



## Unit –I

# Classification, Nomenclature and Isomerism of Organic Compounds

## CLASSIFICATION, NOMENCLATURE, ISOMERISM OF ORGANIC COMPOUNDS. NATURE OF CHEMICAL BONDS.

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## Lecture plan

Classification of bioorganic compounds.

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Nomenclature of bioorganic compounds.

Isomerism of bioorganic compounds.

Electron structure and valency states of the carbon atom.

Interaction of atoms in bioorganic compounds

# Bioorganic compounds

**Organic compounds** are chemical compounds that contain carbon-hydrogen bonds.

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Organic chemistry studies properties, reactions, and syntheses of organic compounds.

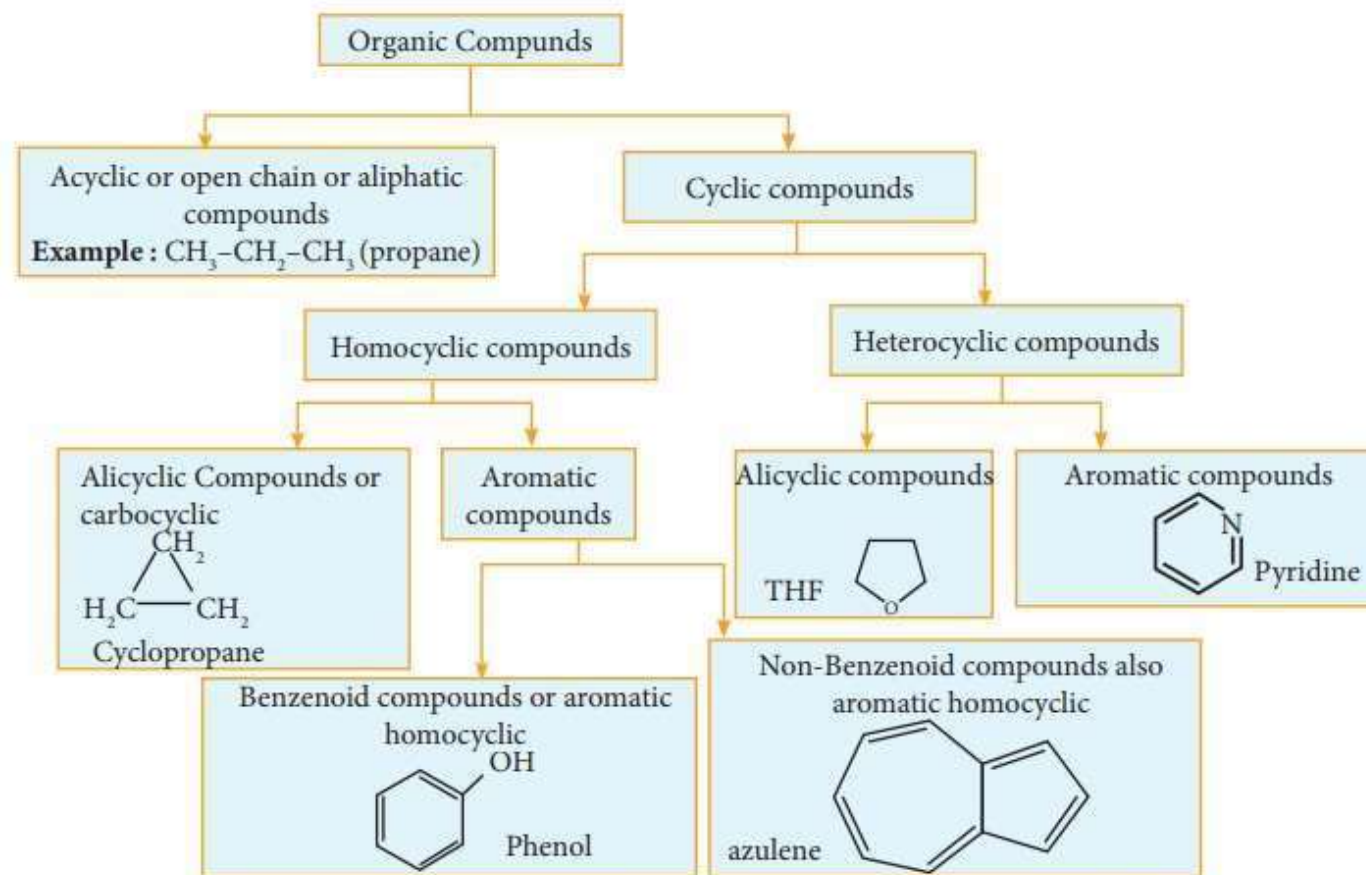
**- Examples of organic compounds:**

- methane ( $\text{CH}_4$ )
- acetylene ( $\text{C}_2\text{H}_2$ )
- ethanol ( $\text{C}_2\text{H}_5\text{OH}$ )
- carbon tetrachloride ( $\text{CCl}_4$ )
- urea [ $\text{CO}(\text{NH}_2)_2$ ]

**- Examples of inorganic compounds:**

- water ( $\text{H}_2\text{O}$ )
- carbon dioxide ( $\text{CO}_2$ )
- bimolecular oxygen ( $\text{O}_2$ )
- sodium chloride ( $\text{NaCl}$ )

# Classification of bioorganic compounds.



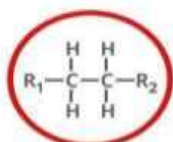
# The functional groups

The functional groups are specific substituents or moieties within molecules that may be responsible for the characteristic chemical reactions of those molecules.

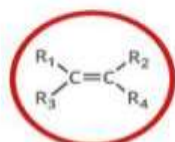
## FUNCTIONAL GROUPS IN ORGANIC CHEMISTRY

FUNCTIONAL GROUPS ARE GROUPS OF ATOMS IN ORGANIC MOLECULES THAT ARE RESPONSIBLE FOR THE CHARACTERISTIC CHEMICAL REACTIONS OF THOSE MOLECULES. IN THE GENERAL FORMULAE SHOWN BELOW FOR EACH FUNCTIONAL GROUP, 'R' REPRESENTS THE REST OF THE MOLECULE, AND 'X' REPRESENTS ANY HALOGEN ATOM.

● HYDROCARBONS ● SIMPLE OXYGEN HETEROATOMICS ● HALOGEN HETEROATOMICS ● CARBONYL COMPOUNDS ● NITROGEN-BASED ● SULFUR-BASED ● AROMATIC



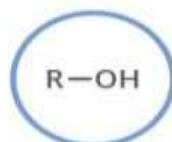
**ALKANE**  
Naming: -ane  
e.g. ethane



**ALKENE**  
Naming: -ene  
e.g. ethene



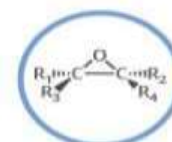
**ALKYNE**  
Naming: -yne  
e.g. ethyne



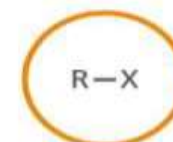
**ALCOHOL**  
Naming: -ol  
e.g. ethanol



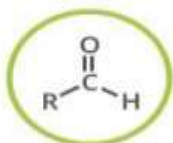
**ETHER**  
Naming: -oxy-ane  
e.g. methoxyethane



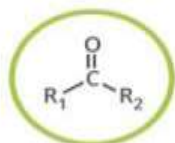
**EPOXIDE**  
Naming: -ene oxide  
e.g. ethene oxide



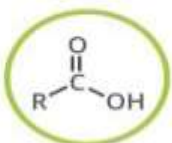
**HALOALKANE**  
Naming: halo-  
e.g. chloroethane



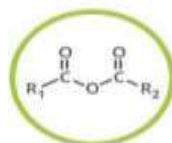
**ALDEHYDE**  
Naming: -al  
e.g. ethanal



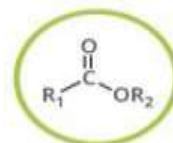
**KETONE**  
Naming: -one  
e.g. propanone



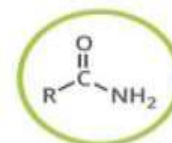
**CARBOXYLIC ACID**  
Naming: -oic acid  
e.g. ethanoic acid



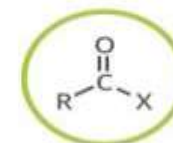
**ACID ANHYDRIDE**  
Naming: -oic anhydride  
e.g. ethanoic anhydride



**ESTER**  
Naming: -yl -oate  
e.g. ethyl ethanoate



**AMIDE**  
Naming: -amide  
e.g. ethanamide



**ACYL HALIDE**  
Naming: -oyl halide  
e.g. ethanoyl chloride



**AMINE**  
Naming: -amine  
e.g. ethanamine



**NITRILE**  
Naming: -nitrile  
e.g. ethanenitrile



**IMINE**  
Naming: -imine  
e.g. ethanimine



**ISOCYANATE**  
Naming: -yl isocyanate  
e.g. ethyl isocyanate



**AZO COMPOUND**  
Naming: -azo-  
e.g. azoethane



**THIOL**  
Naming: -thiol  
e.g. methanethiol



**ARENE**  
Naming: -yl benzene  
e.g. ethyl benzene



## Nomenclature of bioorganic compounds.

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**Nomenclature of organic chemistry** is a method of naming of organic chemical compounds.

3 types of nomenclature are used for naming organic compounds: **trivial/Common names**

**rational and**

**systematic nomenclature - IUPAC nomenclature (IUPAC) –**

*International Union of Pure and Applied Chemistry*

## Nomenclature of bioorganic compounds.

**The trivial** – is a common, (historical) nomenclature is the first type nomenclature. Organic compounds were given random names for the source of formation (oxalic acid, malic acid), color or smell (aromatic compounds), etc.

For example: urea, acetic acid, butyric acid, valeric acid, alanine and many others.

**Rational nomenclature** - organic compounds are named according to the corresponding type of organic compounds (saturated hydrocarbons, ethylenes, acetylenes, alcohols, aldehydes, ketones, acids, etc.). These names contain the name of the main type and the names of the substituents.

For example: methyl alcohol, trimethylacetic aldehyde, dimethyl ketone, chloroacetic acid.

## Nomenclature of bioorganic compounds.

### Systematic nomenclature - IUPAC nomenclature (IUPAC) – International Union of Pure and Applied Chemistry

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A chemical name has three parts in the IUPAC system:

**Prefix-Parent-Suffix**



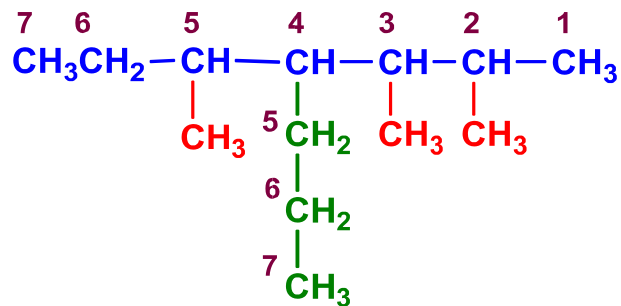
Where are the substituents?



How many carbons?



What family?



2,3,5-Trimethyl-4-propylheptane



## IUPAC rules

Identify the longest carbon chain. This chain is called the parent chain.

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Identify all of the substituents (groups appending from the parent chain).

Number the carbons of the parent chain from the end that gives the substituents the lowest numbers. When comparing a series of numbers, the series that is the "lowest" is the one which contains the lowest number at the occasion of the first difference. If two or more side chains are in equivalent positions, assign the lowest number to the one which will come first in the name.

If the same substituent occurs more than once, the location of each point on which the substituent occurs is given. In addition, the number of times the substituent group occurs is indicated by a prefix (di, tri, tetra, etc.).

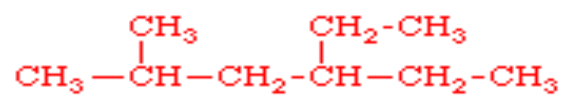
If there are two or more different substituents they are listed in alphabetical order using the base name (ignore the prefixes). The only prefix which is used when putting the substituents in alphabetical order is **iso** as in isopropyl or isobutyl. The prefixes **sec-** and **tert-** are not used in determining alphabetical order except when compared with each other.

If chains of equal length are competing for selection as the parent chain, then the choice goes in series to:

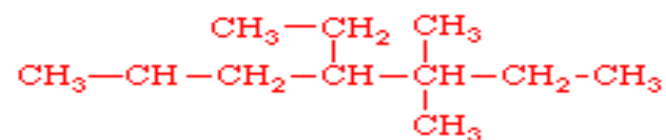
- a) the chain which has the greatest number of side chains.
- b) the chain whose substituents have the lowest- numbers.
- c) the chain having the greatest number of carbon atoms in the smaller side chain.
- d) the chain having the least branched side chains.

A cyclic (ring) hydrocarbon is designated by the prefix **cyclo-** which appears directly in front of the base name.

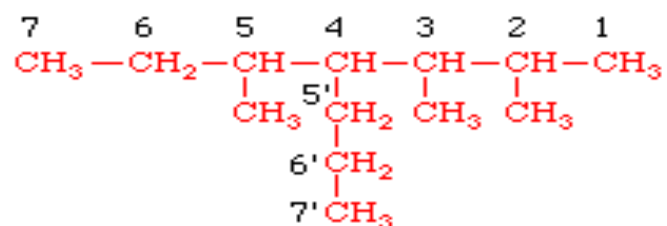
In summary, the name of the compound is written out with the substituents in alphabetical order followed by the base name (derived from the number of carbons in the parent chain). Commas are used between numbers and dashes are used between letters and numbers. There are **no** spaces in the name.



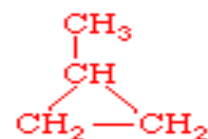
4-ethyl-2-methylhexane



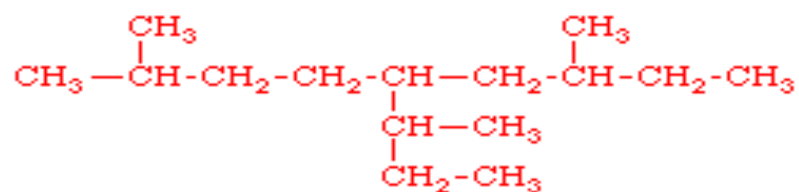
4-ethyl-3,3-dimethylheptane



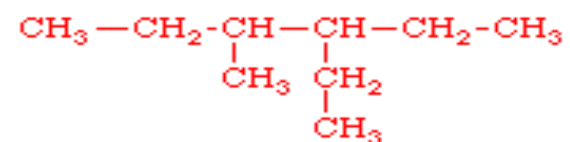
2,3,5-trimethyl-4-propylheptane  
(NOT: 2,3-dimethyl-4-sec-butylheptane)



methylcyclopropane



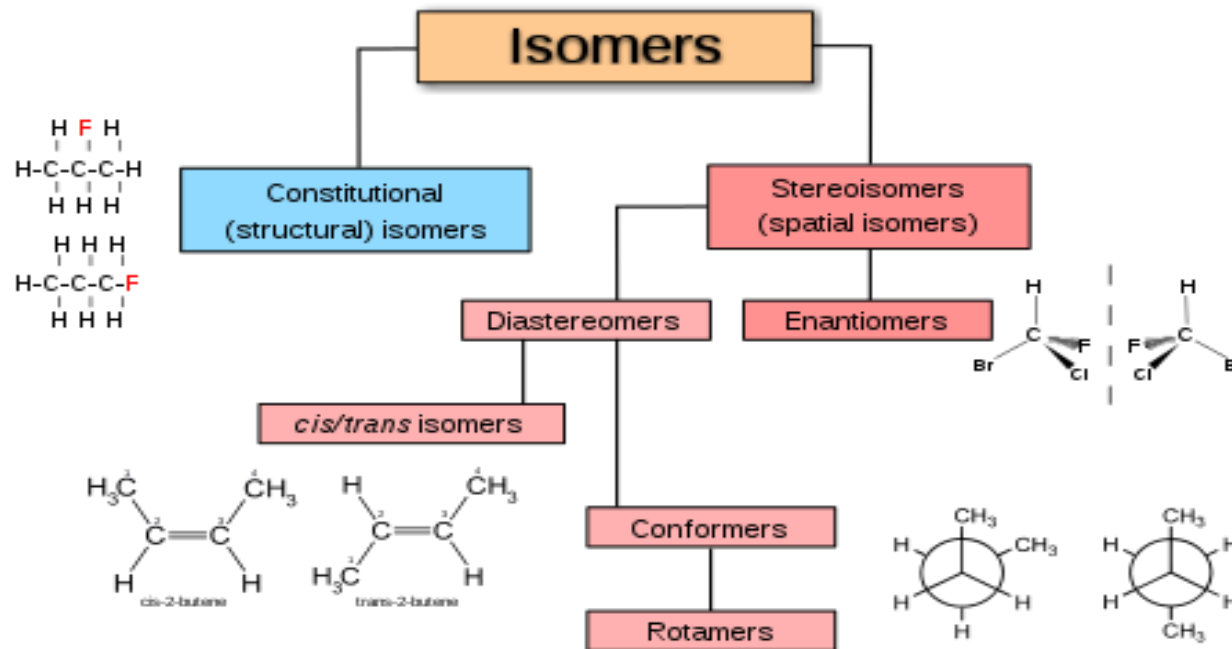
5-sec-butyl-2,7-dimethylnonane



3-ethyl-4-methylhexane

# Isomerism of bioorganic compounds.

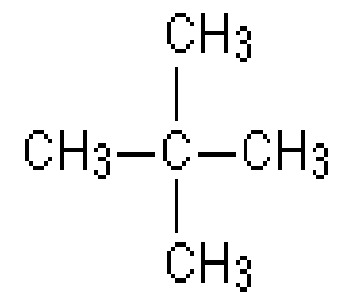
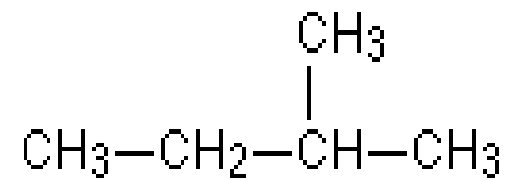
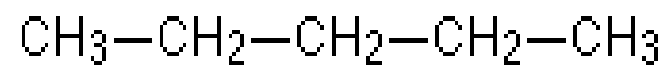
**Isomerism** is the phenomenon in which more than one compounds have the same chemical formula but different chemical structures. Chemical compounds that have identical chemical formulae but differ in properties and the arrangement of atoms in the molecule are called **isomers**.



# Structural isomers

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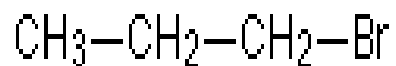
Chain Isomers in Pentane  
Pentane,  $C_5H_{12}$ , has three chain isomers.



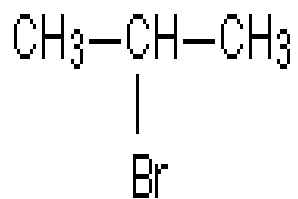
# Structural isomers

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## Positional Isomers of bromopropane



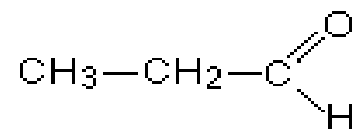
1-bromopropane



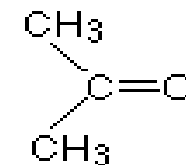
2-bromopropane

## Functional group isomers $\text{C}_3\text{H}_6\text{O}$

A molecular formula  $\text{C}_3\text{H}_6\text{O}$  could be either propanal (an aldehyde) or propanone (a ketone).



propanal



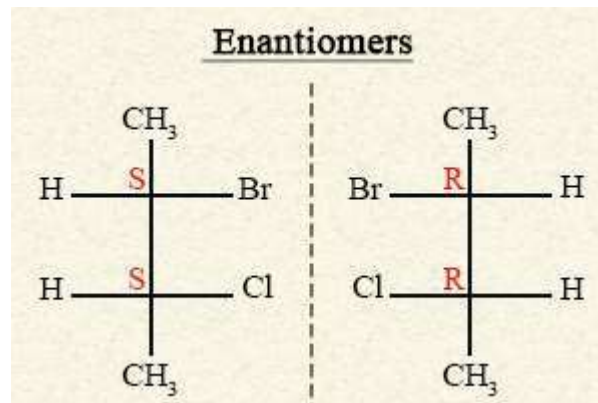
propanone

# Stereoisomers

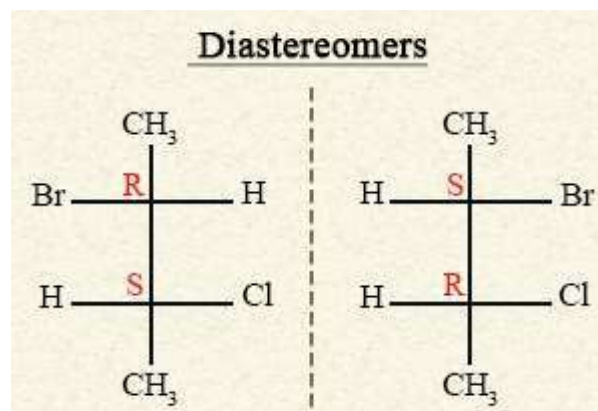
## Enantiomers. Diastereomers.

**Enantiomers** are two molecules that are **nonsuperimposable mirror images**:

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**Diastereomers** are stereoisomers that are not related as object and mirror image and are not enantiomers.

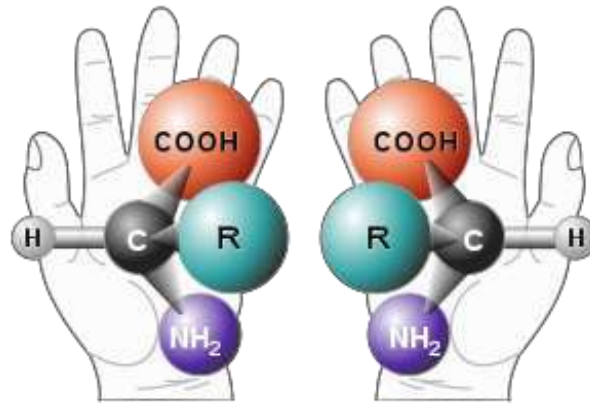


# Chiral carbon. Chirality

Enantiomers contain chiral carbon atom.

~~An **asymmetric carbon atom** (chiral carbon) is a carbon atom that is attached to four different types of atoms or groups of atoms~~

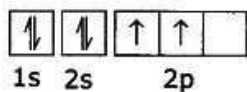
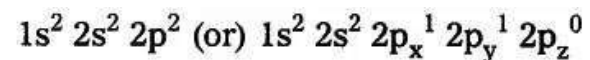
In chemistry, a molecule or ion is called **chiral** (/kaɪˈræl/) if it cannot be superposed on its mirror image by any combination of rotations and translations. This geometric property is called **chirality**.



## Electron structure and valency states of the carbon atom.

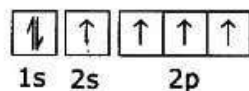
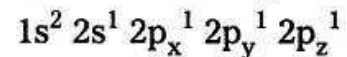
Carbon is an element of second period of periodic table. Its atomic number is 6 and mass number is 12. It is represented as  ${}^{12}_6\text{C}$ .

The ground and excited states of carbon electronic configuration are:



### Carbon (ground state)

Electronic configuration of carbon (excited state) :



### Carbon (excited state)



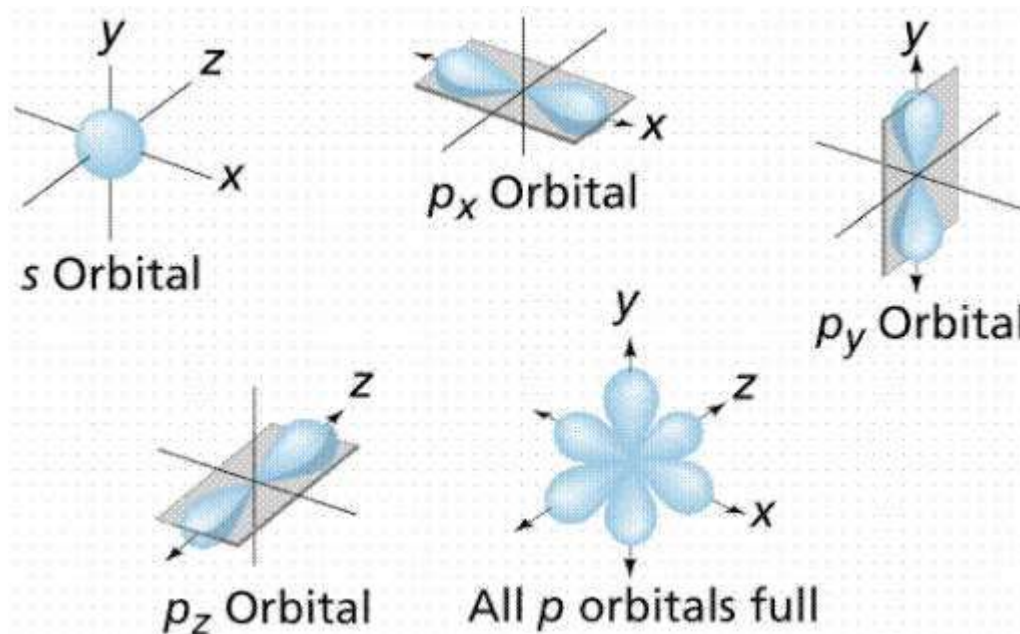
# Types of electron orbitals

In atomic theory and quantum mechanics, an **atomic orbital** is a mathematical function describing the location and wave-like behavior of an electron in an atom. This function can be used to calculate the probability of finding any electron of an atom in any specific region around the atom's nucleus.

The term *atomic orbital* may also refer to the physical region or space where the electron can be calculated to be present, as predicted by the particular mathematical form of the orbital.

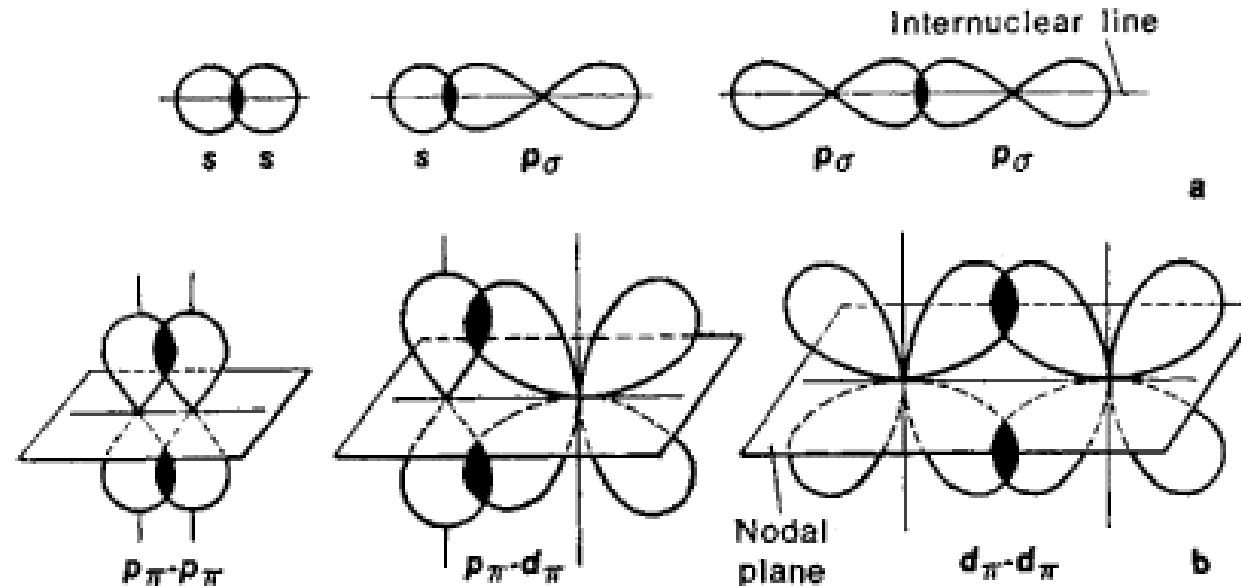
Each orbital in an atom is characterized by a unique set of values of the three quantum numbers  $n$ ,  $\ell$ , and  $m$ , which respectively correspond to the electron's energy, angular momentum, and an angular momentum vector component (the magnetic quantum number).

Each such orbital can be occupied by a maximum of two electrons, each with its own projection of spin. The simple names **s orbital**, **p orbital**, **d orbital**, and **f orbital** refer to orbitals with angular momentum quantum number  $\ell = 0, 1, 2,$  and  $3$  respectively. These names, together with the value of  $n$ , are used to describe the electron configurations of atoms.



## The covalent bonds. $\Sigma$ and $\pi$ bonds.

**Sigma and pi bonds** are types of covalent **bonds** that differ in the overlapping of atomic orbitals. Covalent **bonds** are formed by the overlapping of atomic orbitals. **Sigma bonds** are a result of the head-to-head overlapping of atomic orbitals whereas **pi bonds** are formed by the lateral overlap of two atomic orbitals.

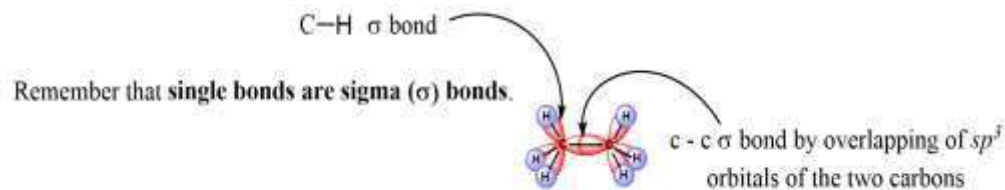
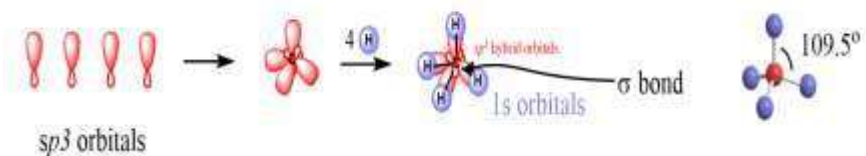
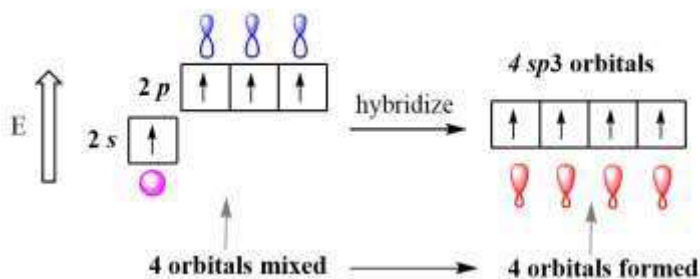


# Hybridization

**Hybridization** is a theory that is used to explain certain molecular geometries that would have not been possible otherwise.

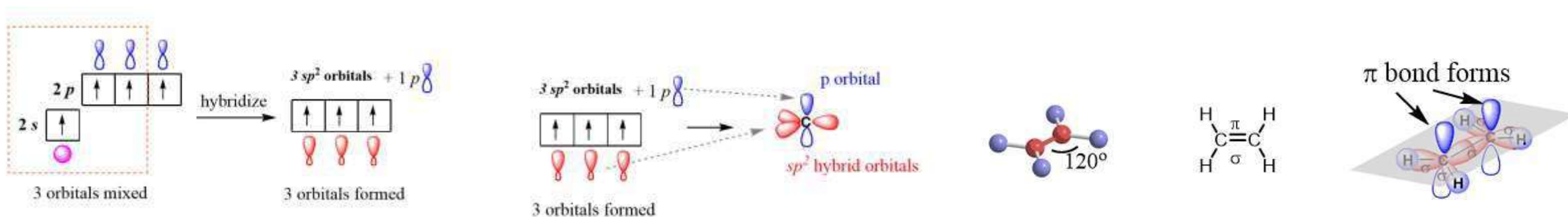
**The  $sp^3$  hybridization** - the **s** and **p** orbitals of the excited state carbon are hybridized to form **four identical** in size, shape and energy orbitals. The four  $sp^3$ -hybridized orbitals arrange in a tetrahedral geometry and make bonds by overlapping with the s orbitals of four hydrogens. This explains the symmetrical geometry of methane ( $CH_4$ ) where all the bonds have the same length and bond angle. All four C-H bonds in methane are single bonds that are formed by **head-on (or end on)** overlapping of  $sp^3$  orbitals of the carbon and s orbital of each hydrogen.

The bonds that form by the head-on overlap of orbitals are called  **$\sigma$  (sigma)** bonds because the electron density is concentrated on the axis connecting the C and H atoms.



# Hybridization

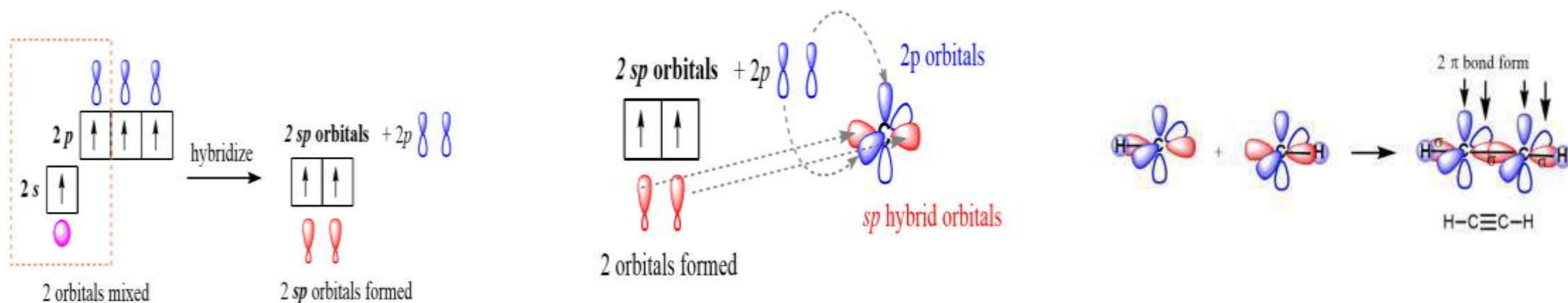
The  $sp^2$  hybridization occurs when the s orbital is mixed with only two p orbitals as opposed to the three p orbitals in the  $sp^3$  hybridization. So, three orbitals are mixed, and the outcome is three hybrid orbitals which are called  $sp^2$  hybrid orbitals.



# Hybridization

## The $sp$ hybridization

In  $sp$  hybridization, the  $s$  orbital of the excited state carbon is mixed with only one out of the three  $2p$  orbitals. It is called  $sp$  hybridization because two orbitals (one  $s$  and one  $p$ ) are mixed:



## Interaction of atoms in bioorganic compounds

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**Electronegativity**, symbol  $\chi$ , measures the tendency of an atom to attract a shared pair of electrons (or electron density). An atom's electronegativity is affected by both its atomic number and the distance at which its valence electrons reside from the charged nucleus. The higher the associated electronegativity, the more an atom or a substituent group attracts electrons.

On the most basic level, electronegativity is determined by factors like the nuclear charge (the more protons an atom has, the more "pull" it will have on electrons) and the number and location of other electrons in the atomic shells (the more electrons an atom has, the farther from the nucleus the valence electrons will be, and as a result, the less positive charge they will experience—both because of their increased distance from the nucleus and because the other electrons in the lower energy core orbitals will act to shield the valence electrons from the positively charged nucleus).

## The mesomeric effect

The **mesomeric effect** in chemistry is a property of substituents or functional groups in a chemical compound. It is defined as the polarity produced in the molecule by the interaction of two pi bonds or between a pi bond and lone pair of electrons present on an adjacent atom. The effect is used in a qualitative way and describes the electron withdrawing or releasing properties of substituents based on relevant resonance structures and is symbolized by the letter **M**. The mesomeric effect is negative (**-M**) when the substituent is an electron-withdrawing group and the effect is positive (**+M**) when the substituent is an electron releasing group.

### **+M EFFECT ORDER :**

$-\text{O}^- > -\text{NH}_2 > -\text{OR} > -\text{ARYAN} > -\text{NHCOR} > -\text{OCOR} > -\text{Ph} > \text{CH}_3 > -\text{F} > -\text{Cl} > -\text{Br} > -\text{I}$

### **-M EFFECT ORDER :**

$-\text{NO}_2 > -\text{CN} > -\text{S(=O)}_2-\text{OH} > -\text{CHO} > -\text{C=O} > -\text{COOCOR} > -\text{COOR} > -\text{COOH} > -\text{CONH}_2 > -\text{COO}^-$

t atom.

## The inductive effect

In chemistry, the **inductive effect** is an effect regarding the transmission of unequal sharing of the bonding electron through a chain of atoms in a molecule, leading to a permanent dipole in a bond. It is present in a  $\sigma$  (sigma) bond as opposed to electromeric effect which is present on a  $\pi$  (pi) bond. The halogen atoms in alkyl halide are electron withdrawing and alkyl groups are electron donating. If the electronegative atom (missing an electron, thus having a positive charge) is then joined to a chain of atoms, usually carbon, the positive charge is relayed to the other atoms in the chain. This is the electron-withdrawing inductive effect, also known as the **-I** effect. In short, alkyl groups tend to donate electrons, leading to the **+I** effect. Its experimental basis is the ionization constant.

### 1) Negative inductive effect (-I):

The electron withdrawing nature of groups or atoms is called as negative inductive effect. It is indicated by -I. Following are the examples of groups in the decreasing order of their -I effect:



### 2) Positive inductive effect (+I):

It refers to the electron releasing nature of the groups or atoms and is denoted by +I. Following are the examples of groups in the decreasing order of their +I effect.





## Sources of information

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[http://www.brainkart.com/article/Classification-of-organic-compounds\\_36452/](http://www.brainkart.com/article/Classification-of-organic-compounds_36452/)

<https://www.compoundchem.com/2014/01/24/functional-groups-in-organic-compounds/>

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[https://en.wikipedia.org/wiki/Chirality\\_\(chemistry\)](https://en.wikipedia.org/wiki/Chirality_(chemistry))

<https://byjus.com/jee/atomic-structure/>

<https://encyclopedia2.thefreedictionary.com/Sigma+and+Pi+Bonds>

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