
| 19. | 1,trans-2, cis-4-trimethyl ,, | ,, | 109.29 | ,, | 10.36* |
| | | | Average Error | | 3.50 |

TABLE 1—(*contd.*)

| | | $T_b$ | | |
|---|---|---|---|---|
| | M | Lit. | Calc. | % Error |
| *VII. Cyclopentenes* : | | | | |
| 1. Cyclopentene | 68.12 | 44.24 | 44.22 | −0.05 |
| 2. 1-Methyl cyclopentene | 82.14 | 75.80 | 72 28 | −4.65 |
| 3. 3-Methyl cyclopentene | ,, | 65 00 | ,, | 11.20* |
| 4. 4-Methyl cyclopentene | ,, | 75.00 | ,, | −3.88 |
| 5. 1-Ethyl cyclopentene | 96.17 | 106.30 | 100.32 | −5.62 |
| 6. 3-Ethyl cyclopentene | ,, | 98.10 | ,, | 2.26 |
| 7. 4-Ethyl cyclopentene | ,, | 106.00 | ,, | −5.37 |
| 8. 1,2-Dimethyl cyclopentene | ,, | 105.80 | ,, | −5.22 |
| 9. 1,3-Dimethyl cyclopentene | ,, | 92.00 | ,, | 9.05 |
| 10. 1,4-Dimethyl cyclopentene | ,, | 93.00 | ,, | 7.65 |
| 11. 1,5-Dimethyl coclopentene | ,, | 102.00 | ,, | −1.65 |
| 12. 3,3-Dimethyl cyclopentene | ,, | 88.00 | ,, | 14.10* |
| 13. 4,4-Dimethyl cyclopentene | ,, | ,, | ,, | 14.10* |
| | | Average Error | ... | 4.54 |
| *VIII Cyclohexanes* : | | | | |
| 1. Cyclohexane | 84.16 | 80.73 | 85.00 | 5.30 |
| 2. Methyl cyclohexane | 98.18 | 100 93 | 101.70 | 0 76 |
| 3. Ethyl cyclohexane | 112.21 | 131.78 | 118.80 | —9.86 |
| 4. 1,1 Dimethyl ayclohexane | ,, | 119.54 | ,, | −0.62 |
| 5. 1,cis-2-Dimethyl cyclohexane | ,, | 129.72 | ,, | −8.43 |
| 6. 1,trans-2-Dimethyl cyclohexane | ,, | 123 41 | ,, | −3.74 |
| 7. 1,cis-3-Dimethyl cyclohexane | ,, | 120.08 | ,, | −1.06 |
| 8. 1,trans-3-Dimethyl cytlohexane | ,, | 124 45 | ,, | −4.54 |
| 9. 1,cis-4-Dimethyl cyclohexane | ,, | 124.32 | ,, | −4.44 |
| 10. 1,trans-4-Dimethyl cyclohexane | ,, | 119.35 | ,, | −0.46 |
| | | Average Error | ... | 3 92 |

TABLE I

| | | $T_b$ | | |
|---|---|---|---|---|
| | M. | Lit. | Calc. | % Error |
| *IX. Cyclohexenes*: | | | | |
| 1. Cyclohexene | 82.14 | 82.97 | 82.28 | −0.84 |
| 2. 1-Methyl cyclohexene | 96.17 | 110.00 | 110.32 | 0.29 |
| 3. 3-Methyl cyclohexene | ,, | 104.00 | ,, | 6.07 |
| 4. 4-Methyl cyclohexene | ,, | 102.74 | ,, | 7.34 |
| 5. 1-Ethyl cyclohexene | 110.19 | 136.00 | 138.38 | 1.75 |
| 6. 3-Ethyl cyclohexene | ,, | 134.00 | ,, | 3.27 |
| 7. 4-Ethyl cyclohexene | ,, | 133.00 | ,, | 4.05 |
| 8. 1,2-Dimethyl cyclohexene | ,, | 137.00 | ,, | 1.05 |
| 9. 1,3-Dimethyl cyclohexene | ,, | ,, | ,, | 1.05 |
| 10. 1,4-Dimethyl cyclohexene | ,, | 128.00 | ,, | 8.10 |
| 11. 1,5-Dimethyl cyclohexene | ,, | 128.00 | ,, | 8.10 |
| 12. 1,6-Dimethyl cyclohexene | ,, | 133.00 | ,, | 4.05 |
| 13. 3,3-Dimethyl cyclohexene | ,, | 119.00 | ,, | 16.30* |
| 14. 4,4-Dimethyl cyclohexene | ,, | 116.00 | ,, | 18.35* |
| | | Average Error | ... | 3.83 |

The error indicated is average % error

TABLE II

Values of Constants in equation (1), $T_b = n_1 (M) + c_1$
Hydrocarbons and related compounds

| | Series | No. considered | $n_1$ | $c_1$ | Average % error |
|---|---|---|---|---|---|
| 1. | Alkanes | 121 | 1.850 | −96 0 | 3.70 |
| 2. | Alkenes | 93 | 1.970 | −101.1 | 4.43 |
| 3. | Alkyl benzenes | 76 | 1.462 | −15.0 | 3.37 |
| 4. | Alkyl Nephthalenes | 35 | 1.100 | +89.0 | 0.97 |
| 5. | Styrenes | 11 | 1 330 | +8.0 | 1.94 |
| 6. | Cyclopentanes | 16 | 1.705 | −71.0 | 3.50 |
| 7. | Cyclopentenes | 10 | 2.000 | −92.0 | 4.54 |
| 8. | Cyclohexanes | 10 | 1.200 | −16 0 | 3.92 |
| 9. | Cyclohexenes | 12 | 2.000 | −82.0 | 3.83 |
| | Total | 384 | Overall Error | | 3.35 |

REFERENCES


1. Das, T. R., Ibrahim, S, B. and Kuloor, N. R. — *Indian Journal of Technology*, Vol. 7, No, 5, p 131.
2. Mathur, B. C. and Kuloor, N. R. ... — *J. Indian Inst. Sc.*, (in Press)
3. Mathur, B. C., Ibrahim, S. H. and Kuloor, N. R. — *Chem Eng*. Mar. 24, 1969, 182.
4. Mathur, B. C. Ibrahim, S. H and ... Kuloor, N. R. — *Ibid.*, May 19, 1969, p. 212.
5. Dreisback, R R. ... ... — "Physical properties of Chemical compounds", Vol. I & III. Advances in Chemistry Series. ACS Publication, 1955.