Tishk International University

Faculty of Dentistry

Department of Basic Science

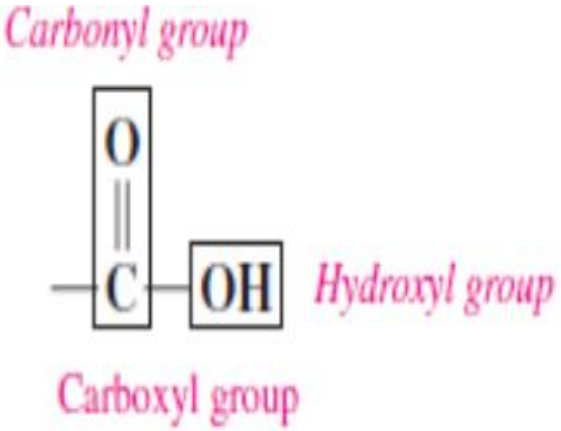
Organic Chemistry

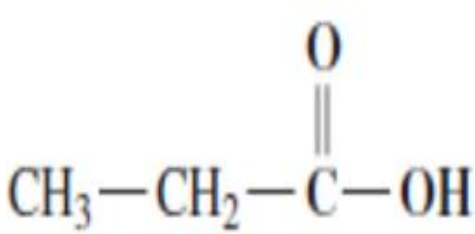
Carboxylic acid & Ester

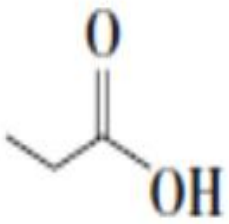
1st grade
8th lecture

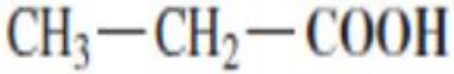
➢ Carboxylic acid:

In a **carboxylic acid**, the carbon atom of a carbonyl group is attached to a hydroxyl group, which forms a **carboxyl group**. Some ways to represent the skeletal and condensed structural formulas for carboxyl group are shown below:







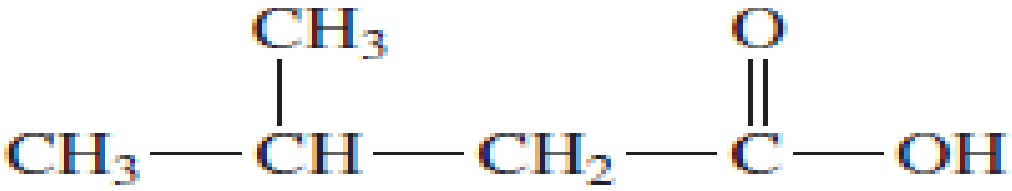


➢ IUPAC naming of Carboxylic acids:

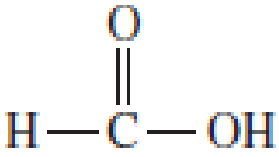
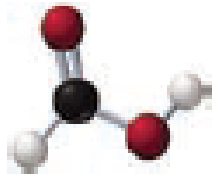
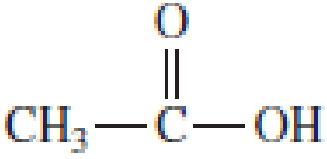
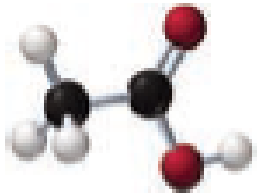
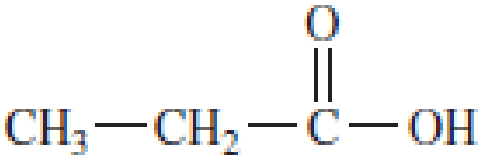
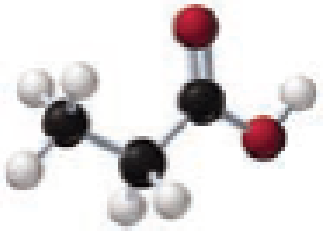
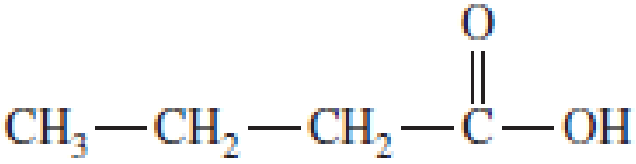
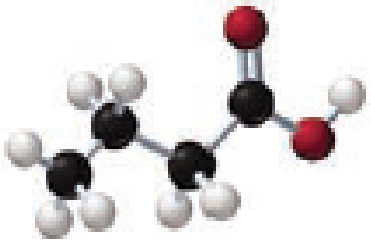
The IUPAC of a carboxylic acid is derived from that of the longest carbon chain that **contains** the **carboxyl** group by dropping the final (**-e)** from the name of the parent alkane and adding the suffix (**-oic)** followed by the **word acid**.

➢ The general formula for an aliphatic carboxylic acid is **(RCOOH)**.

Many carboxylic acids are still named by their common names, which use prefixes: *form*, *acet*, *propion*, *butyr*. When using the common names, the Greek letters **alpha (α), beta (β),** and **gamma (γ)** are assigned to the carbons adjacent to the ***carboxyl carbon***.



IUPAC	4	3	2	1
Common	γ	β	α	

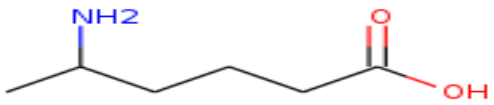
Condensed Structural Formula	IUPAC Name	Common Name	Ball-and-Stick Model
	Methanoic acid	Formic acid	
	Ethanoic acid	Acetic acid	
	Propanoic acid	Propionic acid	
	Butanoic acid	Butyric acid	

In the IUPAC system, a carboxyl group takes precedence over most other functional groups, including hydroxyl groups, amino groups, and the carbonyl groups of aldehydes and ketones. For examples:

- An (**-OH)** group is indicated by the prefix (***hydroxy*-)**;

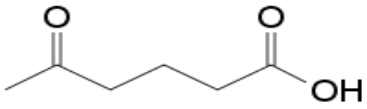
5-Hydroxyhexanoic acid

- An **(-NH_2)** group, by (***amino-)***;



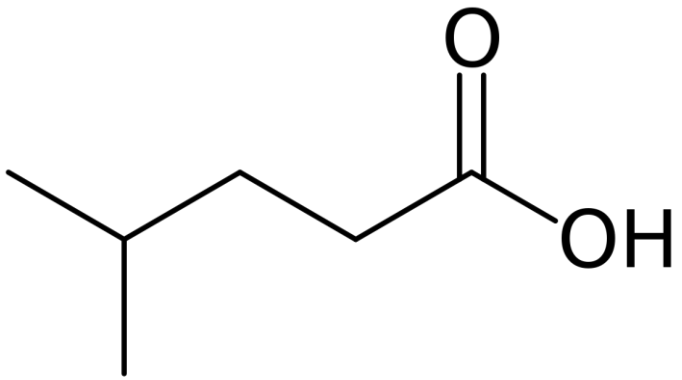
5-Aminohexanoic acid

- The carbonyl group of an aldehyde or ketone, by **(*oxo*-)**.



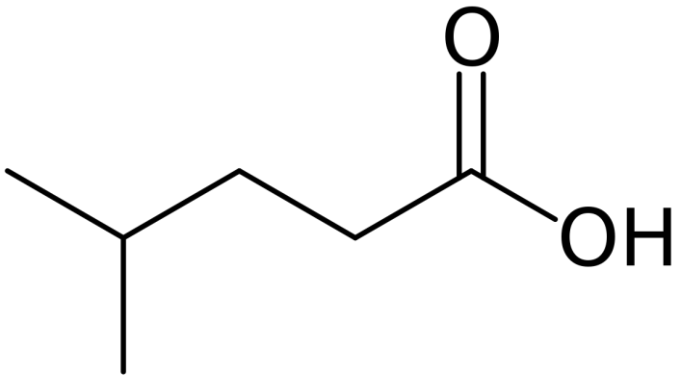
5-Oxohexanoic acid

Example: Give the IUPAC name for the following compound?



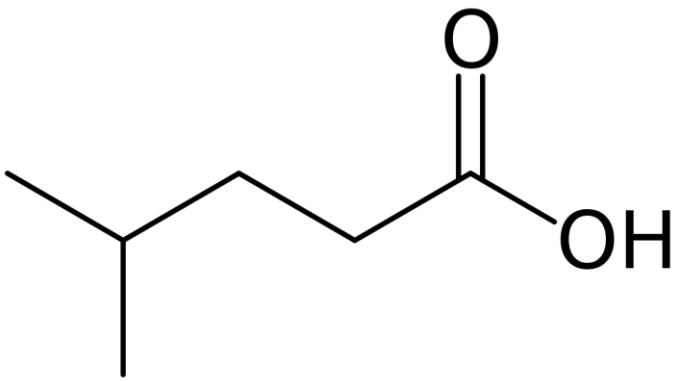
Solution:

Step 1: Name the longest carbon chain that contain carboxyl group and replace the ***(e)*** in the alkane name with ***(-oic acid)***.



Pentanoic acid

Step 2: Name and number any substituents on the carbon chain. Counting from the carboxyl group places the methyl group on carbon 4. The name of the compound according IUPAC system will be:

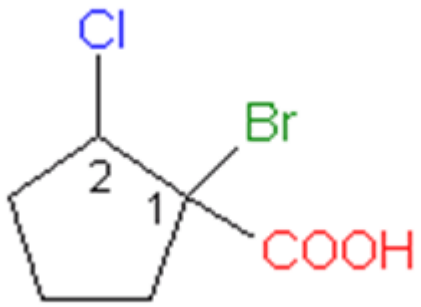


4-Methylpentanoic acid

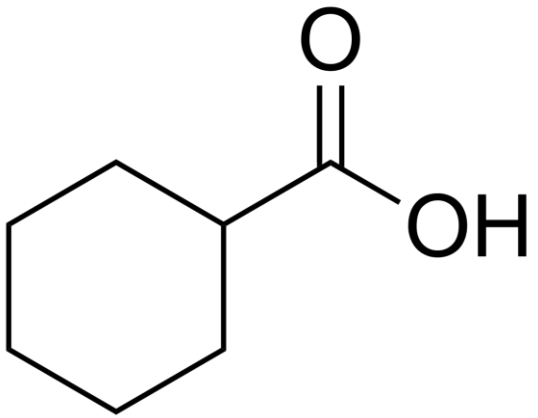
➢ Cyclic carboxylic acids:

A carboxylic acid containing a carboxyl group bonded to a cycloalkane ring is named as **cycloalkane carboxylic acids.** The atoms of the ring are numbered beginning with the carbon attaching to the **-COOH group**.

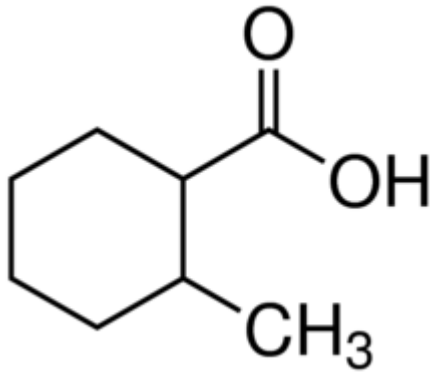
- *(Note: The carboxylic carbon cannot be a ring carbon)*



1-Bromo-2-chlorocyclopentanecarboxylic acid



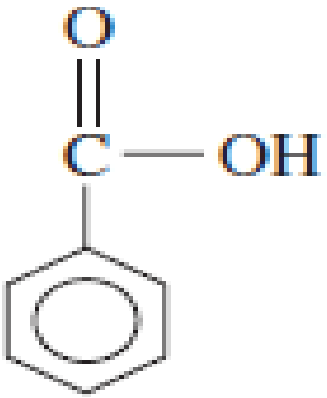
Cyclohexanecarboxylic acid



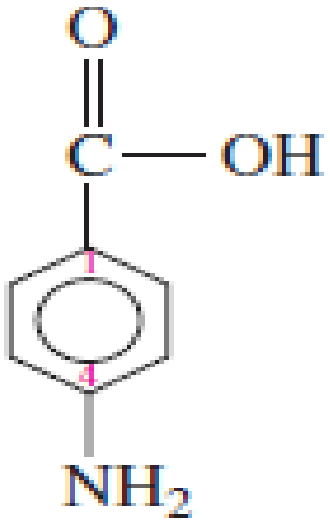
2-Methylcyclohexanecarboxylic acid

➢ Aromatic carboxylic acid:

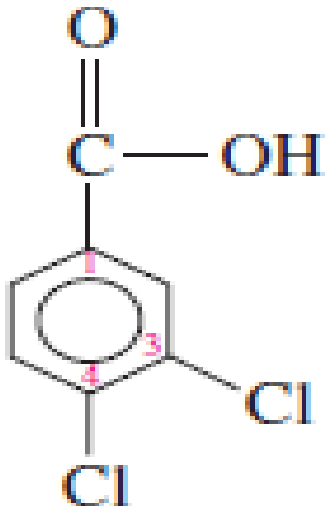
The name of the carboxylic acid of benzene is benzoic acid. The carbon of the carboxyl group is bonded to ***carbon 1*** in the ring and the ring is numbered to give the ***lowest*** possible numbers for any substituents. As before, the prefixes ***ortho, meta,* and *para*** may be used to show the position of one other substituent.



Benzoic acid

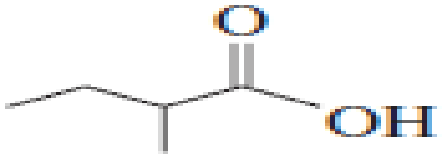


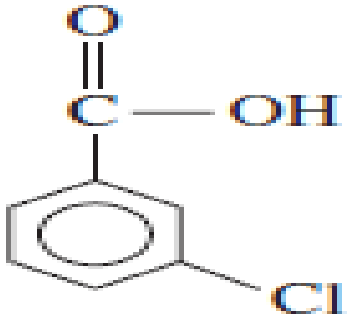
4-Aminobenzoic acid
(*p*-aminobenzoic acid;
PABA)



3,4-Dichlorobenzoic acid

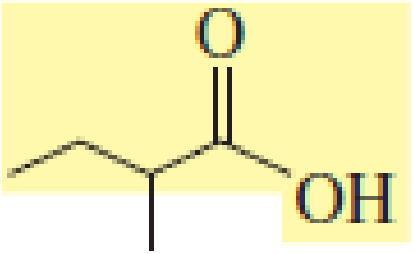
Example: Give the IUPAC and common name, if any, for each of the following carboxylic acids:

a. 

b. 

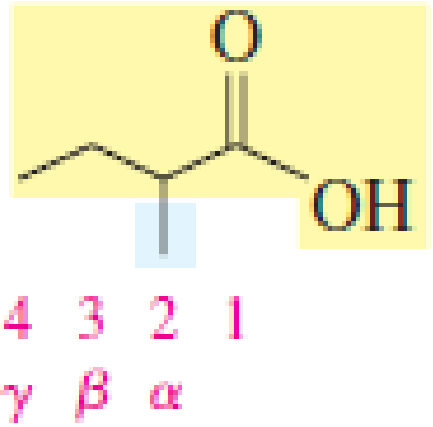
Solution:

a. ***Step1:*** Identify the longest carbon chain contains carboxyl group and replace the **(-*e*)** in the corresponding alkane name with **(-*oic*)** *acid*. A carboxylic acid with four carbon atoms is named **butanoic acid**; the common name is **butyric acid**.



butanoic acid

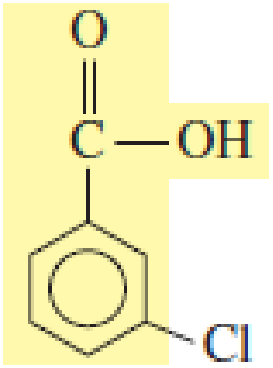
Step2: Give the location and name of each substituent by counting the carboxyl carbon as 1. With a methyl group on the second carbon, the IUPAC name is ***2-methylbutanoic acid***. For the common name, the Greek letter a specifies the carbon atom next to the carboxyl carbon, ***α-methylbutyric acid***.



2-methylbutanoic acid

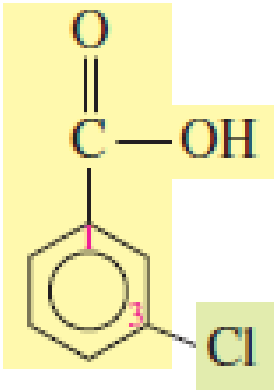
α-methylbutyric acid

b. ***Step1:*** Identify the longest carbon chain and replace the ***(-e)*** in the corresponding alkane name with ***(-oic)*** *acid*. An aromatic carboxylic acid is named as **benzoic acid**.



benzoic acid

Step2: Give the location and name of each substituent by counting the carboxyl carbon as 1 and it gives the IUPAC name as ***3-chlorobenzoic acid***. The common name is ***meta*-chlorobenzoic acid** or ***m*-chlorobenzoic acid**.

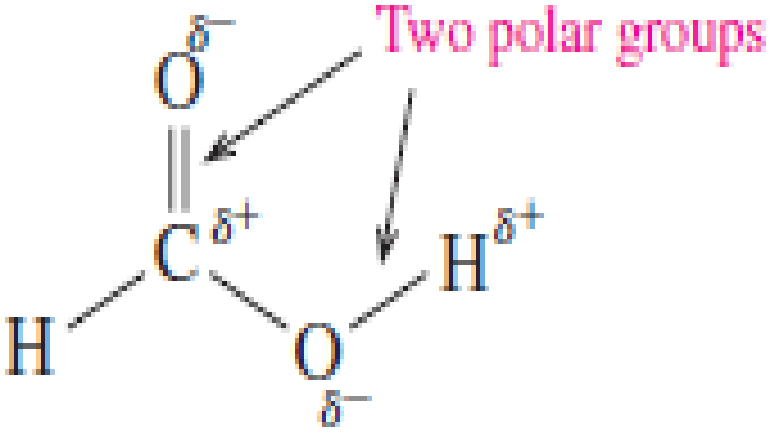


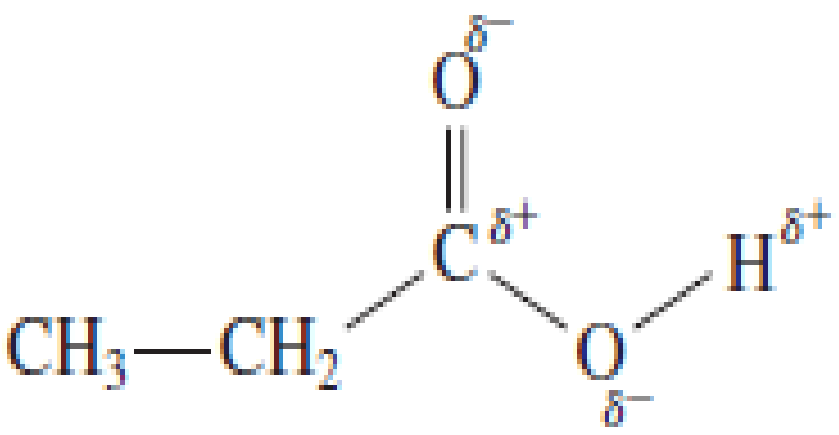
3-chlorobenzoic acid

meta-chlorobenzoic acid

Physical properties of carboxylic acid

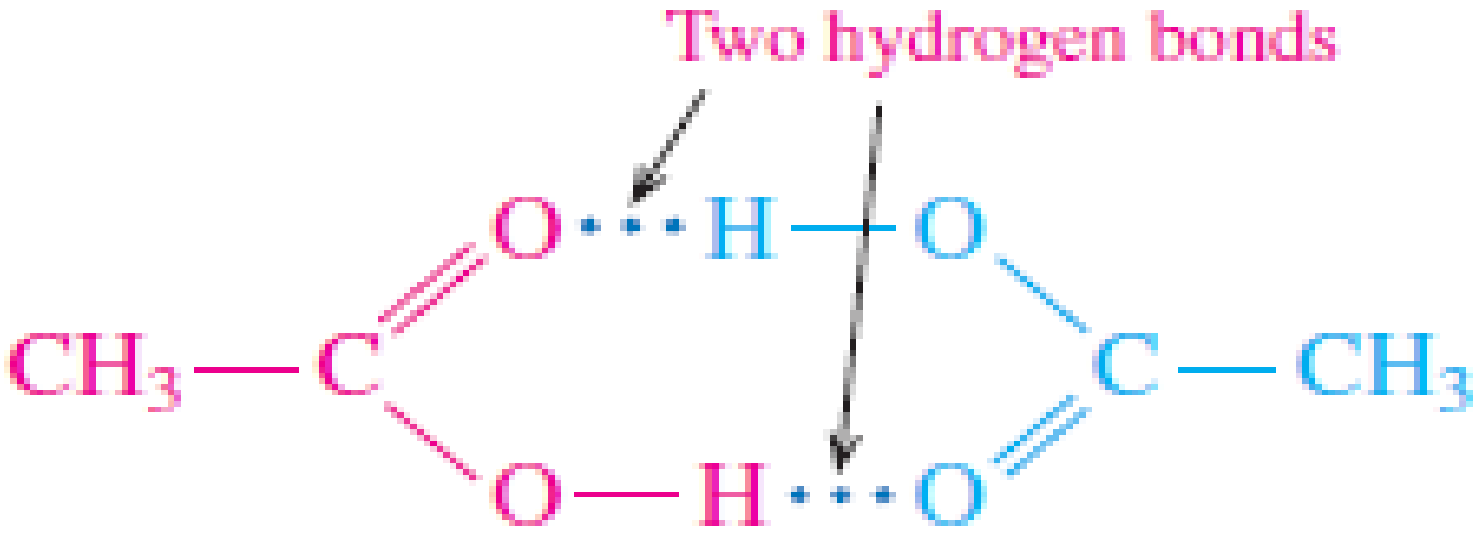
Carboxylic acids are among the ***most polar*** organic compounds because their functional group consists of ***two polar*** groups: a ***hydroxyl*** group and a ***carbonyl*** group. The -OH group is similar to the functional group in **alcohols**, and the carbonyl is similar to the functional group of **aldehydes** and **ketones**.

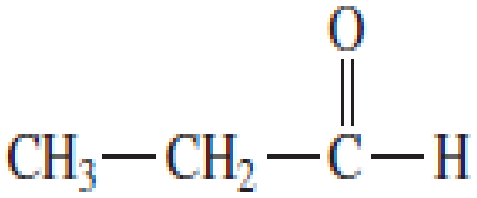


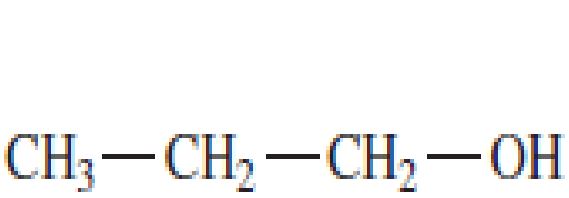


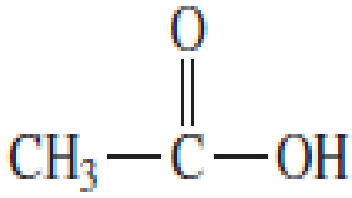
➢ Boiling Points

The polar carboxyl groups allow carboxylic acids to form several ***hydrogen bonds*** with other carboxylic acid molecules. This effect of hydrogen bonds gives carboxylic acids ***higher*** boiling points than **alcohols**, **ketones**, and **aldehydes** of similar molar mass.



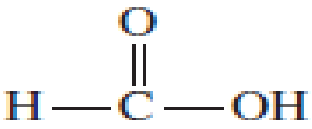
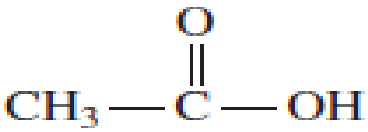
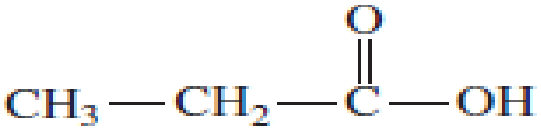
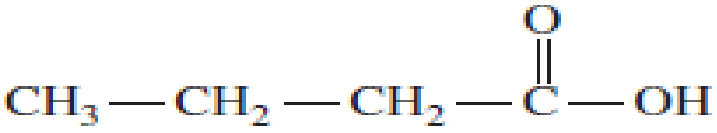
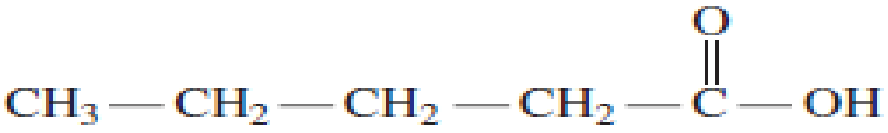
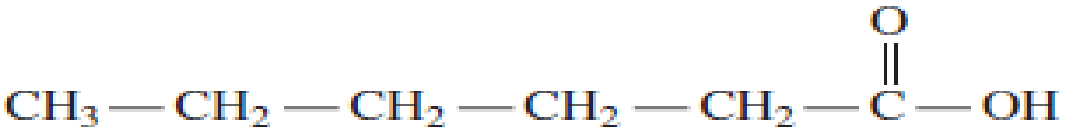
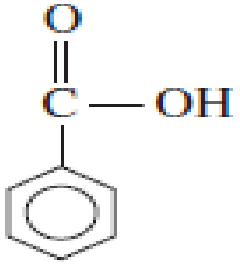






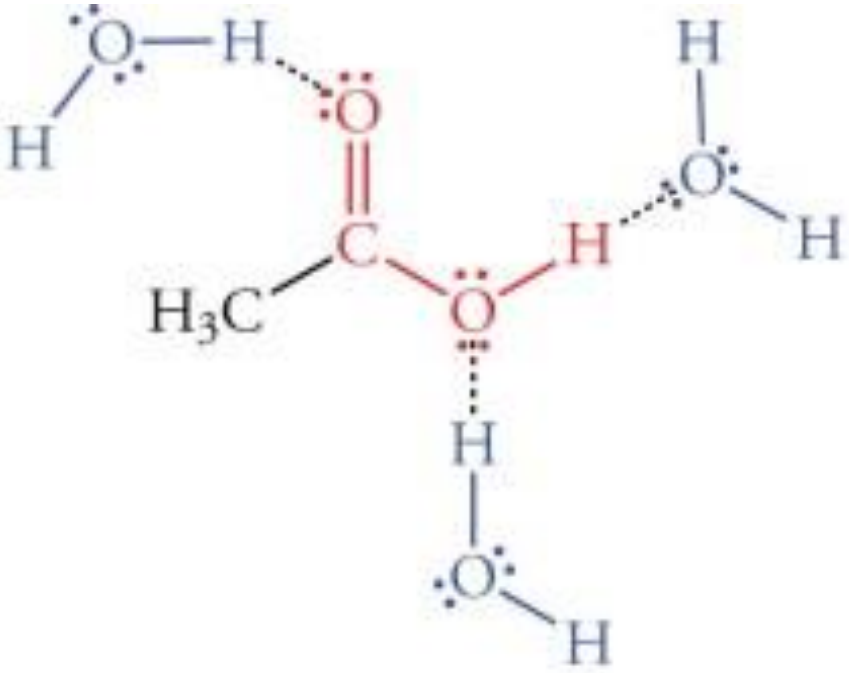
Name	Propanal	1-Propanol	Ethanoic acid
Molar Mass	58	60	60
Family	Aldehyde	Alcohol	Carboxylic acid
bp	49 °C	97 °C	118 °C

- For carboxylic acids, the boiling points increase as the number of carbon atoms in the chain increases.

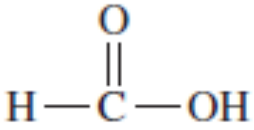
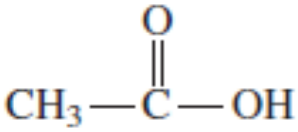
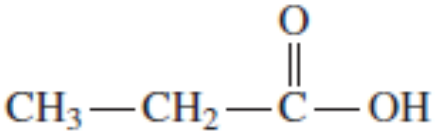
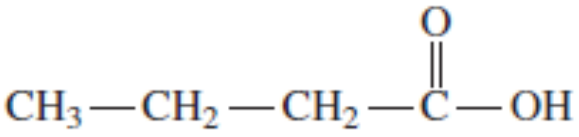
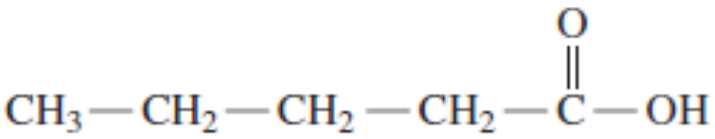
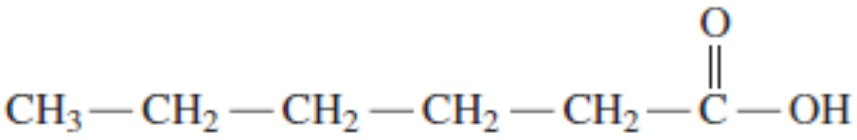
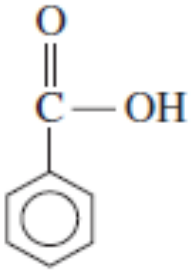
IUPAC Name	Condensed Structural Formula	Boiling Point (°C)
Methanoic acid		101
Ethanoic acid		118
Propanoic acid		141
Butanoic acid		164
Pentanoic acid		187
Hexanoic acid		205
Benzoic acid		250

➢ Solubility of carboxylic acid in Water

Carboxylic acids with ***one to five*** carbons are soluble in water because the carboxyl group forms hydrogen bonds with several water molecules. However, as *the length of the hydrocarbon chain increases*, the ***nonpolar*** portion *reduces* the solubility of the carboxylic acid in water.



hydrogen bonds between acetic acid and water in aqueous solution

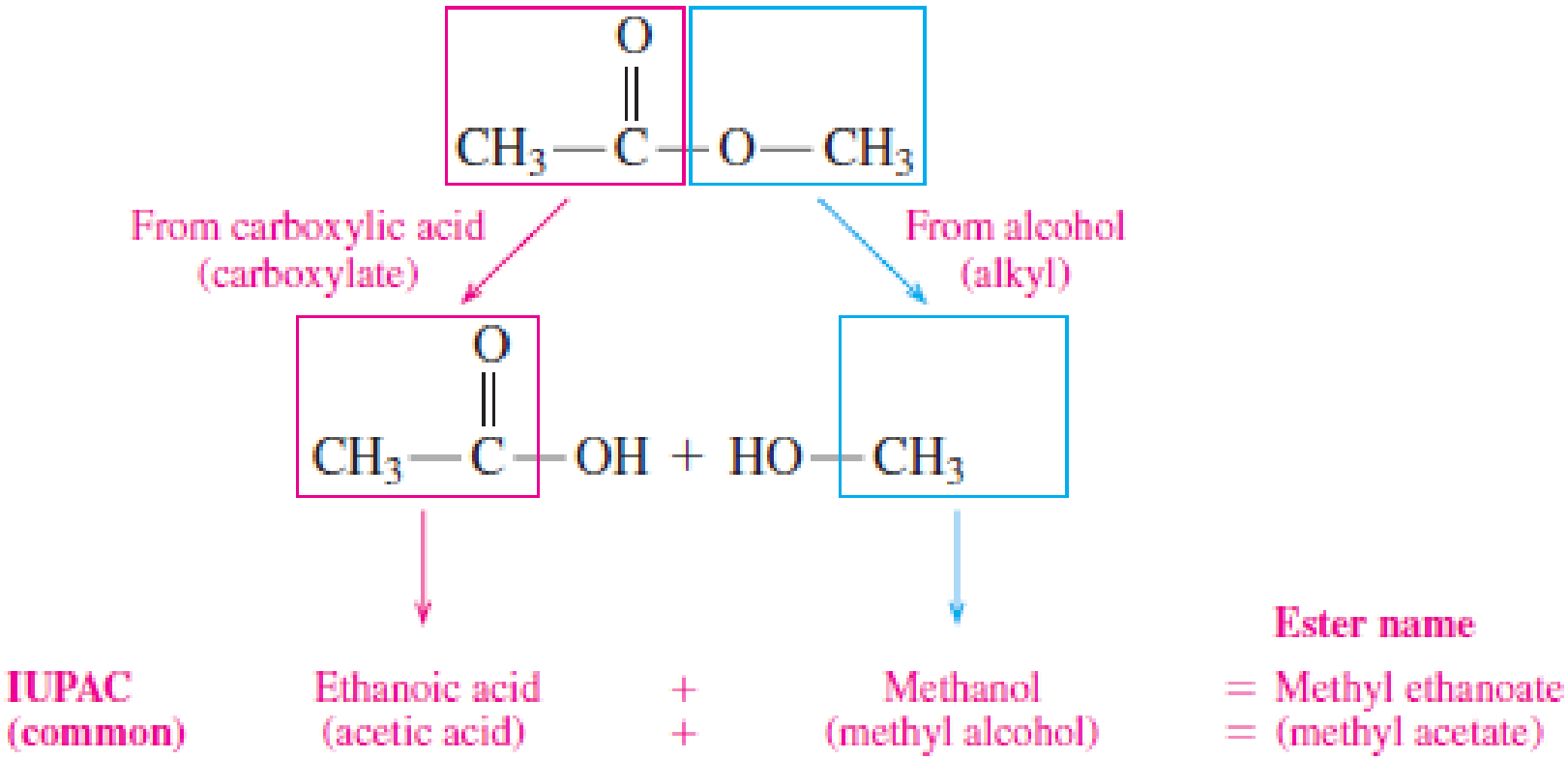
IUPAC Name	Condensed Structural Formula	Boiling Point (°C)	Solubility in Water
Methanoic acid		101	Soluble
Ethanoic acid		118	Soluble
Propanoic acid		141	Soluble
Butanoic acid		164	Soluble
Pentanoic acid		187	Soluble
Hexanoic acid		205	Slightly soluble
Benzoic acid		250	Slightly soluble

➢ Nomenclature of Esters:

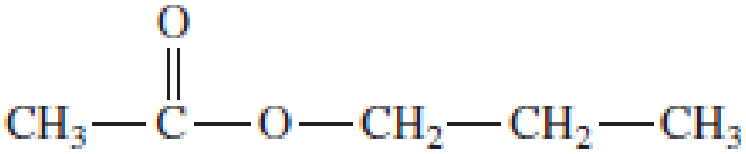
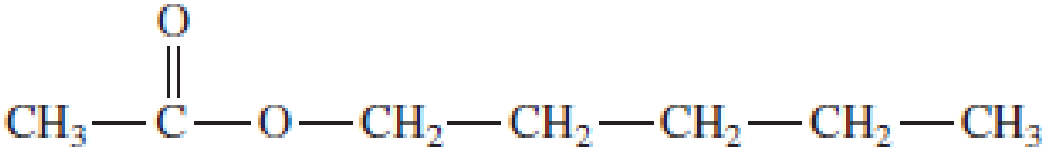
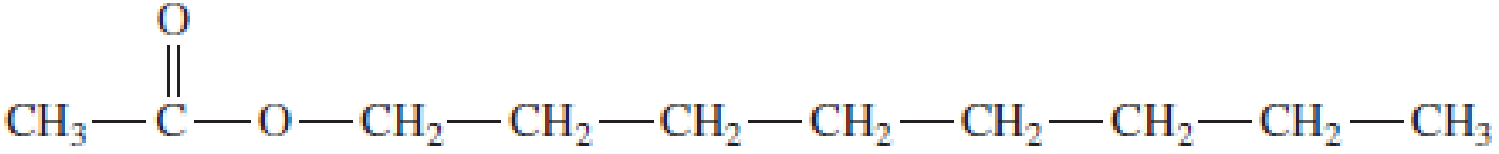
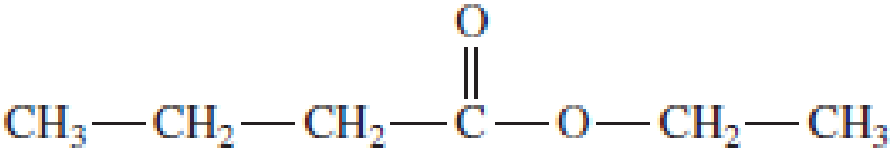
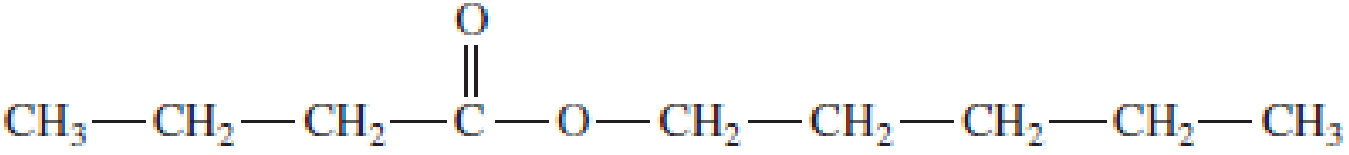
The name of an ester consists of ***two*** words that are derived from the names of the **alcohol** and the **acid** in that **ester**.

- The first word indicates the ***alkyl*** part from the ***alcohol***.
- The second word is the ***carboxylate*** part from the ***carboxylic acid***, *and* change the ***(-ic) acid*** of the acid name to ***(ate)***.
- The general formula for an ester is **(RCOOR′) or (RCO_2R')** .

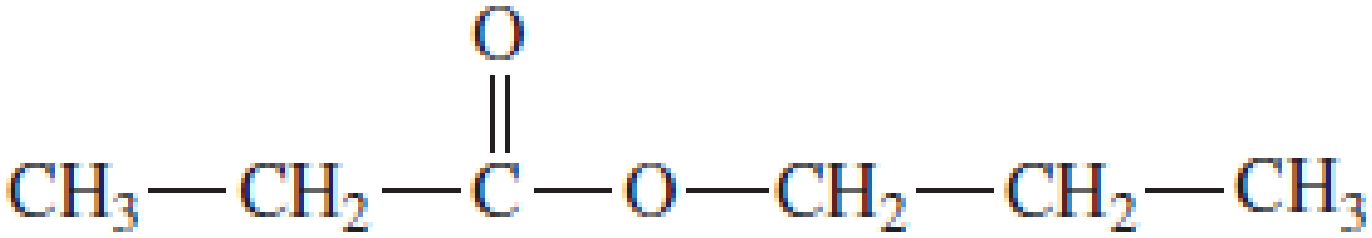
➢ The IUPAC names of esters use the IUPAC names for the carbon chain of the acid, *while the common names of esters use the common names of the acids*.



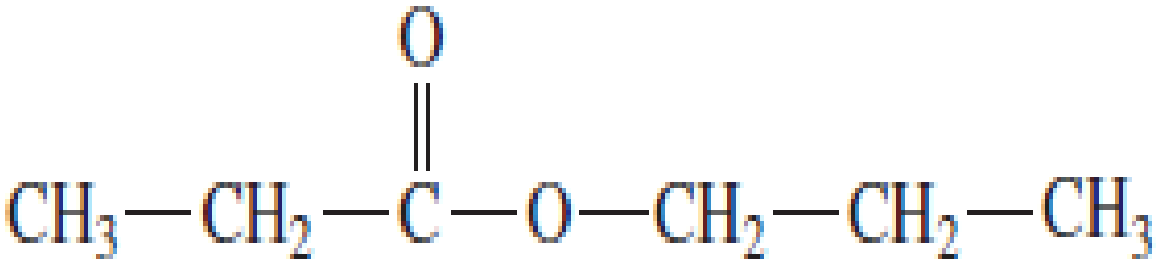
❖ Many of the ***fragrances*** of perfumes and flowers, and the flavors of fruits are due to ***esters***. Small esters are volatile so we can smell them and soluble in water so we can taste them. Several esters and their flavors and odor are listed in the table in next slide:

Condensed Structural Formula and Name	Flavor/Odor
 Propyl ethanoate (propyl acetate)	Pears
 Pentyl ethanoate (pentyl acetate)	Bananas
 Octyl ethanoate (octyl acetate)	Oranges
 Ethyl butanoate (ethyl butyrate)	Pineapples
 Pentyl butanoate (pentyl butyrate)	Apricots

Example: What are the IUPAC and common names of the following ester?

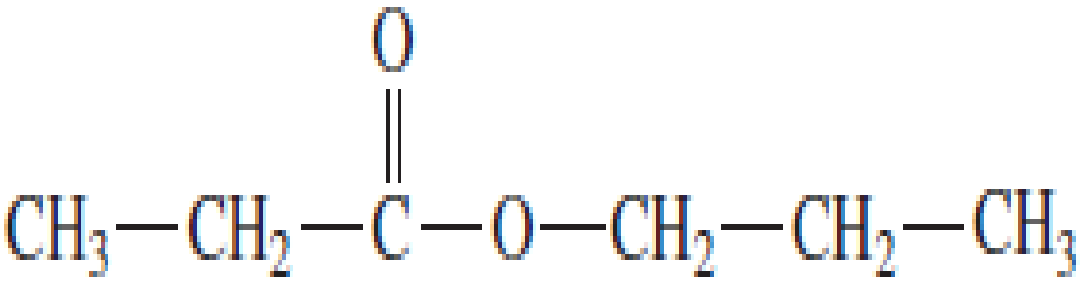


Step 1: Write the name of the carbon chain from the alcohol as an ***alkyl*** group. The alcohol that is used for the ester is **propanol**, which has a three-carbon chain named as **Propyl**.



Propyl

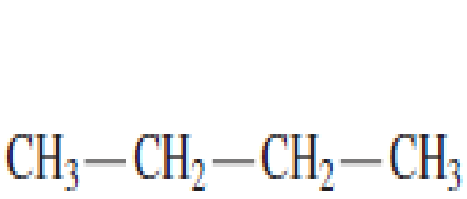
Step 2: The (IUPAC) of carboxylic acid that is used for the ester is **propanoic acid**, which has three carbon atoms. Replacing the ***(-ic)*** *acid* with ***(-ate)*** gives **propanoate**. Thus, the IUPAC name is **Propyl propanoate**. The (common name) of carboxylic acid that is used for the ester is **propionic acid**, which has three carbon atoms. Replacing the ***(-ic)*** *acid* in the common name propionic acid with ***(-ate)*** gives **propionate**. The common name for the ester is **propyl propionate**.

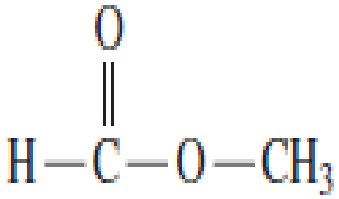


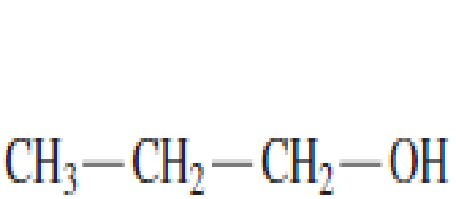
Propyl propanoate (propyl propionate)

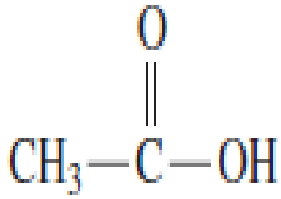
➢ Physical properties of Esters:

Esters have boiling points ***higher*** than those of alkanes and ethers, but ***lower*** than those of alcohols and carboxylic acids of ***similar mass***. Because ester molecules do not have hydroxyl groups, they cannot hydrogen bond to each other.







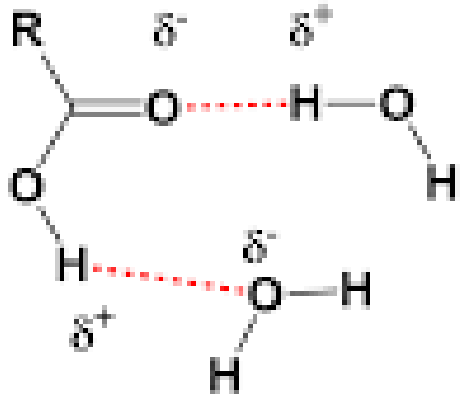


Name	Butane	Methyl methanoate	1-Propanol	Ethanoic acid
Molar Mass	58	60	60	60
Family	Alkane	Ester	Alcohol	Carboxylic acid
bp	0 °C	32 °C	97 °C	118 °C

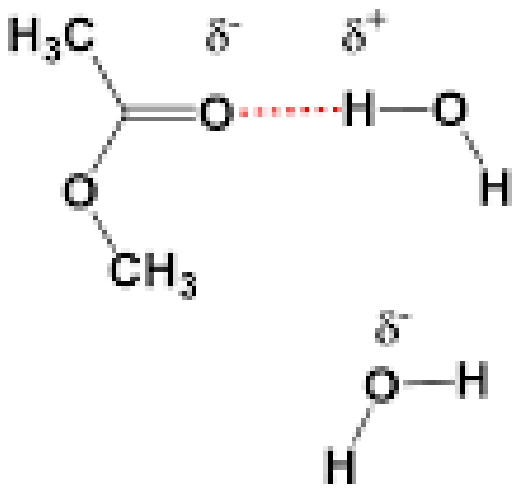
Increase in Boiling Points

➢ Solubility of ester in Water

Esters with ***one to five*** carbon atoms are ***soluble*** in water. The partially negative oxygen of the carbonyl group forms hydrogen bonds with the partially positive hydrogen atoms of water molecules. *The solubility of esters decreases as the number of carbon atoms increases.*



Carboxylic Acid
Hydrogen Bonding with Water



Ester
Hydrogen Bonding with Water

References:

1) Organic chemistry by morrison and boyd.

2) Organic chemistry by solomon and fryhl, 10th Edition, 2011.