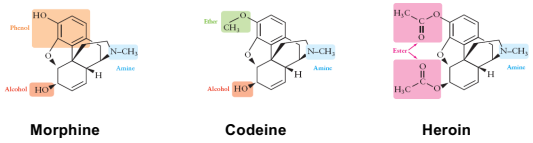
STRUCTURE DETERMINES FUNCTION

- The *function* of complex molecules is largely determined by their chemical *structure*
- The biological activity of complex molecules can be altered by very *subtle chemical changes*
- Consider a class of narcotics called **opioids**….



Morphine **Codeine** **Heroin**

FUNCTIONAL GROUPS

- **Organic compounds** are often "decorated" with atoms other than carbon and hydrogen
  - Atoms other than C or H are **heteroatoms**
  - Common clusters of heteroatoms (with or without carbons) are called **functional groups**
- *Functional groups define a molecule's chemical and physical properties and allow us to organize molecules according to similar structure/function*
  - *For example*: the **opioids** are related compounds with different functional groups

IUPAC NOMENCLATURE RULES

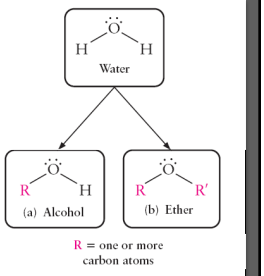
1. ***Assign the root name.*** Use IUPAC rules. The main chain is the longest chain containing the functional group.
2. ***Assign the suffix.*** Match the suffix of the "main chain" to the IUPAC name of the primary functional group.
3. ***Assign a locator number for the functional groups.*** Begin numbering the main chain from the end *closest* to the primary functional group. Place the locator number, followed by a dash, in front of the root name.
4. **Assign prefixes for other substituents**. If the main chain contains "substituents", assign a name and locator number as a prefixes to the root name.

OUTLINE

- 7.1 **C-O Containing Functional Groups: Alcohols and Ethers**
- 7.2 **C=O Containing Functional Groups**
- 7.3 **C-N containing Functional Groups: Amines**
- 7.4 **P=O Containing Functional Groups**

ALCOHOLS AND ETHERS

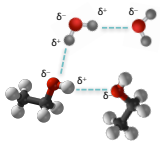
- **Alcohols** and **ethers** are functional groups that contain an oxygen atom with *two single bonds*:
  - In **alcohols**, the O is bound to *one carbon*, always saturated.
  - In **ethers**, it is bound to *two saturated carbons*.
- Both are similar in molecular shape to water:
  - *Implications??*



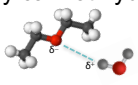
*A chain of carbons of unspecified length is often indicated by the symbol **R***

HYDROGEN BONDING IN ALCOHOLS & ETHERS

- The ***-OH*** group in **alcohols** has the ability to form hydrogen bonds with other alcohols or to water.
  - Alcohol groups (1) increase the solubility of hydrocarbons in water & (2) increase their boiling points
  - The effect of an alcohol group on solubility depends on the size of the hydrocarbon it is bound to

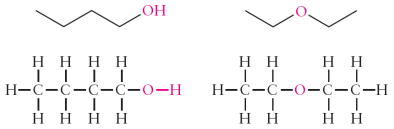


- **Ethers** may form hydrogen bonds to water, but since they have no ***-OH***, they cannot hydrogen bond to each other.



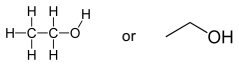
SKELETAL LINE STRUCTURES OF ETHERS AND ALCOHOLS

- Two rules dictate structural representations with heteroatom functional groups:
  1. Heteroatoms (such as oxygen) *must always be indicated with letters* in the skeletal line structures
  2. Hydrogens bound to the heteroatoms must also be indicated.

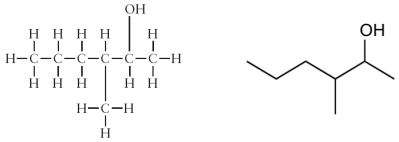


ALCOHOL NOMENCLATURE

- The IUPAC suffix when an **alcohol** is the primary functional group is: ***-anol***
  - The most common "alcohol" is the one consumed in beverages: ***ethanol***

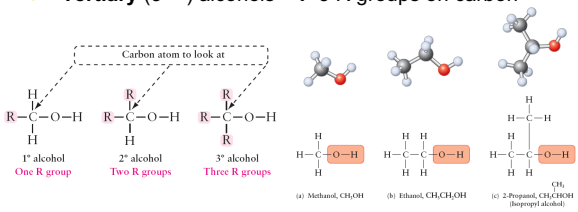


- How would we name the alcohol below?



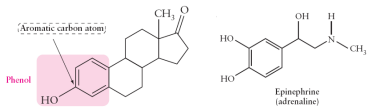
CLASSES OF ALCOHOLS

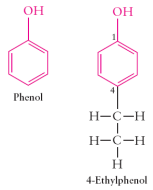
- The alcohol group (**R-OH**) may be bound to a carbon with 1-3 other carbons attached:
  - **Primary** (1°) alcohols → 1 R group on carbon
  - **Secondary** (2°) alcohols → 2 R groups on carbon
  - **Tertiary** (3°) alcohols → 3 R groups on carbon



A SPECIAL KIND OF ALCOHOL: PHENOLS

- Some combinations of specific hydrocarbons with common functional groups have *unique names*
- **Phenols** consist of the alcohol group attached to a carbon within an aromatic ring.

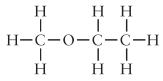




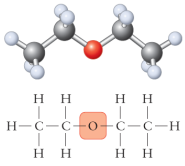
Phenols are commonly found in biologically important molecules

ETHER NOMENCLATURE

- The common name for an **ether** is constructed by:
  1. Naming each substituent R group as though it were a branch in order of priority *(by size)*
  2. Substituents end with ***-yl*** suffix
  3. Appending the name "***ether***"



Ethyl methyl ether



Diethyl ether

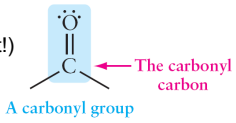
- If the R groups are identical, the prefix "***di***" is added before the name of the R groups.

OUTLINE

- 7.1 **C-O Containing Functional Groups: Alcohols and Ethers**
- 7.2 **C=O Containing Functional Groups**
- 7.4 **P=O Containing Functional Groups**
- 7.3 **C-N containing Functional Groups: Amines**

THE CARBONYL GROUP

- The **carbonyl group** is an oxygen double bonded to a carbon:
  - The carbon is connected to *two* other atoms
  - One of these may be an **R group** and the other may be either an R group, a hydrogen or a heteroatom
- Carbonyl properties:
  - **Trigonal planar** geometry (flat!)
  - **Polar** C=O bond:
    - Intermolecular interactions
    - Solubility in water



CARBONYL-CONTAINING GROUPS

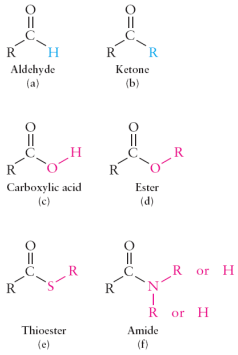
The carbonyl group is not a functional group by itself…

Carbonyls with C or H

- Aldehydes, H
- Ketones, R

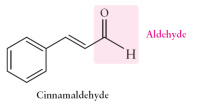
Carbonyls with Heteroatoms

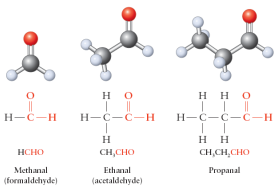
- Carboxylic acids, OH
- Esters, OR
- Thioesters, SR
- Amides, NR_2



ALDEHYDES

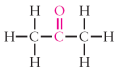
- **Aldehydes** consist of the carbonyl group attached to *at least one hydrogen*.
  - Very common functional group in many biomolecules
- *Nomenclature*:
  - Use IUPAC numbering with *–anal* suffix
  - Molecular formula shorthand is **-CHO**
  - Some simple aldehydes also have common names





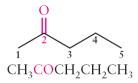
KETONES

- **Ketones** consist of the carbonyl group attached to two R groups.
  - Another common functional group in many biomolecules

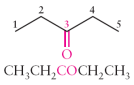


2-Propanone

- *Nomenclature*:
  - Use IUPAC numbering with ***–anone*** suffix
  - *Location* of the ketone group must be specified in the name



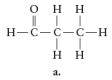
2-Pentanone



3-Pentanone

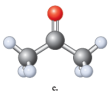
PRACTICE PROBLEMS

1. Name the following aldehydes and ketones.

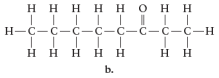


a.

d.



e.



b.

CARBOXYLIC ACIDS

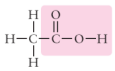
- **Carboxylic acids** combine their carbonyl group (**C=O**) with an alcohol group, **-OH**.

- *Nomenclature*:
  - Use IUPAC numbering with ***–anoic acid*** suffix
  - Molecular formula shorthand is **-COOH**
  - Simple carboxylic acids may have common names

HCOOH

Methanoic acid

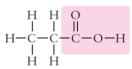
(Formic acid)



CH_3COOH

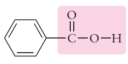
Ethanoic acid

(Acetic acid)



CH_3CH_2COOH

Propanoic acid

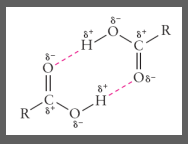


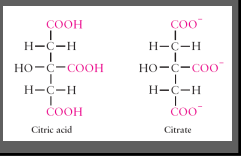
C_6H_5COOH

Benzoic acid

HYDROGEN BONDING

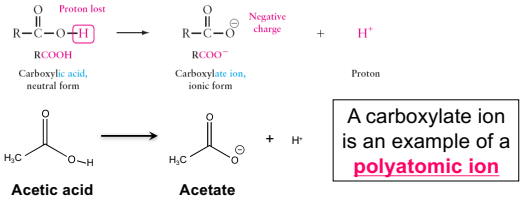
- Carboxylic acids easily form ***hydrogen bonds*** with water or other similar compounds:
  - Increases their solubility in aqueous solution
  - Also increases their boiling points
- The properties of carboxylic acid groups are *additive*:
  - More **–COOH**, more solubility and acidity





IONIZATION OF CARBOXYLIC ACIDS

- The **carboxylic acid** group is called an "acid" because it can "lose" a proton *in aqueous solution*
  - This forms a **carboxylate ion**
  - The name of the ion ends in ***–ate***

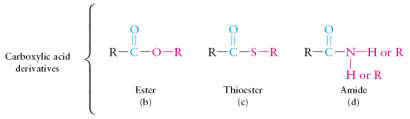


A carboxylate ion is an example of a **polyatomic ion**

CARBOXYLIC ACID DERIVATIVES

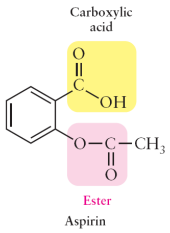
- Carboxylic acid derivatives resemble carboxylic acids in that they have a *heteroatom* connected to the *carbonyl group*.

- We will consider three common derivatives:



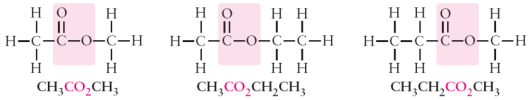
ESTERS

- **Esters** are similar to carboxylic acids except that **–OR** replaces **–OH**
  - *Remember*: R can be any saturated carbon bonded to a further organic group
- *Nomenclature*:
  - Use IUPAC numbering for longest chain with carbonyl carbon
  - Assign the suffix ***–anoate***
  - Assign the prefix for the relevant **R group**



ESTER EXAMPLES

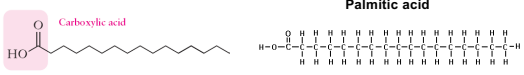
- *How do we name the following esters?*



Many common esters have a very pleasant odor – usually fruity or spicy in quality.

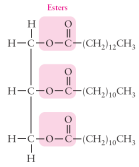
FATTY ACIDS AND FATS

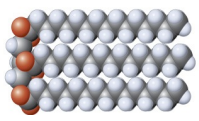
- **Fatty acids** are long hydrocarbon chains containing the carboxylic acid group



Palmitic acid

- Connection of 3 fatty acids to a glycerol molecule by **ester bonds** produces a **triglyceride** (aka. fat)

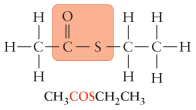




Triglyceride (Fat)

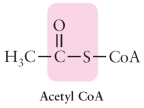
THIOESTERS

- **Thioesters** are like esters, but with an S replacing the O bonded to the R group.
  - Recall the periodic table properties of O and S
  - **Thio** = "sulfur"
- Thioesters are less common than esters:
  - Important in a few biologically relevant molecules



$CH_3COSCH_2CH_3$

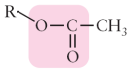
You do NOT need to know the rules for naming this group, just be able to identify it



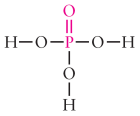
Acetyl CoA

PHOSPHATES

- **Phosphate esters** are compounds derived from phosphoric acid.
  - The **C=O** bond (ester) is replaced with a **P=O** bond (phosphate ester)



Ester

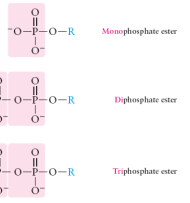


Phosphoric acid, H_3PO_4

- All contain a **P=O** double bond and three **P-O** single bonds.
  - The oxygens in a phosphate ester are joined to up to three **R groups** (either a *saturated* C or H)
  - Phosphate is a common **polyatomic ion** with up to three negative charges (PO_4^{3-})

CLASSES OF PHOSPHATE ESTERS

- **Phosphate esters** are often linked together via their singly-bonded oxygen atoms:
  - The bond between phosphates is a **phosphoanhydride**
  - Up to *three* phosphates may be linked together
- **Phosphoanhydride** bonds are "high energy" chemical bonds:
  - Required to overcome the strong (-) charge repulsion



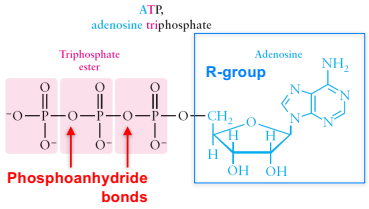
Monophosphate ester

Diphosphate ester

Triphosphate ester

ADENOSINE TRIPHOSPHATE

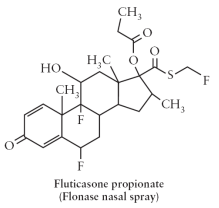
- *The "high energy" bonds in phosphate energy are used to store & transmit energy in cells*
- **ATP** (**adenosine triphosphate**) is the most important of triphosphate esters



PRACTICE PROBLEM

Fluticasone propionate is the active pharmaceutical ingredient in Flonase® nasal spray.

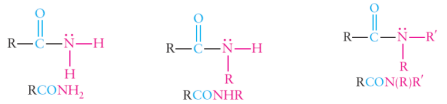
1. Circle and label the thioester and the ester functional groups and explain how they are different from one another.
2. Circle and label the ketones and alcohol functional groups in this molecule.



Fluticasone propionate
(Flonase nasal spray)

AMIDES

- **Amides** consist of a nitrogen bonded to a carbonyl carbon.
  - The *carbonyl* and *nitrogen* behave as a *single unit*.



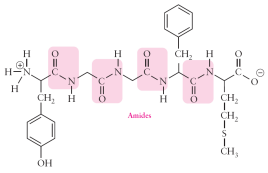
Primary (1°) ***Secondary (2°)*** ***Tertiary (3°)***

- The nitrogen will additionally have up to two hydrogens or R groups attached.
  - *Standard nomenclature for number of R-groups applies*

BIOLOGICALLY RELEVANT AMIDES

- **Amides** are common and biologically important in many molecules:
- *Nomenclature*:
  - Use IUPAC numbering for longest chain with amide
  - Assign the suffix ***–anamide***
  - Assign the prefix for any relevant branches (R-groups)

Proteins & peptides contain an amide bond between individual amino acids



OUTLINE

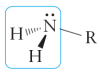
- 7.1 **C-O Containing Functional Groups: Alcohols and Ethers**
- 7.2 **C=O Containing Functional Groups**
- 7.4 **P=O Containing Functional Groups**
- 7.3 **C-N containing Functional Groups: Amines**

AMINES

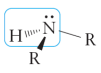
- **Amines** are groups containing nitrogen with three single bonds joined to **hydrogens** or **R groups**.
  - Structurally related to ammonia
  - Geometry is **trigonal pyramidal**

Ammonia 

- Classification system depends on R-group type:
  - The R-group carbons bonded to the N may be *saturated* or *aromatic* *(NOT a carbonyl)*

Amines 

Primary (1°)

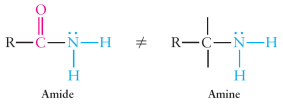


Secondary (2°)

Tertiary (3°)

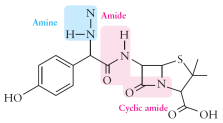
AMINES ARE NOT AMIDES!

- *Do not confuse amines & amides…!*
- Amines *do not have a carbonyl group* directly attached to their nitrogen atom:
  - Amides & amines have distinct chemical properties
  - Amines *can* form ions; amides *cannot* be ionized



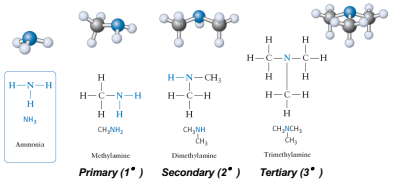
Penicillin antibiotics contain both and amide and an amine, which are *distinct* groups

amoxicillin

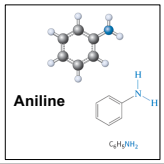


AMINE NOMENCLATURE

1. Longest organic chain receives IUPAC root name and is then followed by the suffix "***amine***"
2. Each R group is treated like a usual substituent & listed in alphabetical order
   - All R group substituents end with ***–yl***
   - Have prefix ***N-*** to denote location (instead of C number)

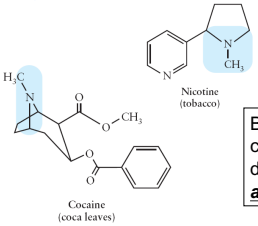


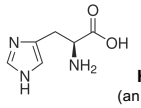
Primary (1°) ***Secondary (2°)*** ***Tertiary (3°)***



AMINES IN ORGANIC RING STRUCTURES

- The R groups attached to an ***amine*** may be part of a larger organic ring structure
- Many biologically important molecules contain ***cyclic amines***



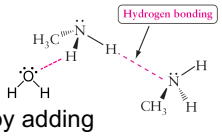


Histidine
(an amino acid)

Biologically active compounds containing amines that are derived from plants are called ***alkaloids***.

AMINES ARE POLAR & CAN BE IONIZED

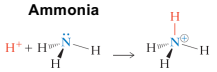
- Amines readily form **hydrogen bonds**
  - With other amines
  - With H_2O & other O-containing molecules



- Amines can also be **ionized** by adding free H^+ to its non-bonding electron pair

Ammonia

Ammonium (polyatomic ion)



Amines are *highly* soluble in water & have high boiling points.