CHAPTER 25: CARBOXYLIC ACIDS AND ESTERS

Organic and Biochemistry Supplement to Enhanced Introductory College Chemistry

by Gregory Anderson; Jen Booth; Caryn Fahey; Adrienne Richards; Samantha Sullivan Sauer; and David Wegman

Chapter 25 Contents

Please visit the web version of Organic and Biochemistry Supplement to Enhanced Introductory College Chemistry (https://ecampusontario.pressbooks.pub/orgbiochemsupplement/) to access the complete book, interactive activities and ancillary resources.

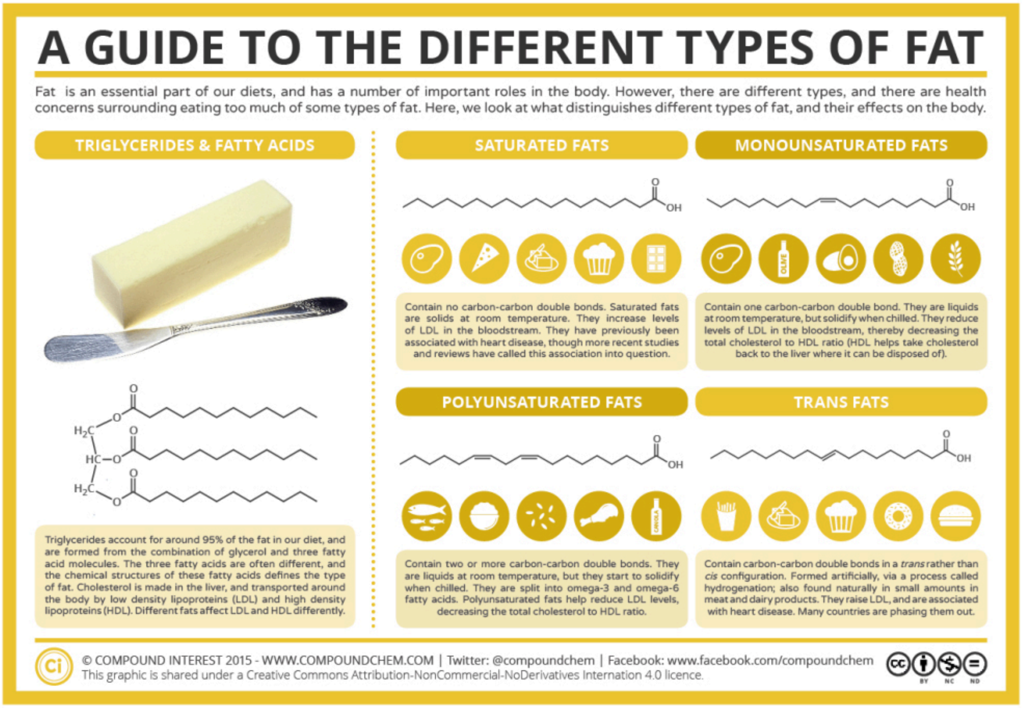
In this chapter, you will learn about:

- Carboxylic acids: what are they? What is their chemical structure? What are the physical and chemical properties of these acids?
- Esters: what are they? What is their chemical structure? What are the physical and chemical properties of esters?

To better support your learning, you should be familiar with the following concepts before starting this chapter:

- Alkanes, Alkenes, and Alkynes (Chapter 20: Alkanes and Akyl Halides and Chapter 22: Alkenes, Alkynes and Aromatics)
- Alcohols and Ethers (Chapter 23: Alcohols and Ethers)
- Aldehydes and Ketones (Chapter 24: Aldehydes and Ketones)
- Functional Groups (Chapter 19.5: Families of Organic Molecules)

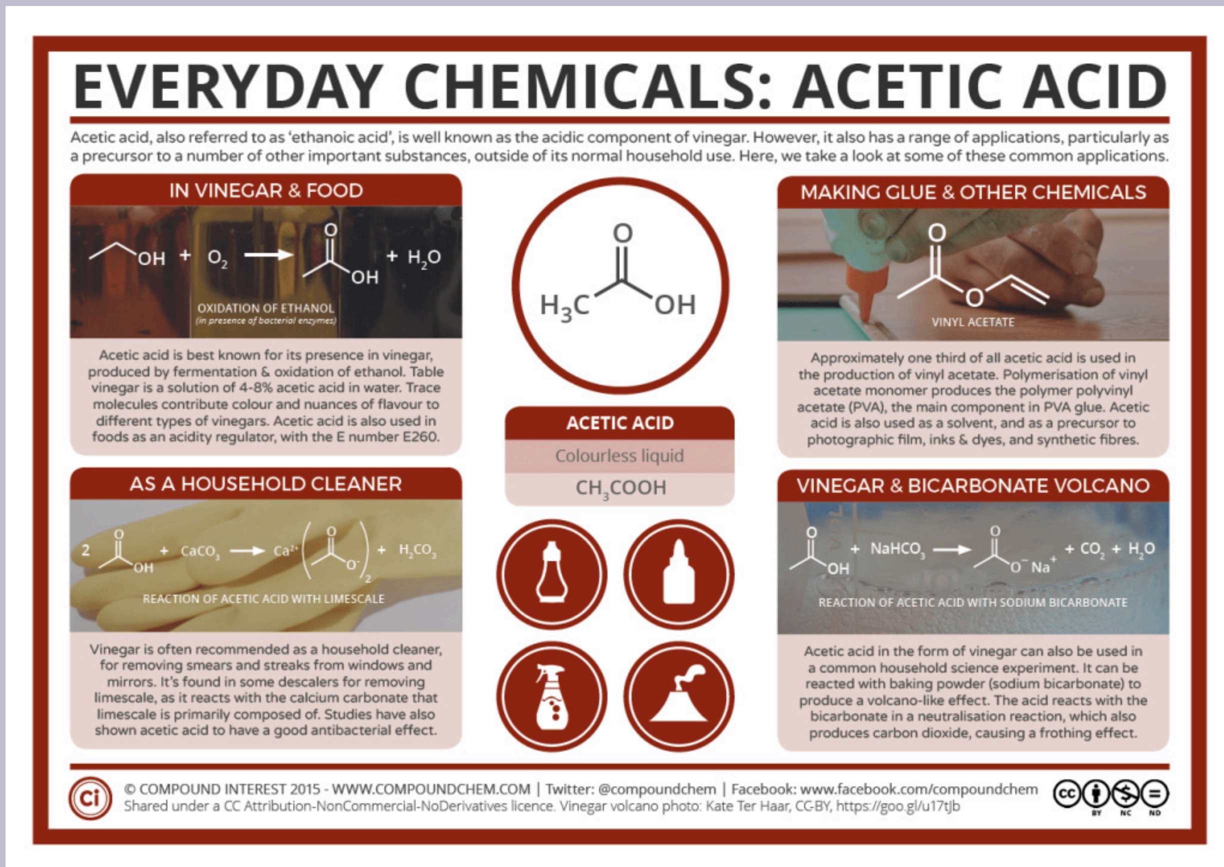
Organic acids have been known for ages. Prehistoric people likely made acetic acid when their fermentation reactions went awry and produced vinegar instead of wine. The Sumerians (2900–1800 BCE) used vinegar as a condiment, a preservative, an antibiotic, and a detergent. Citric acid was discovered by an Islamic alchemist, Jabir Ibn Hayyan (also known as Geber), in the 8th century, and crystalline citric acid was first isolated from lemon juice in 1784 by the Swedish chemist Carl Wilhelm Scheele. Medieval scholars in Europe were aware that the crisp, tart flavour of citrus fruits is caused by citric acid. Naturalists of the 17th century knew that the sting of a red ant's bite was due to an organic acid that the ant injected into the wound. The acetic acid of vinegar (inforgraphic 25.0b), the formic acid of red ants, and the citric acid of fruits all belong to the same family of compounds—carboxylic acids. Soaps are salts of long-chain carboxylic acids. Prehistoric people also knew about organic bases—by smell if not by name; amines are the organic bases produced when animal tissue decays. The organic compounds that we consider in this chapter are carboxylic acids. Soaps are salts of long-chain carboxylic acids. We will also discuss esters which are derived from a carboxylic acid and an alcohol. Fats and oils are esters (see infographic 25.0a.), as are many important fragrances and flavours. The structure of these fats will differ based on the presence of at least one double bond within the carbon chain.



Infographic 25.0a. Read more about "A Guide to Types of Fat and the bonds they contain (https://www.compoundchem.com/2015/08/25/fat/)" by Andy Brunning / Compound Interest, CC BY-NC-ND, or access a text-based summary of infographic 25.0a [New tab]

Spotlight on Everyday Chemistry: Acetic Acid

Acetic acid is a common carboxylic acid which is commonly used in cooking and cleaning practices. Due to its flavour and acidic properties it can be used to regulate the acidity in foods we eat. It is also found to have good antibacterial properties and therefore makes a great household cleaning solution.



Infographic 25.0b. Read more about "Everyday Chemicals: Acetic Acid – Vinegar & Volcanoes (https://www.compoundchem.com/2015/06/11/acetic-acid/)" by Andy Brunning / Compound Interest, CC BY-NC-ND, or access a text-based summary of infographic 25.0b [New tab].

Attribution & References

Except where otherwise noted, this page is adapted by Caryn Fahey from "15.0: Prelude to Organic Acids and Bases and Some of Their Derivatives" In *Basics of General, Organic, and Biological Chemistry (Ball et al.)* by David W. Ball, John W. Hill, and Rhonda J. Scott via LibreTexts, CC BY-NC-SA 4.0./ A LibreTexts version of *Introduction to Chemistry: GOB (v. 1.0),* CC BY-NC 3.0.

25.1 CARBOXYLIC ACIDS - STRUCTURE AND NAMING

Learning Objectives

By the end of this section, you will be able to:

- Name carboxylic acids with common names.
- Name carboxylic acids according to IUPAC nomenclature.

Structure of Carboxylic Acids

Carboxylic acids occur widely in nature, often combined with alcohols or other functional groups, as in fats, oils, and waxes. They are components of many foods, medicines, and household products (Figure 25.1a.). Carboxylic acids are considered weak acids that can neutralize bases and tend to have a sour or tart taste to them. Not surprisingly, many of them are best known by common names based on Latin and Greek words that describe their source.

Figure 25.1a. Carboxylic Acids in the Home. Carboxylic acids occur in many common household items. (a) Vinegar contains acetic acid, (b) aspirin is acetylsalicylic acid, (c) vitamin C is ascorbic acid, (d) lemons contain citric acid, and (e) spinach contains oxalic acid. (**credit** a: Photo by Joe Shlabotnik, CC BY-NC-SA 2.0; b: Photo by U.S. Food and Drug Administration, CC BY-SA 2.0; c: Photo by Pete, PD; d: Photo by eggbank, Unsplash; e: Photo by Willis Lam (https://www.flickr.com/people/85567416@N03), CC BY-SA 2.0)

A carboxylic acid is an organic compound in which a carbon is double bonded to an oxygen atom (referred to as a carbonyl group) while also being single bonded to a hydroxyl group (-OH). This combination of carbonyl group with a hydroxyl group creates what is known as a **carboxyl group**, the functional group found in carboxylic acids.

Indigenous Perspectives: Inuit Love Soy Sauce

Figure 25.1b. Cup of soy sauce (credit: Image by Tim Reckmann (https://www.flickr.com/people/115225894@N07), CC BY 2.0).

Soy sauce was first produced in China about 2,200 years ago. It is now commonly used in Inuit culture as the condiment of choice for Arctic Char also known as *iKaluk* in Inuttut. Spiced soy sauces can contain different carboxylic acids which can add to the flavour profile. A healthy ingredient within soy sauce is Niacin which is an aromatic carboxylic acid (Figure 25.1c.) (Anderson & Rayner-Canham, 2022).

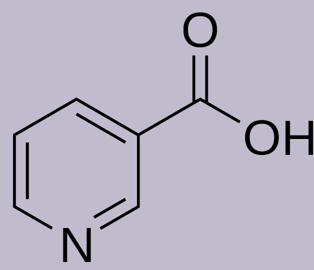


Figure 25.1c. Molecular structure of Niacin (credit: Image by Mysid, PDM)

More information about the use of soy sauce in Inuit culture can be found Soy sauce: An essential Inuit condiment in Chem 13 News Magazine (https://uwaterloo.ca/chem13-news-magazine/fall-2022-special-edition/feature/soy-sauce).

Carboxylic acids, RCO_2H, occupy a central place among carbonyl compounds. Not only are they valuable in themselves, they also serve as starting materials for preparing numerous carboxylic acid derivatives such as acid chlorides, esters, amides, and thioesters (Figure 25.1d.). In addition, carboxylic acids are present in the majority of biological pathways.

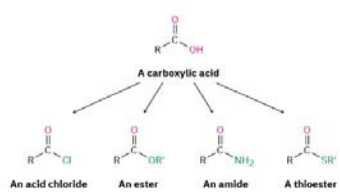


Figure 25.1d. Carboxylic acids, the starting point for formation of several acid derivatives; acid chlorides, esters, amides and thioesters. (**credit:** *Organic Chemistry (OpenStax)*, CC BY-NC-SA 4.0.)

Common Names of Carboxylic Acids

Many carboxylic acids are named using their common names which use the prefixes: *form-, acet-, proprion-, and butyr-.* The simplest carboxylic acid, formic acid (HCOOH), was first obtained by the distillation of ants (Latin *formica*, meaning "ant") (Figure 25.1e.). The bites of some ants inject formic acid, and the stings of wasps and bees contain formic acid (as well as other poisonous materials).

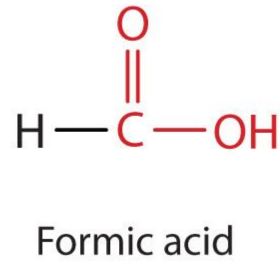


Figure 25.1e. Functional group for carboxylic acids representing formic acid (credit: *Intro Chem: GOB (v. 1.0)*, CC BY-NC-SA 3.0).

The next higher homolog is acetic acid (Figure 25.1f.), which is made by fermenting cider and honey in the presence of oxygen. This fermentation produces vinegar, a solution containing 4%–10% acetic acid, plus a number of other compounds that add to its flavour. Acetic acid is probably the most familiar weak acid used in educational and industrial chemistry laboratories.

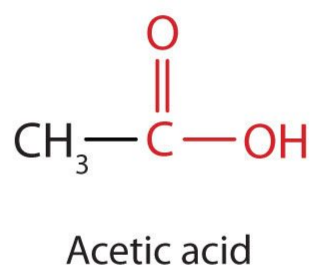
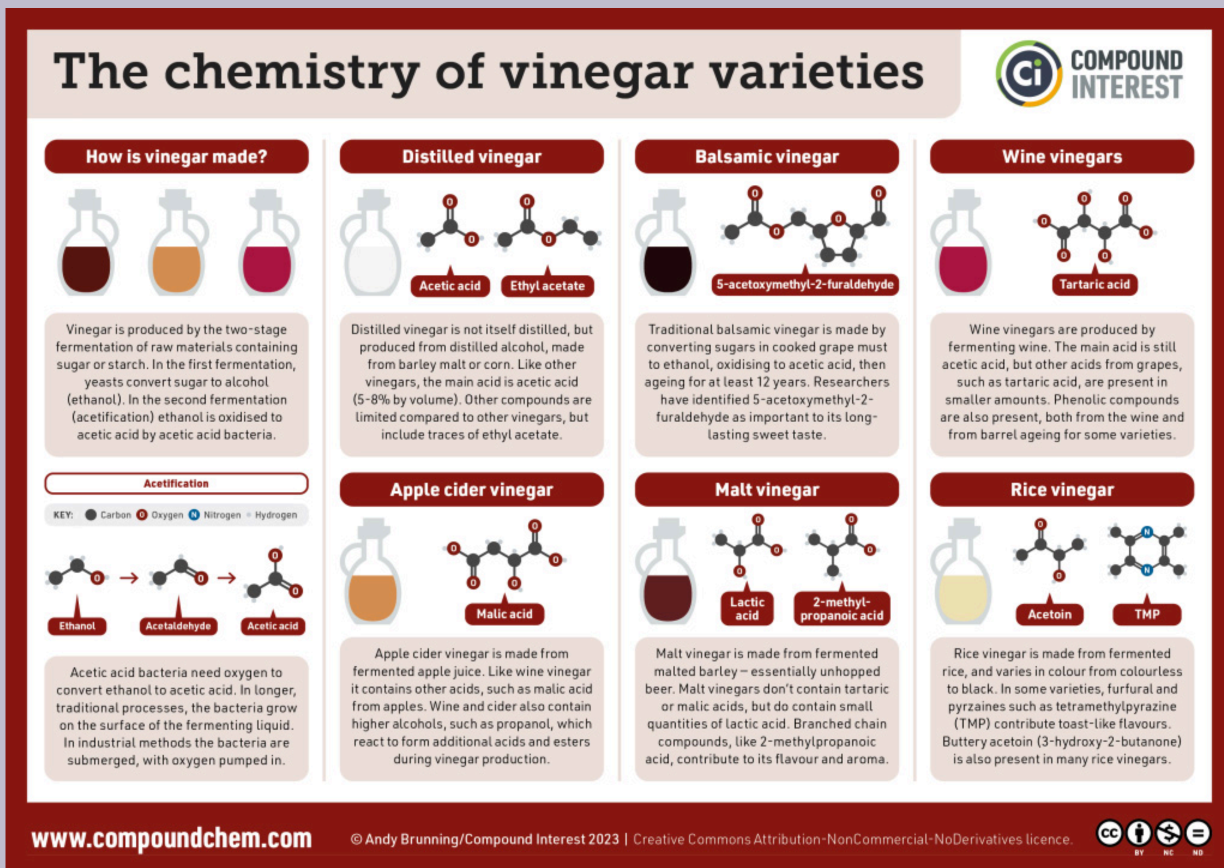


Figure 25.1f. Functional group for carboxylic acids representing acetic acid (credit: *Intro Chem: GOB (v. 1.0)*, CC BY-NC-SA 3.0).

Pure acetic acid solidifies at 16.6°C, only slightly below normal room temperature. In the poorly heated laboratories of the late 19th and early 20th centuries in northern North America and Europe, acetic acid often "froze" on the storage shelf. For that reason, pure acetic acid (sometimes called concentrated acetic acid) came to be known as *glacial acetic acid*, a name that survives to this day. Vinegar comes in a variety of forms which we commonly use in everyday cooking practices. Infographic 25.1a. showcases the changes to chemical structure that provides us with the differing flavours we experience from some of the vinegar varieties.

Spotlight on Everyday Chemistry: Vinegar

Below we can see the chemical structures that make up the varieties of vinegars we use in everyday cooking practice.



Infographic 25.1a. Vinegar or acetic acid is a common carboxylic acid. It comes in a variety of form based on changes to the chemical structure. Read more about "The sour science of vinegar varieties (https://www.compoundchem.com/2023/02/20/vinegar/)" by Andy Brunning / Compound Interest, CC BY-NC-ND, or access a text-based summary of infographic 25.1a [New tab].

The third homolog, propionic acid (CH_3CH_2COOH), is seldom encountered in everyday life. The fourth homolog, butyric acid ($CH_3CH_2CH_2COOH$), is one of the most foul-smelling substances imaginable. It is found in rancid butter and is one of the ingredients of body odour. By recognizing extremely small amounts of this and other chemicals, bloodhounds are able to track fugitives.

Below (Figure 25.1g.) is an example of a carboxylic acid with a substituent group. This acid is named

2-bromo-propanoic acid. 2-bromo-propanoic acid is used in the production of herbicides and the synthesis of pharmaceutical intermediates.

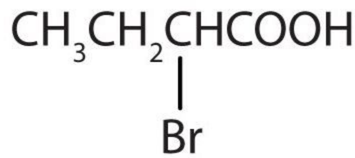
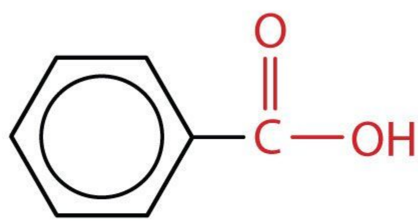


Figure 25.1g. The structural diagram here represents 2-bromo-propanoic acid (credit: *Intro Chem: GOB (v. 1.0)*, CC BY-NC-SA 3.0).

Watch Carboxylic Acids, Typical Acids and Esters – Organic Chemistry – YouTube (4 min) (https://youtu.be/3YeXGpDdgZw?)

The most simplistic aromatic carboxylic acid in which the carboxyl carbon is attached directly to carbon 1 is called benzoic acid (C_6H_5COOH) (Figure 25.1h.). When substituent groups are added to benzoic acid, they are numbered in the direction that gives the smallest numbers possible.



Benzoic acid

Figure 25.1h. Image represents a ring structure containing the functional groups for carboxylic acids (credit: *Intro Chem: GOB (v. 1.0)*, CC BY-NC-SA 3.0).

The *common names* of carboxylic acids use Greek letters (α, β, γ, δ, and so forth), not numbers, to designate the position of substituent groups in acids (Figure 25.1i.). These letters refer to the position of the carbon atom in relation to the carboxyl carbon atom.

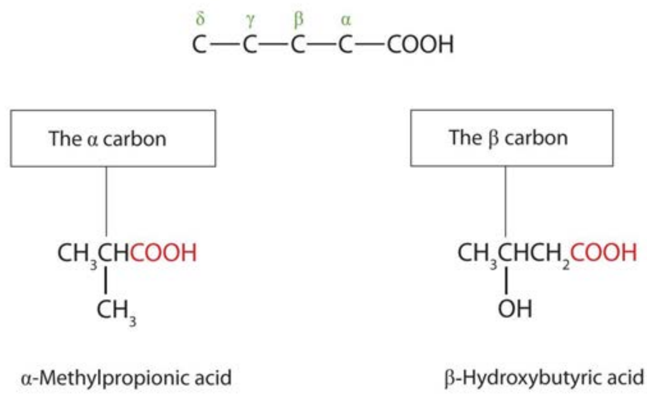


Figure 25.1i. Use of Greek letters to represent the position of substituent groups (credit: *Intro Chem: GOB (v. 1.0)*, CC BY-NC-SA 3.0).

IUPAC Naming of Carboxylic Acids

Here are some basic rules for naming carboxylic acids from the International Union of Pure and Applied Chemistry (IUPAC):

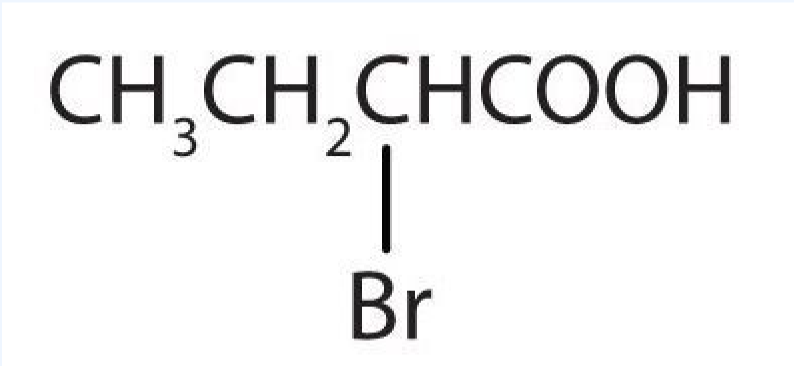
1. Select the longest carbon chain containing the carboxyl group, this is the parent chain. The -e ending of the parent alkane name is replaced by the suffix -oic acid.
2. The carboxyl carbon is always numbered "1" but the number is NOT included in the name.
3. Name the substituents attached to the chain in the usual way (providing you with the lowest numbering possible for these groups).
4. Aromatic carboxylic acids (ie. with a COOH) directly connected to a benzene ring) are named after the parents compound benzoic acid.

In the IUPAC nomenclature system, the parent hydrocarbon is the one that corresponds to the longest continuous chain (LCC) containing the carboxyl group. The –*e* ending of the parent alkane is replaced by the suffix –*oic* and the word *acid*. For example, the carboxylic acid derived from pentane is pentanoic acid ($CH_3CH_2CH_2CH_2COOH$). As with aldehydes, if there are substituents the carboxyl carbon atom is counted first; numbers are used to indicate the substituted carbon atoms in the parent chain.

Greek letters are used with common names; numbers are used with IUPAC names.

Example 25.1a

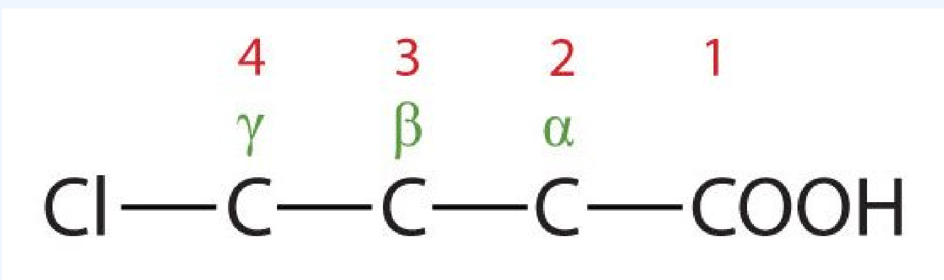
Give the common and IUPAC names for each compound.

1. $ClCH_2CH_2CH_2COOH$
2. 

(Credit: *Intro Chem: GOB (v. 1.0)*, CC BY-NC-SA 3.0).

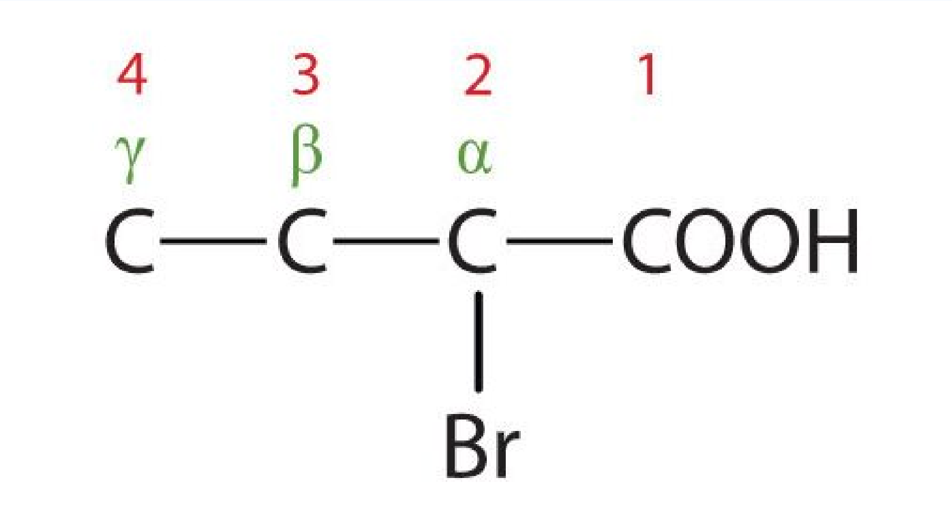
Solution

1. The LCC contains four carbon atoms; the compound is therefore named as a substituted butyric (or butanoic) acid.

   (Credit: *Intro Chem: GOB (v. 1.0)*, CC BY-NC-SA 3.0).

   The chlorine atom is attached to the γ-carbon in the common system or C4 in the IUPAC system. The compound is γ-chlorobutyric acid or 4-chlorobutanoic acid.
2. The LCC contains four carbon atoms; the compound is therefore named as a substituted butyric (or butanoic) acid.



(Credit: *Intro Chem: GOB (v. 1.0)*, CC BY-NC-SA 3.0).

The bromine (Br) atom is at the α-carbon in the common system or C2 in the IUPAC system. The compound is α-bromobutyric acid or 2-bromobutanoic acid.

Exercise 25.1a

Write the condensed structural formula for β-chloropropionic acid.

Check Your Answer[1]

Exercise 25.1b

Give the IUPAC name for each compound.

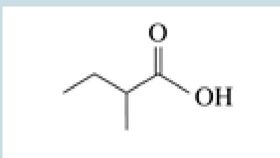
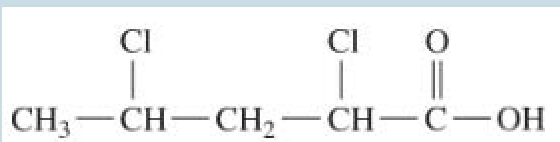
1. $ClCH_2CH_2CH_2CH_2COOH$

2. $(CH_3)_2CHCH_2CHBrCOOH$

Check Your Answers:[2]

Exercise 25.1c

Give the IUPAC name for each compound.

1. 
2. 

Check Your Answer[3]

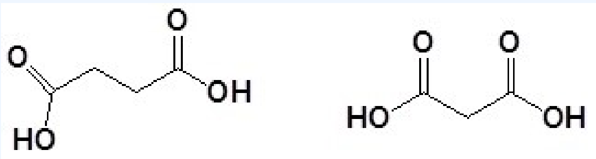
Image source: Adapted from course materials by Caryn Fahey and JR van Haarlem.

Dicarboxylic Acids

A **dicarboxylic acids** is an organic compound containing two carboxyl groups (-COOH) often referred to as a diacid. The general molecular formula for dicarboxylic acids can be written as HO–R–COOH. Dicarboxylic acids are used in the preparation of copolymers such as polyamides and polyesters. The most commonly used diacid in industry is adipic acid, which is a precursor to nylon production. Other examples of diacids include aspartic acid and glutamic acid, both of which are amino acids in the human body.

Example 25.1b

Name the following dicarboxylic acids.



(credit: *Organic Chemistry (Vollhardt & Schore)*, CC BY-NC-SA 4.0

Solution:

a. butanedioic acid
b. propanedioic acid

Example 25.1b source: *Organic Chemistry (Vollhardt & Schore)*, CC BY-NC-SA 4.0

Attribution & References

Except where otherwise noted, this page is adapted by Caryn Fahey from:

- "Why This Chapter?" In Organic Chemistry (Open Stax) by John McMurry licensed under CC BY-NC-SA 4.0. Access for free at Organic Chemistry (Open Stax)
- "15.1: Carboxylic Acids – Structures and Names" In Basics of General, Organic, and Biological Chemistry (Ball et al.) by David W. Ball, John W. Hill, and Rhonda J. Scott via LibreTexts, CC BY-NC-SA 4.0./ A LibreTexts version of Introduction to Chemistry: GOB (v. 1.0), CC BY-NC 3.0.
- "19.1: Naming the Carboxylic Acids" by Steven Farmer & William Reusch In Map: Organic Chemistry (Vollhardt and Schore), CC BY-NC-SA 4.0

References cited in-text

Anderson, C. C., & Rayner-Canham, G. (2022, Fall). *Soy sauce: An essential Inuit condiment* (https://uwaterloo.ca/chem13-news-magazine/fall-2022-special-edition/feature/soy-sauce). *Chem 13 News Magazine.*

Notes

1. Propionic acid has three carbon atoms: C–C–COOH. Attach a chlorine (Cl) atom to the parent chain at the beta carbon atom, the second one from the carboxyl group: Cl–C–C–COOH. Then add enough hydrogen atoms to give each carbon atom four bonds: $ClCH_2CH_2COOH$.

2. a. 5-chloropentanoic acid, b. 1-bromo-5-methylpentanoic acid

3. 1) 2-methylbutanoic acid 2) 2,4-dichloropentanoic acid

25.2 PHYSICAL PROPERTIES OF CARBOXYLIC ACIDS

Learning Objectives

By the end of this section, you will be able to:

- Compare the boiling points of carboxylic acids with alcohols of similar molar mass.
- Compare the solubilities of carboxylic acids in water with the solubilities of comparable alkanes and alcohols in water.

Many carboxylic acids are colourless liquids with disagreeable odours. The carboxylic acids with 5 to 10 carbon atoms all have "goaty" odours (explaining the odour of Limburger cheese). These acids are also produced by the action of skin bacteria on human sebum (skin oils), which accounts for the odour of poorly ventilated locker rooms. The acids with more than 10 carbon atoms are waxlike solids, and their odour diminishes with increasing molar mass and resultant decreasing volatility.

Carboxylic acids exhibit strong hydrogen bonding between molecules. They therefore have high boiling points compared to other substances of comparable molar mass.

The carboxyl group readily engages in hydrogen bonding with water molecules (Figure 25.2a.). The acids with one to four carbon atoms are completely miscible with water. Solubility decreases as the carbon chain length increases because dipole forces become less important and dispersion forces become more predominant. Hexanoic acid [$CH_3(CH_2)_4COOH$] is barely soluble in water (about 1.0 g/100 g of water). Palmitic acid [$CH_3(CH_2)_{14}COOH$], with its large nonpolar hydrocarbon component, is essentially insoluble in water. The carboxylic acids generally are soluble in such organic solvents as ethanol, toluene, and diethyl ether.

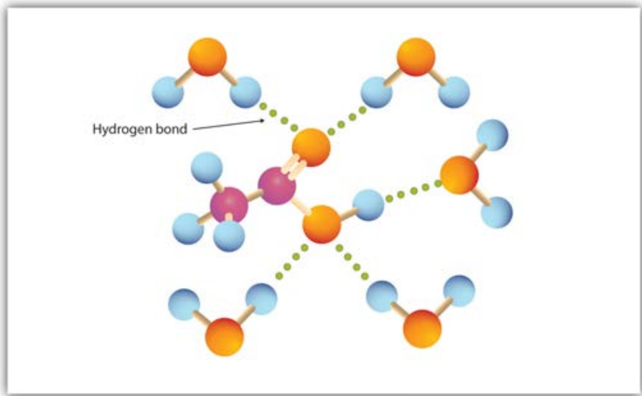


Figure 25.2a. Hydrogen Bonding between an Acetic Acid Molecule and Water Molecules. Carboxylic acids of low molar mass are quite soluble in water (credit: *Intro Chem: GOB (v. 1.0)*, CC BY-NC-SA 3.0).

Table 25.2a. gives a summary of the physical properties for selected carboxylic acids.

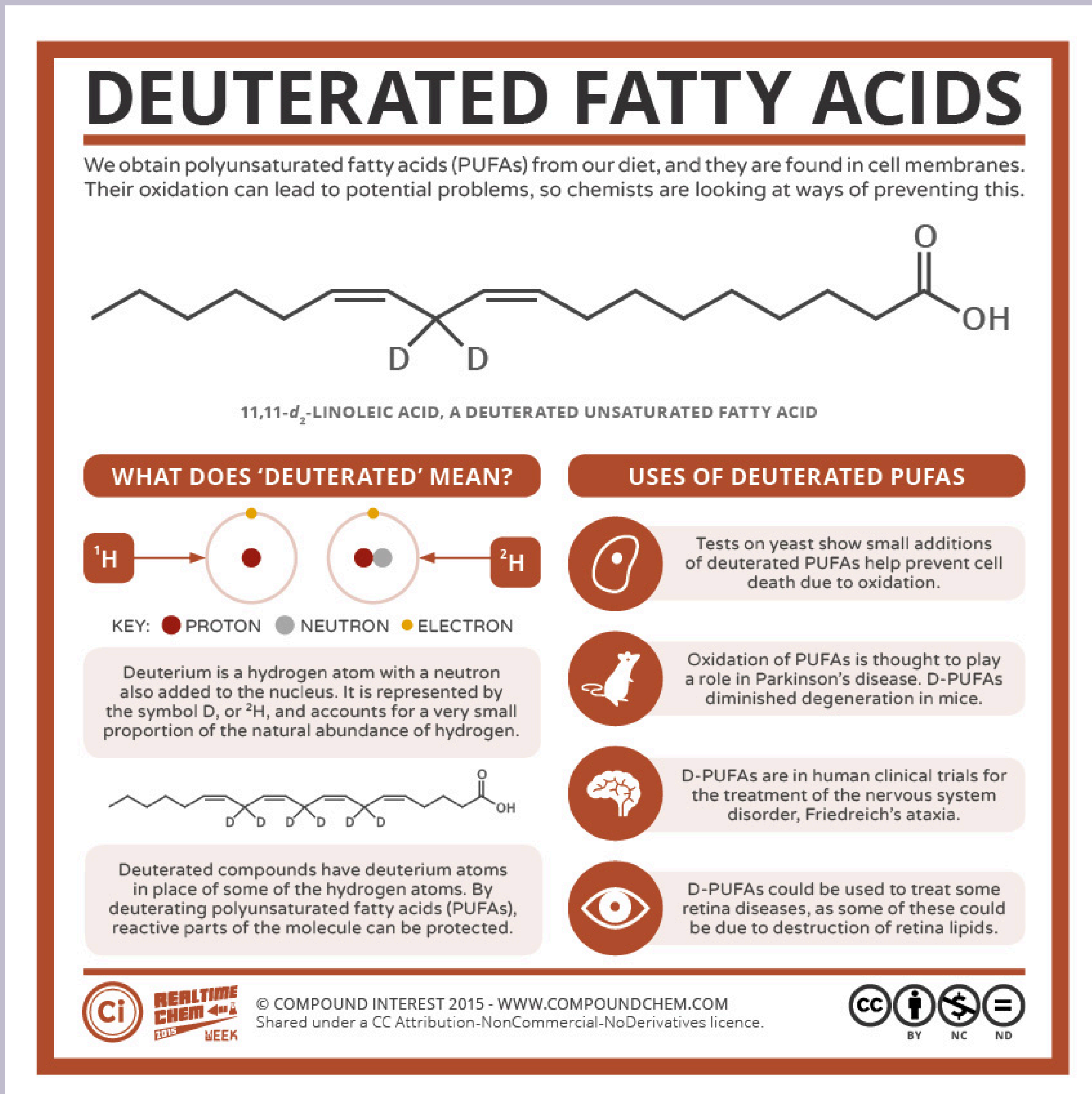
Table 25.2a. Physical Constants of Carboxylic Acids

Condensed Structural Formula	Name of Acid	Melting Point (°C)	Boiling Point (°C)	Solubility (g/100 g of Water)
$HCOOH$	formic acid	8	100	miscible
CH_3COOH	acetic acid	17	118	miscible
CH_3CH_2COOH	propionic acid	−22	141	miscible
$CH_3(CH_2)_2COOH$	butyric acid	−5	163	miscible
$CH_3(CH_2)_3COOH$	valeric acid	−35	187	5
$CH_3(CH_2)_4COOH$	caproic acid	−3	205	1.1
C_6H_5COOH	benzoic acid	122	249	0.29

Table source: "15.3: Physical Properties of Carboxylic Acids" In *Basics of GOB Chemistry (Ball et al.)*, CC BY-NC-SA 4.0.

Spotlight on Everyday Chemistry: Maksim Fomich's Research on Deuterated Fatty Acids

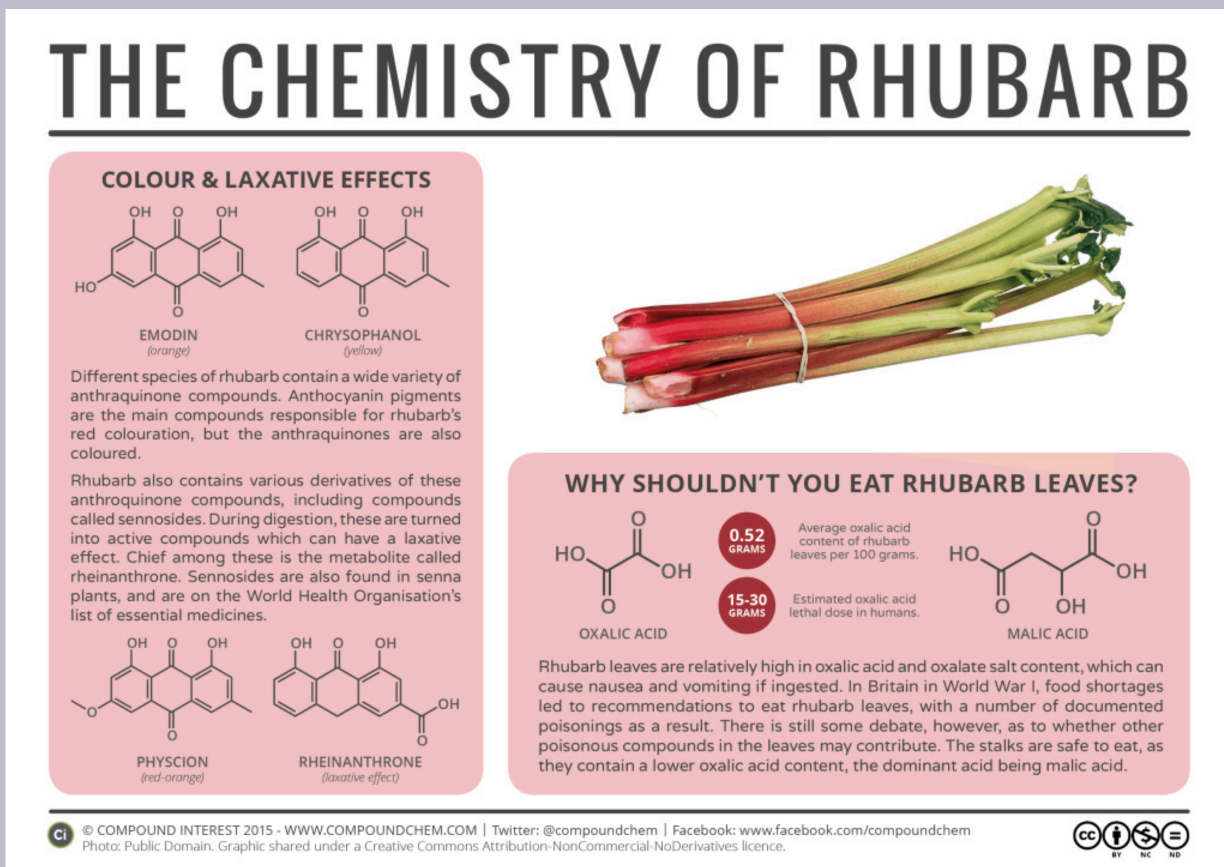
Maksim Fomich is currently looking into creating deuterated polyunsaturated fatty acid compounds, with a view to using them to potentially treat a range of diseases. Here, he explains the premise behind his research.



Infographic 25.2a. Read more about the "RTC Week 2015 – #4: Deuterating Fatty Acids to Treat Diseases (https://www.compoundchem.com/2015/10/22/rtcweek4/)" by Andy Brunning / Compound Interest, CC BY-NC-ND, or access a text-based summary of infographic 25.2a [New tab].

Spotlight on Everyday Chemistry: The Chemistry of Rhubarb

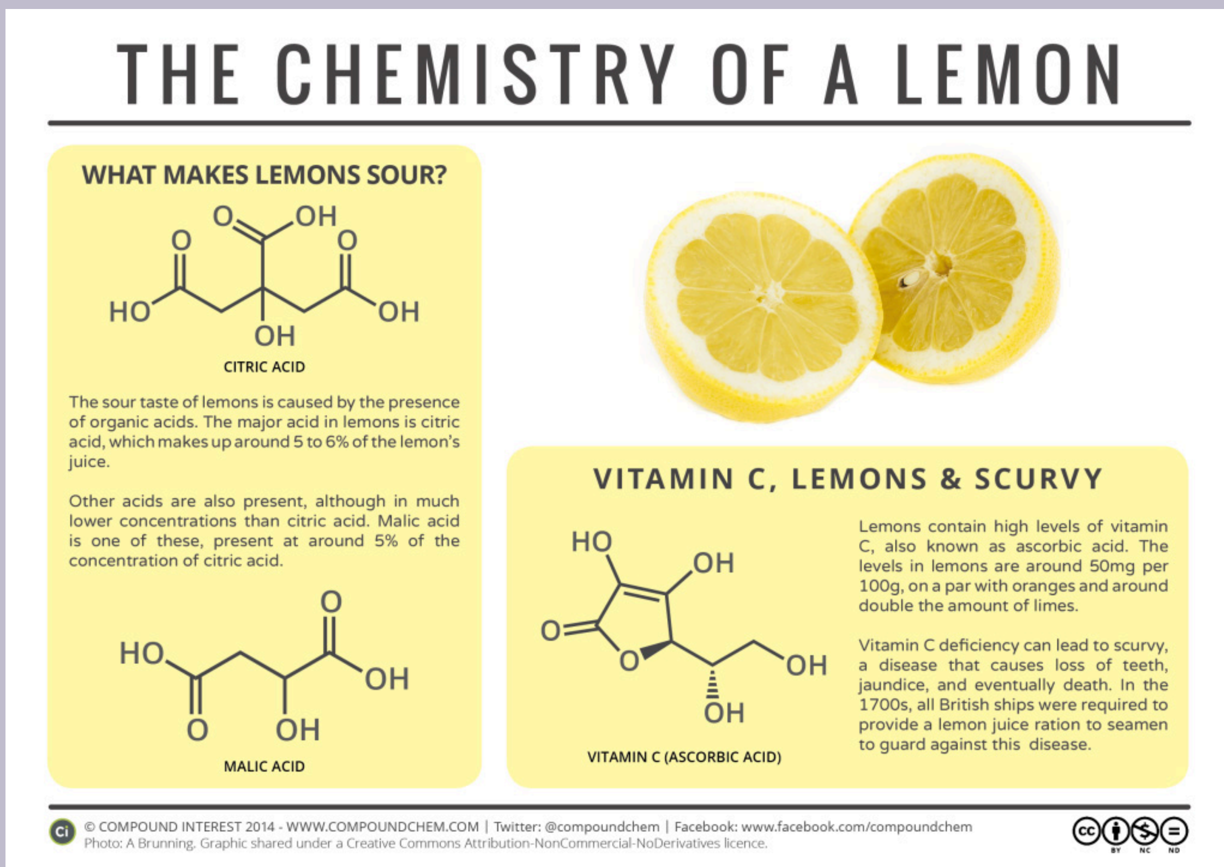
Oxalic acid, an organic compound found in rhubarb leaves, is an example of a dicarboxylic acid. In fact it is the simplest dicarboxylic acid found and is a white crystalline solid that forms a colourless solution in water. Oxalic acid is one component of rhubarb leaves that can be hard on the human stomach if ingested.



Infographic 25.2b. Read more about the "Why Shouldn't You Eat Rhubarb Leaves? – The Chemistry of Rhubarb (https://www.compoundchem.com/2015/04/16/rhubarb/)" by Andy Brunning / Compound Interest, CC BY-NC-ND, or access a text-based summary of infographic 25.2b [New tab].

Spotlight on Everyday Chemistry: The Chemistry of a Lemon

The sour taste of lemons is due in fact to the presence of carboxylic acids. Citric acid is considered to be a tricarboxylic acid, that has a role as a food acidity regulator, an antimicrobial agent and a fundamental metabolite. Malic acid is a dicarboxylic acid that contributes to the sour taste of fruits, plays a role as a food acidity regulator and can be used as a food additive.



Infographic 25.2c. Read more about the "Sourness & Scurvy – The Chemistry of a Lemon (https://www.compoundchem.com/2014/03/03/sourness-scurvy-the-chemistry-of-a-lemon/)" by Andy Brunning / Compound Interest, CC BY-NC-ND, or access a text-based summary of infographic 25.2c [New tab].

Attribution & References

Except where otherwise noted, this page is adapted by Caryn Fahey from "15.3: Physical Properties of

25.3 FORMATION AND REACTIONS OF CARBOXYLIC ACIDS

Learning Objectives

By the end of this section, you will be able to:

- Describe the preparation of carboxylic acids.
- Examine chemical reactions of and with carboxylic acids.

Organic functional groups can be converted into other functional groups through reactions. A map of some of the more common reactions to convert functional groups can be found in Section 19.6 – General Reactions of Carbon in Infographic 19.6a.

Preparation of Carboxylic Acids

Oxidation

Carboxylic acids are the most polar organic compounds because both functional groups are polar. The hydroxyl (-OH) group is similar to that in alcohols while the carbonyl group (C=O) has similarities to aldehydes and ketones. We prepare carboxylic acids by the oxidation of aldehydes or alcohols whose –OH functional group is located on the carbon atom at the end of the chain of carbon atoms in the alcohol (Figure 25.3a.).

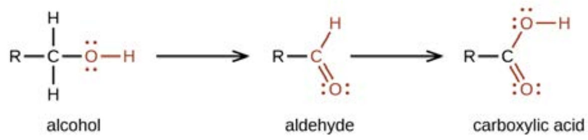


Figure 25.3a. Diagram representing the addition of a double bond to oxygen and then a hydroxyl group to an alcohol to create a carboxylic acid. (credit: *Chemistry (OpenStax)*, CC BY).

For example, in the presence of an oxidizing agent, ethanol is oxidized to acetaldehyde, which is then oxidized to acetic acid (Figure 25.3b.). This process also occurs in the liver, where enzymes catalyze the oxidation of ethanol to acetic acid using dehydrogenase. Acetic acid can be further oxidized to carbon dioxide and water.

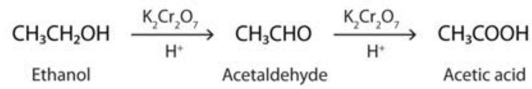


Figure 25.3b. Similar to figure 25.2a. we now see specific examples of an alcohol, aldehyde and carboxylic acid represented. (credit:*Intro to Chem: GOB (v. 1.0)*, CC BY-NC-SA 3.0).

Hydrolysis of Nitriles

Nitriles are organic compounds in which a cyano group (carbon triple bonded to a nitrogen) is attached to a carbon. In Chapter 24, hydrogen cyanide was added to an aldehyde or ketone to form a cyanohydrin. The cyanohydrin contains a nitrile (-C≡N – where ≡ is triple bond). Another method to form a nitrile is shown in Figure 25.3c. Here a primary or secondary alkyl halide will react with sodium cyanide in a substitution reaction to form the alkyl nitrile and sodium halide (Morsch et al, n.d.).

Figure 25.3c. Formation of nitrile through substitution reaction of alkyl bromide with sodium cyanide. (credit: *Organic Chem (Morsch et al.)*, CC BY-SA 4.0).

Nitriles can undergo hydrolysis reactions in the presence of an acidic or basic aqueous solution to form carboxylic acids. In the case of acid catalysts, the nitrile becomes pronated (the addition of a proton or hydrogen cation to an atom forming a conjugate acid). In the case of basic catalysts, the hydroxide anion is capable of direct addition to the carbon-nitrogen triple bond. The examples below outline the reactions taking place during hydrolysis of nitriles. Figure 25.3d. shows the basic reaction for nitriles in an acidic catalyst.

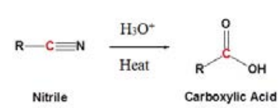


Figure 25.3d. Hydrolysis reaction of a nitrile with an acidic catalyst forming a carboxylic acid (credit: *Organic Chem (Morsch et al.)*, CC BY-SA 4.0).

Figure 25.3e. below is a specific example of acidic hydrolysis using cyclopentanecarbonitrile.

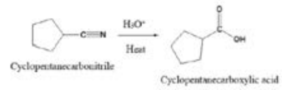


Figure 25.3e. Hydrolysis reaction of a cyclopentanecarbonitrile with an acidic catalyst forming a cyclopentanecarboxylic acid (credit: *Organic Chem (Morsch et al.)*, CC BY-SA 4.0).

Figure 25.3f., shows the basic hydrolysis reaction of nitriles with an alkaline catalyst.

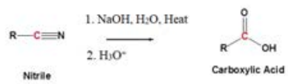


Figure 25.3f. Hydrolysis reaction of a nitrile with a basic catalyst forming a carboxylic acid (credit: *Organic Chem (Morsch et al.)*, CC BY-SA 4.0).

Figure 25.3g. below is a specific example of basic hydrolysis using Butane nitrile.

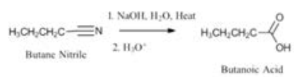


Figure 25.3g. Hydrolysis reaction of butane nitrile with a basic catalyst forming a butanoic acid (credit: *Organic Chem (Morsch et al.)*, CC BY-SA 4.0).

Reactions of Carboxylic Acids

Carboxylic acids are weak acids, meaning they are not 100% ionized in water. Generally, only about 1% of the molecules of a carboxylic acid dissolved in water are ionized at any given time. The remaining molecules are undissociated in solution. They are however considered to be more acidic than most other organic compounds. When carboxylic acids dissociate in water a hydrogen ion is transferred to a water molecule and a carboxylate ion and hydronium ion (H_3O^+) are formed (Figure 25.3h.). Refer back to Infographic 19.6a showing reactions of organic molecules.

$$\mathbf{CH_3COOH + H_2O \rightarrow CH_3COO^- + H_3O^+}$$

Carboxylic Acid + water → Carboxylate Ion + Hydronium Ion

Figure 25.3h. Reaction of a carboxylic acid with water to produce a carboxylate ion and hydronium ion.

Acid-Base Reactions of Carboxylic Acids

Because of the acidic properties of carboxylic acids, they are able to react with bases to form ionic salts. Alkali metal hydroxides and simple amines result in salts with pronounced ionic character that are usually soluble in water. An example of this can be seen in Figure 25.3i. below.

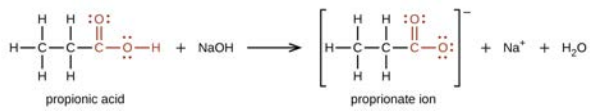


Figure 25.3i. Reaction of a carboxylic acid with a strong base (sodium hydroxide) forming a carboxylate ion, a sodium ion and water. (credit: *Chemistry (OpenStax)*, CC BY).

Heavy metals such as silver, mercury and lead form salts with more covalent characteristics which reduces water solubility, particularly for acids composed of four or more carbon atoms in the chain (Figure 25.3j).

$$RCO_2H + AgOH \rightarrow RCO_2^{\delta(-)} Ag^{\delta(+)} + H_2O$$

Figure 25.3j. Reaction of a heavy metal base with a carboxylic acid.

Esterification

Another reaction which takes place with carboxylic acids is esterification. This reaction type is commonly used to convert carboxylic acids to their ester derivatives. In order to produce an ester from an alcohol and a carboxylic acid, we must heat them in the presence of an acid catalyst such as sulfuric acid (Figure 25.3k. and Figure 25.3l.). This reaction will produce a fragrant ester and water. The reaction is reversible and will reach equilibrium with approximately equivalent amounts of reactants and products. Using excess amounts of alcohol and continuously removing a product, can drive the reaction towards the product side as per LeChatelier's principle.

Figure 25.3k. General esterification reaction with carboxylic acid and alcohol combining to form ester with byproduct of water. (credit: *Organic Chemistry (OpenStax) (https://chem.libretexts.org/Bookshelves/Introductory_Chemistry/Map%3A_Fundamentals_of_General_Organic_and_Biological_Chemistry_(McMurry_et_al.)/17%3A_Carboxylic_Acids_and_their_Derivatives/17.03%3A_Reactions_of_Carboxylic_Acids_-_Ester_and_Amide_Formation)*, CC BY-NC-SA 4.0).

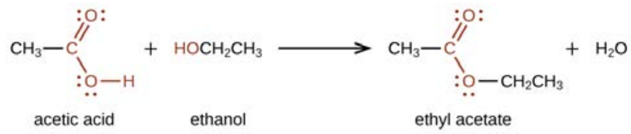


Figure 25.3l. Reaction of acetic acid and an alcohol to produce an ester and water. (credit: *Chemistry (OpenStax)*, CC BY).

Example 25.3a

Preparation of an ester via esterification uses a carboxylic acid and alcohol, heated in the presence of an acid catalyst (Figure 25.3m.). This reaction is reversible and will reach equilibrium with approximately equal amounts of reactants and products.

Write the esterification of acetic acid with 1-butanol.

Solution:

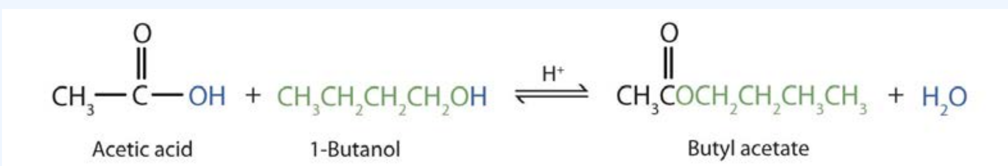


Figure 25.3m. Esterification of acetic acid and 1-butanol forming butyl acetate and water (credit: *Organic Chemistry (OpenStax) (https://chem.libretexts.org/Bookshelves/Introductory_Chemistry/Map%3A_Fundamentals_of_General_Organic_and_Biological_Chemistry_(McMurry_et_al.)/17%3A_Carboxylic_Acids_and_their_Derivatives/17.03%3A_Reactions_of_Carboxylic_Acids_-_Ester_and_Amide_Formation)*, CC BY-NC-SA 4.0).

Amide Formation

Similar to esterification, carboxylic acids will react with ammonia to form a primary amide (Figure 25.3n.). When a carboxylic acid reacts with primary or secondary amines, secondary or tertiary amides are produced, respectively (Figure 25.3o.). Tertiary amines do not form amides when reacted with carboxylic acids.

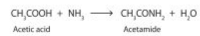


Figure 25.3n. Primary amide formation from reaction of carboxylic acid with ammonia. (credit: *Organic Chemistry (OpenStax) (https://chem.libretexts.org/Bookshelves/Introductory_Chemistry/Map%3A_Fundamentals_of_General_Organic_and_Biological_Chemistry_(McMurry_et_al.)/17%3A_Carboxylic_Acids_and_their_Derivatives/17.03%3A_Reactions_of_Carboxylic_Acids_-_Ester_and_Amide_Formation)*, CC BY-NC-SA 4.0).

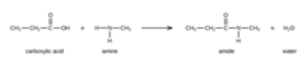


Figure 25.3o. Formation of secondary amide from reaction of carboxylic acid with primary amine. (credit: *Organic Chemistry (OpenStax) (https://chem.libretexts.org/Bookshelves/Introductory_Chemistry/Map%3A_Fundamentals_of_General_Organic_and_Biological_Chemistry_(McMurry_et_al.)/17%3A_Carboxylic_Acids_and_their_Derivatives/17.03%3A_Reactions_of_Carboxylic_Acids_-_Ester_and_Amide_Formation)*, CC BY-NC-SA 4.0).

Exercise 25.3a

Write the product that results from each of the following reactions.

a. methanol + 2-methylbutanoic acid
b. ethanol + pentanoic acid
c. propanoic acid + ammonia

Check Your Answers:[1]

Exercise and image source: Exercise 25.3a questions and answers are created by Samantha Sullivan Sauer, using images from Biovia Draw, licensed under CC BY-NC 4.0

Acid Chloride Formation and Reactions

Carboxylic acids react with thionyl chloride ($SOCl_2$) to form acid chlorides (also known as acyl chlorides) (Figure 25.3p.). During the reaction the hydroxyl group of the carboxylic acid is converted to a chlorosulfite intermediate making it a better leaving group. The chloride anion produced during the reaction acts a nucleophile. Acyl chlorides are extremely reactive, resulting in the chlorine being replaced with something else.

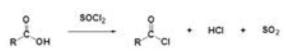


Figure 25.3p. General reaction of carboxylic acid with thionyl chloride to produce acid chloride (credit: *Supplemental Modules (Organic Chemistry*, CC BY-NC-SA 4.0).

An acid chloride will react with a carboxylic acid to form an acid anhydride (Figure 25.3q.), with water to form a carboxylic acid (Figure 25.3r.), with an alcohol to form an ester (Figure 25.3s.) and with ammonia or an amine to form an amide (Figure 25.3t.).

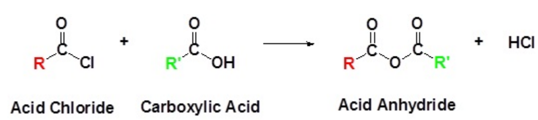


Figure 25.3q. Formation of an acid anhydride from substitution of an acid chloride with a carboxylic acid (credit: *UIS: CHE 269 (Morsch and Andrews)* , CC BY-NC-SA 4.0).

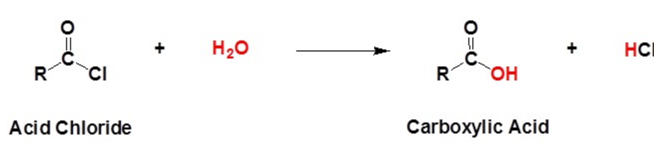


Figure 25.3r. Formation of a carboxylic acid from substitution of an acid chloride with water (credit: *UIS: CHE 269 (Morsch and Andrews)* , CC BY-NC-SA 4.0).

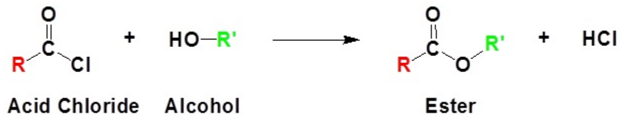


Figure 25.3s. Formation of an ester from substitution of an acid chloride with an alcohol (credit: *UIS: CHE 269 (Morsch and Andrews)* , CC BY-NC-SA 4.0).

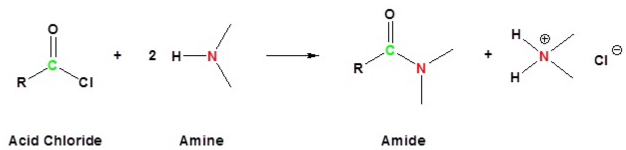
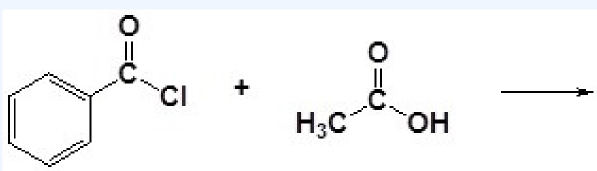
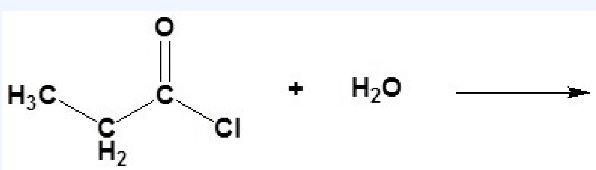


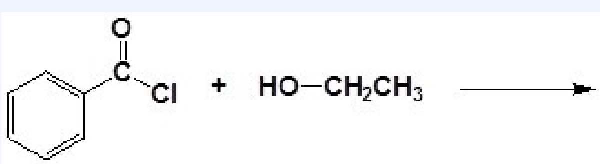
Figure 25.3t. Formation of an amide from substitution of an acid chloride with an amine or ammonia (credit: *UIS: CHE 269 (Morsch and Andrews)* , CC BY-NC-SA 4.0).

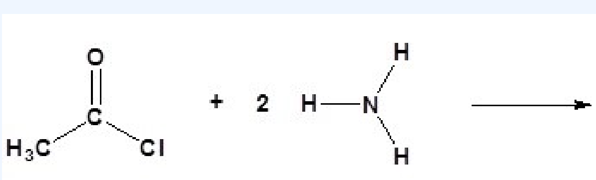
Example 25.3b

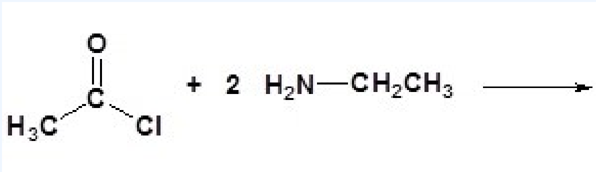
Complete each reaction.

(a) 

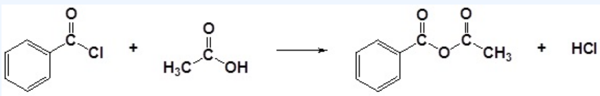
(b) 

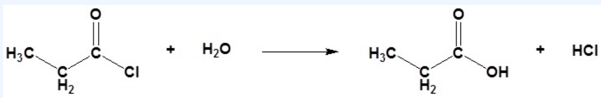
(c) 

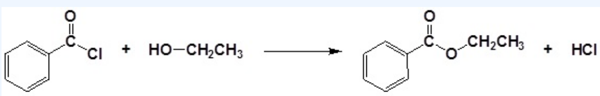
(d) 

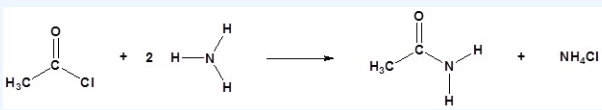
(e) 

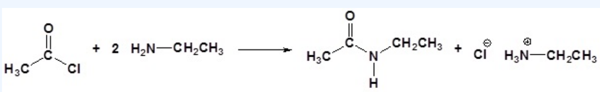
Solutions:

(a) 

(b) 

(c) 

(d) 

(e) 

Example source and images source: *UIS: CHE 269 (Morsch and Andrews)*, CC BY-NC-SA 4.0).

For more advanced understanding of Carboxylic acid structure and reactions check out the videos below.

Watch Crash Course – Organic Chemistry #30 on YouTube (11 min) (https://youtu.be/cA0fGIfALxI?)

Watch Crash Course – Organic Chemistry #31 on YouTube (12 min) (https://youtu.be/VfX2od-AwRo?)

Attribution & References

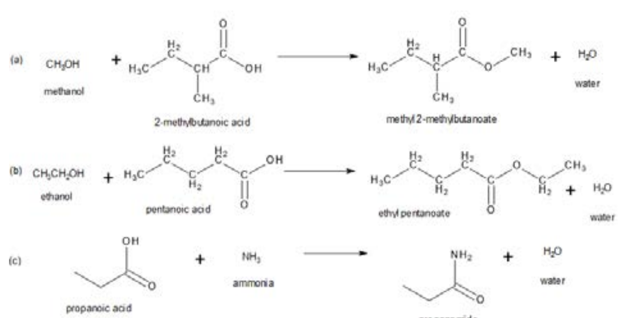
Except where otherwise noted, this page is written and adapted by Caryn Fahey and Samantha Sullivan Sauer from

- “15.2: The Formation of Carboxylic Acids” In *Basics of General, Organic, and Biological Chemistry (Ball et al.)* by David W. Ball, John W. Hill, and Rhonda J. Scott via LibreTexts, licensed under CC BY-NC-SA 4.0. / A derivative authored, remixed, and/or curated by Anonymous via source content that

References cited in-text

Farmer, S., Kennepohl, D., Morsch, L., & Reusch, W. (n.d.). Chemistry of Nitriles (https://chem.libretexts.org/Bookshelves/Organic_Chemistry/Organic_Chemistry_(Morsch_et_al.)/20%3A_Carboxylic_Acids_and_Nitriles/20.07%3A_Chemistry_of_Nitriles). In *Organic Chemistry (Morsch et al.)*. CC BY-SA 4.0.

Notes

1. 

25.4 IONIZATION AND NEUTRALIZATION OF CARBOXYLIC ACIDS

Learning Objectives

By the end of this section, you will be able to:

- Name the typical reactions that take place with carboxylic acids.
- Describe how carboxylic acids react with basic compounds.

Ionization of Carboxylic Acids

The acidic nature of carboxylic acids, compared to other organic molecules, is due to the fact that the carboxyl group contains hydrogen which in solution in water can be transferred to the water molecule. The carboxylic acid in aqueous solutions acts as a weak acid and will only partially dissociate. The dissociated ions include the corresponding carboxylate anion and the hydronium cation (H_3O^+) (Figure 25.4a. and 25.4b.). The carboxylate anions are named by replacing the *–ic acid* ending from the carboxylic acid with *–ate*, see examples below (Kennepohl et al, n.d.).

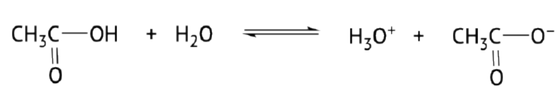


Figure 25.4a. Reaction of acetic acid and water produce hydronium ions and carboxylate ions. (Credit: *Chem 114: Human Chemistry II (Muíño)*, CC BY-NC-SA 4.0).

Figure 25.4b. Reaction of pyruvic acid and water produce pyruvate ions and hydronium ions. (Credit: *Chem 114: Human Chemistry II (Muíño)*,CC BY-NC-SA 4.0).

The extent of dissociation of these weak acids in water is described by K_a values. Remember that a compound with a smaller K_a value will be a weaker acid (Figure 25.4c).

$$RCOOH + H_2O \leftrightarrow RCOO^- + H_3O^+ \quad K_a = \frac{[RCOO^-][H_3O^+]}{[RCOOH]}$$

Figure 25.4c. Dissociation of carboxylic acids and their K_a equation. (Credit: *Chem 114: Human Chemistry II (Muíño)*,CC BY-NC-SA 4.0).

When comparing the acidity of organic and biomolecules, it is useful (and more preferable) to use pK_a values instead of K_a values, which are calculated by taking the negative log of K_a: $pK_a = -\log(K_a)$. When using the pK_a scale, it is important to know that *weaker acids* have *larger* and more positive pK_a values, this is opposite of K_a values. The pK_a values of some typical carboxylic acids are listed in Table 25.4a. (Remember that pK_a is a log expression, which means that every 1 pK_a unit represents a 10-fold change in acidity.)

Table 25.4a. Comparisons of Carboxylic Acid K_a and pK_a Values

Name	Compound	K_a	pK_a
formic acid	HCOOH	$1.8 X 10^{-4}$	3.74
acetic acid	CH_3COOH	$1.8 X 10^{-5}$	4.74
propanoic acid	CH_3CH_2COOH	$1.3 X 10^{-5}$	4.89
butanoic acid	$CH_3CH_2CH_2COOH$	$1.5 X 10^{-5}$	4.82
chloroacetic acid	$ClCH_2COOH$	$1.4 X 10^{-3}$	2.85
trichloroacetic acid	Cl_3CCOOH	$2.3 X 10^{-1}$	0.64
hexanoic acid	$CH_3(CH_2)_4COOH$	$1.3 X 10^{-5}$	4.89
benzoic acid	C_6H_5COOH	$6.5 X 10^{-5}$	4.19
oxalic acid	HOOCCOOH	$5.4 X 10^{-2}$	1.27
	$^-OOCCOOH$	$5.2 X 10^{-5}$	4.28
glutaric acid	$HOOC(CH_2)_3COOH$	$4.5 X 10^{-5}$	4.35
	$^-OOC(CH_2)_3COOH$	$3.8 X 10^{-6}$	5.42

Source: Comparison of Carboxylic acids. (Credit: *Chem 114: Human Chemistry II (Muíño)*,CC BY-NC-SA 4.0).

These water-soluble carboxylic acids ionize to form moderately acidic solutions that exhibit the typical properties of acids, such as changing litmus from blue to red (Figure 25.4d). The anion formed when a carboxylic acid dissociates is called the *carboxylate* anion ($RCOO^-$).

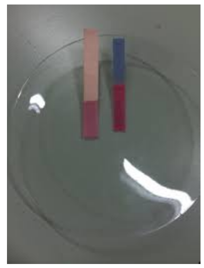


Figure. 25.4d. Litmus paper has been exposed to an acidic solution. (Credit: Photo by Kanesskong, CC BY-SA 4.0)

Neutralization of Carboxylic Acids

Carboxylic acids will react with bases such as sodium hydroxide (NaOH), sodium carbonate (Na_2CO_3), and sodium bicarbonate ($NaHCO_3$) to form water and a carboxylic acid salt:

$$RCOOH + NaOH(aq) \rightarrow RCOO^-Na^+(aq) + H_2O$$

$$2RCOOH + Na_2CO_3(aq) \rightarrow 2RCOO^-Na^+(aq) + H_2O + CO_2(g)$$

$$RCOOH + NaHCO_3(aq) \rightarrow RCOO^-Na^+(aq) + H_2O + CO_2(g)$$

In these reactions, the carboxylic acids act like inorganic acids: they neutralize basic compounds. With solutions of carbonate (CO_3^{2-}) and bicarbonate (HCO_3^-) ions, they also form carbon dioxide gas.

Carboxylic acid salts are named in the same manner as inorganic salts: the name of the cation is followed by the name of the organic anion. The name of the anion is obtained by dropping the –*ic* ending of the acid name and replacing it with the suffix –*ate* (Figure 25.4e). This rule applies whether we are using common names or International Union of Pure and Applied Chemistry (IUPAC) names:

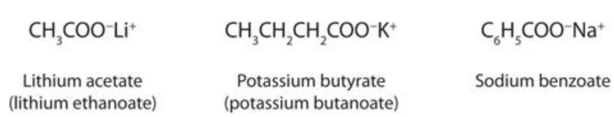


Figure 25.4e. Examples of carboxylate anions – positively charged ions.(Credit: *Intro to Chem: GOB (V. 1.0).*, CC BY-NC-SA 3.0.)

The salts of long-chain carboxylic acids are called soaps (Figure 25.4f). We discuss the chemistry of soaps elsewhere.

$$CH_3(CH_2)_{13}CH_2COO^-Na^+$$

Sodium palmitate (a soap)

Figure 25.4f. Condensed structural formula for sodium palmitate. (Credit: *Intro to Chem: GOB (V. 1.0)*., CC BY-NC-SA 3.0.)

Example 25.4a

Write an equation for each reaction.

1. the ionization of propionic acid in water (H_2O)
2. the neutralization of propionic acid with aqueous sodium hydroxide (NaOH)

Solution:

Propionic acid has three carbon atoms, so its formula is CH_2CH_2COOH.

1. Propionic acid ionizes in water to form a propionate ion and a hydronium (H_3O^+) ion. $CH_3CH_2COOH(aq) + H_2O(\ell) \rightarrow CH_3CH_2COO^-(aq) + H_3O^+(aq)$
2. Propionic acid reacts with NaOH(aq) to form sodium propionate and water. $CH_3CH_2COOH(aq) + NaOH(aq) \rightarrow CH_3CH_2COO^-Na^+(aq) + H_2O(\ell)$

Exercise 25.4a

Write an equation for the reaction of decanoic acid with each compound.

a. aqueous sodium hydroxide (NaOH)
b. aqueous sodium bicarbonate ($NaHCO_3$)

Check Your Answer[1]

Spotlight on Everyday Chemistry: Organic Salts as Preservatives

Some organic salts are used as preservatives in food products. They prevent spoilage by inhibiting the growth of bacteria and fungi. Calcium and sodium propionate, for example, are added to processed cheese and bakery goods; sodium benzoate is added to cider, jellies, pickles, and syrups; and sodium sorbate and potassium sorbate are added to fruit juices, sauerkraut, soft drinks, and wine (Figure 25.4g). Look for them on ingredient labels the next time you shop for groceries.

$(CH_3CH_2COO^-)_2\ Ca^{2+}$

Calcium propionate

$CH_3CH{=}CHCH{=}CHCOO^-K^+$

Potassium sorbate

Figure 25.4g. Examples of carboxylate anions – calcium propionate and potassium sorbate. (Credits: *Intro to Chem: GOB (V. 1.0)*., CC BY-NC-SA 3.0.)

Attribution & References

Except where otherwise noted, this page is adapted by Caryn Fahey from:

- "15.4: Chemical Properties of Carboxylic Acids- Ionization and Neutralization" In *Basics of General,*

References cited in-text

Kennepohl, D., Morsch, L., Farmer, S. Reusch, W. (n.d.). 20.2: Structure and properties of carboxylic acids. In *Organic Chemistry (Morsch et al.)*. LibreTexts. CC BY-SA 4.0.

Notes

1.
    a. Decanoic acid has 10 carbon atoms. It reacts with NaOH to form a salt and water (H_2O). $CH_3(CH_2)_8COOH + NaOH(aq) \rightarrow CH_3(CH_2)_8COO^{-}Na^{+}(aq) + H_2O(\ell)$
    b. With $NaHCO_3$, the products are a salt, H_2O, and carbon dioxide (CO_2). $CH_3(CH_2)_8COOH + NaHCO_3(aq) \rightarrow CH_3(CH_2)_8COO^{-}Na^{+}(aq) + H_2O(\ell) + CO_2(g)$

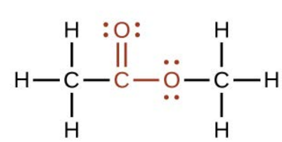
25.5 ESTERS - STRUCTURE, PROPERTIES AND NAMING

Learning Objectives

By the end of this section, you will be able to:

- Identify the general structure for an ester.
- Use common names to name esters.
- Name esters according to the IUPAC system.
- Compare the boiling points of esters with alcohols of similar molar mass.
- Compare the solubilities of esters in water with the solubilities of comparable alkanes and alcohols in water.

Esters contain a carbonyl group with a second oxygen atom bonded to the carbon atom in the carbonyl group by a single bond. In an ester, the second oxygen atom bonds to another carbon atom (Figure 25.5a.). The names for esters include prefixes that denote the lengths of the carbon chains in the molecules and are derived following nomenclature rules similar to those for inorganic acids and salts. The functional groups for an ester are shown in red below.



methyl ethanoate
(methyl acetate)

Figure 25.5a. Condensed structural formula for an ester highlighting the carbonyl group and a single oxygen bonded to another carbon (credit: *Chemistry (OpenStax)*, CC BY).

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 25.5b. shows models for two common esters.

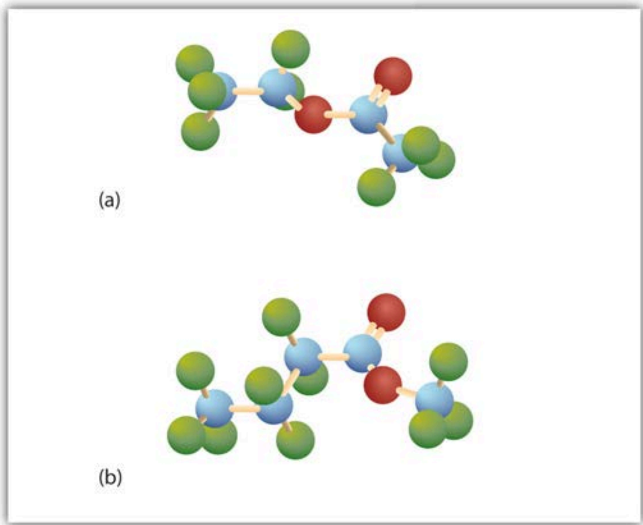


Figure 25.5b. The Structure of Esters. Esters feature a carbon-to-oxygen double bond that is also singly bonded to a second oxygen atom, which is then joined to an alkyl or an aryl group. The esters shown here are ethyl acetate (a) and methyl butyrate (b). (credit: *Intro Chem: GOB (V. 1.0).*, CC BY-NC-SA 3.0.)

Esters are produced by the reaction of acids with alcohols. For example, the ester ethyl acetate, $CH_3CO_2CH_2CH_3$, is formed when acetic acid reacts with ethanol (Figure 25.5c.).

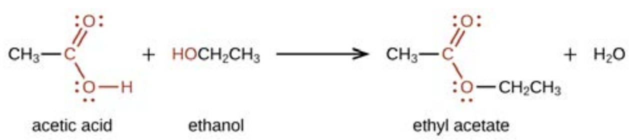


Figure 25.5c. Chemical reaction of acetic acid and ethanol to produce an ester: ethyl acetate (credit: *Chemistry (OpenStax)*, CC BY 4.0).

Properties of Esters

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

Ester molecules are polar but have no hydrogen atom attached directly to an oxygen atom. They are therefore incapable of engaging in intermolecular hydrogen bonding with one another and thus have considerably lower boiling points than their isomeric carboxylic acids counterparts. Because ester molecules can engage in hydrogen bonding with water molecules, however, esters of low molar mass are somewhat soluble in water. Borderline solubility occurs in those molecules that have three to five carbon atoms. Table 25.5a. lists the physical properties of some common esters.

Esters are common solvents. Ethyl acetate is used to extract organic solutes from aqueous solutions—for example, to remove caffeine from coffee. It also is used to remove nail polish and paint. Cellulose nitrate is dissolved in ethyl acetate and butyl acetate to form lacquers. The solvent evaporates as the lacquer "dries," leaving a thin film on the surface. High boiling esters are used as softeners (plasticizers) for brittle plastics.

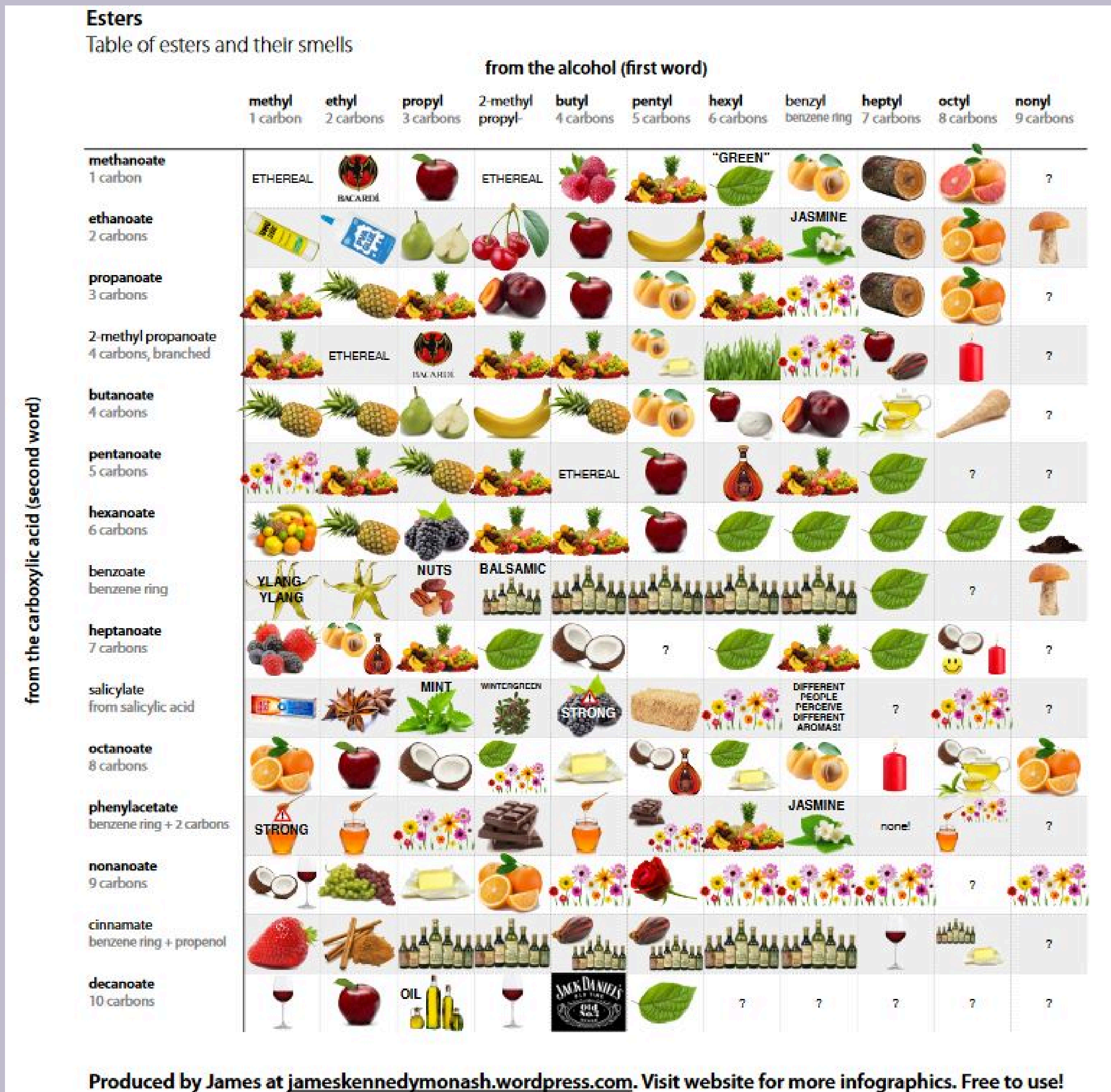
Table 25.5a. *Physical Properties of Some Esters*

Condensed Structural Formula	Name	Molar Mass	Melting Point (°C)	Boiling Point (°C)	Aroma
$HCOOCH_3$	methyl formate	60	−99	32	
$HCOOCH_2CH_3$	ethyl formate	74	−80	54	rum
CH_3COOCH_3	methyl acetate	74	−98	57	
$CH_3COOCH_2CH_3$	ethyl acetate	88	−84	77	
$CH_3CH_2CH_2COOCH_3$	methyl butyrate	102	−85	102	apple
$CH_3CH_2CH_2COOCH_2CH_3$	ethyl butyrate	116	−101	121	pineapple
$CH_3COO(CH_2)_4CH_3$	pentyl acetate	130	−71	148	pear
$CH_3COOCH_2CH_2CH(CH_3)_2$	isopentyl acetate	130	−79	142	banana
$CH_3COOCH_2C_6H_5$	benzyl acetate	150	−51	215	jasmine
$CH_3CH_2CH_2COO(CH_2)_4CH_3$	pentyl butyrate	158	−73	185	apricot
$CH_3COO(CH_2)_7CH_3$	octyl acetate	172	−39	210	orange

Source: "15.6: Physical Properties of Esters" In *Basics of GOB Chemistry (Ball et al.)*, CC BY-NC-SA 4.0.

Spotlight of Everyday Chemistry: Esters and Their Smells

The infographic below represents some of the common smells produced by esters. We find that several fruity smells we are familiar with in the foods we eat and cook with are produced by esters.



The distinct smell we can imagine when we walk through a Christmas tree farm is due to an ester found in the oils of conifer trees. Similar to Christmas trees, mangoes have a distinct aroma. This smell is due to an ester which provides the fruity notes found in mangoes.

Visit the Compound Interest website by Andy Brunning to read more about the "Aroma Chemistry: The Aroma of Christmas Trees [New tab] (https://www.compoundchem.com/2014/12/19/christmastrees/)" or the "The Chemistry of Mangos: What Do They Have in Common with Poison Ivy? [New tab] (https://www.compoundchem.com/2017/06/13/mango/)"

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.

Here are some basic rules for naming esters from the International Union of Pure and Applied Chemistry (IUPAC):

1. Write the name for the carbon chain from the alcohol as an *alkyl group.* For example if the alcohol is ethanol, the first word in ester naming will be ethyl.
2. The second word for naming an ester involves naming the acid but substituting the *-oic* ending for *-oate.* For example if the acid is ethanoic acid, the second word in the name becomes ethanoate.

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 25.5b.).

Table 25.5b. Nomenclature of Esters

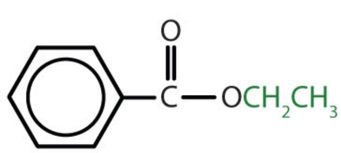
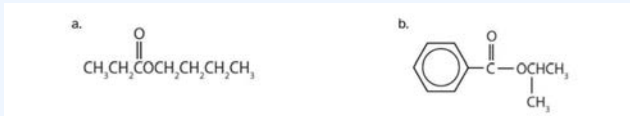
Condensed Structural Formula	Common Name	IUPAC Name
$HCOOCH_3$	methyl formate	methyl methanoate
CH_3COOCH_3	methyl acetate	methyl ethanoate
$CH_3COOCH_2CH_3$	ethyl acetate	ethyl ethanoate
$CH_3CH_2COOCH_2CH_3$	ethyl propionate	ethyl propanoate
$CH_3CH_2CH_2COOCH(CH_3)_2$	isopropyl butyrate	isopropyl butanoate
	ethyl benzoate	ethyl benzoate

Table and image credit: *Intro Chem: GOB (V. 1.0).*, CC BY-NC-SA 3.0.

Example 25.5a

Give the common and IUPAC names for each compound.



(credit: *Intro Chem: GOB (V. 1.0).*, CC BY-NC-SA 3.0).

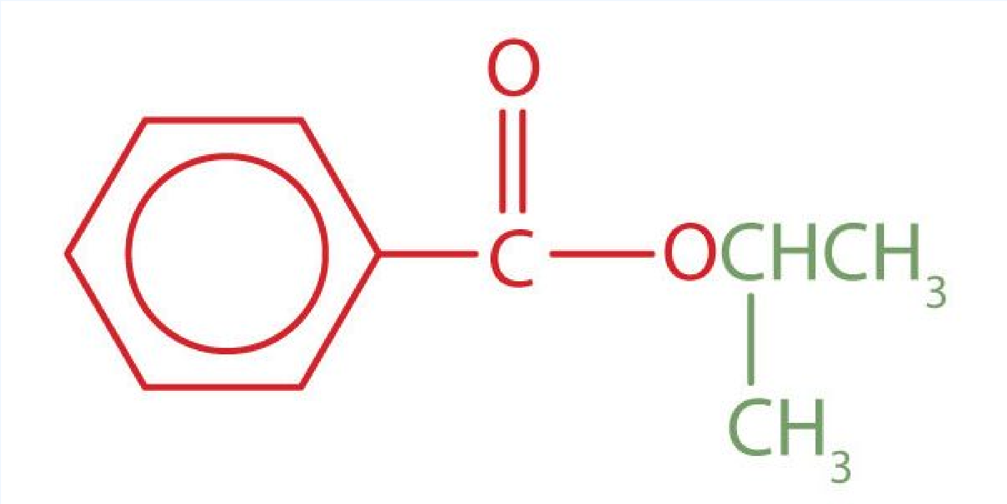
Solution:

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

(credit: *Intro Chem: GOB (V. 1.0).*, CC BY-NC-SA 3.0).

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).

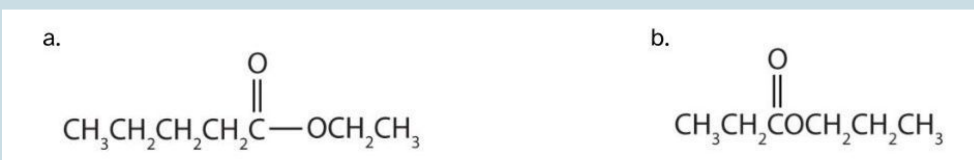


(credit: *Intro Chem: GOB (V. 1.0).*, CC BY-NC-SA 3.0).

Exercise & Image credits: *Intro Chem: GOB (V. 1.0).*, CC BY-NC-SA 3.0

Exercise 25.5a

Give the common and IUPAC names for each compound.



(Credit: *Intro Chem: GOB (V. 1.0).*, CC BY-NC-SA 3.0.)

Check Your Answers:[1]

Exercise & Image credits: *Introduction to Chemistry: GOB.*, CC BY-NC-SA 3.0.

Exercise 25.5b

Draw the structure for ethyl pentanoate.

Check Your Answer[2]

Exercise & solution image credits: *Introduction to Chemistry: GOB.*, CC BY-NC-SA 3.0.

Indigenous Perspectives: The Strawberry

The strawberry or *ken'niiohontésha* in Mohawk language, is a symbol of importance in woman's medicine and for naming babies in the longhouse. The strawberry is one of several festivals in Haudenosaunee's cycle of ceremonies to give thanks to the natural world.

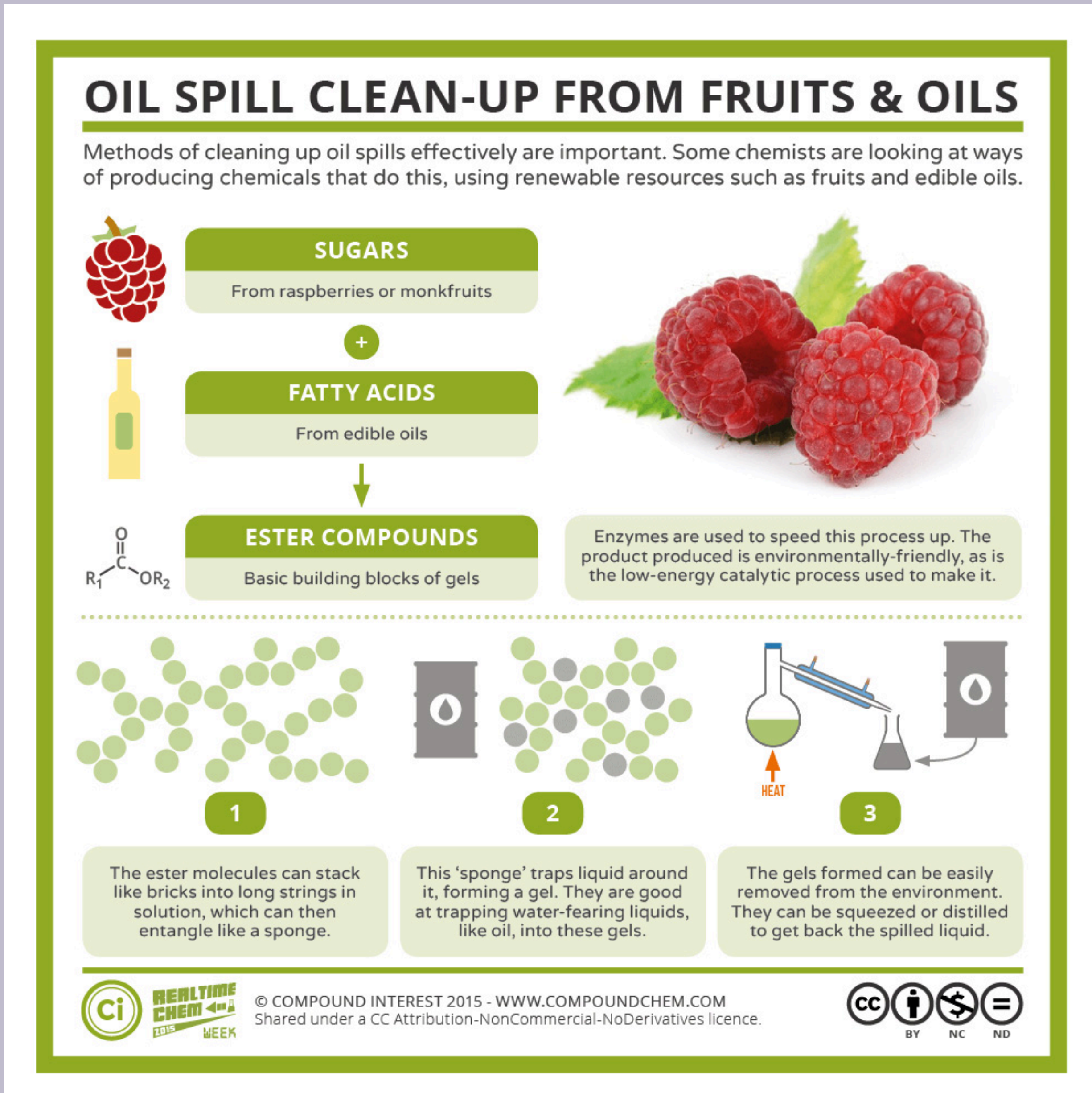
Figure 25.5d. Over 350 different volatile molecules (many members of the ester family) have been identified in strawberries. (credit: Photo by Rebecca Siegel, *Chemistry (OpenStax) (https://openstax.org/books/chemistry/pages/1-introduction)*, CC BY 4.0).

For more details on the importance of the strawberry read: CBC News – Strawberry harvest has cultural and ceremonial significance for Kahnawake community [New tab] (https://www.cbc.ca/news/indigenous/kahnawake-mohawk-community-garden-strawberries-1.4728940). The interview below with Elder Duke Redbird also looks at the importance of the strawberry "heart berry": City News – The Indigenous story of the Strawberry Moon [New tab] (https://www.youtube.com/watch?v=RSi39qSrVYI).

Spotlight on Everyday Chemistry: Julian Silverman's Research on Oil Spill

Cleanup


JULIAN SILVERMAN
PhD CANDIDATE, THE CITY COLLEGE OF NEW YORK



Infographic 25.5b. Read more about "RTC Week 2015 – #2: Oil Spill Clean-Ups Using Fruits & Oils (https://www.compoundchem.com/2015/10/20/rtcweek2/)" by Andy Brunning / Compound Interest, CC BY-NC-ND, or access a text-based summary of infographic 25.5b [New tab].

Attribution & References

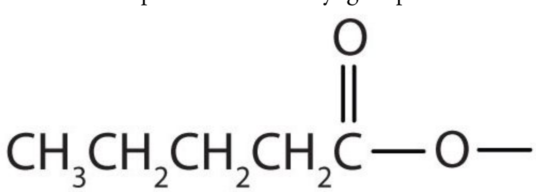
Except where otherwise noted, this page is adapted by Caryn Fahey from:

- "18.3 Aldehydes, Ketones, Carboxylic Acids, and Esters" In *General Chemistry 1 & 2* by Rice University, a derivative of *Chemistry (Open Stax)* by Paul Flowers, Klaus Theopold, Richard Langley & William R. Robinson and is licensed under CC BY 4.0. Access for free at *Chemistry (OpenStax) (https://openstax.org/books/chemistry/pages/1-introduction)*
- "15.5: Esters – Structures and Names" & "15.6: Physical Properties of Esters" In Basics of General, Organic, and Biological Chemistry (Ball et al.)by David W. Ball, John W. Hill, and Rhonda J. Scott via LibreTexts, CC BY-NC-SA 4.0./ A LibreTexts version of *Introduction to Chemistry: GOB (v. 1.0),* CC BY-NC 3.0.

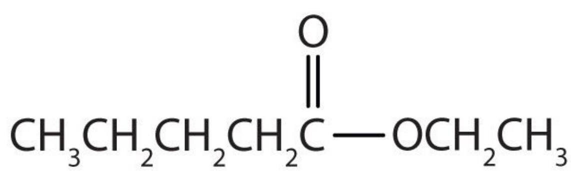
Notes

1. a. ethyl pentanoate, b. propyl propanoate.

2. 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.



25.6 REACTIONS OF ESTERS

Learning Objectives

By the end of this section, you will be able to:

- Identify and describe the substances from which most esters are prepared.
- Describe the typical reaction that takes place with esters.
- Identify the products of an acidic hydrolysis of an ester.
- Identify the products of a basic hydrolysis of an ester.

Preparation of Esters

Some esters can be prepared by esterification, a reaction in which a carboxylic acid and an alcohol, heated in the presence of a mineral acid catalyst, form an ester and water (Figure 25.6a.).

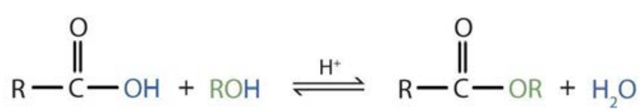


Figure 25.6a. Chemical reaction of an alcohol and a carboxylic acid forming an ester and water (credit: *Intro Chem: GOB (V. 1.0).*, CC BY-NC-SA 3.0).

The reaction is reversible. As a specific example of an esterification reaction, butyl acetate can be made from acetic acid and 1-butanol (Figure 25.6b.).

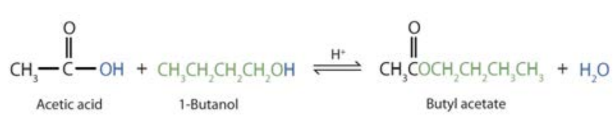
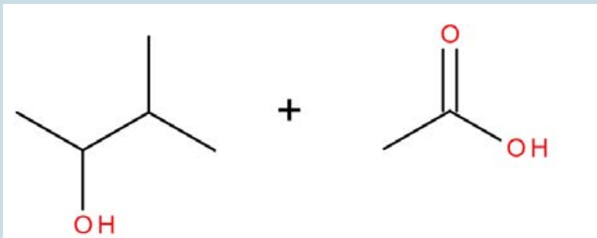


Figure 25.6b. Chemical reaction of an alcohol and a carboxylic acid forming an ester and water (credit: *Intro Chem: GOB (V. 1.0).*, CC BY-NC-SA 3.0).

Exercise 25.6a

What is the major product when the following reaction occurs?



Check Your Answer:[1]

Source: Exercise 25.6a by Samantha Sullivan Sauer, drawn using Biovia Draw, CC BY-NC 4.0

The video below outlines the basic structure of esters as well as examining how they are formed. **Watch GCSE Chemistry – Esters #59 On YouTube (2 mins) (https://youtu.be/cYgRd4rXY6I?)**

Video Source: GCSE Chemistry. (2020, March 26). *GCSE Chemistry – Esters #59 (youtube.com)* [Video]. YouTube.

Reactions of Esters

Esters are neutral compounds, unlike the acids from which they are formed. In typical reactions, the alkoxy (OR′) group of an ester is replaced by another group. One such reaction is hydrolysis, literally "splitting with water." The hydrolysis of esters is catalyzed by either an acid or a base.

Acidic hydrolysis is simply the reverse of **esterification**. The ester is heated with a large excess of water containing a strong-acid catalyst (Figure 25.6c.). Like esterification, the reaction is reversible and does not go to completion.

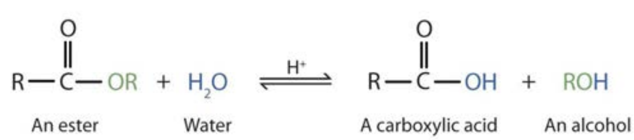


Figure 25.6c. A chemical reaction of an ester with water is the reverse of the production of an ester (esterification) (credit: *Intro Chem: GOB (V. 1.0).*, CC BY-NC-SA 3.0).

As a specific example, butyl acetate and water react to form acetic acid and 1-butanol (Figure 25.6d.). The reaction is reversible and does not go to completion.

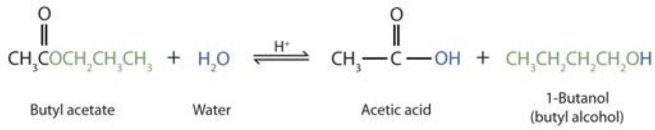


Figure 25.6d. An example of acidic hydrolysis of butyl acetate (credit: *Intro Chem: GOB (V. 1.0).*, CC BY-NC-SA 3.0).

Links to Enhanced Learning

For more detailed hydrolysis reactions involving esters click on the video link below.

Khan Academy – Ester Hydrolysis Reactions [New tab] (https://www.youtube.com/watch?v=l_WuC4vpTsY)

Example 25.6a

Write an equation for the acidic hydrolysis of ethyl butyrate ($CH_3CH_2CH_2COOCH_2CH_3$) and name the products.

Solution

Remember that in acidic hydrolysis, water (HOH) splits the ester bond. The H of HOH joins to the oxygen atom in the OR part of the original ester, and the OH of HOH joins to the carbonyl carbon atom. The products are butyric acid (butanoic acid) and ethanol.

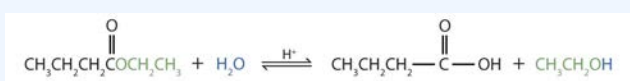


Figure 25.6e. Chemical reaction for the acidic hydrolysis of ethyl butyrate (credit: *Intro Chem: GOB (V. 1.0).*, CC BY-NC-SA 3.0).

Exercise 25.6b

Write an equation for the acidic hydrolysis of methyl butanoate and name the products.

Check Your Answer[2]

When a base (such as sodium hydroxide [NaOH] or potassium hydroxide [KOH]) is used to hydrolyze an ester, the products are a carboxylate salt and an alcohol (Figure 25.6f.). Because soaps are prepared by the alkaline hydrolysis of fats and oils, alkaline hydrolysis of esters is called **saponification** (Latin *sapon*, meaning "soap," and *facere*, meaning "to make"). In a saponification reaction, the base is a reactant, not simply a catalyst. The reaction goes to completion:

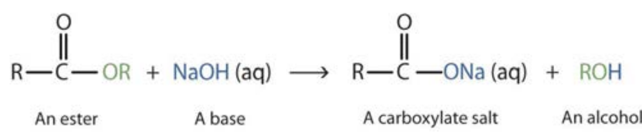


Figure 25.6f. Reaction of an ester with a base (credit: *Intro Chem: GOB (V. 1.0).*, CC BY-NC-SA 3.0).

As a specific example, ethyl acetate and NaOH react to form sodium acetate and ethanol (Figure 25.6g.).

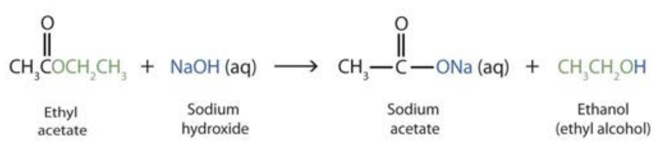


Figure 25.6g. Chemical reaction of ethyl acetate with sodium hydroxide (credit: *Intro Chem: GOB (V. 1.0).*, CC BY-NC-SA 3.0).

Example 25.6b

Write an equation for the hydrolysis of methyl benzoate in a potassium hydroxide solution.

Solution

In basic hydrolysis, the molecule of the base splits the ester linkage. The acid portion of the ester ends up as the *salt* of the acid (in this case, the potassium salt). The alcohol portion of the ester ends up as the free alcohol.

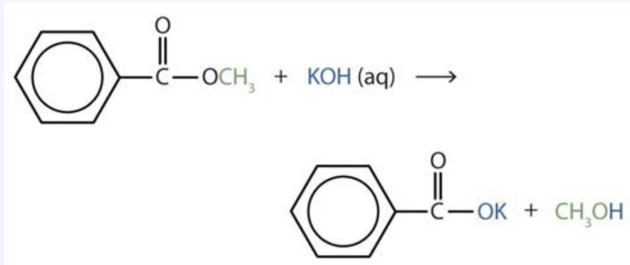


Figure 25.6h. Hydrolysis of methyl benzoate in potassium hydroxide (credit: *Intro Chem: GOB (V. 1.0).*, CC BY-NC-SA 3.0).

Exercise 25.6c

Write the equation for the hydrolysis of ethyl propanoate in a sodium hydroxide solution.

Check Your Answer[3]

Spotlight on Everyday Chemistry: Soap and Stains

Figure 25.6i. Various bars of soap (credit: Image by Baba79, CC BY-SA 4.0).

Household soaps such as, hand soap, bar soap, dish soap and shampoo are among some of the common personal items we use on a daily basis. The modern processes for creating these hygiene products, include the use of methyl esters as a key ingredient. Methyl esters are fatty acids which have important physical and chemical properties such as excellent solubility and lubricity. They are also sustainable and biodegradable which make them great components of cleaning products. These esters are derived from natural products such as vegetable oil or animal fats which are heated with a base (such as sodium hydroxide), hydrolyzed to form a salt of the carboxylic acid and eventually used in soap production (Cremer North America, 2022). For more information about soap production and the variety of hygiene products we produce and use everyday, visit Compound Interest: Soaps versus body wash – in C&EN [New tab] (https://www.compoundchem.com/2018/05/14/soap-vs-body-wash/).

Soy methyl esters commonly found in eco-friendly stain removers can be combined with natural essential oils to effectively clean fabrics and are commonly used in natural or eco-friendly laundry products. For more information on stain removal see Compound Interest: The Chemistry of Stain Removal [New tab] (https://www.compoundchem.com/2015/06/18/stain-removal/).

Not all laundry soaps are created equal and laundry pods tend to be far more concentrated in chemical components than regular liquid detergents. Higher concentrations of alcohols and esters within these cleaning solutions caused them to be highly alkaline which can lead to chemical burns if ingested. For more information on laundry pods and the dangers of ingestion see, Compound Interest: The chemistry behind why you shouldn't eat laundry pods [New tab] (https://www.compoundchem.com/2018/01/25/laundry-pods/).

Attribution & References

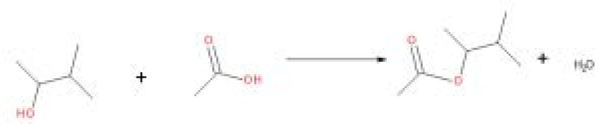
Except where otherwise noted, this page is adapted by Caryn Fahey from

- "15.7: Preparation of Esters" & "15.8: Hydrolysis of Esters" In *Basics of General, Organic, and Biological Chemistry (Ball et al.)* by David W. Ball, John W. Hill, and Rhonda J. Scott via LibreTexts, CC BY-NC-SA 4.0./ A LibreTexts version of *Introduction to Chemistry: GOB (v. 1.0)*, CC BY-NC 3.0.

References cited in-text

Cremer North America. (2022, July 6). *How methyl esters play a key role in making soap (https://www.petercremerna.com/how-methyl-esters-play-a-key-role-in-making-soap/).*

Notes

1. 

2. $CH_3CH_2COOCH_3$ + H_2O → CH_3CH_2COOH + CH_3OH Products are propanoic acid and methanol.
3. $CH_3CH_2COOCH_2CH_3$ + NaOH → CH_3CH_2COOH + CH_3CH_2OH Products are propanoic acid and ethanol.

CHAPTER 25 - SUMMARY

25.1 Carboxylic acids: Structure and Naming

A carboxylic acid (RCOOH) contains the functional group COOH, called the carboxyl group, which has an OH group attached to a carbonyl carbon atom. There are many familiar carboxylic acids. The R group may be a hydrogen atom (as in formic acid, HCOOH), an alkyl group (as in acetic acid, CH_2COOH), or an aryl group (as in benzoic acid, C_6H_5COOH). Simple carboxylic acids are best known by common names based on Latin and Greek words that describe their source (e.g., formic acid, Latin formica, meaning "ant"). Greek letters, not numbers, designate the position of substituted acids in the common naming convention. IUPAC names are derived from the LCC of the parent hydrocarbon with the -e ending of the parent alkane replaced by the suffix -oic and the word acid.

25.2 Physical Properties of Carboxylic Acids

Many carboxylic acids are colourless liquids. Carboxylic acids are highly polar molecules and readily engage in hydrogen bonding, so they have relatively high boiling points compared to other substances of comparable molar mass. Boiling points increase with molar mass. Carboxylic acids having one to four carbon atoms are completely miscible with water. Solubility decreases with molar mass. Carboxylic acids have strong, often disagreeable, odours.

25.3 Formation and Reactions of Carboxylic Acids.

A carboxylic acid is formed by the oxidation of an aldehyde with the same number of carbon atoms. Because aldehydes are formed from primary alcohols, these alcohols are also a starting material for carboxylic acids. Carboxylic acids are considered to be some of the most acidic organic compounds however are still considered weak acids. This means they do not dissociate 100% in water. They partially dissociate to form carboxylate salts and hydronium ions. They react with bases to form salts and with carbonates and bicarbonates to form carbon dioxide gas and the salt of the acid. Carboxylic acids also undergo a reaction known as esterification which allows them to react with alcohols to form esters and water.

25.4 Ionization and Neutralization of Carboxylic Acids

Soluble carboxylic acids are weak acids in aqueous solutions. They will partially dissociate to form carboxylate anions and hydronium cations. Since they are moderately acidic, they will turn litmus paper from blue to red. Carboxylic acids neutralize bases to form carboxylate acid salts. When reacting with solutions of carbonate and bicarbonate they also form carbon dioxide gas.

25.5 Esters: Structure, Properties and Naming

Esters contain a carbonyl group with a second oxygen atom bonded to the carbon atom in the carbonyl group by a single bond. 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). The names for esters include prefixes that denote the lengths of the carbon chains in the molecules and are derived following nomenclature rules similar to those for inorganic acids and salts. Esters are produced by the reaction of acids with alcohols.

25.6 Reactions of Esters

Esters are produced by the reaction of acids with alcohols.

Esters are pleasant-smelling compounds that are responsible for the fragrances of flowers and fruits. Ester molecules are polar but have no hydrogen atom attached directly to an oxygen atom. They are therefore incapable of engaging in intermolecular hydrogen bonding with one another and thus have considerably lower boiling points than their isomeric carboxylic acids counterparts. Because ester molecules can engage in hydrogen bonding with water molecules, however, esters of low molar mass are somewhat soluble in water. Esters are common solvents.

Esters can be synthesized by esterification, in which a carboxylic acid and an alcohol are combined under acidic conditions.

Esters are neutral compounds that undergo hydrolysis, a reaction with water. Hydrolysis is the most important reaction of esters. Under acidic conditions, hydrolysis is essentially the reverse of esterification and gives a carboxylic acid and alcohol. When carried out under basic conditions, the process is called saponification and gives a carboxylate salt and an alcohol. Inorganic acids also react with alcohols to form esters. Some of the most important esters in biochemistry are those formed from phosphoric acid.

Attribution & References

Except where otherwise noted, this page is adapted by Caryn Fahey from “15.S: Organic Acids and Bases and

CHAPTER 25 - REVIEW

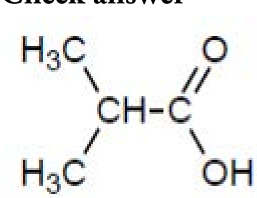
25.1 Carboxylic Acids – Structure and Naming

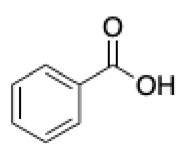
1. Give IUPAC names for the following substances:

The structure shows an acid chloride with a five-carbon chain. A methyl group is attached to C 4 The chlorine atom is attached to the carbonyl carbon.

(credit: *Organic Chemistry (OpenStax) (https://openstax.org/books/organic-chemistry/pages/21-1-naming-carboxylic-acid-derivatives)*, CC BY-NC-SA 4.0)

a. **Check answer**[1]

b.  **Check answer**[2]

c.  **Check answer**[3]

The structure shows an ester with seven carbon atoms. An isopropyl group is attached to the carbonyl carbon and another isopropyl group is attached to the ester oxygen.

(credit: *Organic Chemistry (OpenStax) (https://openstax.org/books/organic-chemistry/pages/21-1-naming-carboxylic-acid-derivatives)* CC BY-NC-SA 4.0)

d.

Check answer[4]

The structure shows a benzene ring attached to a carbonyl group enclosed in parentheses with a subscript two. The carbonyl carbon is single-bonded to an oxygen atom.

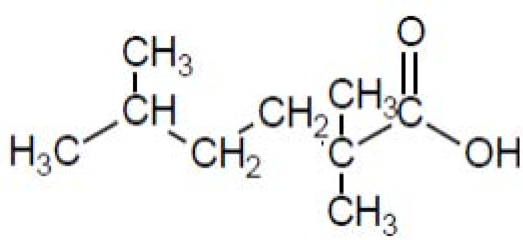
(credit: *Organic Chemistry (OpenStax) (https://openstax.org/books/organic-chemistry/pages/21-1-naming-carboxylic-acid-derivatives)*, CC BY-NC-SA 4.0)

e. **Check answer**[5]

The structure of an ester shows a cyclopentane ring attached to a carbonyl group which in turn is attached to an oxygen atom bound to an isopropyl group.

(credit: *Organic Chemistry (OpenStax) (https://openstax.org/books/organic-chemistry/pages/21-1-naming-carboxylic-acid-derivatives)*, CC BY-NC-SA 4.0)

f. **Check answer**[6]

g. 

Check answer[7]

2. Draw structures corresponding to the following names:
   a. 2,2-dimethylpropanoic acid **Check answer**[8]
   b. 2,3-difluorobutanic acid **Check answer**[9]
   c. 4,4-dimethylpentanoic acid **Check answer**[10]
   d. Phenyl benzoate **Check answer**[11]
   e. 2,4-Dimethylpentanoyl chloride **Check answer**[12]

25.2 Physical Properties of Carboxylic Acids

1. Fatty acids are carboxylic acids that have long hydrocarbon chains attached to a carboxylate group. How does a saturated fatty acid differ from an unsaturated fatty acid? How are they similar? **Check answer**[13]
2. What carboxylic acid is responsible for the pain of an ant sting? **Check answer**[14]
3. What carboxylic acid is found in vinegar? **Check answer**[15]

25.3 Formation and Reactions of Carboxylic Acids

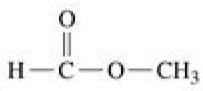
1. Write the balance chemical equation for the dissociation of propanoic acid in water. **Check answer**[16]
2. Write the balanced equations for each of the following reactions;
   a. ethanol reacts with propionic acid
   b. benzoic acid, $C_6H_5CO_2H$, is added to a solution of sodium hydroxide

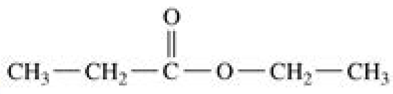
25.4 Chemical Properties of Carboxylic Acids – Ionization and Neutralization

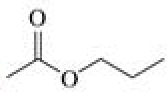
1. Write the balanced chemical equation for the neutralization of propanoic acid with sodium hydroxide. **Check answer**[17]
2. Write the balanced chemical equation for the reaction of each of the following carboxylic acids with NaOH:
   a. formic acid **Check answer**[18]
   b. 3-chloropropanoic acid **Check answer**[19]

25.5 Esters – Structure, Properties and Naming

1. Draw the condensed structural formula for the ester formed when each of the following reacts with methyl alcohol:
   a. acetic acid **Check answer**[20]
   b. pentanoic acid **Check answer**[21]
2. Write the IUPAC and common names, if any, for each of the following:

a. 

b. 

c. 

Check answer[22]

25.6 Reactions of Esters

1. How do acidic hydrolysis and basic hydrolysis of an ester differ in terms of products obtained? **Check answer**[23] And the extent of reaction? **Check answer**[24]
2. An ester that has the smell of pineapple can be synthesized from butanoic acid and methanol. Write the balanced chemical equation for the formation of this ester. **Check answer**[25]
3. Write an equation for the acidic hydrolysis of ethyl butyrate ($CH_3CH_2CH_2COOCH_2CH_3$) and name the products. **Check answer** [26]
4. Write an equation for the hydrolysis of methyl benzoate in a potassium hydroxide solution. **Check answer**[27]

Links to Enhanced Learning

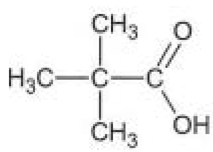
Create your own organic nomenclature quiz to identify, name and draw carboxylic acids and esters using Organic Nomenclature [New tab] (https://orgchem101.com/nom/en/index.php). You can customize the types of questions you receive and get instant feedback. Khan Academy [New tab] (https://www.khanacademy.org/) reviews Carboxylic Acids [New tab] (https://www.khanacademy.org/science/organic-chemistry/carboxylic-acids-derivatives)

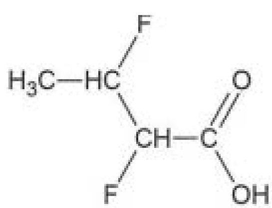
Attribution & References

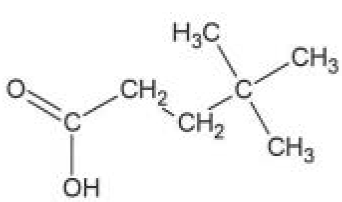
Except where otherwise noted, this page (including images in solutions) is adapted by Caryn Fahey from:

- "Naming Carboxylic Acids Derivatives" In *Organic Chemistry* by John McMurray, CC BY-NC-SA 4.0. Access for free at *Organic Chemistry (OpenStax)* (https://openstax.org/books/organic-chemistry/pages/1-why-this-chapter)
- "18.3 Aldehydes, Ketones, Carboxylic Acids, and Esters" In *General Chemistry 1 & 2* by Rice University, a derivative of *Chemistry (Open Stax)* by Paul Flowers, Klaus Theopold, Richard Langley & William R. Robinson and is licensed under CC BY 4.0. Access for free at *Chemistry (OpenStax) (https://openstax.org/books/chemistry/pages/1-introduction)*
- Images that are not marked otherwise are adapted from course materials by Caryn Fahey and JR van Haarlem
- Images in solutions are from the original source, except:
  - 25.6 Question 3, 4: *Intro Chem: GOB (V. 1.0).*, CC BY-NC-SA 3.0

Notes

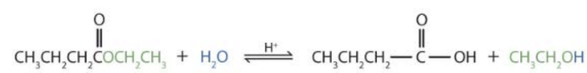
1. 4-Methylpentanoyl chloride
2. 2-methylpropanoic acid
3. benzoic acid
4. Isopropyl 2-methylpropanoate
5. Benzoic anhydride
6. Isopropyl cyclopentanecarboxylate
7. 2,2,5-trimethylhexanoic acid
8. 

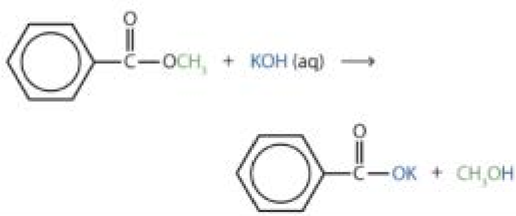
9. 

10. 

11. $C_6H_5CO_2C_6H_5$
12. $(CH_3)_2CHCH_2CH(CH_3)COCl$
13. Since they are both carboxylic acids, they each contain the –COOH functional group and its characteristics. The

difference is the hydrocarbon chain in a saturated fatty acid contains no double or triple bonds, whereas the hydrocarbon chain in an unsaturated fatty acid contains one or more multiple bonds.

14. formic acid
15. acetic acid
16. The dissociation of propanoic acid produces a carboxylate ion and a hydronium ion.
17. A chemical equation for the neutralization of a carboxylic acid includes the reactants, a carboxylic acid and a base, and the products, a carboxylate salt and water.
18. $HCOOH + NaOH = HCOONa + H_2O$
19. $C_3H_5ClO_2 + NaOH = C_3H_4ClO_2 + Na^+ + H_2O$
20. $CH_3COOH + CH_3OH = C_3H_6O_2$
21. $CH_3CH_2CH_2CH_2COOH + CH_3OH = C_6H_{12}O_2$
22. a. Acetic acid or ethanoic acid (IUPAC), b. ethyl propanoate, c. propyl ethanoate
23. acidic hydrolysis: carboxylic acid + alcohol; basic hydrolysis: carboxylate salt + alcohol
24. basic hydrolysis: completion; acidic hydrolysis: incomplete reaction
25. The ester formed is methyl butanoate. It has a fruity pineapple smell. Reaction: $CH_3CH_2CH_2COOH + CH_3OH = CH_3CH_2CH_2COOCH_3$
26. The products are butyric acid (butanoic acid) and ethanol. 
27. In basic hydrolysis, the molecule of the base splits the ester linkage. The acid portion of the ester ends up as the salt of the acid (in this case, the potassium salt). The alcohol portion of the ester ends up as the free alcohol.



CHAPTER 25 - INFOGRAPHIC DESCRIPTIONS

Infographics used in Chapter 25

- 25.0a A Guide to Types of Fat and the bonds they contain
- 25.0b Everyday Chemicals: Acetic Acid – Vinegar & Volcanoes
- 25.1a The sour science of vinegar varieties
- 25.2a RTC Week 2015 – #4: Deuterating Fatty Acids to Treat Diseases
- 25.2b Why Shouldn't You Eat Rhubarb Leaves? – The Chemistry of Rhubarb
- 25.2c Sourness & Scurvy – The Chemistry of a Lemon
- 25.5a Table of Esters and Their Smells v2
- 25.5b RTC Week 2015 – #2: Oil Spill Clean-Ups Using Fruits & Oils

25.0a A Guide to Types of Fat and the bonds they contain

Fat is an essential part of our diets, and has a number of important roles in the body. However, there are different types, and there are health concerns surrounding eating too much of some types of fat. Here, we look at what distinguishes different types of fat, and their effects on the body.

Triglycerides and fatty acids: Triglycerides account for around 95% of the fat in our diet, and are formed from the combination of glycerol and three fatty acid molecules. The three fatty acids are often different, and the chemical structures of these fatty acids defines the type of fat. Cholesterol is made in the liver, and transported around the body by low density lipoproteins (LDL) and high density lipoproteins (HDL). Different fats affect LDL and HDL differently.

Saturated fats: Contain no carbon-carbon double bonds. Saturated fats are solids at room temperature. They increase levels of LDL in the bloodstream. They have previously been associated with heart disease, though more recent studies and reviews have called this association into question.

Monosaturated fats: Contain one carbon-carbon double bond. They are liquids at room temperature, but solidify in while chilled. They reduce levels of LDL in the bloodstream, thereby decreasing the total cholesterol to HDL ratio (HDL helps take cholesterol back to the liver where it can be disposed of).

Polyunsaturated fats: Contain two ore more carbon-carbon bonds. They are liquids at room temperature, but they start to solidify when chilled. They are split into omega-3 and omega-6 fatty acids. Polyunsaturated fats help reduce LDL levels, decreasing the total cholesterol to HDL ratio.

Trans fats: Contain carbon-carbon double bond in a *trans* rather then *cis* configuration. Formed artificially, via a process called hydrogenation; also found naturally in small amounts in meat and dairy products. They raise LDL, and are associated with heart disease. Many countries are phasing them out.

Read more about "A Guide to Types of Fat and the bonds they contain [New tab] (https://www.compoundchem.com/2015/08/25/fat/)" by Andy Brunning / Compound Interest, CC BY-NC-ND

25.0b Everyday Chemicals: Acetic Acid – Vinegar & Volcanoes

Acetic acid also known as 'ethanoic acid' or the acid component of vinegar.

Acetic acid: colourless liquid, CH3COOH.

Acetic acid is best known for its presence in vinegar, produced by fermentation and oxidation of ethanol. Table vinegar is a solution of 4-8% acetic acid in water. Trace molecules contribute colour and nuances of flavour to different types of vinegars. Acetic acid also used in food as an acidity regulator, with the E number E260.

Vinegar often recommended as household cleaner: removing smears/streaks from windows/mirrors and it contains descalers for removing limescale, reacting with the calcium carbonate that limescale is primarily composed of. Studies show acetic acid has antibacterial effect.

Approximately 1/3 of all acetic acids are used in production of vinyl acetate. Polymerisation of vinyl acetate monomer produces polymer polyvinyl acetate (PV), the main component of PVA glue. Acetic acid also used as solvent and precursor to photographic film, inks and dyes, and synthetic fibres.

Acetic acid in the form of vinegar can be used in household science experiments to create volcano-like effect. Acid reacts with baking soda (sodium bicarbonate) in a neutralization reaction creating carbon dioxide and causing a frothing effect.

Read more about "Everyday Chemicals: Acetic Acid – Vinegar & Volcanoes [New tab] (https://www.compoundchem.com/2015/06/11/acetic-acid/)" by Andy Brunning / Compound Interest, CC BY-NC-ND

25.1a The sour science of vinegar varieties

Vinegar is produced by the two-stage fermentation of raw materials containing sugar or starch. In the first fermentation, yeasts convert sugar to alcohol (ethanol). In the second fermentation (acetification) ethanol is oxidized to acetic acid by acetic acid bacteria.

Acetification: Acetic acid bacteria need oxygen to convert ethanol to acetic acid. In longer, traditional processes, the bacteria grow on teh surface of the fermentation liquid. In industrial methods the bacteria are submerged, with oxygen pumped in.

Distilled vinegar: Distilled vinegar is not itself distilled, but produced from distilled alcohol, made from barley malt or corn. Like other vinegars, the main acid is acetic acid (5-8% by volume). Other compounds are limited compared to other vinegars, but include traces of ethyl acetate.

Apple cider vinegar: Apple cider vinegar is amde from fermented apple juice. Like wine vinegar it contains other acids, such as malic acid from apples, Wine and sider also contain higher alcohols, such as propanol, which react to form additional acids and esters during vinegar production.

Balsamic vinegar: Traditional balsamic vinegar is made by converting sugars in cooked grape must be ethanol, oxidizing to acetic acid, then ageing for at least 12 years. Researchers have identified 5-acetoxymenthyl-2-furaledhyde as important to its long-lasting sweet taste.

Mal vinegar: Malt vinegar is made from fermented malted barely – essentially unhopped beer. Malt vinegars don't contain tartaric or malic acids, but do contain small quantities of lactic acid. Branched chain compounds, like 2-methylpropanoic acid, contribute to its flavour and aroma.

Wine vinegar: Wine vinegar are produced by fermenting wine. The main acid is still acetic acid, but other acids from grapes, such as tartaric acid, are present in smaller amounts. Phenolic compounds are also present, both from the wine and from barrel ageing from some varieties.

Rice vinegar: Rice vinegar is made from fermented rice and varies in colour from colourless to black. In some varieties, furfural and pyrazines such as tetramethylpyrazine (TMP) contribute toast-like flavours. Buttery acetoin (3-hydroxy-2-butanone) is also present in many rice vinegars.

Read more about "The sour science of vinegar varieties [New tab] (https://www.compoundchem.com/2023/02/20/vinegar/)" by Andy Brunning / Compound Interest, CC BY-NC-ND

25.2a RTC Week 2015 – #4: Deuterating Fatty Acids to Treat Diseases

Maksim Fomich, research at the Institute of Physical Organic Chemistry in Belarus, is looking into deuterated fatty acids.

Polyunsaturated fatty acids (PUFAs) are obtained from diet and can be found in cell membranes. Their oxidation can lead to potential problems.

A deuterated unsaturated fatty acid: 11,11-*d*2-Linoleic acid

Deuterium is a hydrogen atom with a neutron also added to the nucleus, represented by the symbol D, or 2H, and accounts for a very small proportion of the natural abundance of hydrogen. Deuterated compounds have deuterium atoms in place of some of the hydrogen atoms. By deuterating polyunsaturated fatty acids (PUFAs), reactive parts of the molecule can be protected.

Uses of deuterated PUFAs:

- Tests on yeast show small additions of deuterated PUFAs help prevent cell death dur to oxidation.
- Oxidation of PUFAs is thought to play a role in Parkinson's disease. D-PUFAs diminished degeneration in mice.

- D-PUFAs are in human clinical trials for the treatment of Friedreich's ataxia, a nervous system disorder.
- D-PUFAs could be used to treat some retina diseases, as some of these could be due to destruction of retina lipids.

Read more about the "RTC Week 2015 – #4: Deuterating Fatty Acids to Treat Diseases [New tab] (https://www.compoundchem.com/2015/10/22/rtcweek4/)" by Andy Brunning / Compound Interest, CC BY-NC-ND

25.2b Why Shouldn't You Eat Rhubarb Leaves? – The Chemistry of Rhubarb

Different species of rhubarb contains a wide variety of anthraquinone compounds. Ahthocyanin pigments are the main compounds responsible for rhubarb red colouration, anthraquinone also coloured. Emodin (orange colour), Chrysophanol (yellow colour), Physcion (red-orange colour).

Rhubarb also contains various derivatives of anthraquinone compounds including sennosides. During digestion these are turned into active compounds which have a laxative effect. Chief among these is the metabolite called rheinanthrone. Sennosides are found in senna plants and are on the World Health Organizatio's (WHO) list of essential medicines.

Rhubarb leaves are high in oxalic acid (0.52g per 100g) and oxalate salt (15-30g lethal dose in humans) content, which can cause nausea and vomiting if ingested. Debate if other poisonous compounds in the leaves may contribute. The stalk is sage to eat as it contains lower oxalic acid content, the dominant acid being malic acid.

Read more about the "Why Shouldn't You Eat Rhubarb Leaves? – The Chemistry of Rhubarb [New tab] (https://www.compoundchem.com/2015/04/16/rhubarb/)" by Andy Brunning / Compound Interest, CC BY-NC-ND

25.2c Sourness & Scurvy – The Chemistry of a Lemon

The sour taste of lemons is caused by the presence of organic acids. The major acid in lemons is citric acid, which makes up around 5-6% of the lemon's juice. Other acids in lower concentrations then citric acid: malic acid is present around 5% of the concentration of citric acid.

Lemons contain high levels of vitamin C (ascorbic acid): 50mg per 100g, on par with oranges and around double the amount of limes.

Vitamin C deficiency can lead to scurvy, a disease that cause loss of teeth, jaundice, eventually death. In the 1700s, all British ships required to provide lemon juice ration to seamen to guard against the disease.

Read more about the "Sourness & Scurvy – The Chemistry of a Lemon [New tab]

25.5a Table of Esters and Their Smells v2

Table of esters and their smells: column, from the alcohol (first word) ; rows, from the carboxylic acid (sec

	Methyl (1 carbon)	Ethyl (2 carbon)	Propyl (3 carbons)	2-Methyl (propyl-)	Butyl (4 carbons)	Pentyl (5 carbons)	Hexyl (6 carbons)	Benzyl (benzene ring)	Hepty (7 carbo
Methanoate (1 carbon)	Ethereal	Bacardi	Apples	Ethereal	Raspberries	Fruits	Green Leaf	Peaches	Wood
Ethanoate (2 carbons)	Glue stick(UHU stick)	PVA glue	Pears	Cherries	Apples	Banana	Fruits	Jasmine	Wood
Propanoate (3 carbons)	Fruits	Pineapple	Fruits	Plums	Apples	Peaches	Fruits	Flowers	Wood
2-Methyl Propanoate (4 carbons, branched)	Fruits	Ethereal	Bacardi	Fruits	Fruits	Peaches, Butter	Grass	Flowers	Apple coca bean
Butanoate (4 carbons)	Pineapple	Pineapple	Pears	Banana	Pineapple	Peaches	Apple, soap	Plums	Tea
Pentanoate (5 carbons)	Flowers	Fruits	Pineapple	Fruits	Ethereal	Apple	Cognac	Fruits	Green Leaf
Hexanoate (6 carbons)	Citrus fruits, banana, pineapple	Pineapple	Blackberries	Fruits	Fruits	Apple	Green Leaf	Green Leaf	Green Leaf
Benzoate (benzene ring)	Ylang-ylang	Ylang-ylang	Nuts	Balsamic	Balsamic	Balsamic	Balsamic	Balsamic	Green Leaf
Heptanoate (7 carbons)	Berries	Peaches, cognac	Fruits	Green leaf	Coconut	?	Green leaf	Fruits	Green Leaf
Salicylate (from salicylic acid)	Deep heat rub	Star anise	Mint	Wintergreen	Blackberry (strong)	Hay	Flowers	Different people perceive different aromas	?
Octanoate (8 carbons)	Oranges	Apples	Coconut	Green leaf, flowers	Butter	Coconut, cognac	Green leaf, butter	Peaches	Candl
Phenylacetate (benzene ring + 2 carbons)	Honey (strong)	Honey (strong)	Flowers	Chocolate	Honey	Chocolate flowers	Fruits	Jasmine	None
Nonanoate (9 carbons)	Coconut, red wine	Grapes	Butter	Oranges	Flowers	Roses	Flowers	Flowers	Flowe

Cinnamate (benzene ring + propenol)	Strawberries	Cinnamon	Balsamic	Balsamic	Balsamic, cocoa bean	Balsamic, cocoa bean	Balsamic	Balsamic	Red wine
Decanoate (10 carbons)	Red wine	Apples	Oil	Red wine	Jack Daniels	Green Leaf	?	?	?

Read more about the "Table of Esters and Their Smells v2 [New tab] ()" by James Kennedy, shared with permission under CC BY-ND 4.0.

25.5b RTC Week 2015 – #2: Oil Spill Clean-Ups Using Fruits & Oils

Julian Silverman, PhD candidate in the City College of New York researching this topic.

Sugars (from raspberries or monkfruits) plus fatty acids (from edible oils) crate ester compounds (basic building blocks of gels). Enzymes are used to speed this process up. The product produced is environmentally friendly, using a low energy catalytic process to make it.

1. The ester molecules can stack like bricks into long strings in solution, which can then entangle like a sponge.
2. This 'sponge' traps liquid around it forming a gel, which is good at trapping water-fearing liquids (oil).
3. The gel formed is easily removed from the environment and can be squeezed/distilled to get back the spilled liquid.

Read more about "RTC Week 2015 – #2: Oil Spill Clean-Ups Using Fruits & Oils [New tab] ()" by Andy Brunning / Compound Interest, CC BY-NC-ND

Attribution & References

Compound Interest infographics are created by Andy Brunning and licensed under CC BY-NC-ND

Except where otherwise noted, content on this page has been created as a textual summary of the infographics used within our OER. Please refer to the original website (noted below each description) for further details about the image.