

4.5: Esters

Learning Objectives

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

Esters are carboxylic acid derivatives formed by replacing the H in the hydroxyl group with a carbon group. Esters have the general formula 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 *not* a hydrogen atom (if it were a hydrogen atom, the compound would be a carboxylic acid). Figure 4.5.1 shows the general structure for an ester, with the functional group shown in red.

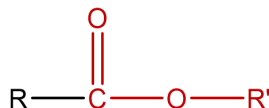


Figure 4.5.1: The structure of an ester. Esters feature a carbon-oxygen double bond that is also singly bonded to a second oxygen atom, which is then joined to an alkyl or an aryl group.

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.

Naming Esters

Although esters are covalent compounds and salts are ionic, esters are named in a manner similar to that used for naming salts.

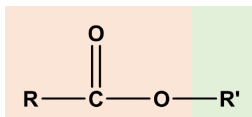
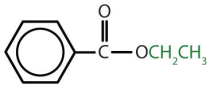


Figure 4.5.2: Guide for naming esters.

The common and International Union of Pure and Applied Chemistry (IUPAC) rules for naming esters are similar. In both systems, the identity of the R' carbon group (that replaced the hydrogen) is given and is followed by the name of the acid portion. Another similarity among the systems is that the *-ic acid* ending of the parent acid is replaced by the suffix *-ate* (Table 4.5.1).

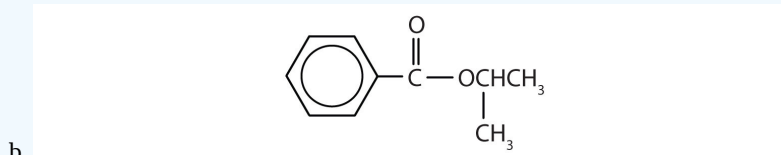
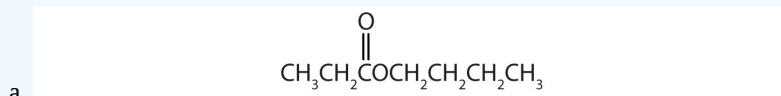
If the ester molecule has substituents, as with carboxylic acids, the carbonyl carbon atom is always assigned to C1. It is unnecessary to designate this group by number.

Table 4.5.1: Nomenclature of Esters

Condensed Structural Formula	Common Name	IUPAC Name
HCOOCH_3	methyl formate	methyl methanoate
$\text{CH}_3\text{COOCH}_3$	methyl acetate	methyl ethanoate
$\text{CH}_3\text{COOCH}_2\text{CH}_3$	ethyl acetate	ethyl ethanoate
$\text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}_3$	ethyl propionate	ethyl propanoate
$\text{CH}_3\text{CH}_2\text{CH}_2\text{COOCH}(\text{CH}_3)_2$	isopropyl butyrate	isopropyl butanoate
	ethyl benzoate	ethyl benzoate

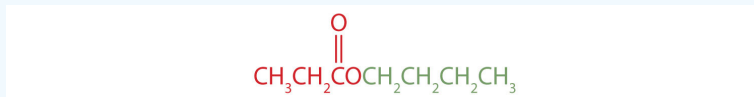
✓ Example 4.5.1

Give the common and IUPAC names for each compound.



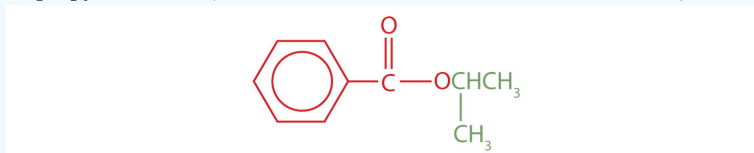
Solution

a. The alkyl group attached directly to the oxygen atom is a butyl group (in green).



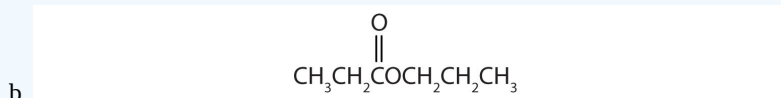
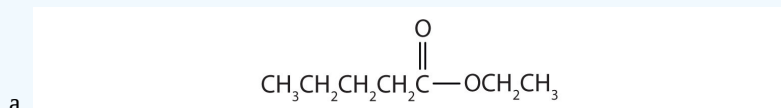
The part of the molecule derived from the carboxylic acid (in red) has three carbon atoms. It is called propionate (common) or propanoate (IUPAC). The ester is therefore butyl propionate or butyl propanoate.

b. 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 4.5.1

Give the common and IUPAC names for each compound.

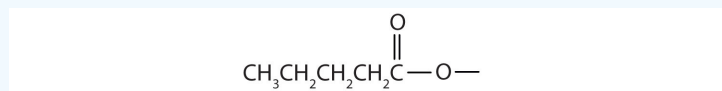


✓ Example 4.5.2

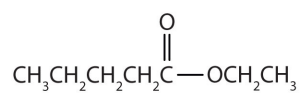
Draw the structure for ethyl pentanoate.

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 4.5.2

Draw the structure for phenyl pentanoate.

Key Takeaway

- An ester has an OR' group attached to the carbon atom of a carbonyl group.
- The R' cannot be H, because this will represent a carboxylic acid.
- The common and IUPAC names for esters identify the R' group that replaced the H followed by the name of the acid portion of the molecule.

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