Activity One

Hydrocarbon Boiling Points

Chemists often gather data regarding physical and chemical properties of substances. Although these data can be organized in many ways, the most useful ways uncover trends or patterns among the values. These patterns often trigger attempts to explain regularities.

The development of the periodic table is a good example of this approach. Recall that you predicted a property of one element from values of that property for neighboring elements on the periodic table.

In a similar vein, we seek patterns among boiling point data for some hydrocarbons. During evaporation and boiling, individual molecules in the liquid state gain enough energy to overcome intermolecular forces and enter the gaseous state.

table 1  Hydrocarbon boiling points

<table>
<thead>
<tr>
<th>Hydrocarbon</th>
<th>boiling point (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Butane</td>
<td>-0.5</td>
</tr>
<tr>
<td>Decane</td>
<td>174.0</td>
</tr>
<tr>
<td>Ethane</td>
<td>-88.6</td>
</tr>
<tr>
<td>Heptane</td>
<td>98.4</td>
</tr>
<tr>
<td>Hexane</td>
<td>68.7</td>
</tr>
<tr>
<td>Methane</td>
<td>-161.7</td>
</tr>
<tr>
<td>Nonane</td>
<td>150.8</td>
</tr>
<tr>
<td>Octane</td>
<td>125.7</td>
</tr>
<tr>
<td>Pentane</td>
<td>36.1</td>
</tr>
<tr>
<td>Propane</td>
<td>-42.1</td>
</tr>
</tbody>
</table>

Answer the following questions about boiling point data given in table 1 above.

1. a. In what pattern or order are Table 1 data organized?
   b. Is this a useful way to present the information? Why?

2. Assume we want to search for a trend or pattern among these boiling points.
   a. Propose a more useful way to arrange these data.
   b. Reorganize the data table based on your idea.

3. Use your new data table to answer these questions:
   a. Which substance(s) are gases (have already boiled) at room temperature (22 C)?
   b. Which substance(s) boil between 22 C (room temperature) and 37 C (body temperature)?

4. What can you infer about intermolecular attractions in decane compare to those in butane?

5. Intermolecular forces also help explain other liquid properties such as viscosity and freezing points.
   a. Based on their intermolecular attractions, try to rank pentane, octane, and decane in order of increasing viscosity. Assign "1" to the least viscous ("thinnest") of the three.
   b. Check with your teacher to see whether you are correct.
Activity Two

Alkane Boiling points: Trends^1

Boiling is a physical change whereby a liquid is converted into a gas. Boiling occurs when the vapor pressure of a liquid is equal to the atmospheric pressure pushing on the liquid. But what other factors affect the boiling point of a liquid?

To explain relative boiling points we must take into account a number of properties for each substance. The properties include molar mass, structure, polarity and hydrogen bonding ability. All of these properties can effect the boiling point of a liquid. In this exploration we will investigate the boiling points for the first ten straight chain alkane hydrocarbons. We are most interested in the effect of molecular size (mass) upon a substance’s relative boiling point.

1. Listed in table 1 below is boiling point data for the first ten straight chain alkanes. Enter the data into your calculator for analysis by assigning:
   L1 = carbon number
   L2 = boiling point

2. Construct a scatterplot of carbon number vs. boiling point and sketch the graph in your lab report.

3. Use your graph to determine the average change in boiling point (in degrees Celsius) when a carbon atom and two hydrogen atoms are added to a given alkane chain.

4. Describe the relationship between the number of carbons and the boiling point by using one of the following terms (# of carbon atoms and boiling point “°C”):
   vary directly
   vary inversely
   directly proportional
   inversely proportional

Table 1 Hydrocarbon Boiling Points

<table>
<thead>
<tr>
<th>Hydrocarbon</th>
<th>Formula</th>
<th>Boiling Point (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Butane</td>
<td>C₄H₁₀</td>
<td>-0.5</td>
</tr>
<tr>
<td>Decane</td>
<td>C₁₀H₂₂</td>
<td>174.0</td>
</tr>
<tr>
<td>Ethane</td>
<td>C₂H₆</td>
<td>-88.6</td>
</tr>
<tr>
<td>Heptane</td>
<td>C₇H₁₆</td>
<td>98.4</td>
</tr>
<tr>
<td>Hexane</td>
<td>C₆H₁₄</td>
<td>68.7</td>
</tr>
<tr>
<td>Methane</td>
<td>CH₄</td>
<td>-161.7</td>
</tr>
<tr>
<td>Nonane</td>
<td>C₉H₂₀</td>
<td>150.8</td>
</tr>
<tr>
<td>Octane</td>
<td>C₈H₁₈</td>
<td>125.7</td>
</tr>
<tr>
<td>Pentane</td>
<td>C₅H₁₂</td>
<td>36.1</td>
</tr>
<tr>
<td>Propane</td>
<td>C₃H₈</td>
<td>-42.1</td>
</tr>
</tbody>
</table>
5. The pattern of boiling points among the first ten alkanes allows you to predict the boiling points of other alkanes. Let’s assume the relationship is linear and proportional. Use the calculator to calculate the regression equation for the data. Enter the equation into Y1 and plot the line of “best fits”. Record the regression equation and sketch the calculator screen in your lab report.

Directions for the TI-82/83

\[
\text{Regression Equation: } Y = \text{__________________________}
\]

6. From your graph, extrapolate the boiling points of undecane \(\text{C}_{11}\text{H}_{24}\), dodecane \(\text{C}_{12}\text{H}_{26}\) and tridecane \(\text{C}_{13}\text{H}_{28}\).

Directions for the TI-82/83

\[
\begin{align*}
\text{Window:} \\
X_{\text{min}} &= 0 \\
X_{\text{max}} &= 15 \\
X_{\text{scl}} &= 1.5 \\
Y_{\text{min}} &= -200 \\
Y_{\text{max}} &= 500 \\
Y_{\text{scl}} &= 70 \\
\text{Graph} \\
\text{Calc} \\
\text{Value} \\
Y = \\
\text{Eval X}=11 \\
\text{Enter}
\end{align*}
\]

7. Compare your predicted boiling points to actual values provided by your teacher. Calculate the percentage error for each value. Suggest reasons, both mathematical and chemical for any differences in your predictions.

8. We have already noted that a substance’s boiling point depends on its intermolecular forces—that is, on attractions among its molecules. In a summary paragraph discuss how intermolecular attractions are related to the number of carbon atoms in each molecule for alkanes you have studied.
Activity Three

Alkane Boiling Points: Isomers

You have already observed the boiling points of straight chain alkanes are related to the number of carbon atoms in their molecules. Increased intermolecular attractions are related to the greater molecule-molecule contact possible for larger alkanes.

For example, consider the boiling points of some isomers

1. Boiling points for two sets of isomers are listed below.

C5H12 Isomers

CH3 — CH2 — CH2 — CH2 — CH3  

<table>
<thead>
<tr>
<th>Boiling Point (C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>36.1</td>
</tr>
</tbody>
</table>

CH3 — CH — CH2 — CH3  

<table>
<thead>
<tr>
<th>Boiling Point (C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>27.8</td>
</tr>
</tbody>
</table>

CH3 — C — CH3  

<table>
<thead>
<tr>
<th>Boiling Point (C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.5</td>
</tr>
</tbody>
</table>

Some C8H12 Isomers

CH3 — CH2 — CH2 — CH2 — CH2 — CH2 — CH2 — CH3  

<table>
<thead>
<tr>
<th>Boiling Point (C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>125.6</td>
</tr>
</tbody>
</table>

CH3 — CH2 — CH2 — CH2 — CH2 — CH — CH3  

<table>
<thead>
<tr>
<th>Boiling Point (C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>117.7</td>
</tr>
</tbody>
</table>

CH3 — CH — CH2 — C — CH3  

<table>
<thead>
<tr>
<th>Boiling Point (C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>99.2</td>
</tr>
</tbody>
</table>

2. Within a given series, how does the boiling point change as the number of carbon side-changes increase?
3. Match each boiling point to the appropriate C$_7$H$_{16}$ isomer: 98.4 C, 92.0 C, 79.2 C.

   \[ \text{CH}_3 - \text{CH}_2 - \text{CH} - \text{CH}_2 - \text{CH}_2 - \text{CH}_3 \]

   a. \[ \begin{array}{c}
   \text{CH}_3 \\
   \mid \\
   \text{CH}_3 \\
   \mid \\
   \text{CH}_3
   \end{array} \]

   b. \[ \begin{array}{c}
   \text{CH}_3 \\
   \mid \\
   \text{CH}_3 \\
   \mid \\
   \text{CH}_3
   \end{array} \]

   c. \[ \begin{array}{c}
   \text{CH}_3 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_3
   \end{array} \]

4. This is a C$_8$H$_{18}$ isomer.

   \[ \begin{array}{c}
   \text{CH}_3 \\
   \mid \\
   \text{CH}_3 - \text{CH}_2 - \text{C} - \text{CH}_2 - \text{CH}_2 - \text{CH}_3 \\
   \mid \\
   \text{CH}_3
   \end{array} \]

   a. Compare it to each C$_8$H$_{18}$ isomer listed in table 3. Predict whether it would have a higher or lower boiling point than each of these other C$_8$H$_{18}$ isomers.

   b. Would the C$_8$H$_{18}$ isomer shown above have a higher or lower boiling point than each of the three C$_5$H$_{12}$ isomers shown in table 3?

4. Write a summary paragraph explaining what you have learned in activity one, two and three with regards to the following terms:

   hydrocarbons  boiling point  isomers

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1Adopted from ChemCom: Chemistry in the Community, second edition, 1995, American Chemical Society