Learning Objectives

- Identify the general structure for an ester.
- Use common names to name esters.
- Name esters according to the IUPAC system.

Esters have the general formula \( \text{RCOOR}' \), where \( R \) may be a hydrogen atom, an alkyl group, or an aryl group, and \( R' \) may be an alkyl group or an aryl group but \textit{not} a hydrogen atom. (If it were hydrogen atom, the compound would be a carboxylic acid.) Figure \( \PageIndex{1} \) shows models for two common esters.

![Figure \( \PageIndex{1} \): The Structure of Esters. Esters feature a carbon-to-oxygen double bond that is also singly bonded to a second oxygen atom, which is then joined to an alkyl or an aryl group. The esters shown here are ethyl acetate (a) and methyl butyrate (b).](image)

Esters occur widely in nature. Unlike carboxylic acids, esters generally have pleasant odors and are often responsible for the characteristic fragrances of fruits and flowers. Once a flower or fruit has been chemically analyzed, flavor chemists can attempt to duplicate the natural odor or taste. Both natural and synthetic esters are used in perfumes and as flavoring agents.

Fats and vegetable oils are esters of long-chain fatty acids and glycerol. Esters of phosphoric acid are of the utmost importance to life.

Names of Esters

Although esters are covalent compounds and salts are ionic, esters are named in a manner similar to that used for naming salts. The group name of the alkyl or aryl portion is given first and is followed by the name of the acid portion. In both common and International Union of Pure and Applied Chemistry (IUPAC) nomenclature, the -\textit{ic} ending of the parent acid is replaced by the suffix -\textit{ate} (Table \( \PageIndex{1} \)).
Table 1: Nomenclature of Esters

<table>
<thead>
<tr>
<th>Condensed Structural Formula</th>
<th>Common Name</th>
<th>IUPAC Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCOOCH₃</td>
<td>methyl formate</td>
<td>methyl methanoate</td>
</tr>
<tr>
<td>CH₃COOCH₃</td>
<td>methyl acetate</td>
<td>methyl ethanoate</td>
</tr>
<tr>
<td>CH₃COOCH₂CH₃</td>
<td>ethyl acetate</td>
<td>ethyl ethanoate</td>
</tr>
<tr>
<td>CH₃CH₂COOCH₂CH₃</td>
<td>ethyl propionate</td>
<td>ethyl propanoate</td>
</tr>
<tr>
<td>CH₃CH₂CH₂COOCH(CH₃)₂</td>
<td>isopropyl butyrate</td>
<td>isopropyl butanoate</td>
</tr>
<tr>
<td>ethyl benzoate</td>
<td>ethyl benzoate</td>
<td></td>
</tr>
</tbody>
</table>

Example

Give the common and IUPAC names for each compound.

1. \[
\text{CH₃CH₂COCH₂CH₂CH₂CH₃}
\]
   - The alkyl group attached directly to the oxygen atom is a butyl group (in green).
   - The part of the molecule derived from the carboxylic acid (in red) has three carbon atoms. It is called propionate (common) or propanoate (IUPAC). The ester is therefore butyl propionate or butyl propanoate.

2. \[
\text{CH₃C-OCHCH₃}
\]
   - An alkyl group (in green) is attached directly to the oxygen atom by its middle carbon atom; it is an isopropyl group.
   - The part derived from the acid (that is, the benzene ring and the carbonyl group, in red) is benzoate. The ester is
therefore isopropyl benzoate (both the common name and the IUPAC name).

Exercise \(\PageIndex{1}\)

Give the common and IUPAC names for each compound.

a.  

\[
\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{C} \equiv \text{OCH}_2\text{CH}_3
\]

b.  

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

Example \(\PageIndex{2}\)

Draw the structure for ethyl pentanoate.

Solution

Start with the portion from the acid. Draw the pentanoate (five carbon atoms) group first; keeping in mind that the last carbon atom is a part of the carboxyl group.

Then attach the ethyl group to the bond that ordinarily holds the hydrogen atom in the carboxyl group.

Exercise \(\PageIndex{2}\)

Draw the structure for phenyl pentanoate.

Concept Review Exercises

1. From what carboxylic acid and what alcohol can isopropyl hexanoate be made?
2. From what carboxylic acid and what alcohol can cyclobutyl butyrate be made?

Answers

1. hexanoic acid and isopropyl alcohol
2. butyric acid and cyclobutyl alcohol

Key Takeaway

- An ester has an OR group attached to the carbon atom of a carbonyl group.

Exercises

1. Draw the structure for each compound.
   a. methyl acetate
   b. ethyl pentanoate
   c. phenyl acetate
   d. isopropyl propionate

2. Draw the structure for each compound.
   a. ethyl hexanoate
   b. ethyl benzoate
   c. phenyl benzoate
   d. ethyl 3-methylhexanoate

3. Name each compound with both the common name and the IUPAC name.
   a. 
   b. 

4. Name each compound with both the common name and the IUPAC name.
   a. 

Answers

1. d.  

3. a. methyl formate; methyl methanoate  
   b. ethyl propionate; ethyl propanoate