

# BIO-ORGANIC CHEMISTRY

(Organic Chemistry for Biology Students)  
(SQBS 1603)

## Organic Compounds Containing Oxygen

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# Physical properties of the alkanes



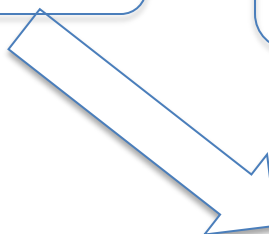
Alkanes are insoluble in water



The alkanes have few direct roles in biological systems



Biological systems are aqueous (water based)



## Adding functional groups

## What is functional group?

Molecules possessing the same functional group belong to the same family of organic compounds.

The chemical components that are added to the simple skeleton of an organic compound.

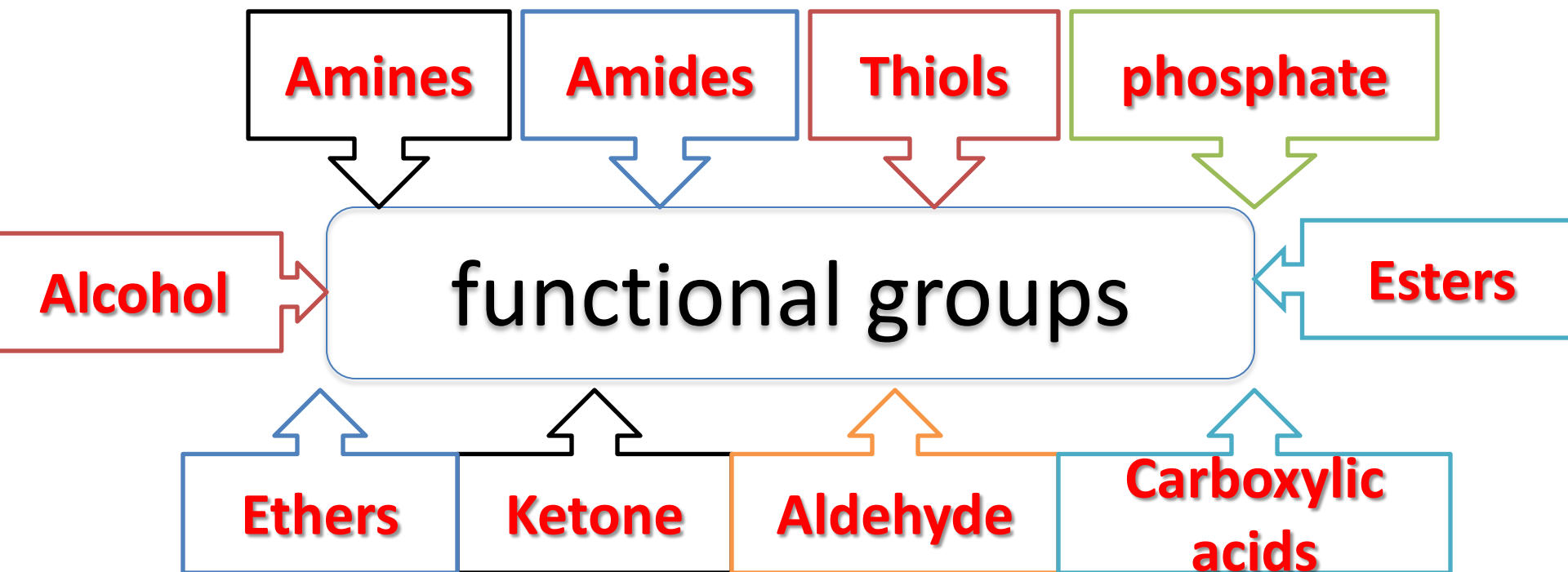
To generate chemical diversity and functionality.

Hydrocarbon

Groups containing oxygen

Groups containing nitrogen

Groups containing phosphorus and sulfur



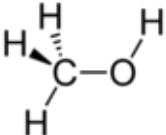
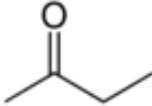
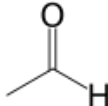
# Functional groups

## Biological importance of functional group

Functional group	Biological importance
Alcohol	Lipids, carbohydrates
Ethers	Archael plasma membranes
Ketone	Metabolic intermediates
Aldehyde	Reducing sugars such as glucose
Carboxylic acids	Lipids, proteins
Ester	Bacterial and eukaryotic plasma membranes
Amines	Proteins, nucleic acids DNA and RNA
Amides	Proteins, nucleic acids DNA and RNA
Thiol	Protein structure, Energy metabolism
Phosphate	ATP, DNA

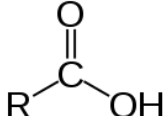
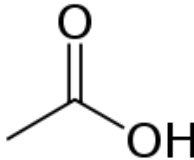
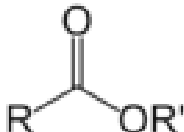
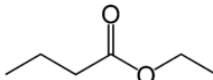
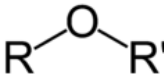
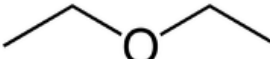
# Functional groups

## Groups containing oxygen

Chemical class	Group	Formula	Structural Formula	Prefix	Suffix	Example
<b>Alcohol</b>	Hydroxyl	ROH	$\begin{array}{c} \text{R}-\text{O} \\   \\ \text{H} \end{array}$	hydroxy-	-ol	Methanol 
<b>Ketone</b>	Carbonyl	RCOR'	$\begin{array}{c} \text{O} \\    \\ \text{R}^1-\text{C}-\text{R}^2 \end{array}$	keto-, oxo-	-one	Methyl ethyl ketone <i>(Butanone)</i> 
<b>Aldehyde</b>	Aldehyde	RCHO	$\begin{array}{c} \text{O} \\    \\ \text{R}-\text{C}-\text{H} \end{array}$	aldo-	-al	Acetaldehyde <i>(Ethanal)</i> 

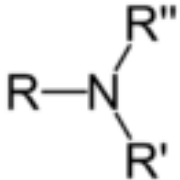

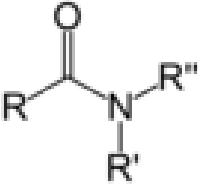
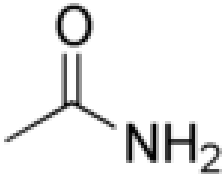
# Functional groups

## Groups containing oxygen

Chemical class	Group	Formula	Structural Formula	Prefix	Suffix	Example
<b>Carboxylate (Carboxylic acid)</b>	Carboxyl	RCOOH		Carboxy-	-oic acid	Acetic acid 
<b>Esters</b>	Ester	RCOOR'			alkyl alkanoate	Ethyl butyrate <i>(Ethyl butanoate)</i> 
<b>Ethers</b>	ether	ROR		Di-	-ether	Diethyl ether 

# Functional groups


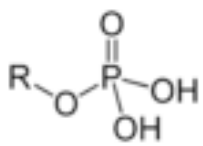
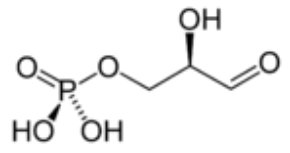
## Groups containing **nitrogen**

Chemical class	Group	Formula	Structural Formula	Prefix	Suffix	Example
<b>Amines</b>	Amino	$\text{RNH}_2$ $\text{R}_2\text{NH}$ $\text{R}_3\text{N}$		amino-	-amine	Dimethylamine 
<b>Amide</b>	Amide	$\text{RCONH}_2$ $\text{RCONHR}'$ $\text{RCONR}_2$		Carboxamide-	-amide	Acetamide 



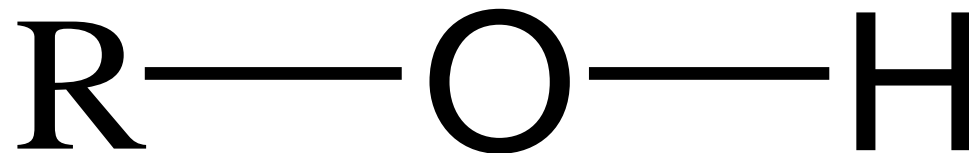
# Functional groups

## Groups containing **sulphur and phosphorus**

Chemical class	Group	Formula	Structural Formula	Prefix	Suffix	Example
<b>Thiol</b>	Sulfhydryl	RSH	$\begin{array}{c} \text{R}-\text{S} \\   \\ \text{H} \end{array}$	Mercapto- Sulfanyl-	-thiol	Ethanathiol (Ethyl mercaptan) 
<b>Phosphate</b>	phosphate	$\text{ROP}(=\text{O})(\text{OH})_2$		phospho-		Glyceraldehyde 3-phosphate 

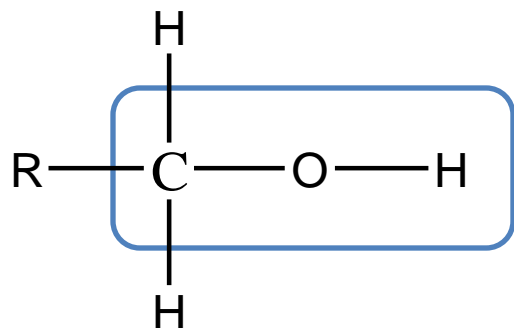
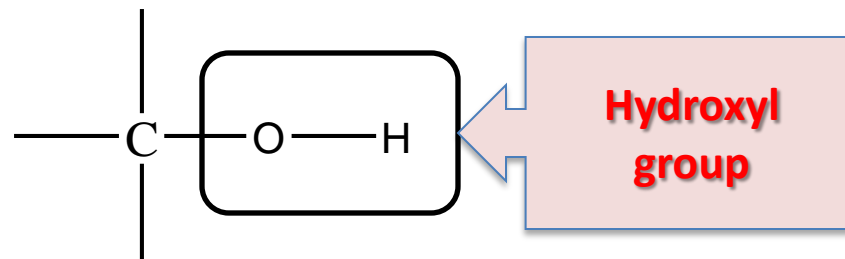
# Alcohol

- Alcohol
  - Hydroxyl group : -OH functional group
  - Generic formula: R-OH
  - General structure

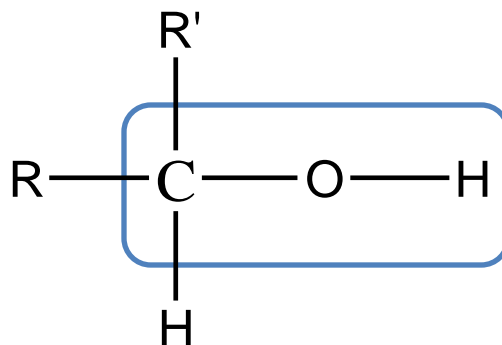


# Alcohol

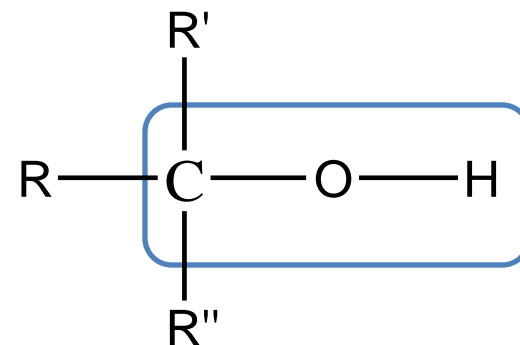
- Classification



**Primary (1°)**

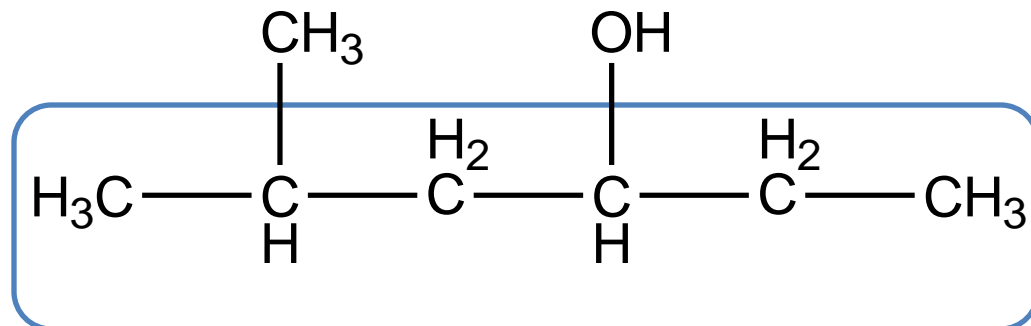
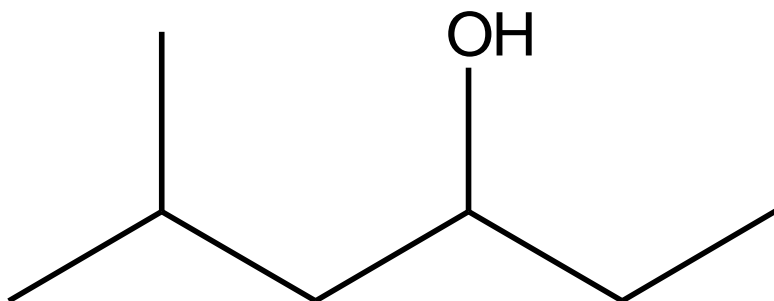


**Secondary (2°)**



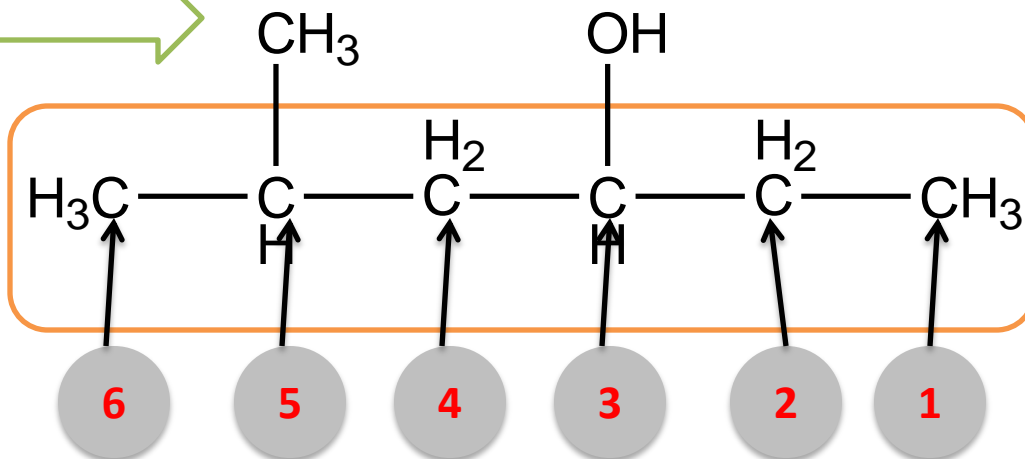
**Tertiary (3°)**

# Naming Alcohols



C : 6 → hexane → hexanol

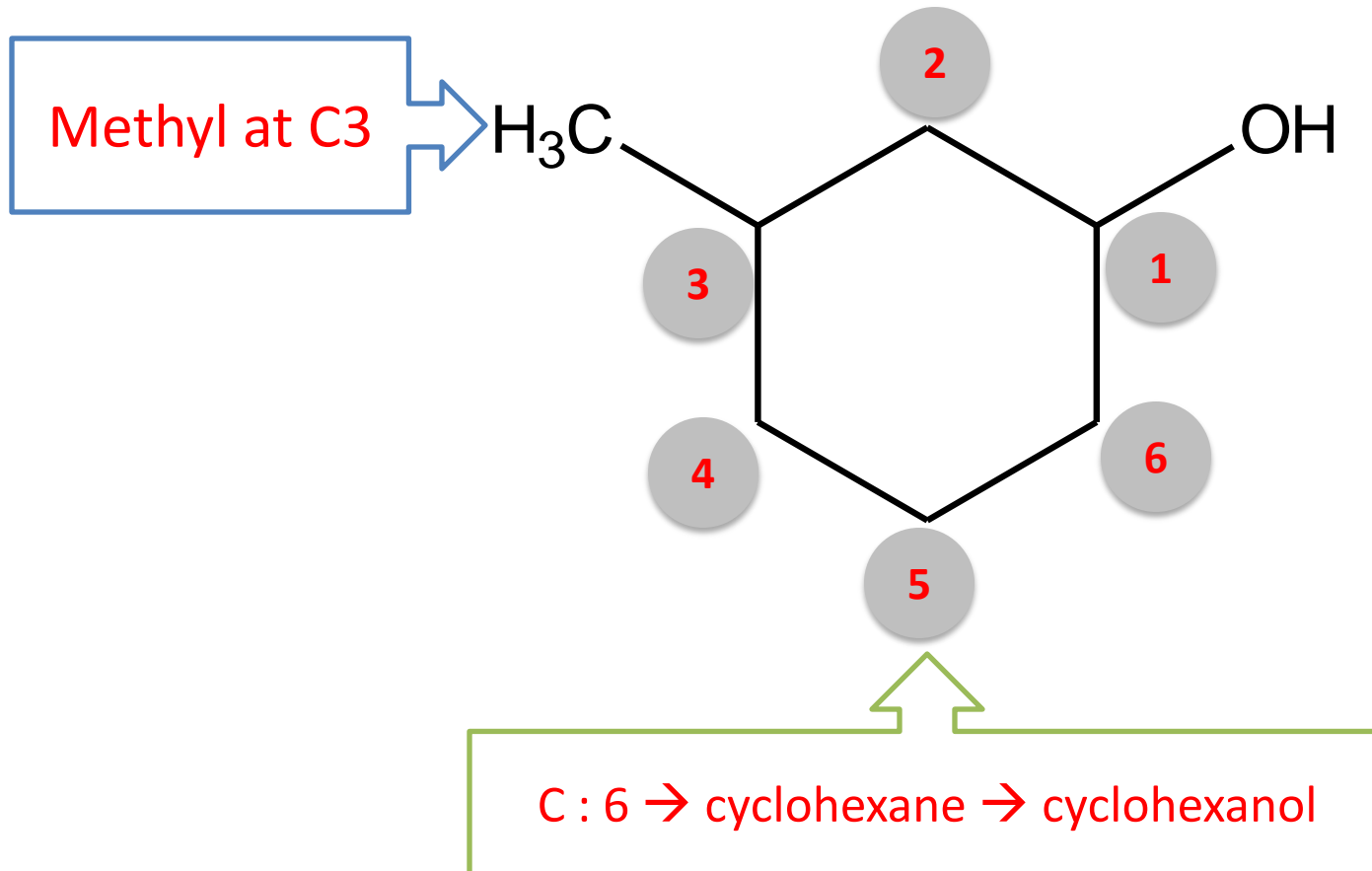
Methyl at C5



**5-methyl-3-hexanol**

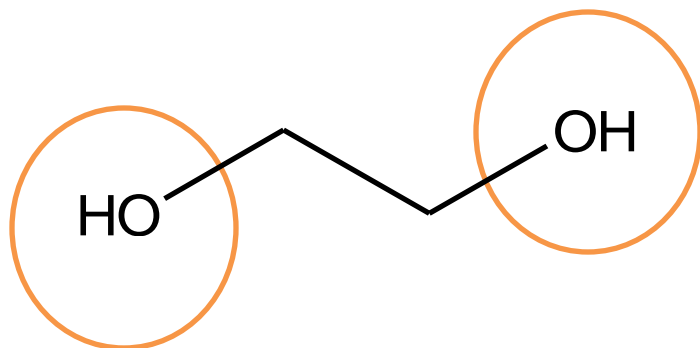
# Naming Alcohols

- Give the IUPAC name of the following alcohol

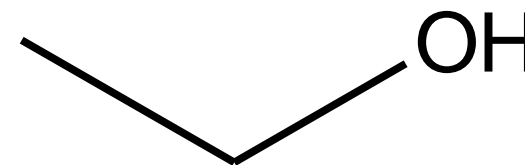


**3-methyl-cyclohexanol**

# Naming Alcohols



-diol



Ethanol

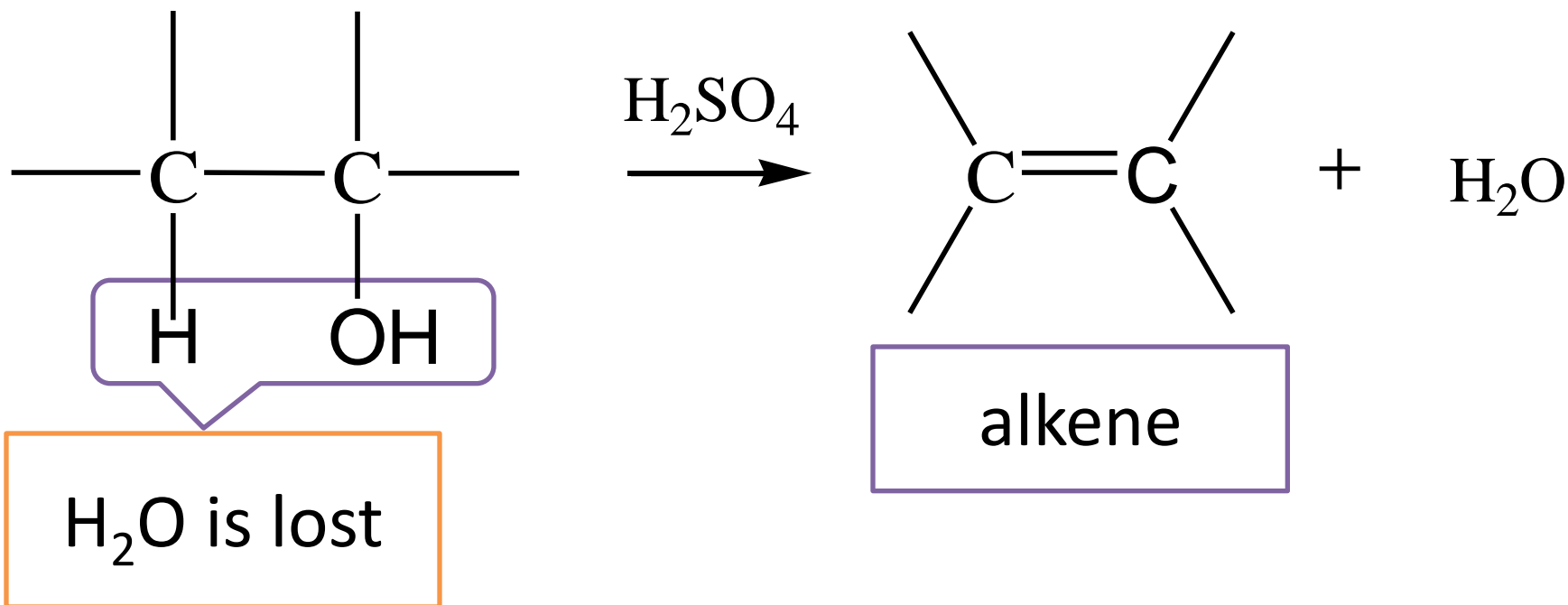
**IUPAC name: 1,2-ethanediol or Ethane-1,2-diol**  
**Common name: ethylene glycol**

# Reactions of alcohol

- Dehydration
- Oxidation

# Dehydration

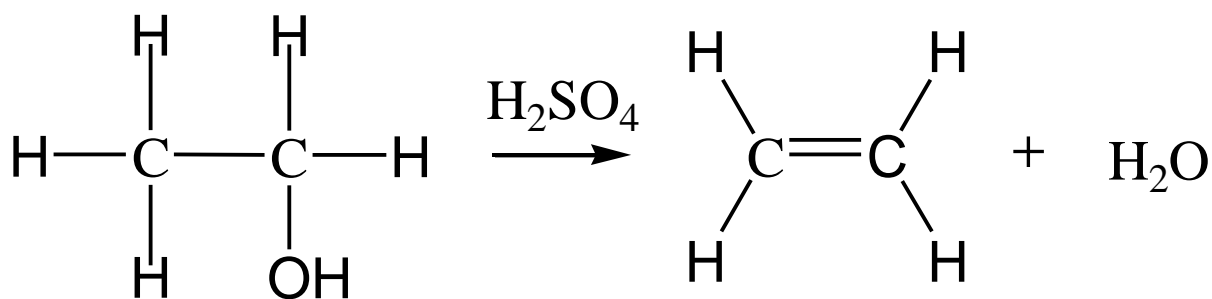
- Loss of water ( $\text{H}_2\text{O}$ )
- Elimination reaction
  - Elements of the starting material are lost and a new multiple bond is formed





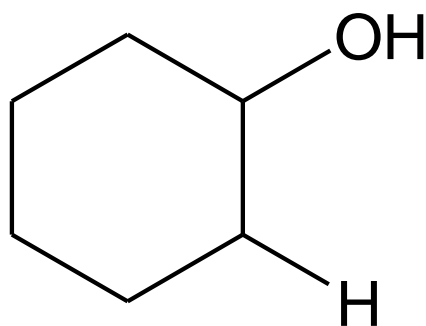
# Dehydration

- Examples

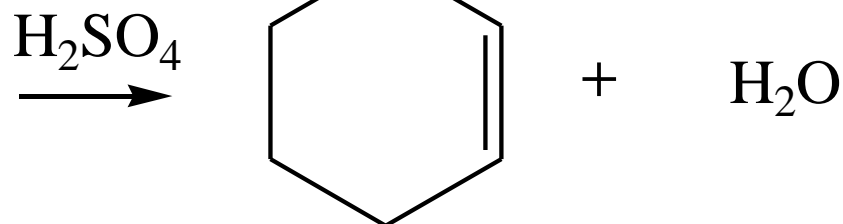


Ethanol

Ethene



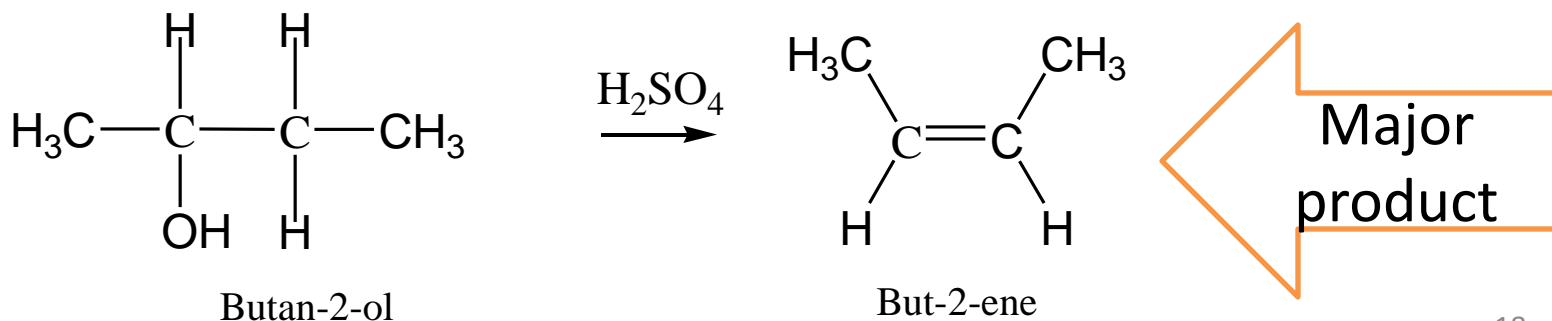
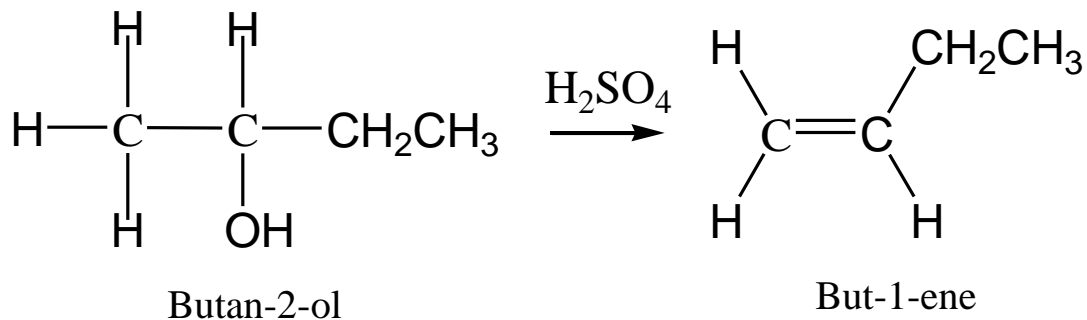
Cyclohexanol



Cyclohexene

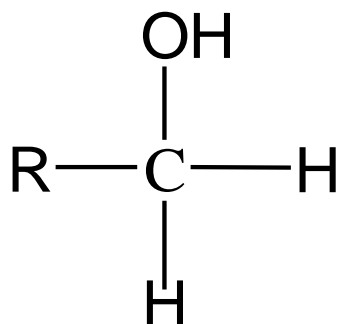
# Dehydration

- **Zaitsev** rule
  - The major product in elimination is the alkene that has more alkyl groups bonded to it.

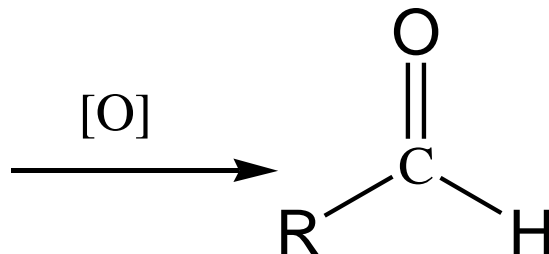


# Oxidation

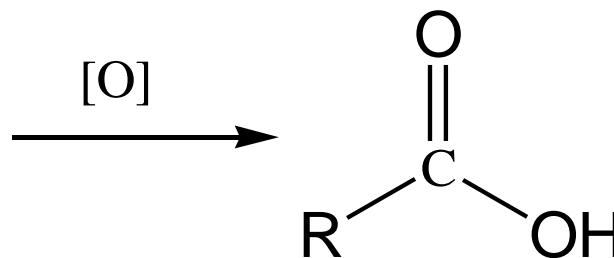
- Primary ( $1^\circ$ ) alcohols
  - Oxidized to aldehydes (RCHO)
  - And further oxidized to carboxylic acids (RCOOH)



alcohol



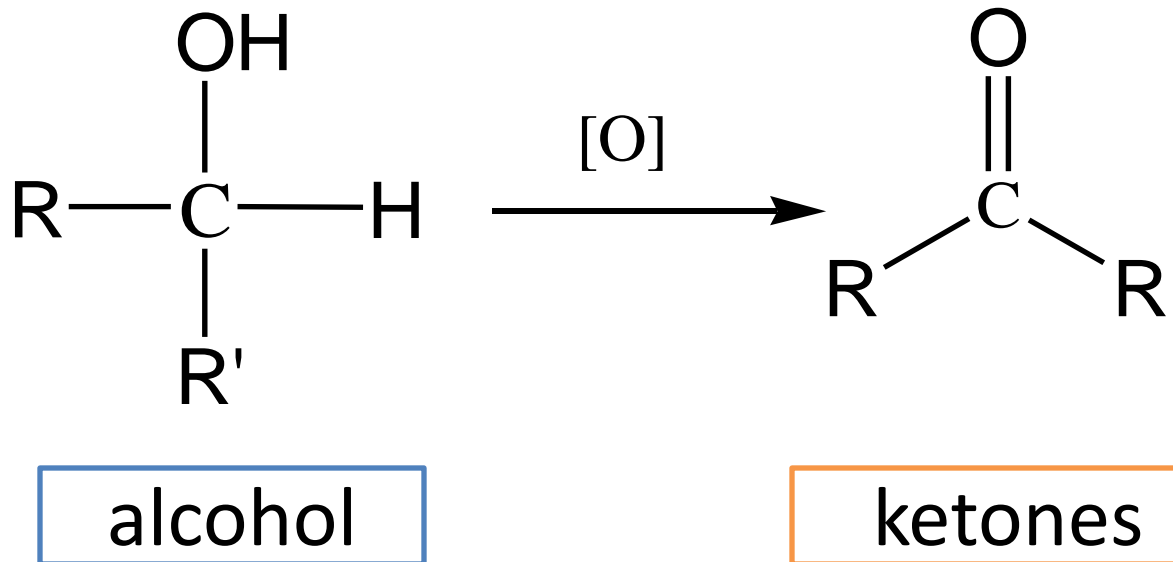
aldehyde



Carboxylic  
acid

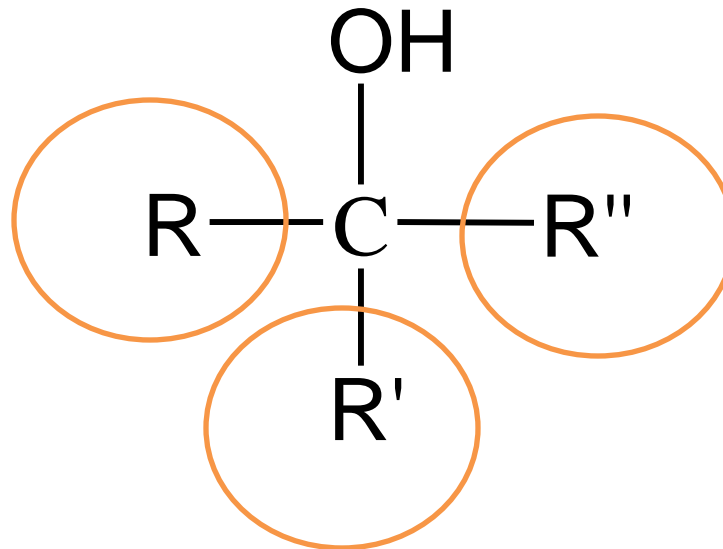
# Oxidation

- Secondary ( $2^\circ$ ) alcohols
  - Oxidized to ketones ( $R_2CO$ )

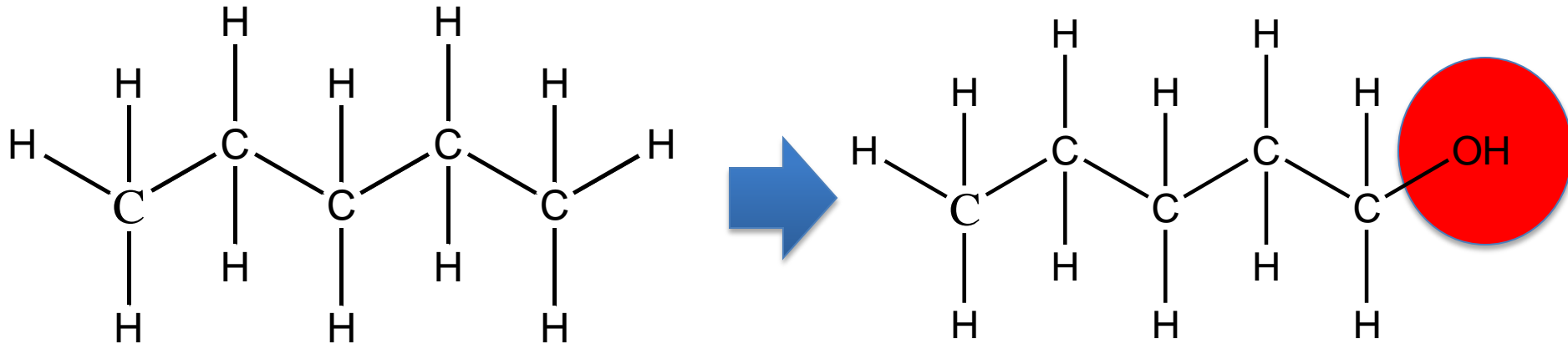


# Oxidation

- Tertiary( $3^\circ$ ) alcohols
  - They are not oxidized



# Physical properties of alcohols



**hydroxyl group → oxygen + hydrogen → highly electronegative atom → polar molecules**

# Physical properties of alcohols

hydroxyl group  $\rightarrow$  oxygen + hydrogen

highly  
electronegative  
atom

polar  
molecules

dipolar  
interaction

dispersion  
forces

hydrogen  
bonding

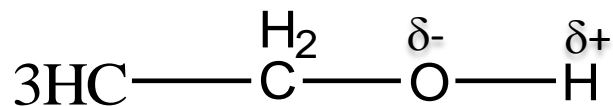
soluble in  
water in  
small  
quantity

Strong non-covalent forces

Exhibit higher melting and boiling  
points than alkanes

# Physical properties of alcohols

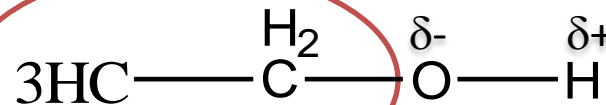
Ethanol



Electron pulls towards highly electronegative oxygen atom

Low electron density

high electron density



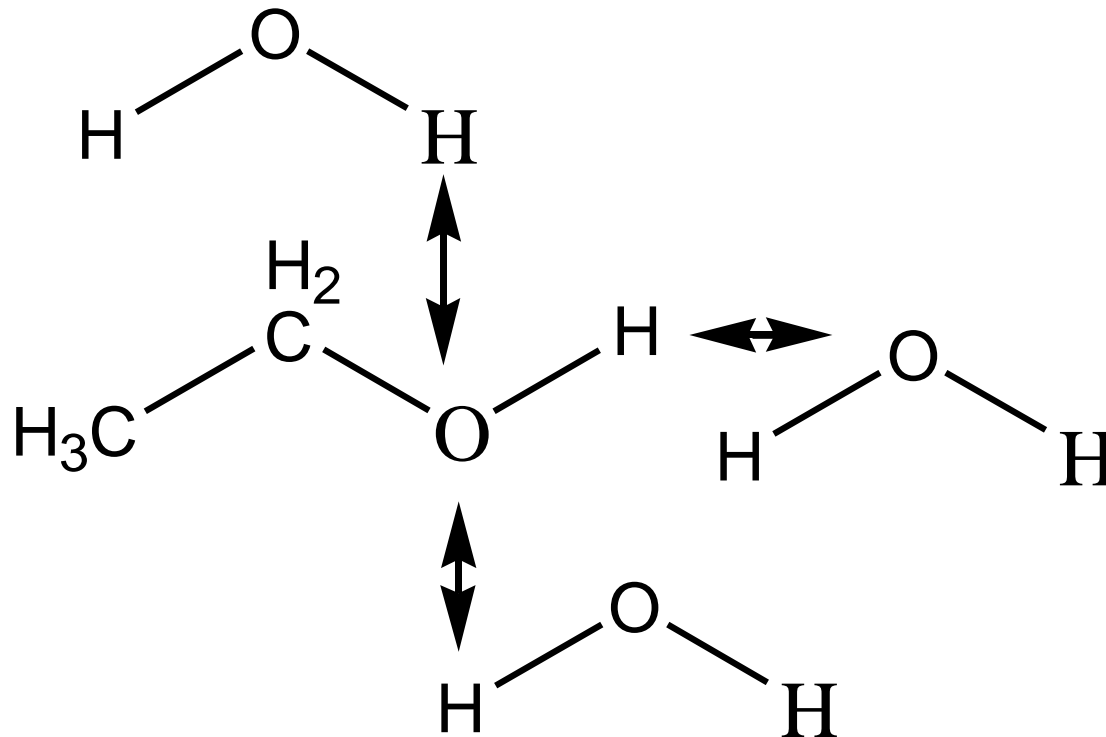
The distribution of electrons within the molecules is **unequal**

The molecule is **polar**



# Physical properties of alcohols

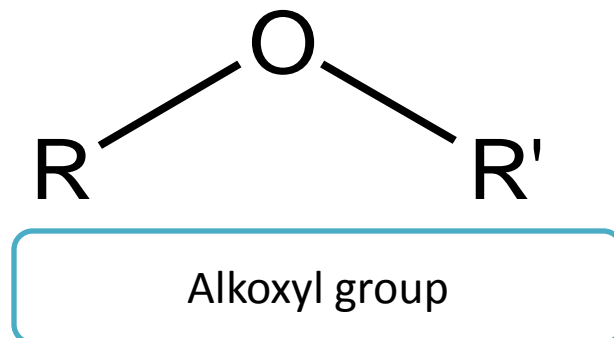
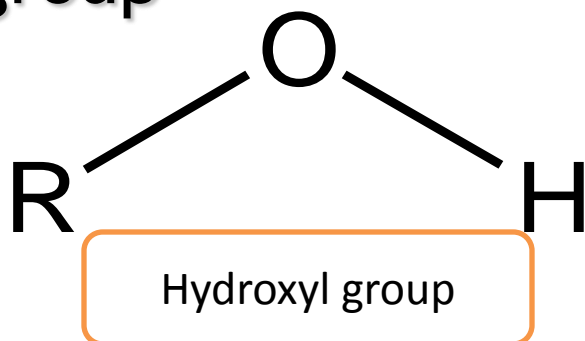
## hydrogen bonding



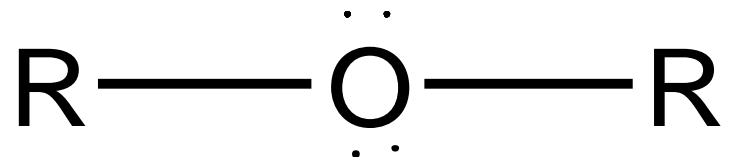
Ethanol is attracted to the water molecules through hydrogen bonds

# Ether

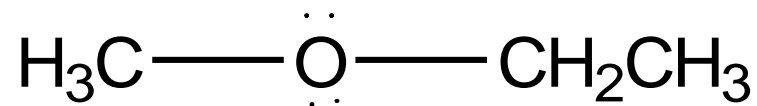
- Alkoxy group : combination of an alkyl group and oxygen atom (alkyl + oxygen = alkoxy)
- Generic formula:  $R-O-R'$
- Similar to alcohol (hydroxyl group), except that the H atom is replaced with an alkyl group



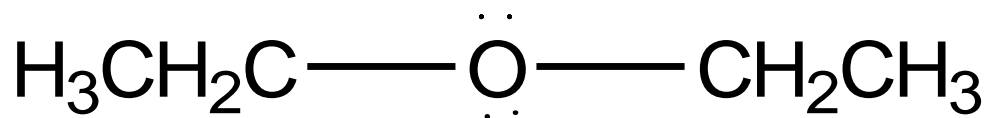
# Ether



R groups are the  
same

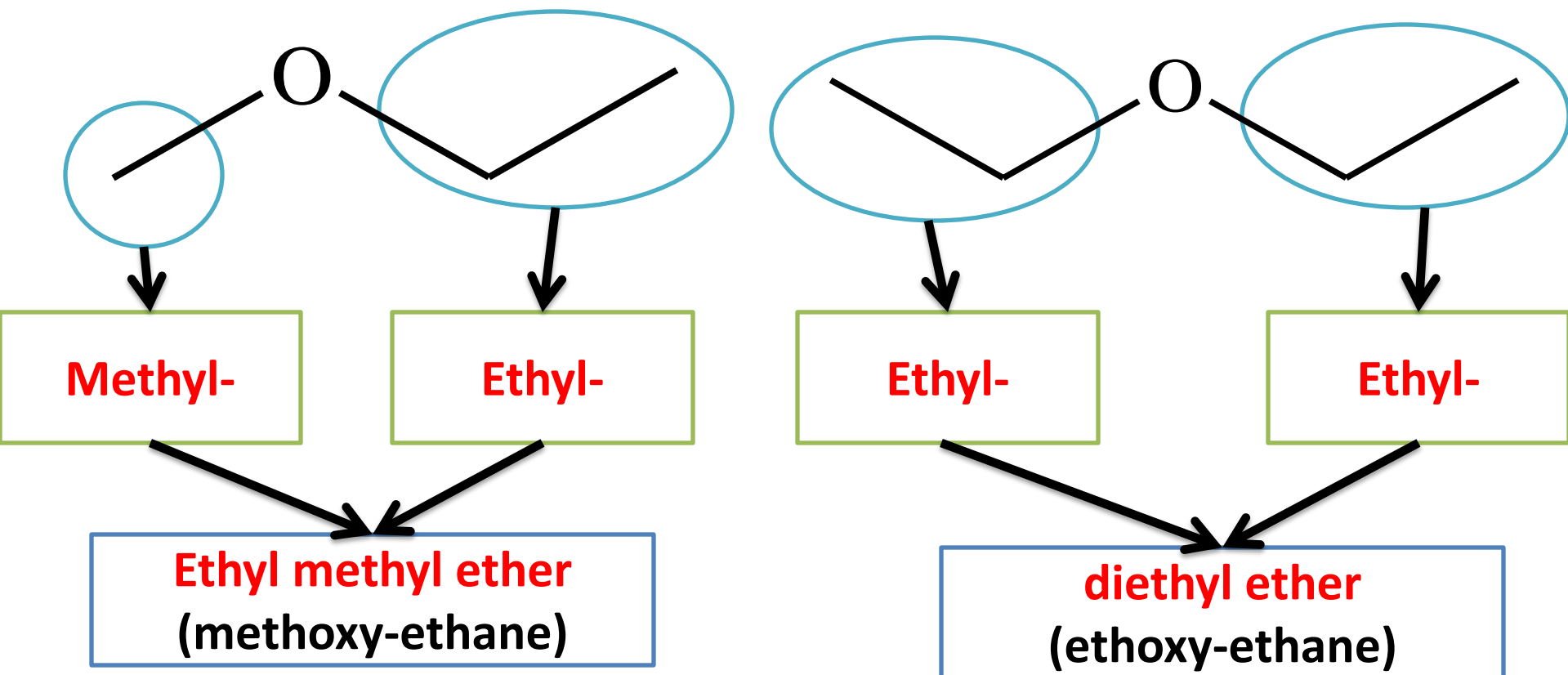


R groups are  
different



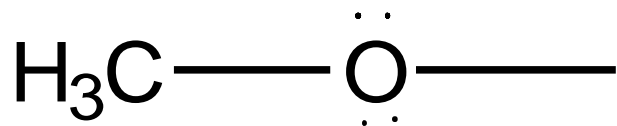
# Naming Ether

Simple ethers: Usually assigned common names

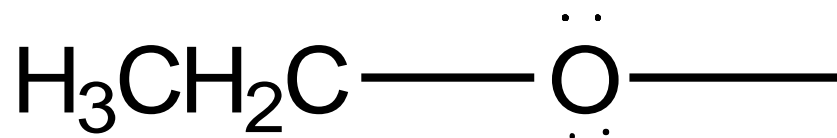


# Naming Ether

More complex ethers: IUPAC name

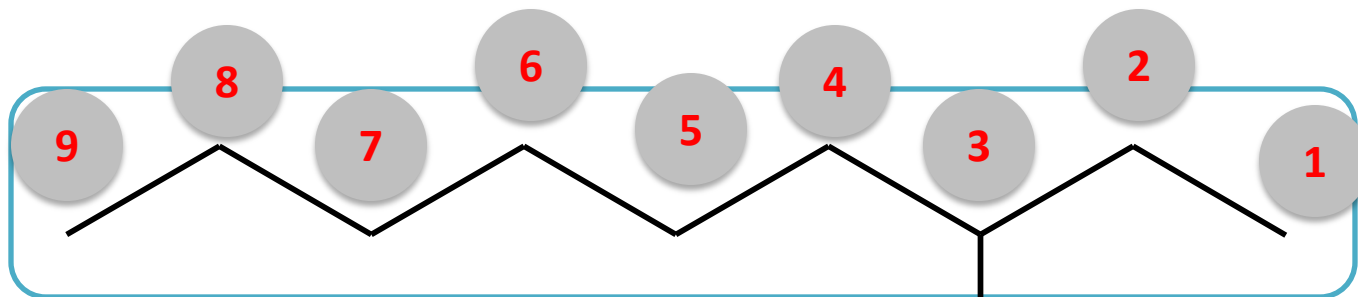


**Methoxy-**

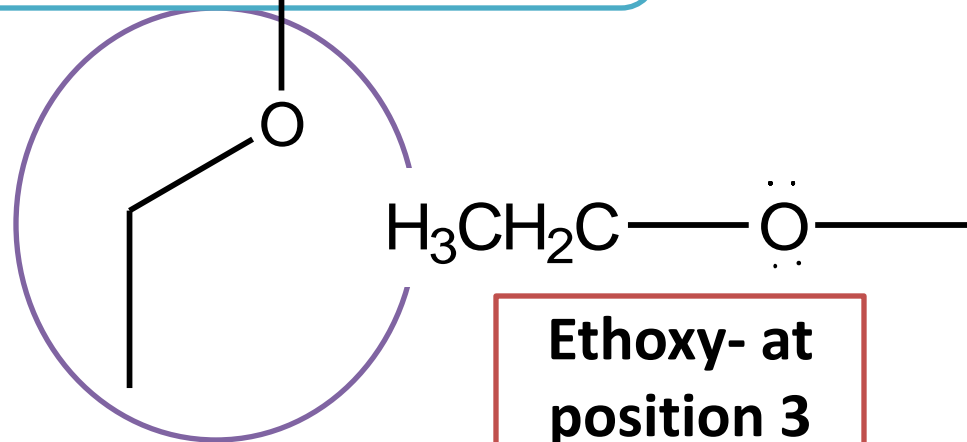


**Ethoxy-**

# Naming Ether



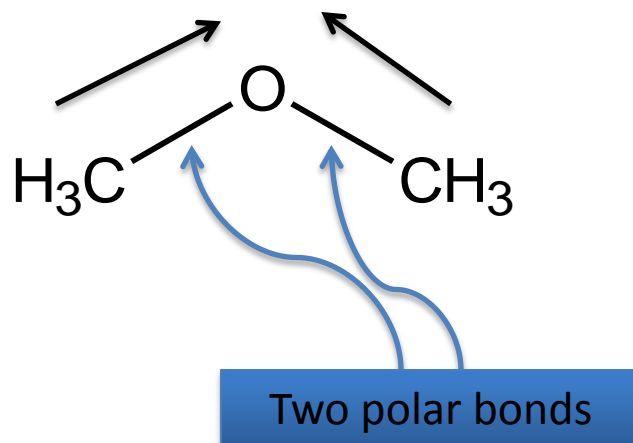
9 C → nonane



**3-ethoxy-nonane**

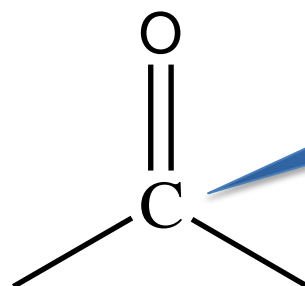
# Physical properties of ethers

**Presence of oxygen → polar molecules**



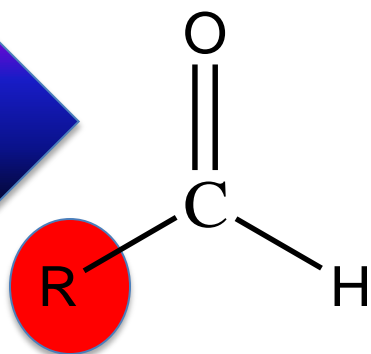
# Aldehydes and Ketones

**Carbonyl group**

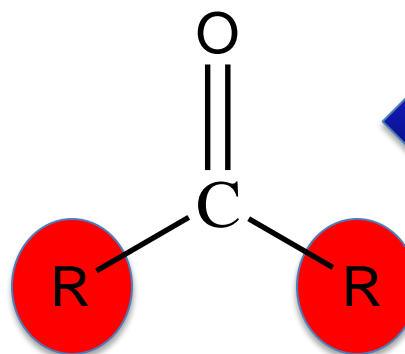


Carbonyl carbon

**Aldehyde**



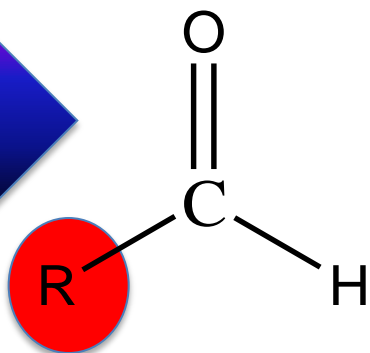
**Ketone**



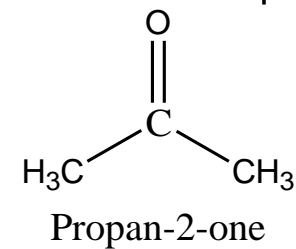
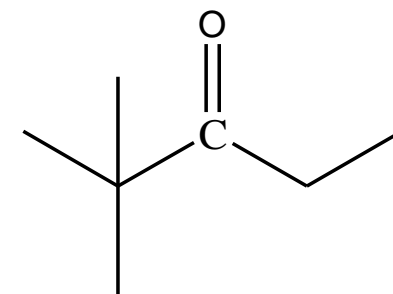
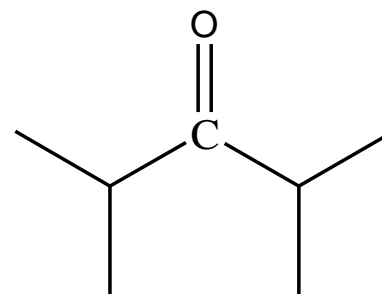
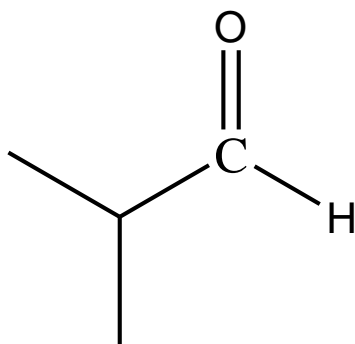
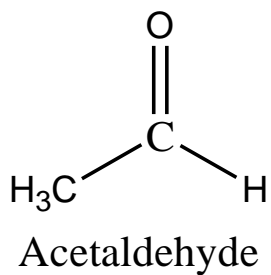
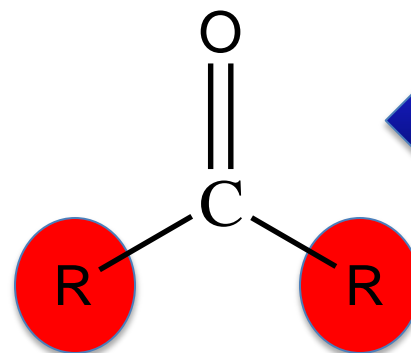


# Aldehydes and Ketones

**Aldehyde**

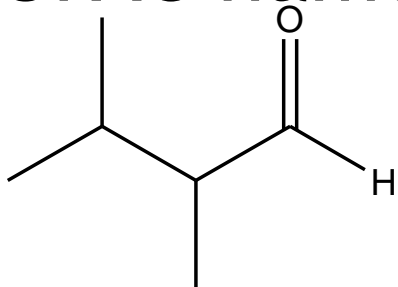


**Ketone**



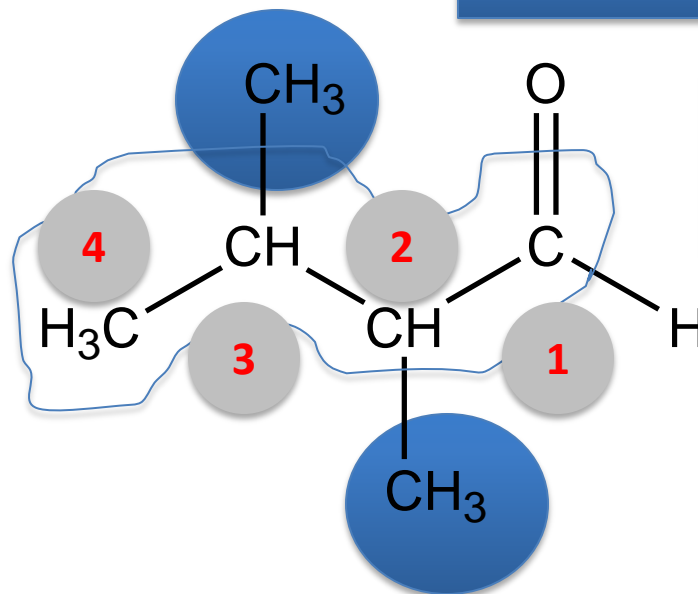
# Naming aldehydes

IUPAC name



4 C → butane → butanal

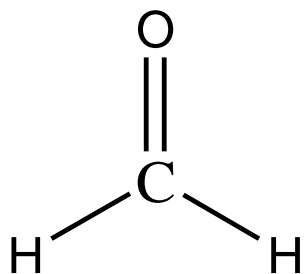
Methyl → at 2 and 3 → dimethyl



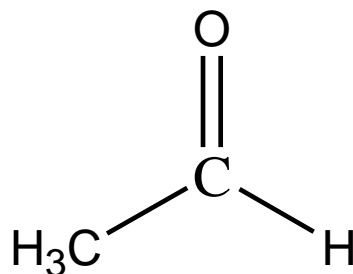
**2,3-dimethylbutanal**

# Naming aldehydes

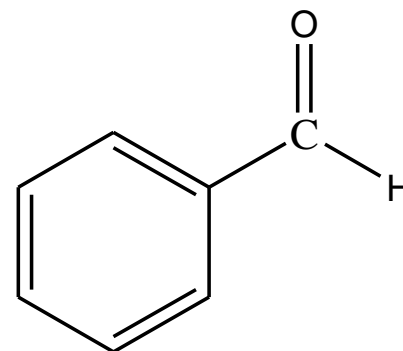
- Simple aldehydes have common names that are widely used
- Examples:



Formaldehyde



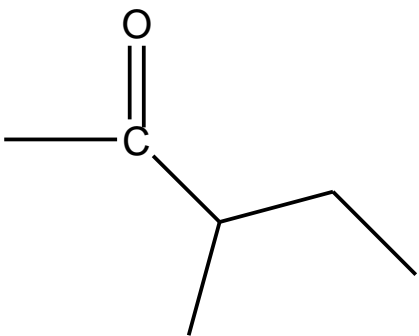
Acetaldehyde



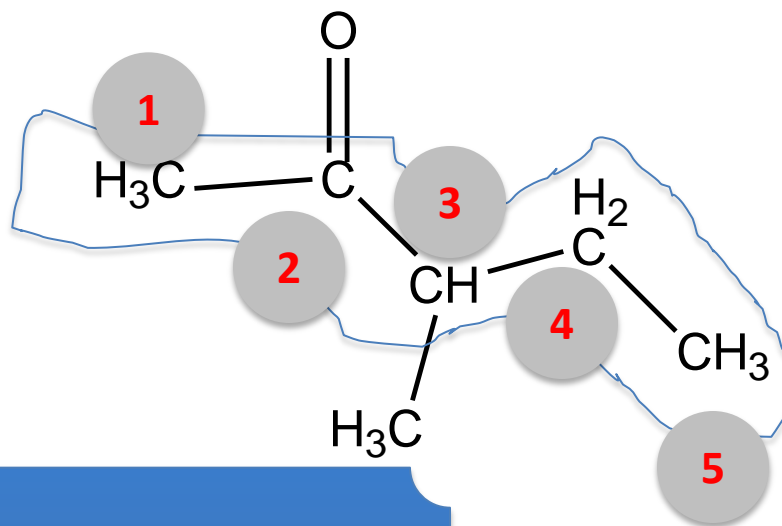
Benzaldehyde

# Naming Ketones

IUPAC name



5 C → pentane → pentanone

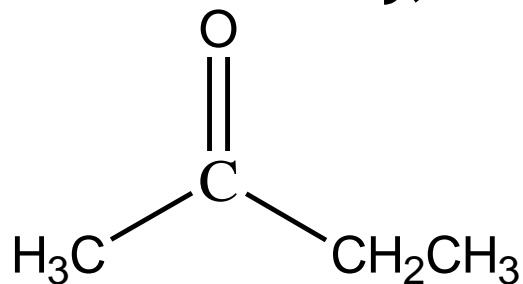


**3-methyl-2-pentanone**

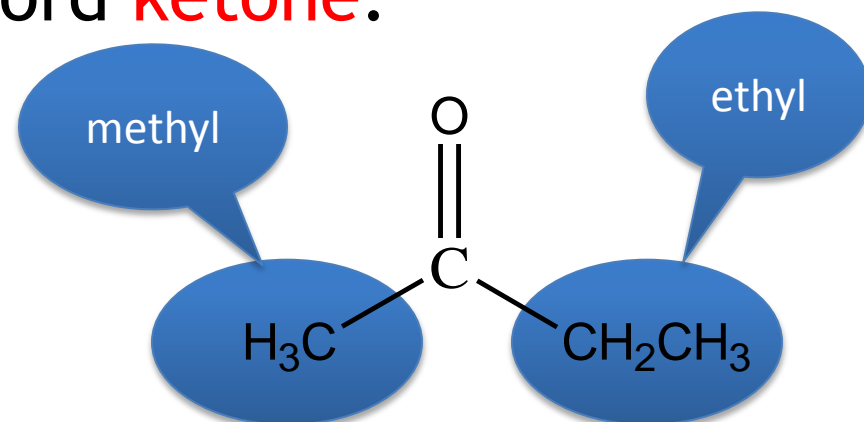
Carbonyl → position 2  
Methyl → position 3

# Naming Ketones

- Common names for ketones:
  - Naming **both alkyl group** on the carbonyl carbon.
  - Arranging them **alphabetically**.
  - Finally, adding the word **ketone**.



**IUPAC name: 2-butanone**

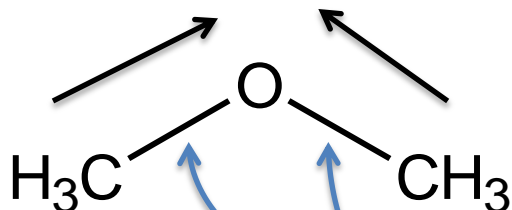


**common name:  
Ethyl methyl ketone**

# Physical properties of aldehydes and ketones

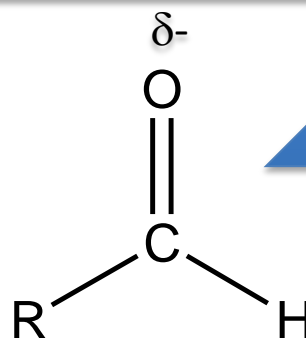
Presence of oxygen  $\rightarrow$  polar molecules

Ether

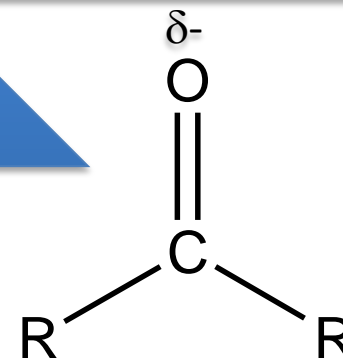


Two polar bonds

Aldehyde



ketone

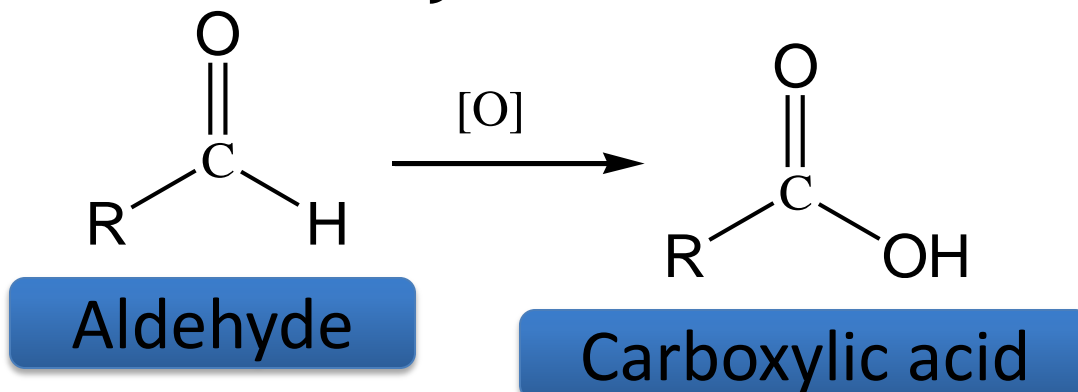


Electrons  
pulled  
towards  
highly  
electronegative  
oxygen  
atom

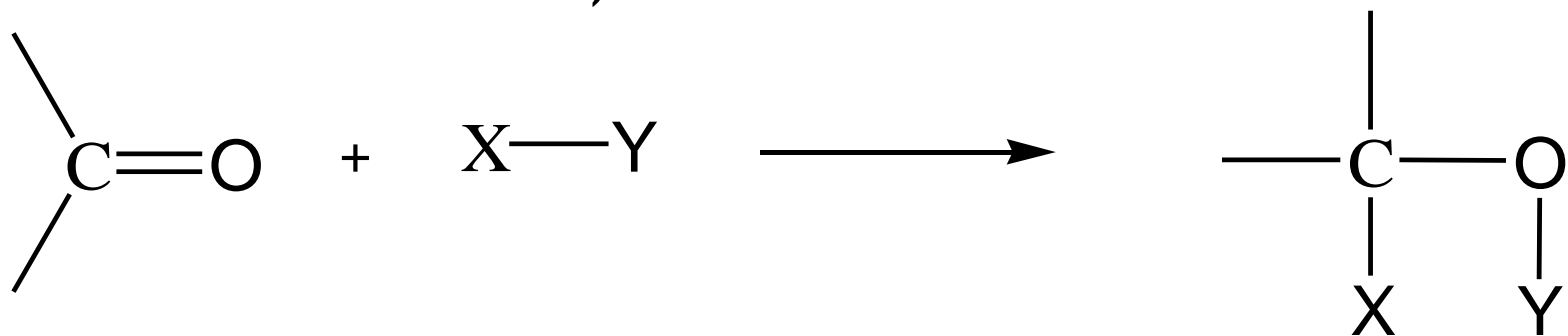
.....generating an uneven  
distribution of electron: polar  
molecule

# Reactions of aldehydes and ketones

## 1. Oxidation of aldehydes

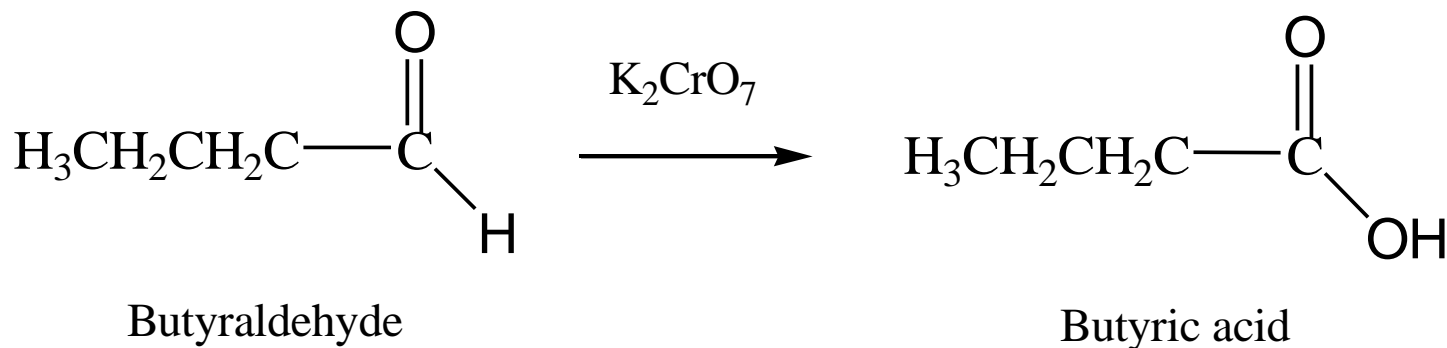


## 2. Reduction of aldehydes and ketones (addition reaction)

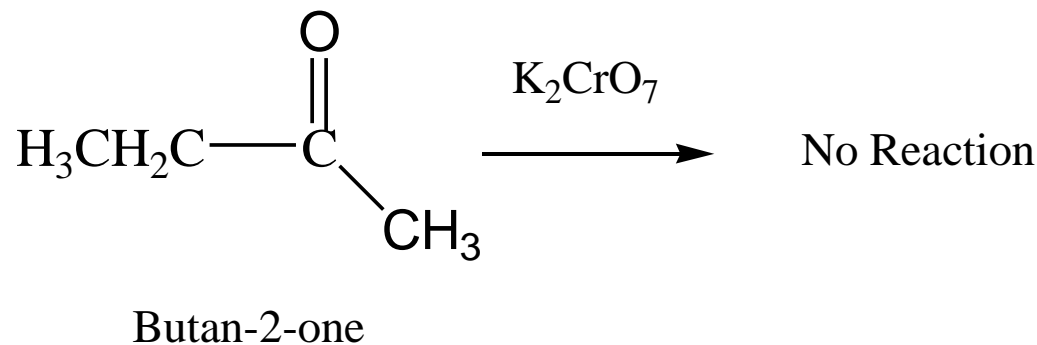


# Oxidation of aldehydes

- Examples



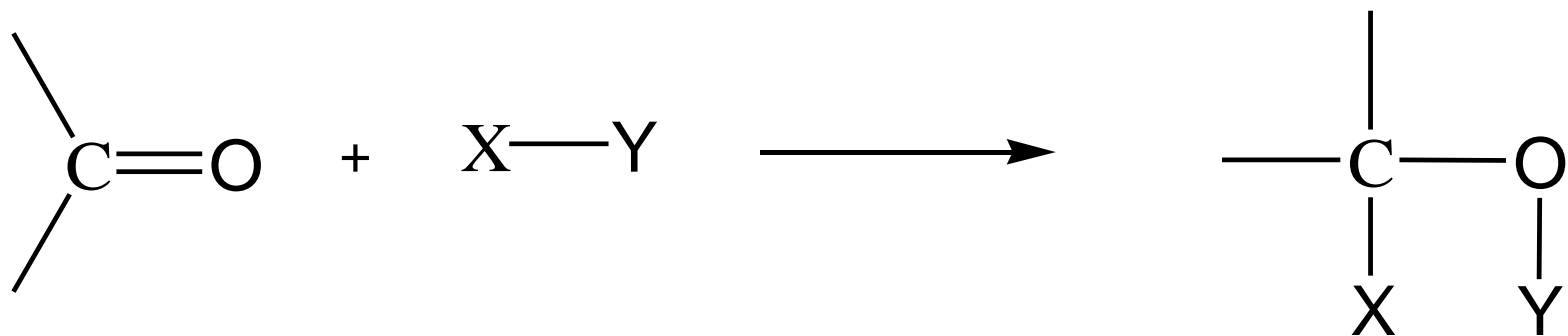
- How about ketones?





# Reduction of aldehydes and ketones (addition reaction)

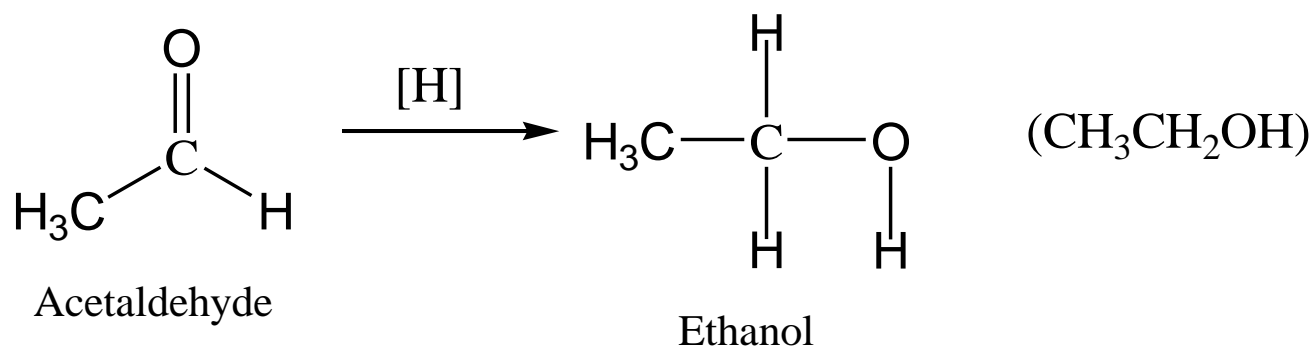
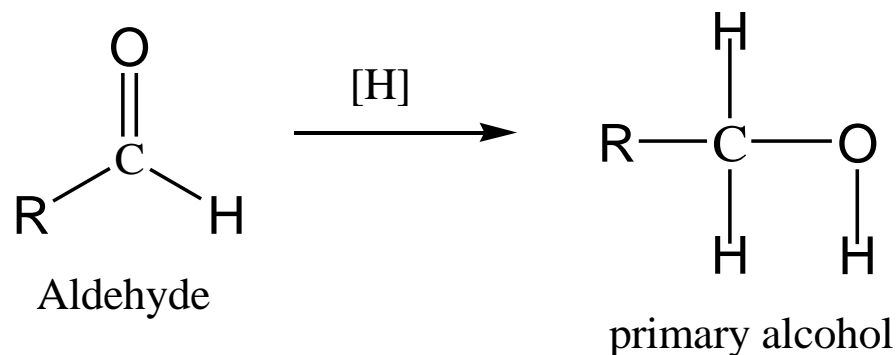
- Reduction
  - Decrease in the number of C-O
  - Increase in the number of C-H bonds
- The conversion of a carbonyl group (C=O) to an alcohol is a reduction.
  - The starting material has more C-O bonds than the product



# Reduction of aldehydes and ketones (addition reaction)

- Aldehydes

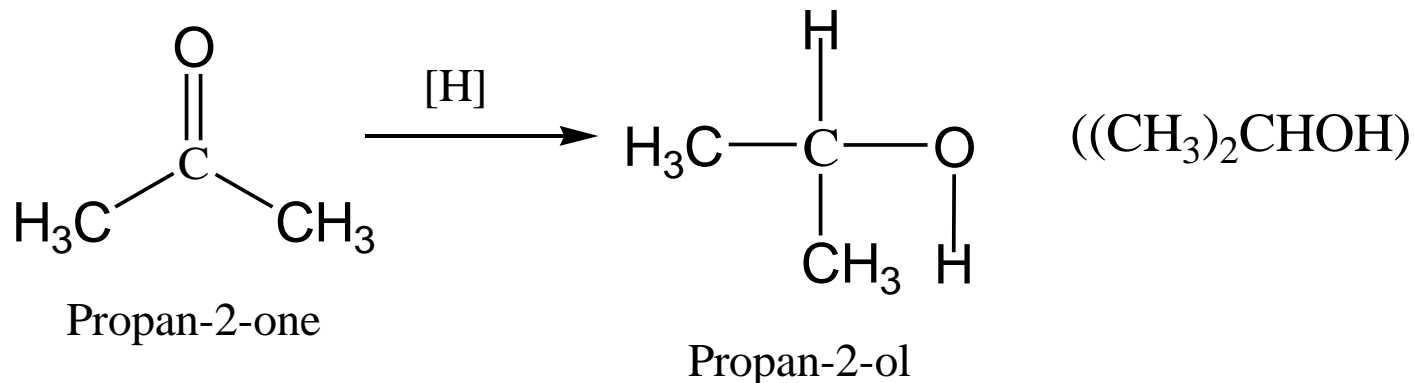
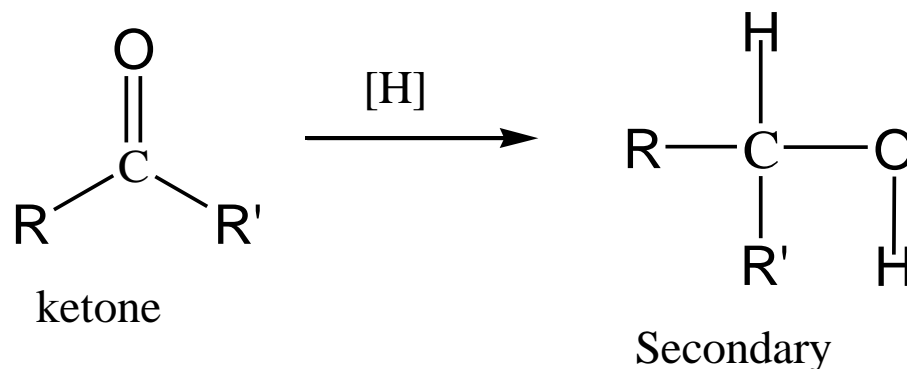
- Reduce to primary ( $1^\circ$ ) alcohol



# Reduction of aldehydes and ketones (addition reaction)

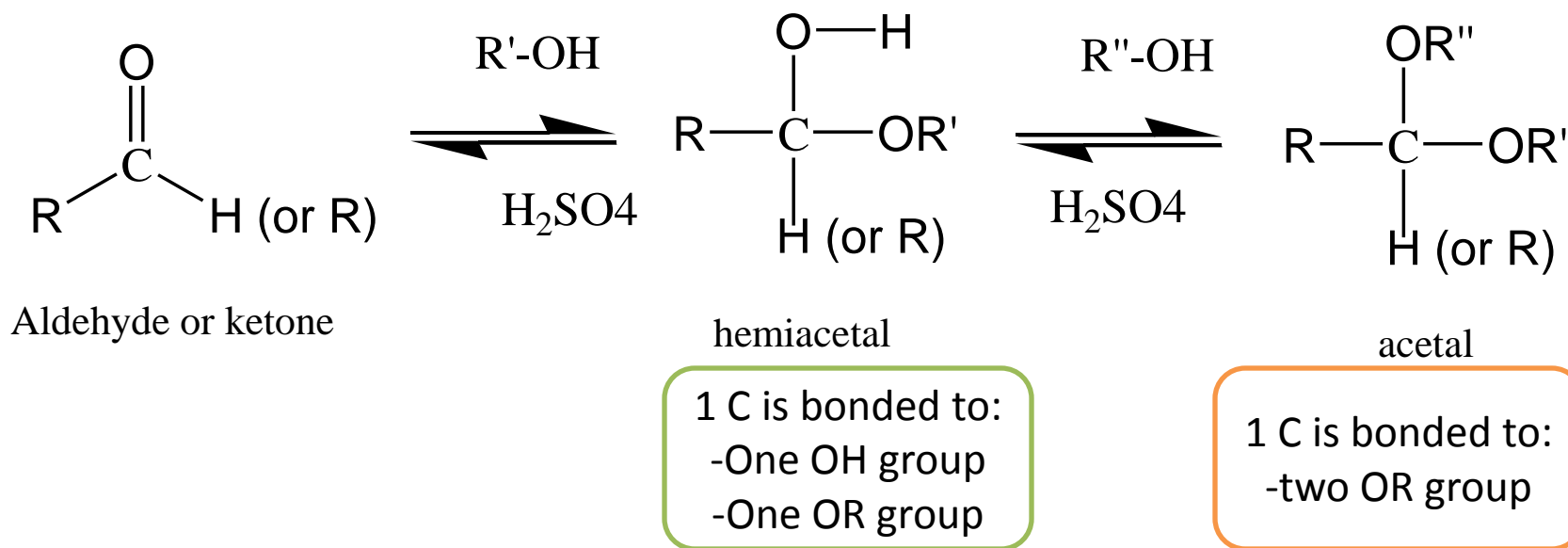
- Ketones

- Reduce to secondary ( $2^\circ$ ) alcohol



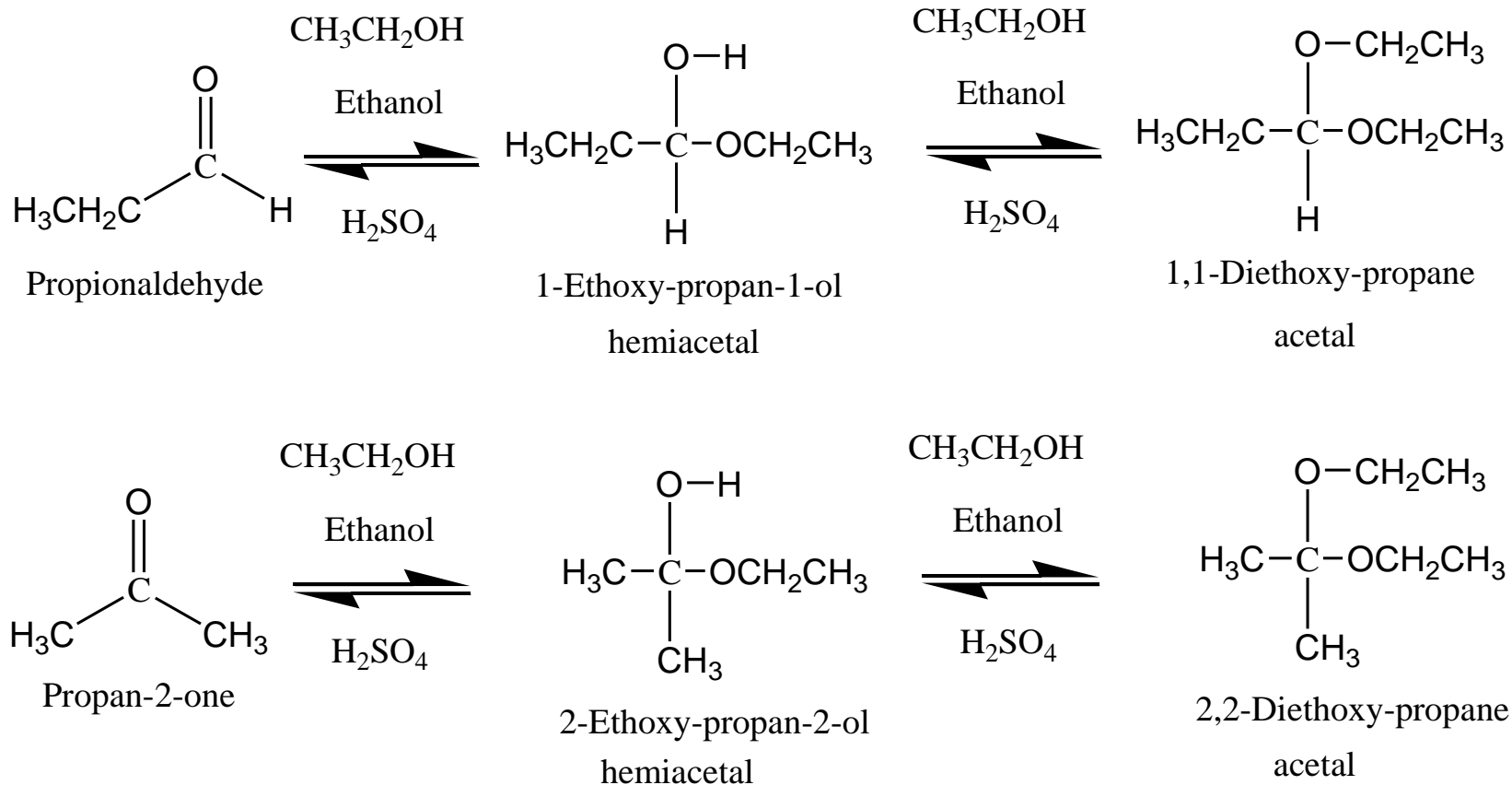
# Acetal formation

- Aldehydes and ketones undergo addition reaction with alcohols to form **hemiacetals** and **acetals**.



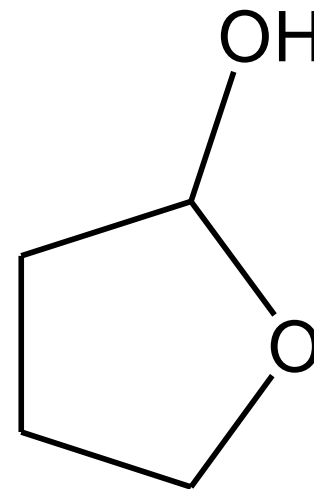
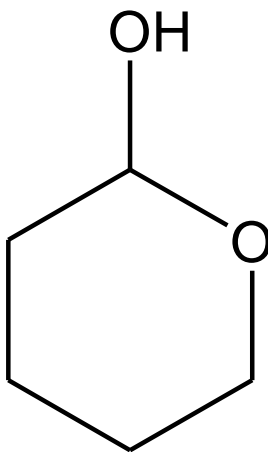
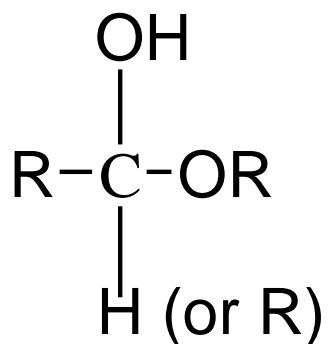
# Acetal formation

- Example



# Cyclic hemiacetals

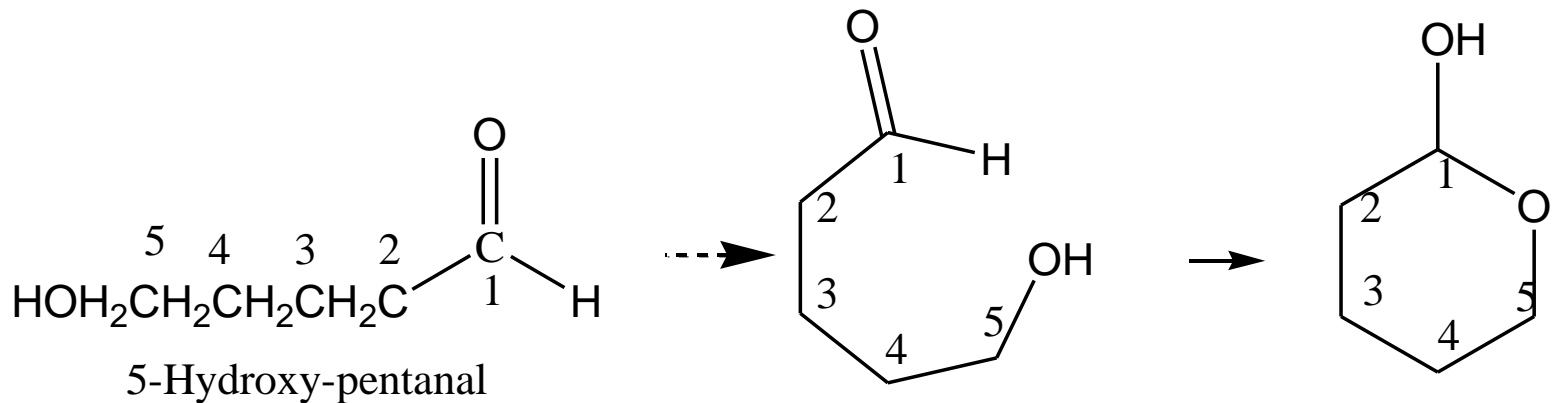
1 C is bonded to:  
-One OH group  
-One OR group



1 C is bonded to:  
-One OH group  
-An OR group that is part of a ring

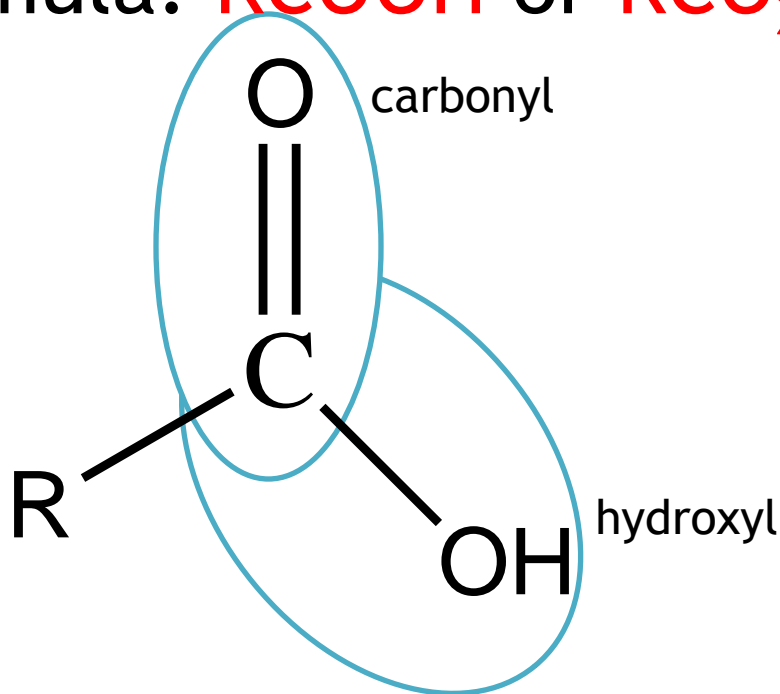
# Cyclic hemiacetals

- Formation of cyclic hemiacetals
  - **Intramolecular reaction** of a compound that contain both a **hydroxyl group (-OH)** and **aldehyde or ketone**.



# Carboxylic Acids

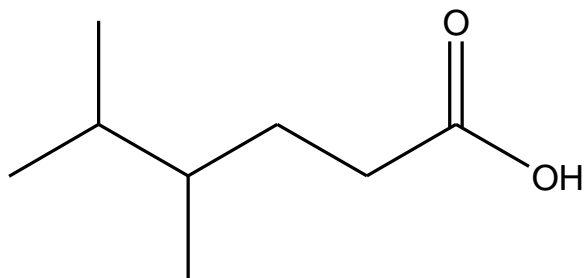
- **Carboxyl group**: Combining the hydroxyl and carbonyl.
- Generic formula: **RCOOH** or **RCO<sub>2</sub>H**



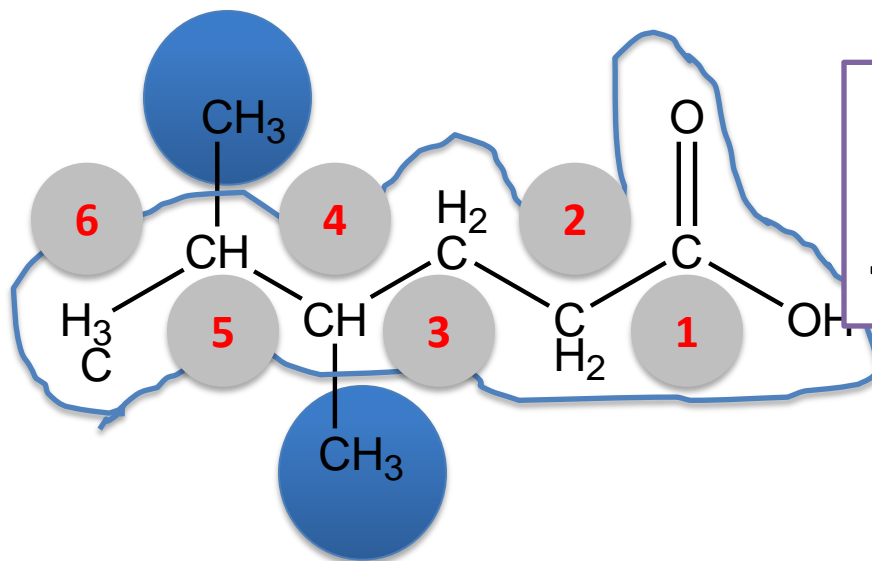


# Naming Carboxylic acids

- IUPAC system → suffix *-oic acid*



6 C → hexane →  
hexanoic acid

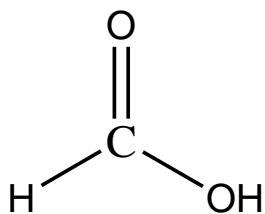


2 methyl at  
position 4 and 5  
→ 4,5-dimethyl-

**4,5-dimethylhexanoic acid**

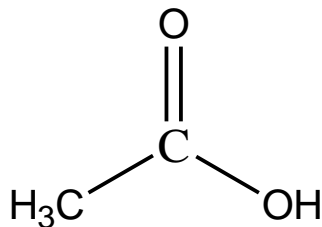
# Naming Carboxylic acids

- Many simple carboxylic acids are often referred to by their common names.



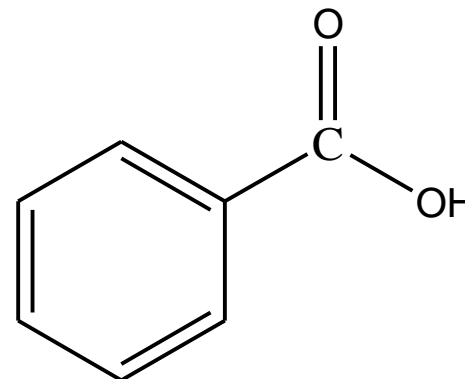
Formic acid

IUPAC name:  
methanoic acid



Acetic acid

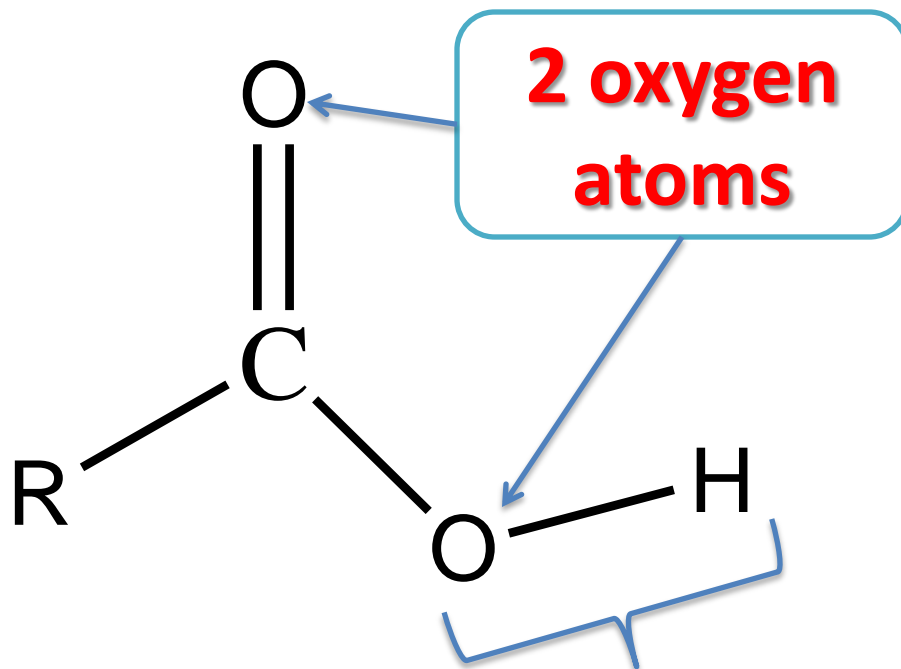
IUPAC name:  
ethanoic acid



Benzoic acid

IUPAC name:  
benzenecarboxylic  
acid

# Physical properties of carboxylic acids

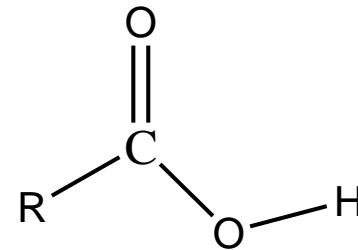


**2 oxygen atoms**

**2 very electronegative atoms attach with each other**

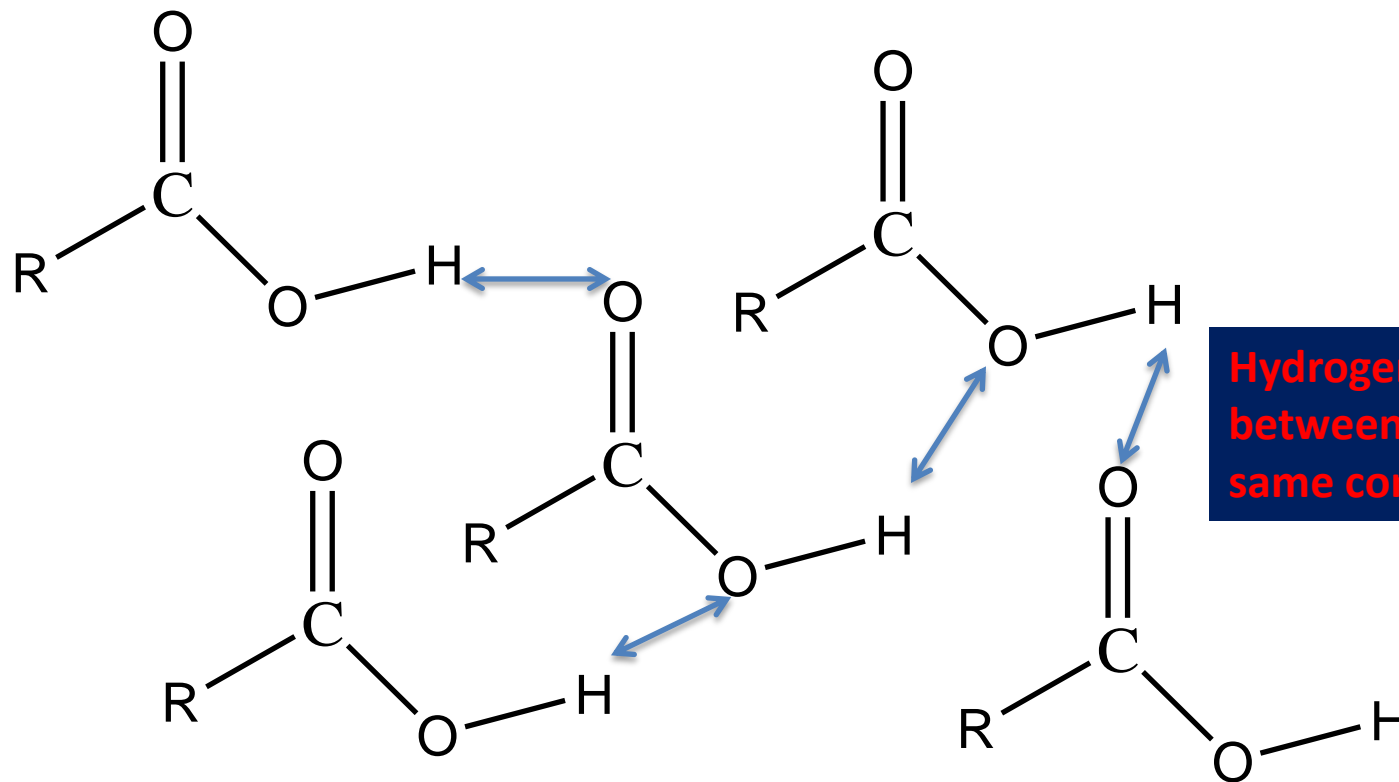
# Physical properties of carboxylic acids

- Polarity?
- Dipolar interaction?
- Hydrogen bonding between molecules of same compound?
- Hydrogen bonding with water?
- Solubility in water?
- Boiling point?



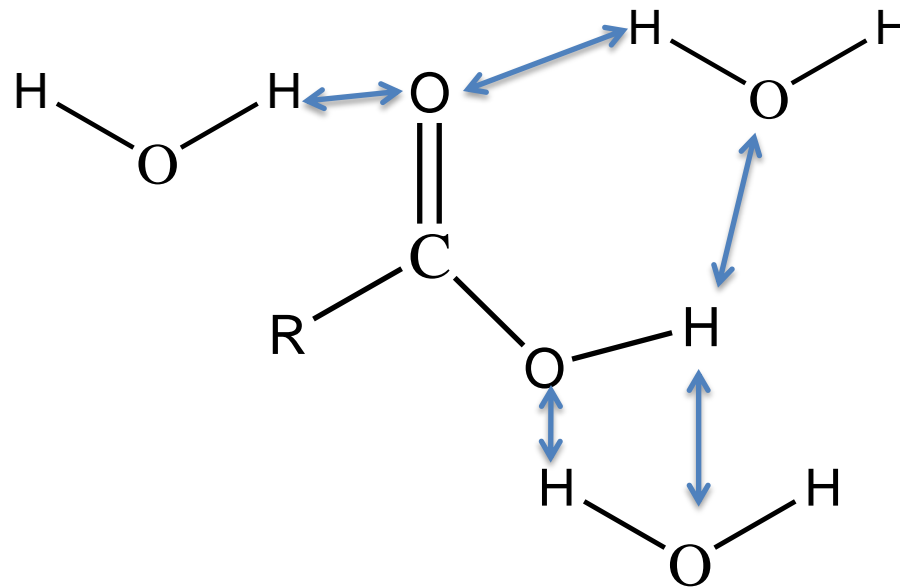
# Physical properties of carboxylic acids

Presence of oxygen + hydrogen  
(carbonyl and hydroxyl group) → polar molecules

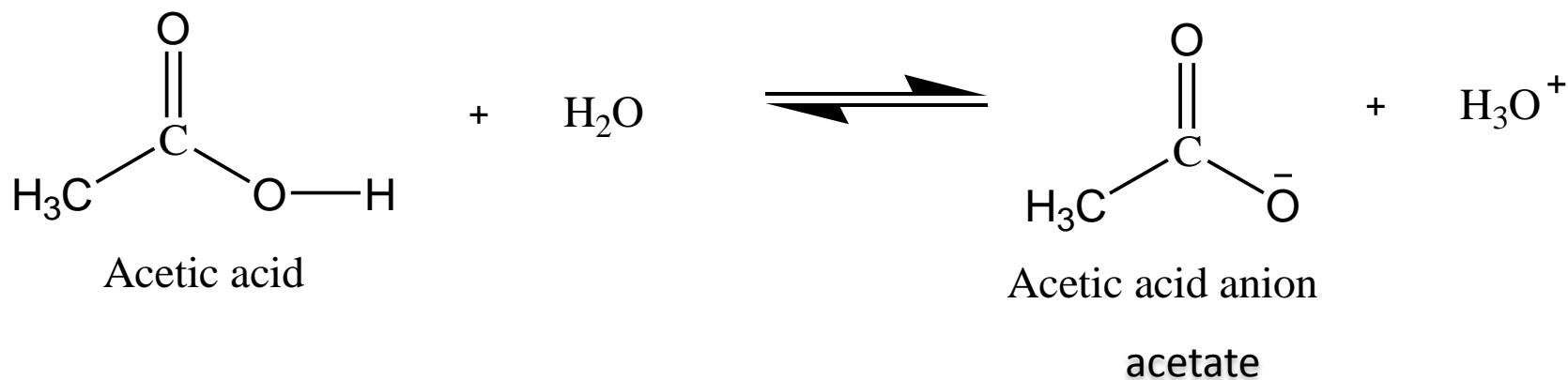
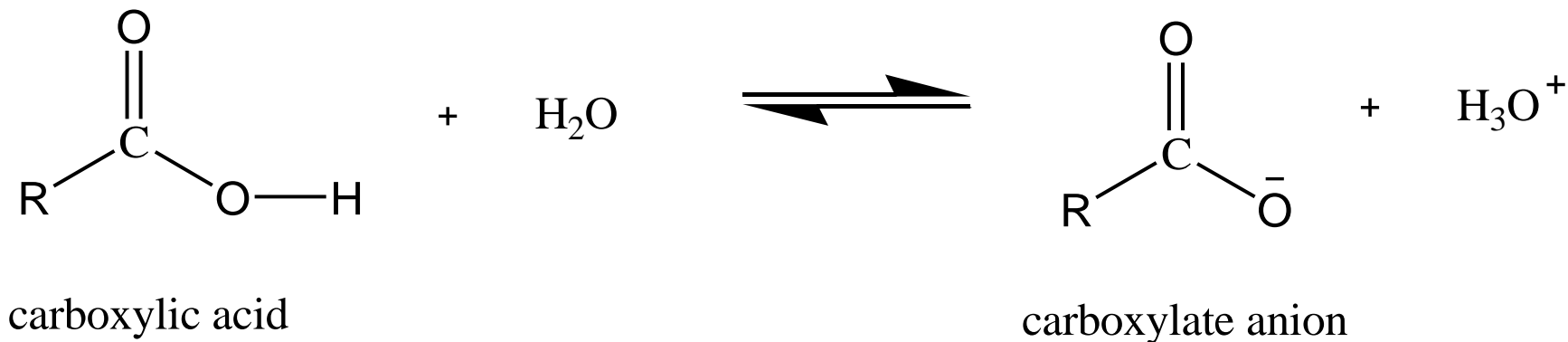


# Physical properties of carboxylic acids

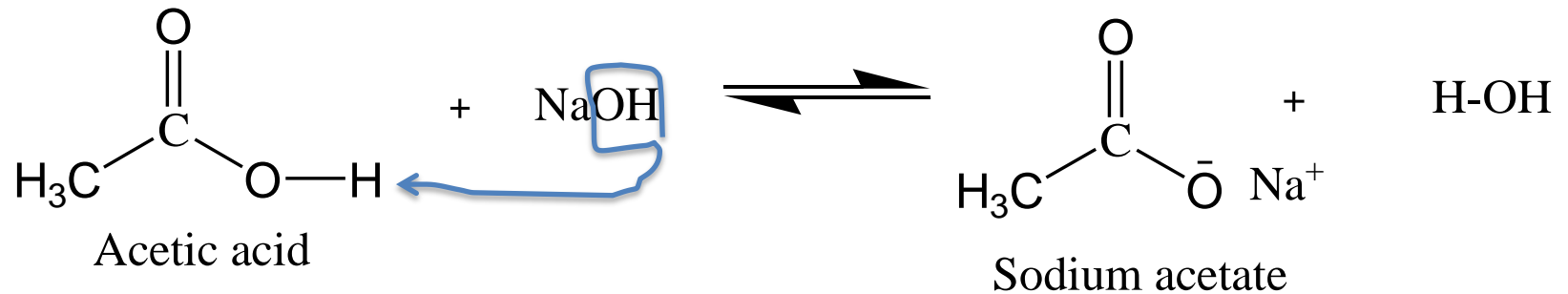
- Hydrogen bonding with water?
- Solubility in water?



# The acidity of carboxylic acids



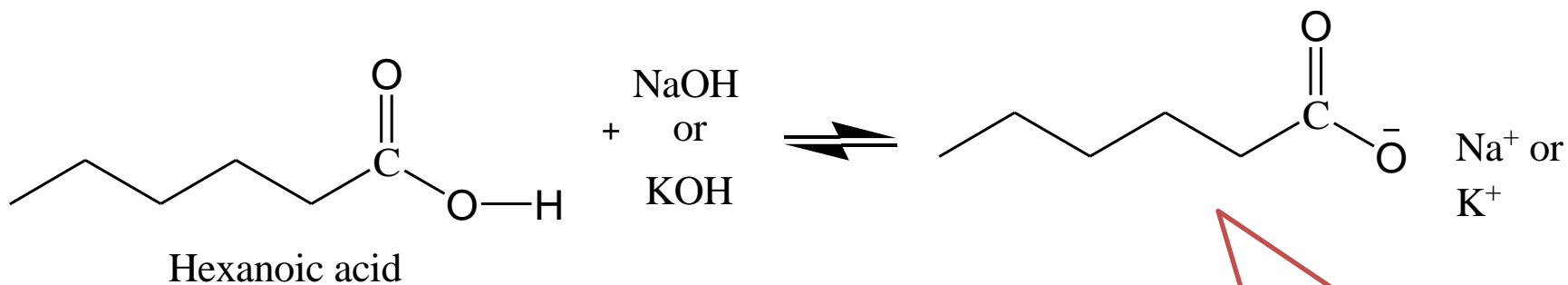
# Reaction with bases



Carboxylate  
anions



# Carboxylate anions



Carboxylate anions:  
sodium or potassium hexanoate

Name of the  
metal cation  
(e.g: sodium)

+

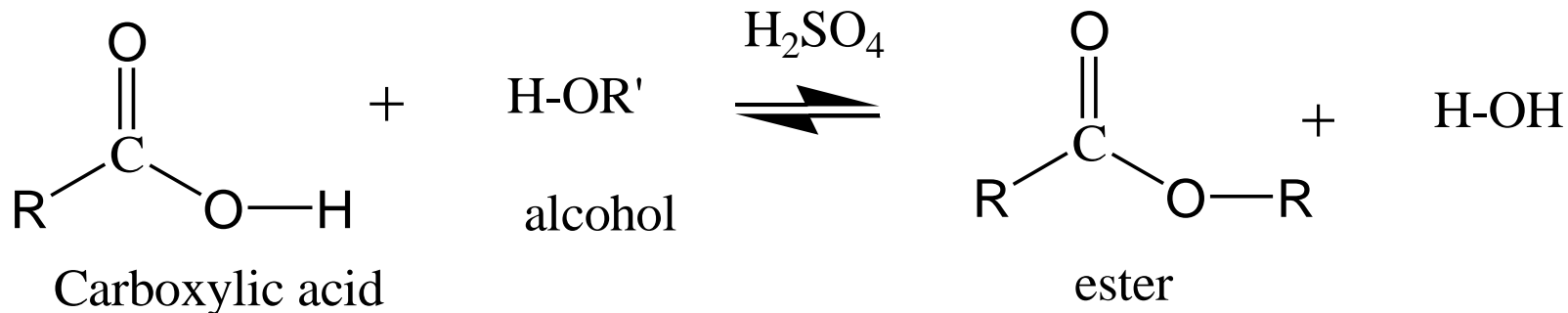
Parent  
(e.g. hexane)

+

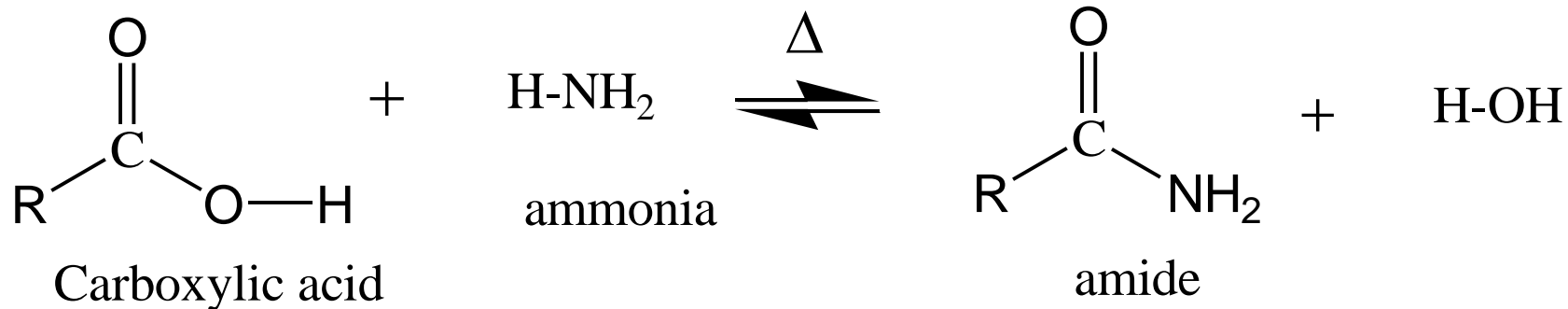
-ate (suffix)

# Conversion of carboxylic acids to esters and amides

Formation of ester

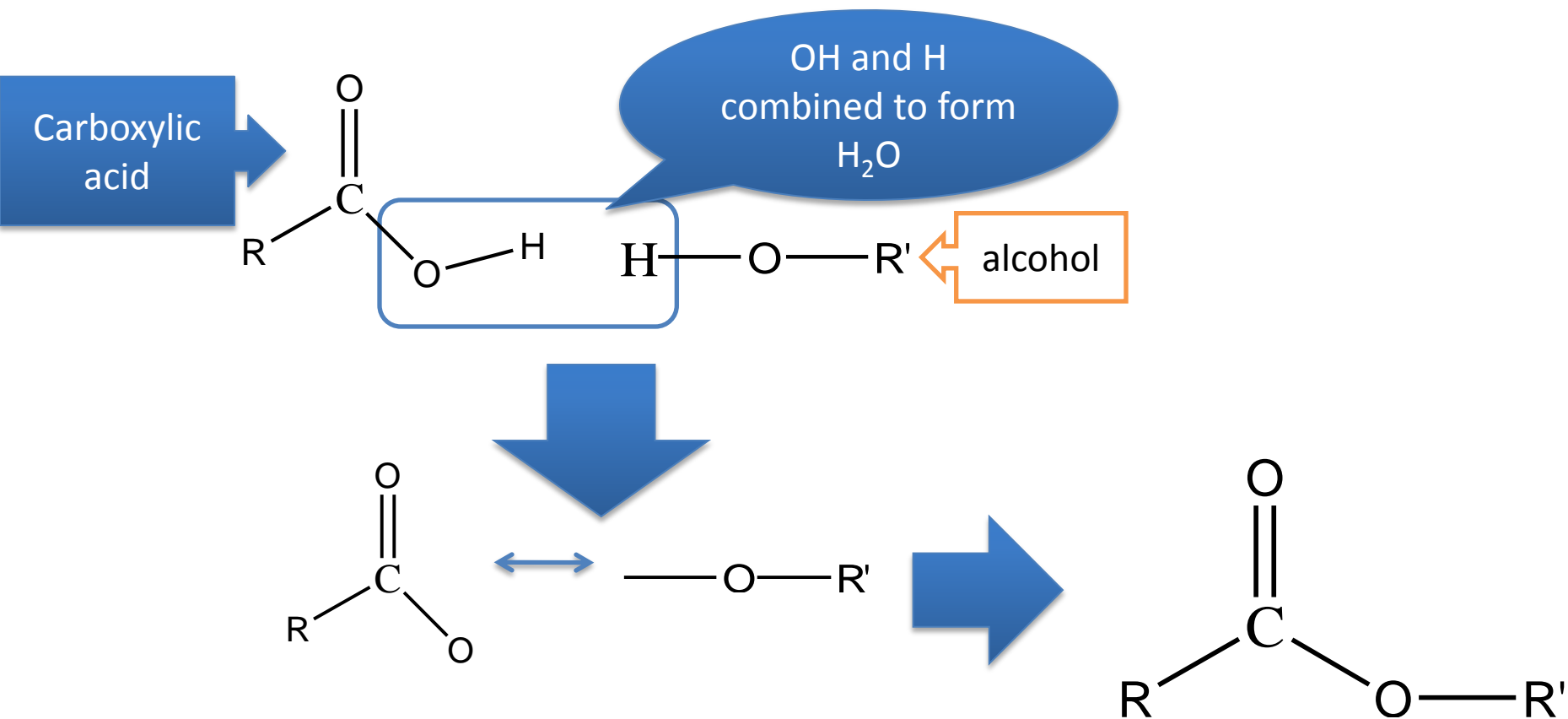


Formation of amide



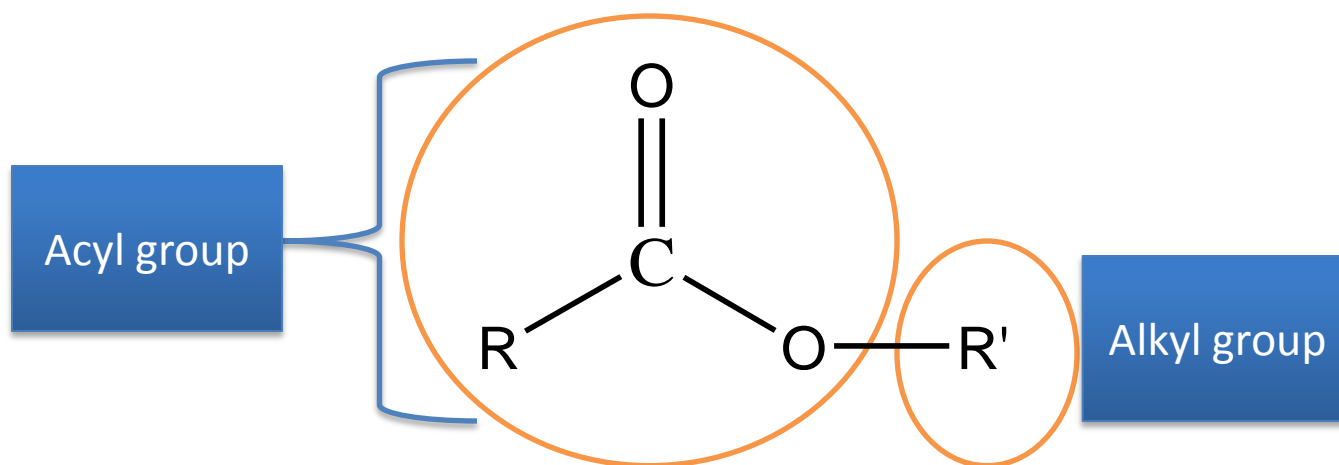
# Esters

- A modified carboxyl group
- Generic formula: **RCOOR'**

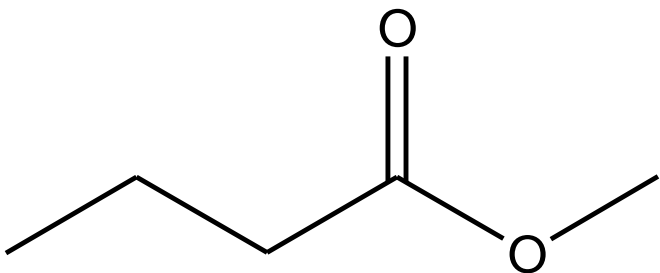


# Naming esters

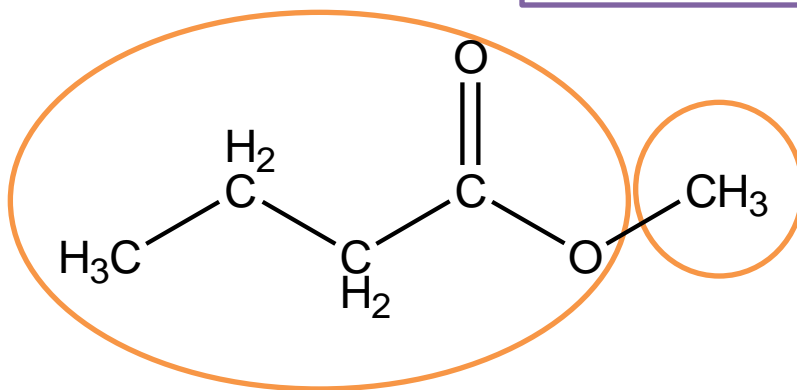
- IUPAC system → suffix *-ate*
- Two parts
  1. Name the acyl group (RCO-) by changing the *-ic* ending of the parent carboxylic acid to the suffix *-ate*.
  2. Name the R' group bonded to the oxygen atom as an alkyl group.



# Naming esters



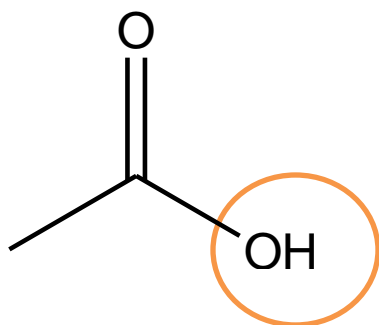
4 C → butanoic acid  
→ butanoate



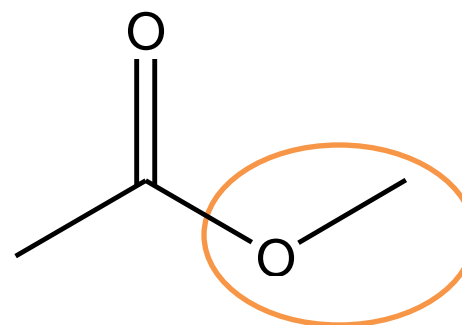
**R' = methyl**

**Methyl butanoate**

# Physical properties of esters



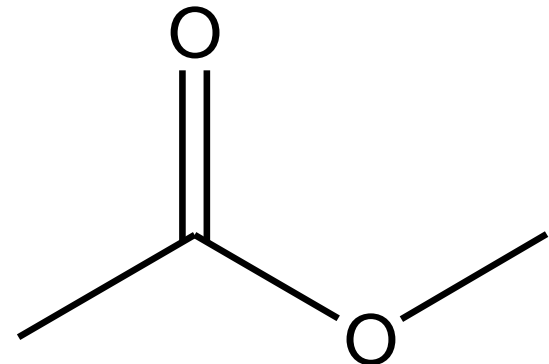
Carboxylic  
acid



ester

# Physical properties of esters

- Polarity?
- Dipolar interaction?
- **Hydrogen bonding between molecules of same compound?**
- Hydrogen bonding with water?
- Solubility in water?
- Boiling point?



# Ester formation from carboxylic acids

- **Substitution**

- All acyl (RCO) compounds.



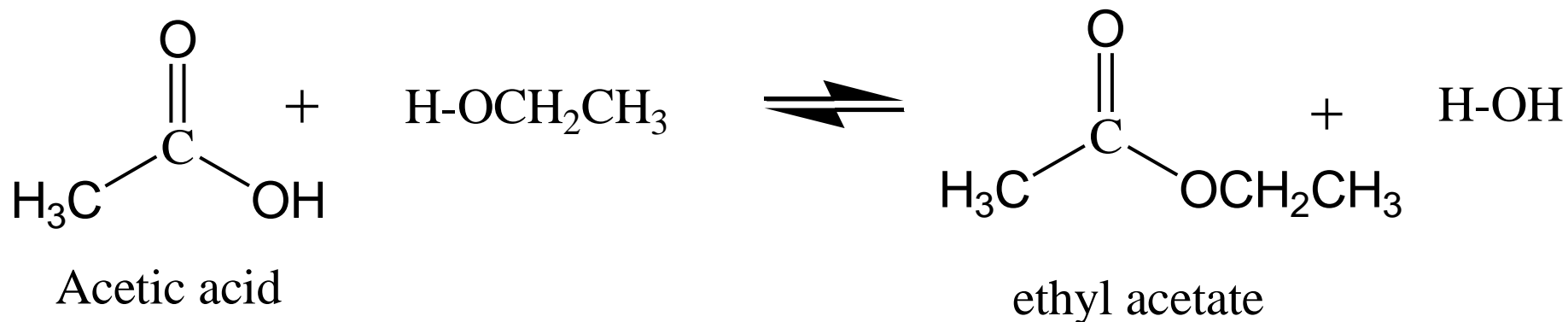


# Ester formation

- Fischer esterification

- Treatment of carboxylic acid (RCOOH) with an alcohol (R'OH) in the presence of an acid catalyst forms an ester (RCOOR').

- example



# REFERENCES

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- Horton, H.R., Moran, L.A., Scrimgeour, K.G., Perry, M.D. and Rawn J.D. (2006). *Principles of Biochemistry*, 4<sup>th</sup> Edition. Pearson International Edition.
- Smith, J.G. (2010). *General, Organic and Biological Chemistry*. McGraw-Hill Higher Education.
- Denniston, K.J., Topping, J.J. and Caret, R.L. (2008). *General, Organic and Biochemistry*, 6<sup>th</sup> edition. McGraw-Hill Higher Education.

# MY PROFILE



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Website: <http://www.staff.blog.utm.my/niknizam/>