Organic and Biological (Slide 1)

§1 General Characteristics of Organic Molecules

1. Structure

1° Carbon makes 4 bonds.

2° All single bonds: tetrahedral (正四面体); sp^3 hybridized (杂化)

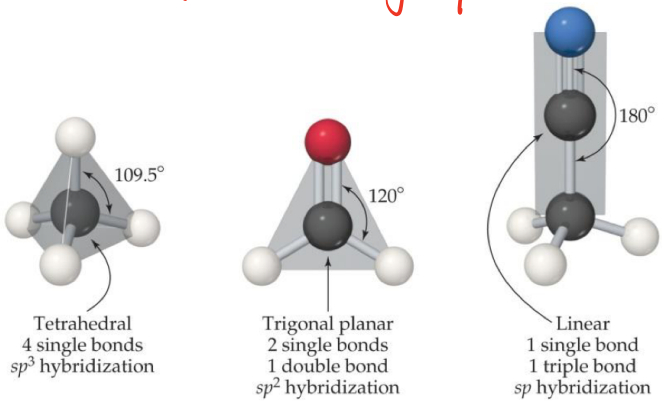
3° One double bond: trigonal planar (平面三角形); sp^2 hybridized

4° One triple bond: linear; sp hybridized

5° C-H are most common

6° C forms stable (strong) bonds with many elements, including C, H, O, N, and the halogens. (卤族)

7° Groups of atoms that determine how an organic molecule reacts are called functional groups. (官能团)

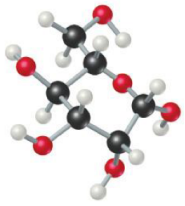


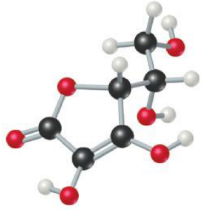
2. Solubility

1° Most prevalent bonds are C-C and C-H, which are nonpolar (非极性); solubility in water is low for many organic compounds.

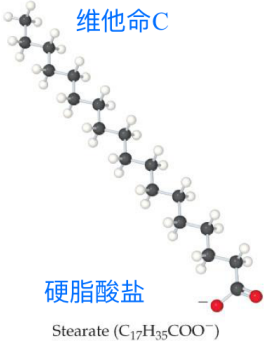
2° Organic molecules, such as glucose, that have polar groups are soluble in polar solvents.

3° Molecules with long nonpolar regions and polar regions act as surfactants (表面活性剂),


Glucose ($C_6H_{12}O_6$)


Ascorbic acid ($HC_6H_7O_6$)

维他命C


硬脂酸盐

Stearate ($C_{17}H_{35}COO^-$)

bringing nonpolar material into aqueous solution.

3. Acid-Base Properties

1° Many organic molecules contain acidic or basic functional groups.

2° Carboxylic acids ($-COOH$) are the most common acids.

3° Amines ($-NH_2$, $-NHR$, or $-NR_2$, where R is an organic group made up of C and H atoms) are the most common bases.

§2 Hydrocarbons (烃)

1. Types

1° Hydrocarbons consist of only carbon and hydrogen

2° They are grouped based on the number of bonds between carbon atoms.

3° Four basic types:

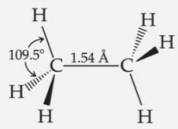
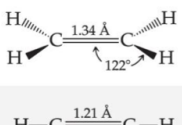
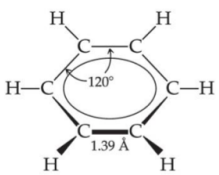
Alkanes (烷烃)

Alkenes (烯烃)

Alkynes (炔烃)

Aromatic hydrocarbons (芳香烃)

Table 24.1 The Four Hydrocarbon Types with Molecular Examples

Type	Example			
Alkane	Ethane	CH_3CH_3		
Alkene	Ethylene	$CH_2{=}CH_2$		
Alkyne	Acetylene	$CH{\equiv}CH$		
Aromatic	Benzene	C_6H_6		

2. Properties Common to Hydrocarbons

1° Nonpolar. Insoluble in water, but soluble in nonpolar solvents.

2° Melting points and boiling points are determined by dispersion forces (low molar mass hydrocarbons are gas; moderate molar mass hydrocarbons are liquids; high molar mass hydrocarbons are solids)

Table 24.2 First Ten Members of the Straight-Chain Alkane Series

Molecular Formula	Condensed Structural Formula	Name	Boiling Point (°C)
CH_4	CH_4	Methane	−161
C_2H_6	CH_3CH_3	Ethane	−89
C_3H_8	$CH_3CH_2CH_3$	Propane	−44
C_4H_{10}	$CH_3CH_2CH_2CH_3$	Butane	−0.5
C_5H_{12}	$CH_3CH_2CH_2CH_2CH_3$	Pentane	36
C_6H_{14}	$CH_3CH_2CH_2CH_2CH_2CH_3$	Hexane	68
C_7H_{16}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_3$	Heptane	98
C_8H_{18}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	Octane	125
C_9H_{20}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	Nonane	151
$C_{10}H_{22}$	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	Decane	174

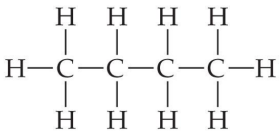
Nomenclature relevant to carbon molecules in organic molecules

1- meth
2- eth
3- prop
4- but
5- pent
6- hex
7- hept
8- oct
9- non
10- dec

3. Writing Formulas

1° Structural formulas show how atoms are bonded to each other.

2° Condensed structure fomulas don't show all C-H; they condense them to groupings, like CH_3.



$H_3C—CH_2—CH_2—CH_3$

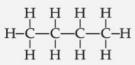
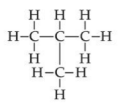
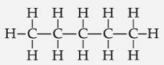
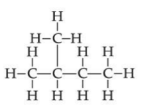
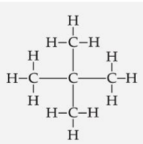
or

$CH_3CH_2CH_2CH_3$

4. Structure Isomers (同分异构体)

Same molecular formula but different connections of atoms.

Table 24.3 Isomers of C_4H_{10} and C_5H_{12}

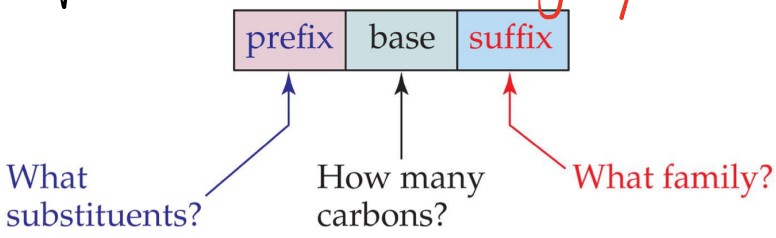
Systematic Name (Common Name)	Structural Formula	Condensed Structural Formula	Space-filling Model	Melting Point (°C)	Boiling Point (°C)
Butane (*n*-butane)		$CH_3CH_2CH_2CH_3$		−138	−0.5
2-Methylpropane (isobutane)		$CH_3—CH(CH_3)—CH_3$		−159	−12
Pentane (*n*-pentane)		$CH_3CH_2CH_2CH_2CH_3$		−130	+36
2-Methylbutane (isopentane)		$CH_3—CH(CH_3)—CH_2—CH_3$		−160	+28
2,2-Dimethylpropane (neopentane)		$CH_3—C(CH_3)_2—CH_3$		−16	+9

5. Systematic Nomenclature of Organic Compounds

1° Base: This tells how many carbons are in the longest continuous chain.

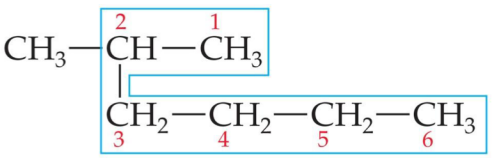
2° Suffix: This tells what type of compound it is.

3° Prefix: This tells what groups are attached to the chain.



6. How to Name a Compound

1° Find the longest continuous chain of C atoms, and use this as the base name.



2-Methyl*hexane*

2° Number of the chain from the end nearest the first substituent encountered.

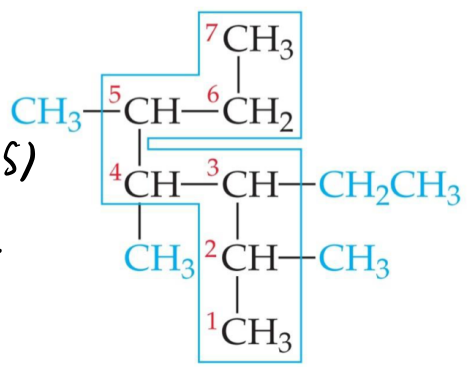
3° Name each substituent. (Side chains that are based on alkanes are called alkyl groups)

Table 24.4 Condensed Structural Formulas and Common Names for Several Alkyl Groups

Group	Name
CH_3-	Methyl
CH_3CH_2-	Ethyl
$CH_3CH_2CH_2-$	Propyl
$CH_3CH_2CH_2CH_2-$	Butyl
$(CH_3)_2CH-$	Isopropyl
$(CH_3)_3C-$	*tert*-Butyl

4° Begin the name with the number(s) on the C atom(s) to which each substituent is bonded.

5° When two or more substituents are present, list them alphabetically.



3-Ethyl-2,4,5-trimethylheptane

7. Saturated vs. Unsaturated (飽合 VS 不飽合)

1° Hydrocarbons with single bonds only are called saturated hydrocarbons. These are called alkanes.

2° Alkenes, alkynes, and aromatic hydrocarbons are called unsaturated hydrocarbons.

3° Unsaturated hydrocarbons are more reactive than saturated hydrocarbons.

§3 Alkanes

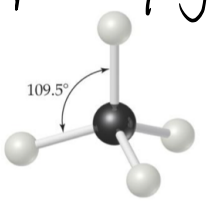
1. Use of Some Simple Alkanes

1° Methane (CH_4): in natural gas (heating fuel)

2° Propane (C_3H_8): in bottled gas (heating and cooking fuel)

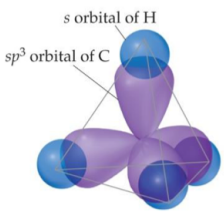
3° Butane (C_4H_{10}): in disposable lighters and fuel canisters for camping.

4° Alkanes with 5 to 12 C atoms: gasoline



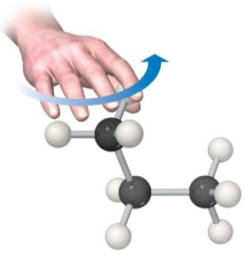
2. Structure of Alkanes

1° Carbons in alkanes are sp^3 hybridized, tetrahedral, and have 109.5° bond angles.



2° Straight chain form.

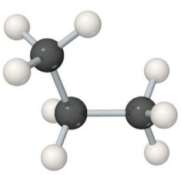
3° C can make 4 bonds, so a carbon atom can bond to 3 or 4 C atoms, making a branched alkane.



3. Cycloalkanes

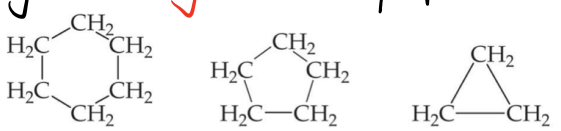
1° Alkanes that form rings or cycles.

2° sp^3 hybridization requires 109.5° angles, so three or four-C ring is not very stable.



3° Five-C and more have room for proper bond angle.

4° Naming: add cyclo- as a prefix to alkane name.



4. Reactions of Alkanes

1° Alkanes are relatively unreactive due to the lack of polarity and presence of only C–C and C–H σ bonds, which are very stable.

2° The do not react with acids, bases, or oxidizing agents.

3° The most important reaction observed is combustion.

$2\,C_2H_6(g) + 7\,O_2(g) \longrightarrow 4\,CO_2(g) + 6\,H_2O(l)$

(exothermic! (放热) $\Delta H^\circ = -2885\,kJ$)

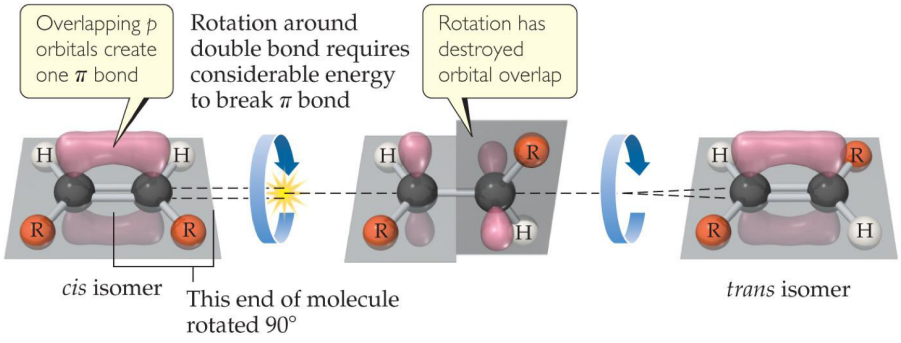
§4 Alkenes & Alkynes

1. Alkenes

1° Contain at least one C=C bond

2° No free rotation about the double bond

3° Naming: longest chain must include both carbon atoms that share the double bond; end name in -ene; lowest number possible given to double-bond carbon atoms; isomers also indicated.



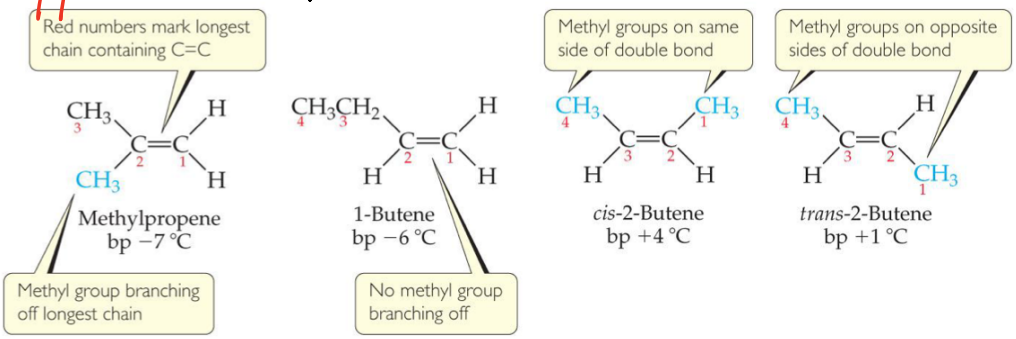
2. Geometric Isomers (几何异构体)

1° Since there is no free rotation around the double bond, the direction of the longest chain can differ for four or more C atoms.

2° Compounds that have all atoms connected to the same atoms but differ in three-dimensional arrangement are geometric

isomers.

3° Alkanes have cis (same side of the double bond) or trans (opposite side of the double bond) isomers



3. Alkynes

1° Contain at least one C≡C

2° Unsaturated

3° Naming: longest continuous chain containing both carbon atoms in the triple bond; name ends in -yne (instead of -ane or -ene); give C atoms in triple bond lowest number.

4. Additional Reaction of Alkenes and Alkynes

1° Add atoms to the double or triple bond, making it saturated or more saturated.

2° π bonds are broken and electrons form σ bonds to added atoms.

3° Work with H_2 (hydrogenation), HX (hydrogen halides or water), or X_2 (halogenation)

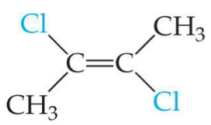
$$H_2C{=}CH_2 + Br_2 \longrightarrow H_2C(Br){-}CH_2(Br)$$

$$CH_3CH{=}CHCH_3 + H_2 \xrightarrow{Ni,\ 500\ ^\circ C} CH_3CH_2CH_2CH_3$$

$$CH_2{=}CH_2 + H_2O \xrightarrow{H_2SO_4} CH_3CH_2OH$$

$$CH_3C{\equiv}CCH_3 + Cl_2 \longrightarrow$$

2-Butyne



trans-2,3-Dichloro-2-butene

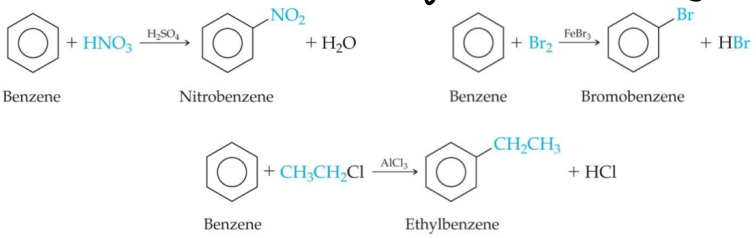
§5 Aromatic Hydrocarbons (芳香烃)

1. Structure of Aromatic Hydrocarbons

Aromatic hydrocarbons have six-membered rings containing localized and delocalized electrons.

2. Substitution Reaction

The π ring is much more stable than a π bond. So, aromatic hydrocarbons are much less reactive than alkenes and alkynes. They undergo substitution reactions: groups replace H on a ring (e.g. nitration, halogenation, alkylation).



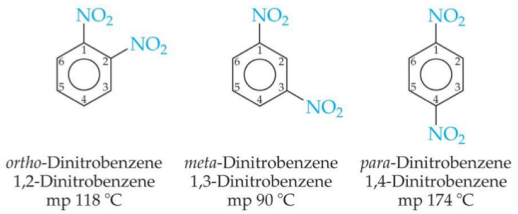
3. Aromatic Nomenclature

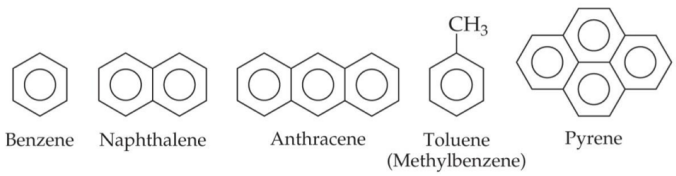
1° Many aromatic hydrocarbons are known by their common names.

2° Others are named as derivatives of benzene.

3° Substitution position for two substituents:

1,2 = ortho- 1,3 = meta- 1,4 = para





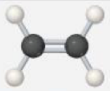
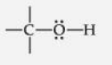
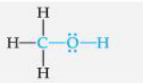
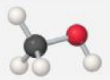
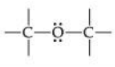
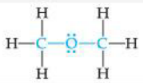
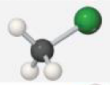
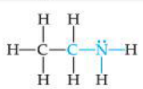
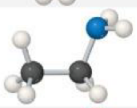
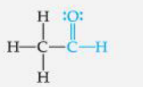
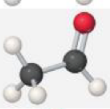
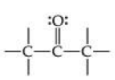
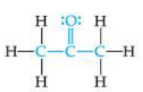
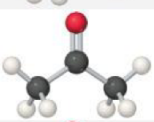
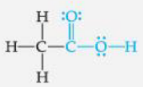
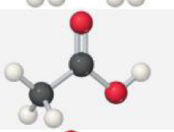
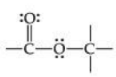
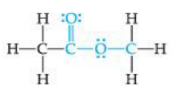
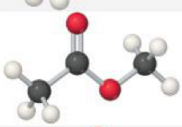
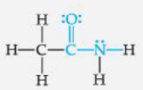
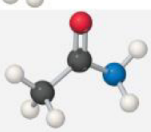
§6 Function Groups

1. The chemistry of an organic molecule is largely determined by

the functional groups it contains.

2. R represents the alkyl portion (C, H) of an organic molecule.

Table 24.6 Common Functional Groups

Functional Group	Compound Type	Suffix or Prefix	Example: Structural Formula	Example: Ball-and-stick Model	Example: Systematic Name (common name)
	Alkene	*-ene*			Ethene (Ethylene)
—C≡C—	Alkyne	*-yne*	H—C≡C—H		Ethyne (Acetylene)
	Alcohol 羟基	*-ol*			Methanol (Methyl alcohol)
	Ether 醚基	*ether*			Dimethyl ether
 (X = halogen)	Alkyl halide or haloalkane 卤代烷	*-ide*			Chloromethane (Methyl chloride)
	Amine 氨基	*-amine*			Ethylamine
	Aldehyde 醛基	*-al*			Ethanal (Acetaldehyde)
	Ketone 酮基	*-one*			Propanone (Acetone)
	Carboxylic acid 羧基	*-oic acid*			Ethanoic acid (Acetic acid)
	Ester 脂基	*-oate*			Methyl ethanoate (Methyl acetate)
	Amide 酰胺基	*-amide*			Ethanamide (Acetamide)

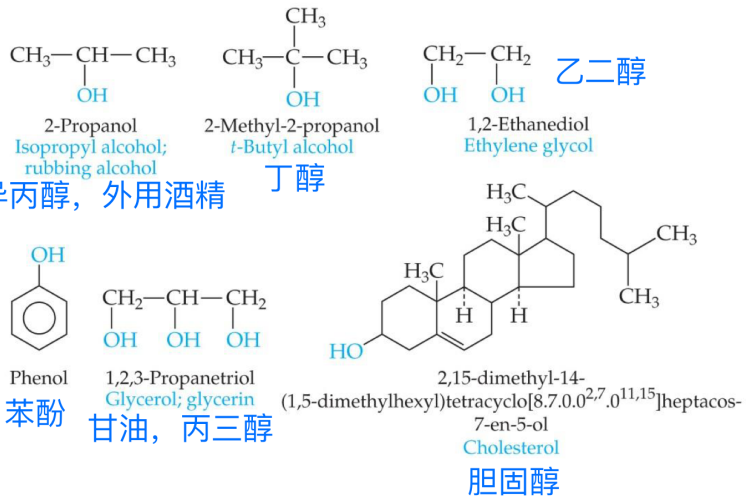
§7. Alcohols (醇类)

1. Structures

Alcohols contain one or more –OH group (the alcohol group or the hydroxyl group)

2. Naming

They are named from the parent hydrocarbon, the suffix is changed to -ol and a number designates the carbon to which the -OH group is attached.



3. Properties and Uses of Alcohols

1° Polar molecules: lead to water solubility and higher boiling points.

2° Methanol: used as a fuel addictive

3° Ethanol: in alcoholic beverages

4° Ethylene glycol: in antifreeze

5° Glycerol: cosmetic skin softener and food moisturizer.

6° Phenol: making plastics and dyes; topical anesthetic in throat sprays

7° Cholesterol: important biomolecule in membranes, but can precipitate and form gallstones of block blood vessels

§8 Ethers (醚类)

1. Structure

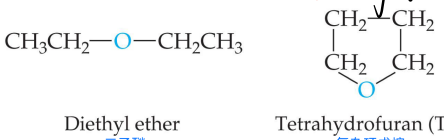
1° R-O-R

2° Formed by dehydration between alcohol molecules

2. Properties and Uses

1. Not very reactive (except combustion)

2. Used as solvents for organic reactions



§9 Aldehydes and Ketones (醛类和酮类)

1. Structure of aldehydes

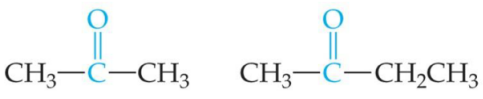
Aldehydes have at least one hydrogen atom attached to the carbonyl (C=O 羰基) carbon atom.

Methanal
Formaldehyde
甲醛

Ethanal
Acetaldehyde
乙醛

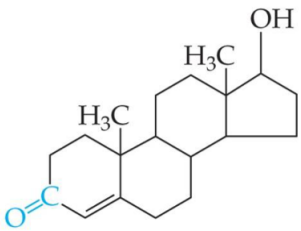
2. Structure of Ketones

Ketones have two R groups attached to the carbonyl carbon atom.



Propanone
Acetone
丙酮

2-Butanone
Methyl ethyl ketone
丁酮



Testosterone
睾酮，雄性激素

3. Important Aldehydes and Ketones

- Many aldehydes are natural flavorings: vanilla (香草), cinnamon (肉桂), spearmint (绿薄荷), and caraway (香菜) are from aldehydes.
- Ketones are used extensively as solvents; the most important solvent other than water is acetone (丙酮), which dissolves in water and dissolves many organic compounds.

§10. Carbonxylic Acids

1. Structure

hydroxyl group bonded to the carbonyl group.

2. Properties and Uses

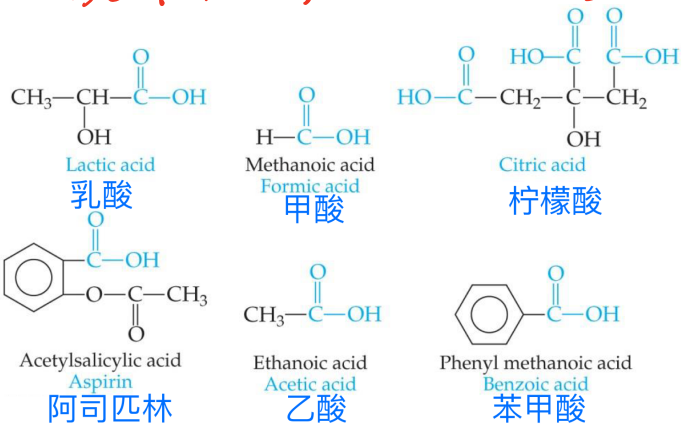
1° H on the hydroxyl group is weakly acidic.

2° Important in manufacturing polymers for films, fibers and paints.

3° Oxidation product of alcohols (some make aldehydes)

$$CH_3CH_2OH + (O) \longrightarrow CH_3\overset{\overset{O}{\|}}{C}H + H_2O$$

$$CH_3\overset{\overset{O}{\|}}{C}H + (O) \longrightarrow CH_3\overset{\overset{O}{\|}}{C}OH$$

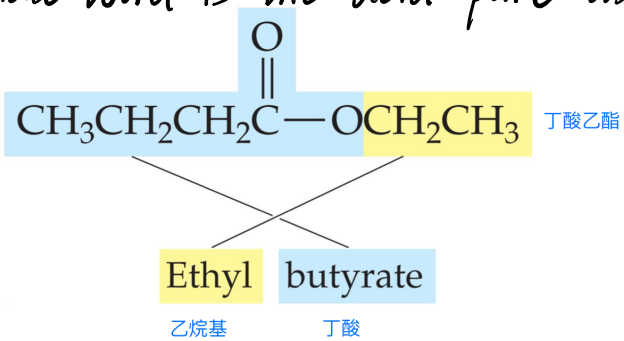


§11 Esters (酯类)

1. Esters are the products of reactions between carbonxylic acids and alcohols.
2. They are found in many fruits and perfumes.
3. Naming:

Name the alcohol part as an alkyl name.

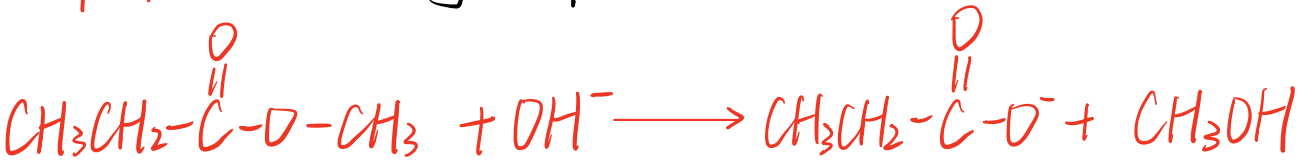
Separate word is the acid part as an -ate anion.



4. Decomposition of Esters

1° Heating an ester in the presence of an acid catalyst and water can decompose the ester.
(This is the reverse reaction of the preparation of an ester; it is a equilibrium.)

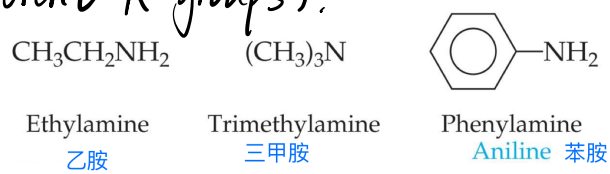
2° Heating an ester in the presence of a base results in saponification (making soap).



§12 Nitrogen Containing Organic Compounds

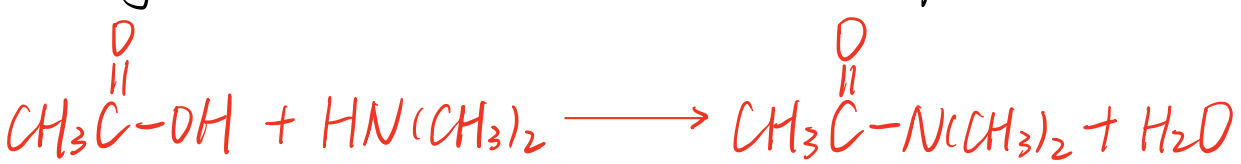
1. Amines (氨基)

Amines are organic derivatives of ammonia (NH_3). One, two or all three H atoms can be replaced by R groups (the same or different R groups).



2. Amide (酰胺基)

If H in NH_3 or an amine is replaced by a carbonyl group (N directly attached to C=O), an amide is formed.

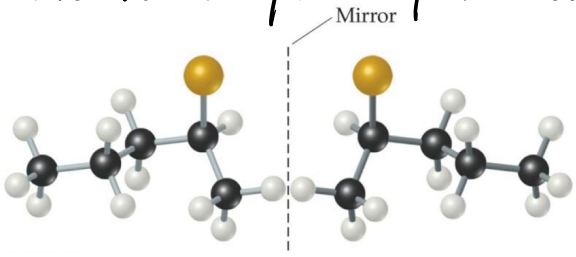


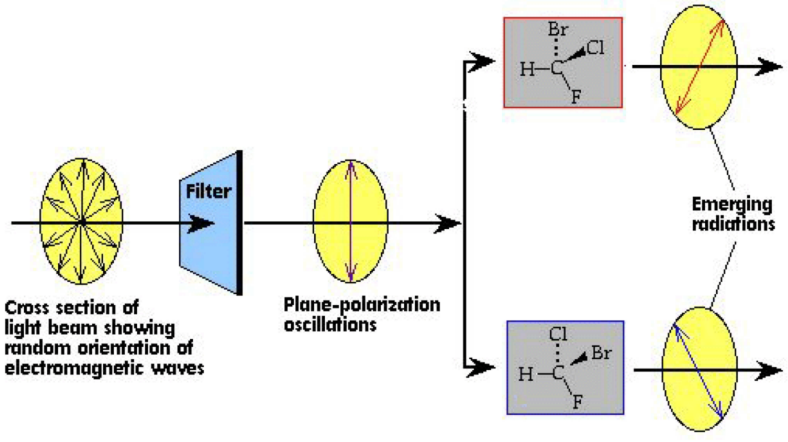
§13 Chirality

1. Carbons with four different groups attached to them are chiral.
2. These are optical isomers, or enantiomers. (光学/对映异构体)

3. Enantiomers have the same physical and chemical properties when they react with nonchiral reagents.

4. Enantiomers rotate plane-polarized light in opposite directions.

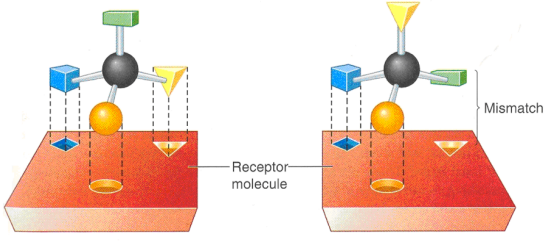


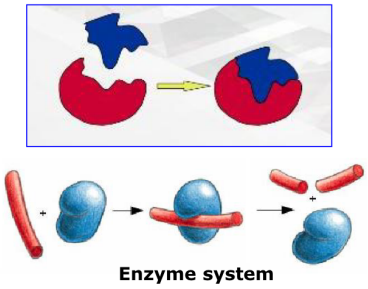


§14 Stereochemistry

1. Molecular recognition

Molecular recognition is carried out by some special biomolecules (e.g. receptors or enzymes) that are themselves spatially arranged in a specific direction





Most biomolecules are handness and their binding sites can thus distinguish between the right-hand or left-hand compounds.

2. Isomers

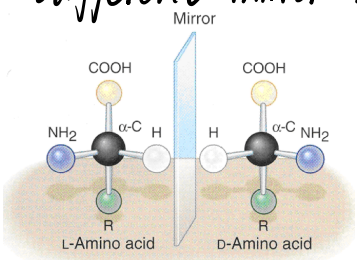
(Constitutional (Structure) isomerism

Geometrical isomerism
Optical isomerism
} Stereochemistry

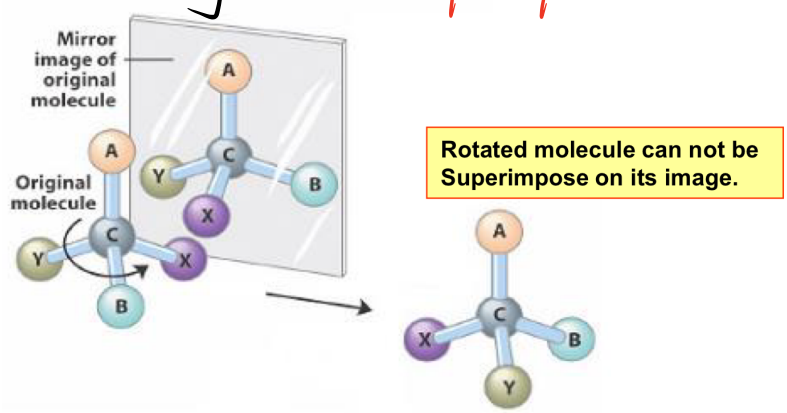
3. Optical isomer

1° Carbon atoms that are bound to four different atoms or groups are said to be asymmetric.

2° The bonds formed by an asymmetric carbon can be arranged in two different mirror images of each other.



3° The test for stereoisomers is one of superimposability. Molecules that can exist as enantiomers (对映异构体) are said to be chiral. They are non-superimposable on their mirror images.

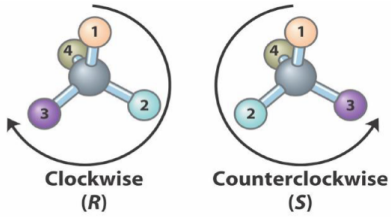


4° A collection containing only one enantiomeric form of a chiral molecule is called Enantiopure or Optically Pure.

5° Enantiomers have identical physical properties and consequently are difficult to separate and quantitate.

4. Chirality (手性)

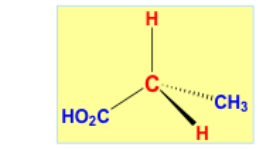
1° C atom (sp^3 hybridization) attached with 4 inequivalent substituents is called: Chiral center



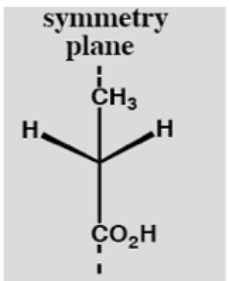
Rotate direction: Clockwise , prefix the name with (R);
Counter clockwise, (S)

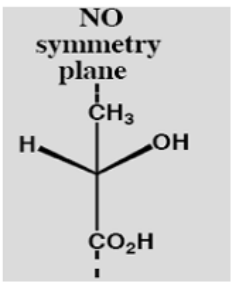
2° In general:

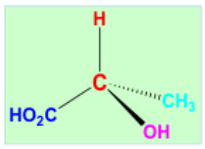
① There is no internal mirror plane (no symmetry), hence the carbon is chiral (R or S)



Propanic acid (achiral)







Lactic acid (chiral)

② The more symmetry elements a compound has, the more likely the compound will be achiral (非手性的)

5. Priority Rules

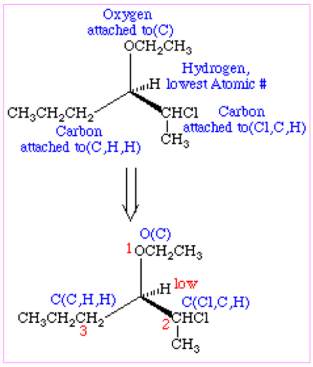
1° Each atom bounded to the chiral center is assigned a priority based on atomic number, the higher the atomic number, the higher the priority.

$$I > Br > Cl > SH > OH > NH_2 > CH_3 > H$$

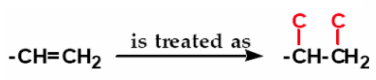
2° If the priority cannot be assigned as per atom bonded to chiral center, look to the next set of atom(s); priority is assigned at the first point of difference.

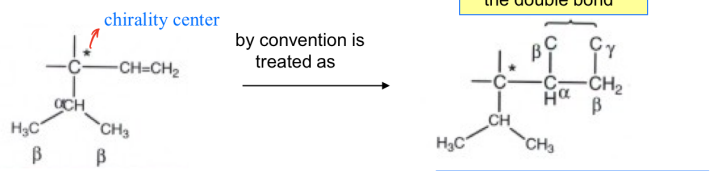
$$-CH_2-H < -CH_2-CH_3 < -CH_2-NH_2 < -CH_2-OH$$

3° Atoms participating in a double or triple bond to be an equivalent number of similar atoms by single bonds are considered to be bonded.



If a decision regarding the priority cannot be reached, compare the atomic numbers of the **second** atom(s) in each substituent, then the **third**, etc.





The isopropyl group has 1 alpha and 2 beta carbons

The simulated double bond has a Alpha and 2 beta carbons, like the Isopropyl group, but it also has a Gamma carbon

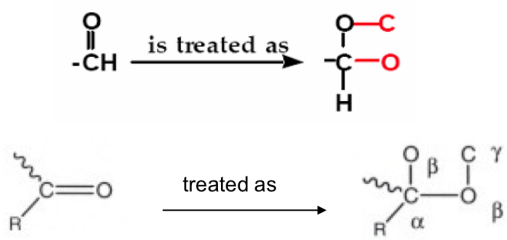
The Counts is: α, β, β

The Counts is: α, β, β, γ

Lower priority

Higher priority

Nomenclature priority treatment for carbonyl double bond



In this way, two C-O bonds are shown for both C and O

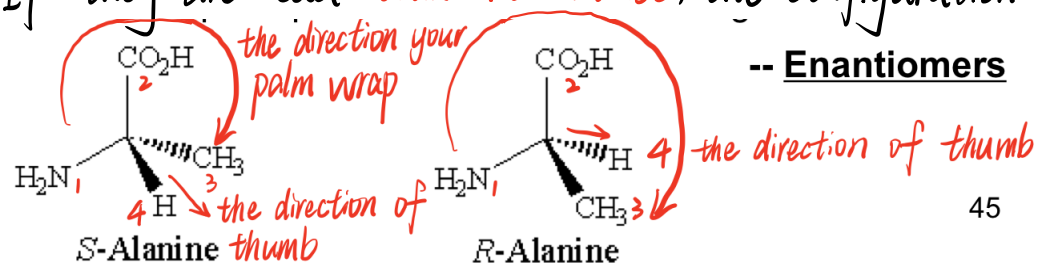
b. R,S Nomenclature for chiral center

1° Locate the chiral center, identify its four substituents and assign priority from 1 (highest) to 4 (lowest) to each substituent.

2° Orient the molecule so that the group of lowest priority (4) is directed away from you.

3° Read the three groups projecting toward you in order from highest (1) to lowest priority (3)

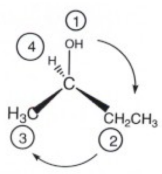
4° If the groups are read clockwise, the configuration is R (right)
If they are read counterclockwise, the configuration is S (left)



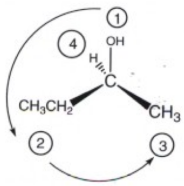
-- Enantiomers

45

Name the chirality for 2-butanol

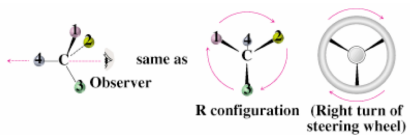


(R)-2-butanol



(S)-2-butanol

- There are four different groups on α-carbon (most close to –**OH**), no symmetry plane.
- Priority (based on atomic number):



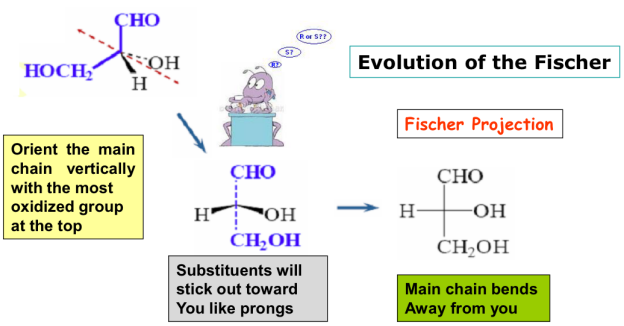
-OH > -CH_2CH_3 > -CH_3 > -H

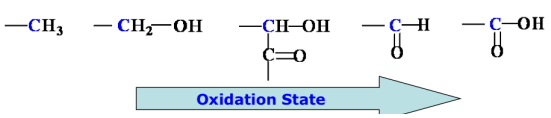
- Orient -**H** away from you and read the three groups from highest (-**OH**) to lowest priority (-CH_3)

51

- Clockwise: R; Counterclockwise: S

7. How to draw a chiral center



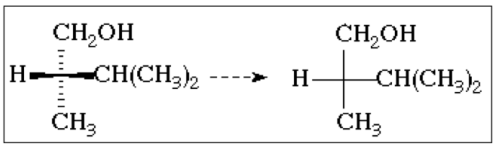


费歇尔投影式

Fischer projections and the "exchange method"

省略

- The central carbon is always omitted.
- Rotating the molecules so that the "**top**" and "**bottom**" groups are oriented back, away from you.
- Placing the "**right**" and "**left**" groups in a position where they are projecting outwards you, as in a "**bow-tie**".
- All bonds are drawn as simple lines.



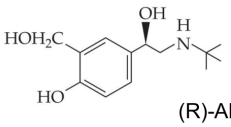
8. Asymmetric carbons are present in most biological molecules

1° Asymmetric carbons are key features of amino acid and carbonhydrates

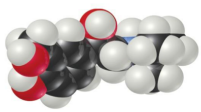
2° Protein (and other biomolecules) are stereospecific, because they also are chiral and their binding sites can thus distinguish between enantiomers.

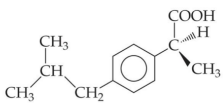
3° Many drugs are chiral compounds.

4° Equal mixtures of enantiomers is called a racemic mixture. Often only one enantiomer is clinically active; the other can be inert OR harmful.



(R)-Albuterol





(S)-Ibuprofen