MATERIALS: 250 mL beaker, small test tubes, test tube holders, thermometer, 2 50 mL beakers, hot plate, boiling sticks, various bottles containing smelling substances (Part B and C).

PURPOSE: The purpose of this experiment is study the chemistry involved in smell.

LEARNING OBJECTIVES: By the end of this experiment, the student should be able to demonstrate these proficiencies:
1. Identify functional groups in chemical structures
2. Understand how an ester is formed from the condensation reaction of a carboxylic acid and alcohol
3. Understand how chemical structure is related to smell

PRE-LAB: Complete the pre-lab on page E39B-6 before lab.

DISCUSSION: The sense of smell (or olfaction) is very complex and not fully understood. Smell relies on chemical and biochemical reactions occurring in our nose. Chemical compounds that are volatile are most easily detected as these interact best with the receptors in our nose. Different smells can result from substances containing different chemical structures or functional groups. Below is a summary of some common functional groups:

<table>
<thead>
<tr>
<th>Functional Group</th>
<th>Functional Group Name</th>
<th>Example of Functional Group</th>
</tr>
</thead>
<tbody>
<tr>
<td>-OH</td>
<td>Alcohol</td>
<td>CH₃OH, methanol</td>
</tr>
<tr>
<td>O</td>
<td>Carboxylic acid</td>
<td>CH₃COOH, acetic acid</td>
</tr>
<tr>
<td>R₁-C-O-R₂</td>
<td>Ester</td>
<td>CH₃COOCH₃, methyl acetate</td>
</tr>
<tr>
<td>O</td>
<td>Aldehyde</td>
<td>CH₃COH, acetaldehyde</td>
</tr>
<tr>
<td>R₁-C-O-R₂</td>
<td>Ketone</td>
<td>CH₃COCH₃, acetone</td>
</tr>
<tr>
<td>-NH₂</td>
<td>Amine</td>
<td>CH₃NH₂, methylamine</td>
</tr>
<tr>
<td></td>
<td>Aromatic</td>
<td>C₇H₈, toluene</td>
</tr>
</tbody>
</table>

In a condensation reaction, a carboxylic acid and an alcohol combine to form an ester and water.

\[
\text{Carboxylic acid} + \text{alcohol} \rightarrow \text{ester} + \text{water}
\]
Esters have the general structure of $\overset{\text{O}}{\text{R}_1}\overset{\text{O}}{\text{C}}\overset{\text{O}}{\text{R}_2}$ where the R1 and R2 groups represent any organic moiety. (For example, R1 is CH$_3$CH$_2$CH$_2$, and R2 is CH$_3$ in the ester shown above.) Esters generally have a sweet smell.

**PROCEDURE: (Work in pairs)**

**Part A: Synthesis of Esters**

1. You will be synthesizing two of three esters from the chemical reaction of a carboxylic acid and an alcohol. The goal is to identify the ester that produces the wintergreen, banana, and cherry smells.

   Ester A: Salicylic acid (solid) and Methanol (liquid)
   Ester B: Benzoic acid (solid) and 1-Propanol (liquid)
   Ester C: Acetic acid (liquid) and 3-Methyl-1-butanol (liquid)

   Group 1 is assigned Esters A and B
   Group 2 is assigned Esters B and C
   Group 3 is assigned Esters A and C

   Circle the 2 esters your group has been assigned.

   These assignments will allow some replicate samples in case there are experimental errors.

   **CAUTION:** Glacial acetic acid and concentrated sulfuric acid are corrosive. Always use care when handling.

2. Assemble a hot water bath by half filling a 250 mL beaker with water and heating it on a hot plate to 80-85°C. Place a thermometer held by a clamp into the water to monitor the temperature. (For some hot plates, start with a setting of 6 and when it reaches 70°C, turn it back to 4.)

3. In a clean test tube labeled with your assigned ester letter (A, B, or C), add the following, in this order:
   a. either add 0.2 g (solid) or 10 drops (liquid) of your assigned carboxylic acid
   b. 20 drops of your assigned alcohol
   c. 5 drops of sulfuric acid

   Mix the solution with a wooden stick until the solid dissolves. Leave the stick in the test tube (even during heating). Repeat this process with your other assigned ester making sure to label the test tube.

4. Place the test tubes in the 80-85°C water bath, using test tube holders to keep the tubes from floating or tipping in the beaker. Heat for about 20 minutes mixing the solution from time to time and maintaining the temperature between 80-85°C. The water should NOT be boiling. If your water bath becomes too hot, remove the test tubes until the water is in the appropriate temperature range.

   While your esters are heating, answer the questions below the data table for Part A.

5. After heating, remove the test tubes from the water bath. Pour each ester into a separate beaker containing about 2 mL of distilled water (this helps with releasing the vapors). Make sure you know which ester is in each beaker.

6. Cautiously smell each ester, by wafting the vapors to your nose. Describe the smell in the data section.

7. Go to the other groups to smell the other esters. Check that replicate esters smell the same.

8. Based on your data, classify the 3 esters (A, B, C) as wintergreen, banana, or cherry smelling esters. Consult with your lab partner. Do your smells agree?

9. Dispose of the esters in the proper waste beaker in the instructor hood. Dispose of your test tubes in the broken glassware box. Unplug the hot plate. Clean up your lab station. Wash your hands to remove chemicals.
Experiment 39B
THE CHEMISTRY OF SMELL

Part A:
Circle the 2 esters you were assigned to synthesize:
- Ester A: Salicylic acid and Methanol
- Ester B: Benzoic acid and 1-Propanol
- Ester C: Acetic acid and 3-Methyl-1-butanol

<table>
<thead>
<tr>
<th>Ester</th>
<th>Description of Smell</th>
<th>Identification (Wintergreen, Banana, or Cherry)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

What is the name of the type of reaction used in Part A (carboxylic acid reacted with an alcohol) to synthesize an ester?

______________________________

Draw the structures of the 2 products formed from the reaction of benzoic acid and ethanol:

\[
\text{\begin{diagram}
\text{\includegraphics[width=0.5\textwidth]{benzoic_acid_reaction.png}}
\end{diagram}}
\]

Sometimes people “smell” the same substance differently or may describe the same smell differently. Why do you think this is the case?

Part B: Identifying Common Smells

1. Obtain the Part B set of common smells from your instructor.
2. Smell the contents of the containers making sure not to overload your nose. Recap the containers after you smell them. Do not mix up the caps and bottles.
3. Describe the smell (not as easy as it sounds) and the appearance of the substance in the table below.
4. Identify the contents of each container based on your observations.
Below is a list of possible substances for the Part B smells. Based on the smell, identify each sample. Then, for each structure, circle the functional group(s) and name the functional group(s) present. For each substance, only the main chemical component of that smell is shown below; some contain mixtures of various compounds. Note that not all carbons and hydrogens are shown in the drawings; lone pairs are not shown as these are not full Lewis structures.

<table>
<thead>
<tr>
<th>ID #</th>
<th>Chemical Structure, Chemical Name, and Substance</th>
<th>Name of Functional Group(s) Present</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td><img src="image1.png" alt="Cinnamaldehyde" /> Cinnamaldehyde, Cinnamon</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td><img src="image2.png" alt="Naphthalene" /> Naphthalene, Moth balls</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td><img src="image3.png" alt="Acetic acid" /> Acetic acid, Vinegar</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td><img src="image4.png" alt="Methyl butyrate" /> Methyl butyrate, Apple</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td><img src="image5.png" alt="S-Carvone" /> S-Carvone, Caraway seeds</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td><img src="image6.png" alt="Isopropanol" /> Isopropanol, Rubbing alcohol</td>
<td></td>
</tr>
</tbody>
</table>

E39B-4
Part C: Comparison of Smells

1. R-Carvone and S-Carvone are special isomers of each other. They have the same chemical formula and very similar structures, but they have distinct smells. R-Carvone has a minty smell, while S-Carvone smells like caraway seeds (as you’ve seen in Part B) or dill. The difference in smell is subtle for some people. Obtain the C-1 and C-2 bottles and identify which is R-Carvone and S-Carvone. Remember to waft the vapors and not overload your nose. Cap bottles when done.

<table>
<thead>
<tr>
<th>Description of Smell</th>
<th>Identification</th>
</tr>
</thead>
<tbody>
<tr>
<td>C-1</td>
<td></td>
</tr>
<tr>
<td>C-2</td>
<td></td>
</tr>
</tbody>
</table>

R-Carvone and S-Carvone are known as enantiomers, they are non-superimposable mirror images of each other. They have the same boiling point, melting point, solubility behavior, etc., however, they have different optical activity (they respond to polarized light differently). This makes them chiral.

Look at the structures and circle the areas where there are differences.

Your nose is very sensitive to small chemical differences. To be able to distinguish chiral compounds, some of your odor receptors must be chiral.

2. Some smells are found in nature and some smells can be generated by chemicals synthesized in the lab (like your esters). Smell bottles C-3 and C-4. One bottle contains pure vanilla extract, which comes from the vanilla orchid. The other bottle contains vanillin which is the main flavor component of vanilla and synthesized in a lab. This is sometimes sold in stores as “artificial” or “imitation” vanilla and is considerably cheaper than pure vanilla extract. Identify which bottle contains pure vanilla (natural) and which contains vanillin (fake).

<table>
<thead>
<tr>
<th>Description of Smell</th>
<th>Identification</th>
</tr>
</thead>
<tbody>
<tr>
<td>C-3</td>
<td></td>
</tr>
<tr>
<td>C-4</td>
<td></td>
</tr>
</tbody>
</table>

Vanillin is a chemical component found in the extract of the vanilla orchid and contributes most to the smell and flavor of vanilla. Why do samples of the pure vanilla extract and vanillin smell different?

Cost per ounce:
Imitation = $0.30/oz
Pure = $0.82/oz
Fancy gourmet = $2.25/oz
Vanilla bean = $2.73/oz

In the structure of vanillin, identify the 2 functional groups.
Expt. 39B – The Chemistry of Smell
Name ________________________________

Pre-lab

1. a. Draw the structure of acetic acid. What functional group is present in acetic acid? _______________________

b. Draw the structure of methanol. What functional group is present in methanol? __________________________

c. Acetic acid and methanol react in a **condensation reaction** producing an ester and water. Draw the structures of the two products of this reaction.

2. a. What do you think your nose is detecting when you smell something?

b. What makes it possible for you to distinguish different odors?

c. Why might two substances smell different or similar to each other?

3. a. Putrescine has the smell of decaying fish. Circle and identify (name) the functional group in putrescine.

   ![Putrescine structure]

b. Alanine is an amino acid. It does not have a smell. Circle and identify (name) the functional groups in alanine.

   ![Alanine structure]