

12.10: Esters - Structures and Names

Learning Objectives

- Describe the general structure for an ester.
- Determine whether a compound is an ester from a molecular structure and a name.

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 hydrogen atom, the compound would be a carboxylic acid.) Figure 12.10.1 shows models for two common esters.

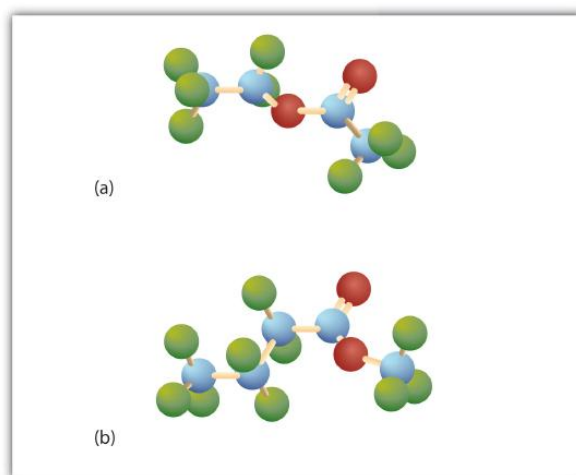


Figure 12.10.1: The Structure of Esters. Esters feature a carbon-to-oxygen double bond that is also singly bonded to a second oxygen atom, which is then joined to an alkyl or an aryl group. The esters shown here are ethyl acetate (a) and methyl butyrate (b).

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.

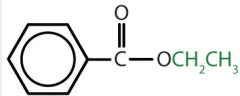
Fats and vegetable oils are esters of long-chain fatty acids and glycerol. Esters of phosphoric acid are of the utmost importance to life.

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 *-ic* ending of the parent acid is replaced by the suffix *-ate* (Table 12.10.1).

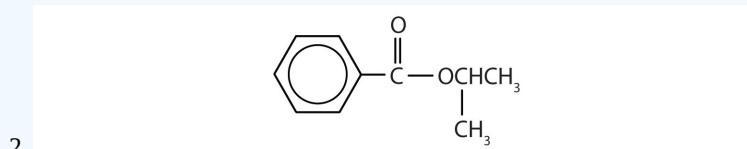
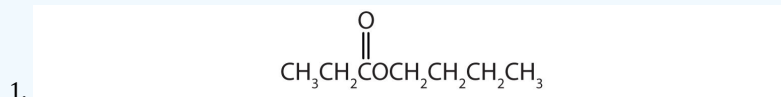
Table 12.10.1: Nomenclature of Esters

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

Condensed Structural Formula	Common Name	IUPAC Name
	ethyl benzoate	ethyl benzoate

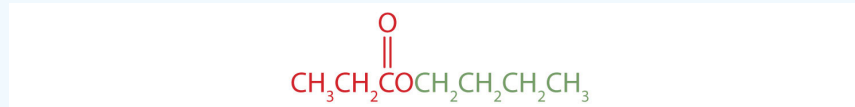
✓ Example 12.10.1

Give the common and IUPAC names for each compound.



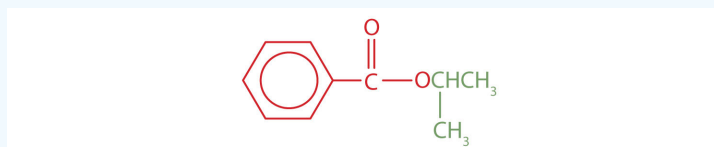
Solution

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



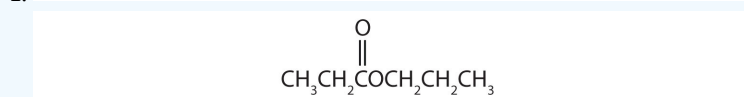
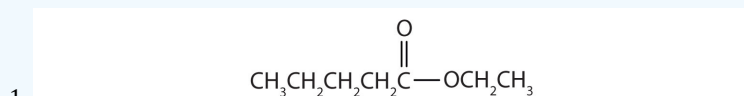
The part of the molecule derived from the carboxylic acid (in red) has three carbon atoms. It is called propionate (common) or propanoate (IUPAC). The ester is therefore butyl propionate or butyl propanoate.

1. 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 12.10.1

Give the common and IUPAC names for each compound.

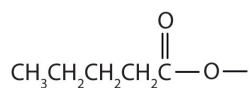


✓ Example 12.10.2

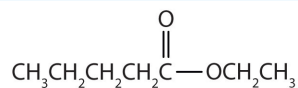
Draw the structure for ethyl pentanoate.

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 12.10.2

Draw the structure for phenyl pentanoate.

Key Takeaway

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

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