Organic Chemistry
244 CHEM

Bonding, Structural Formulas, and Molecular Shapes

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Organic Chemistry: Definition

- **Organic Chemistry** is unique in that it deals with vast numbers of substances, both natural and synthetic.

  - *The clothes, the petroleum products, the paper, rubber, wood, plastics, paint, cosmetics, insecticides, and drugs*

- But, from the chemical makeup of organic compounds, it was recognized that one constituent common to all was *the element carbon*.

- **Organic chemistry** is defined as *the study of carbon/hydrogen-containing compounds and their derivatives.*

The Uniqueness of Carbon

- What is unique about the element *carbon*?
- Why does it form so many compounds?
  - *The answers lie in*
    - The **structure** of the *carbon* atom.
    - The **position** of *carbon* in the periodic table.
- These factors enable it to form strong bonds with
  - other carbon atoms
  - and with other elements (hydrogen, oxygen, nitrogen, halogens,…etc).
- Each organic compound has its own characteristic set of physical and chemical properties which depend on the *structure of the molecule*.

Atomic Structure

- **Atoms consist of three main particles: neutrons (have no charge), protons (positively charged) and electrons (negatively charged).**
  - **Neutrons and protons are found in the nucleus.**
  - **Electrons are found outside the nucleus.**

    Electrons are distributed around the nucleus in successive *shells* (*principal energy levels*).

- **Atom is electrically neutral.**

  i.e. Number of electrons = Number of protons

- **Atomic number of an element is the number of protons.**

Atomic Structure

- The energy levels are designated by capital letters (*K, L, M, N*, ..) or whole numbers (*n*).

- The maximum capacity of a shell = $2n^2$ electrons.
  n = number of the energy level.

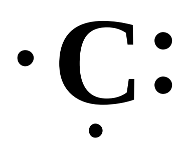
- For example, the element carbon (atomic number 6)
  6 electrons are distributed about the nucleus as

Shell	K	L	M	N
Number of electrons	2	4	0	0

Atomic Structure

Valance Electrons: Electron-Dot Structures

- **Valance Electrons** are those electrons located in the *outermost energy level* (*the valance shell*).
- **Electron-dot structures**
  - The symbol of the element represents the core of the atom.
  - The valance electrons are shown as dots around the symbol.



Chemical Bonding

- **In 1916 G.N. Lewis pointed out that:**

  the noble gases were stable elements and he ascribed their lack of reactivity to their having their valence shells filled with electrons.

  - **2 electrons in case of helium.**
  - **8 electrons for the other noble gases.**

- **According to Lewis,**

  in interacting with one another atoms can achieve a greater degree of stability

  by rearrangement of the valence electrons

  to acquire the outer-shell structure of the closest noble gas in the periodic table.

Chemical Bonding

- **This can be achieved in either of two ways:**

A) Ionic Bonding

through transfer of electrons between atoms.

B) Covalent Bonding

through sharing of electrons between atoms.

C) Coordinate Covalent Bonding

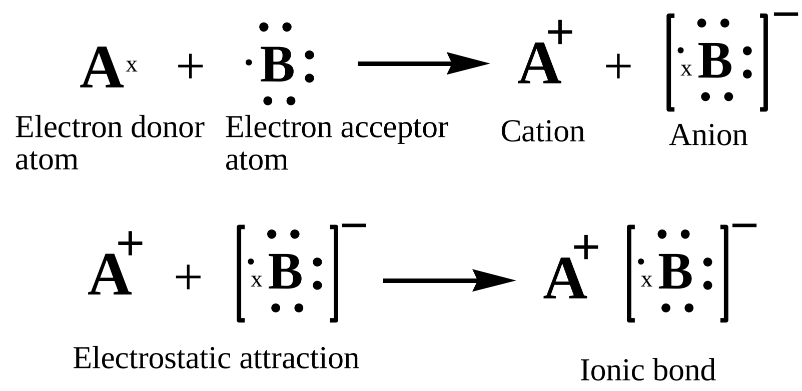
It is a covalent bond (a shared pair of electrons) in which both electrons come from the same atom.

Chemical Bonding

A) Ionic Bonding

- Elements at the left of the periodic table give up their valance electrons and become +*ve charged ions* (*cations*).
- Elements at the right of the periodic table gain the electrons and become -*ve charged ions* (*anions*).
- **Ionic bond**

  The electrostatic force of attraction between oppositely charged ions.



- The majority of ionic compounds are *inorganic substances*.

Electronegativity measures the ability of an atom to attract electrons.

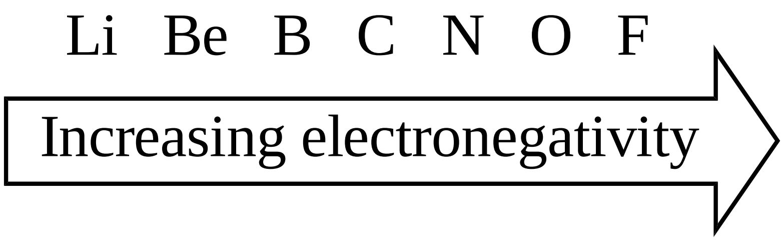
- Electronegativities of Some of Elements

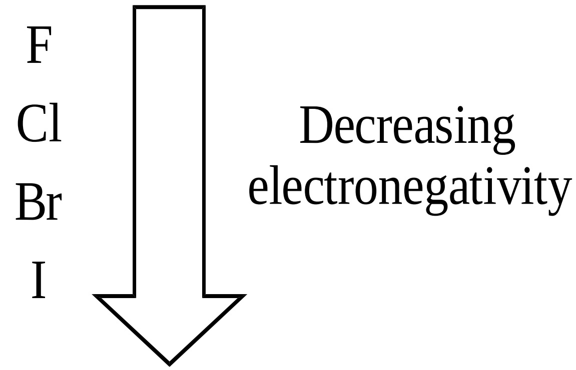
H							
2.1							
Li	**Be**		**B**	**C**	**N**	**O**	**F**
1	1.5		2	2.5	3	3.5	4
Na	**Mg**		**Al**	**Si**	**P**	**S**	**Cl**
0.9	1.2		1.5	1.8	2.1	2.5	3
K							**Br**
0.8							2.8

We notice that:

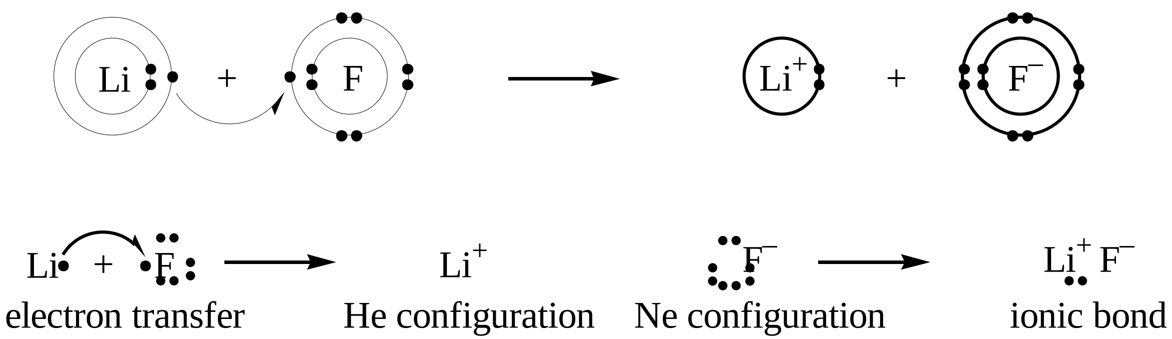
a) The electronegativity increases across a horizontal row of the periodic table from left to right;

b)The electronegativity decreases go down a vertical column:





Example:

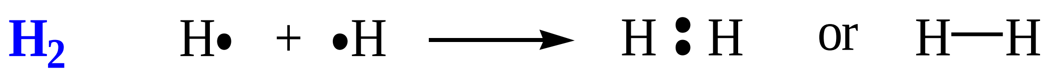


c) Ionic substances, because of their strong internal electrostatic forces, are usually very high melting solids, often having melting points above 1,000 °C.

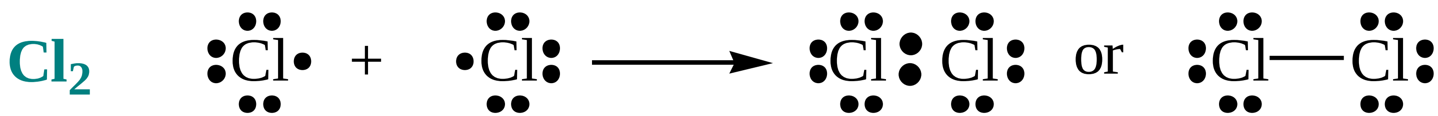
d) In polar solvents, such as water, the ions are solvated, and such solutions usually conduct an electric current.

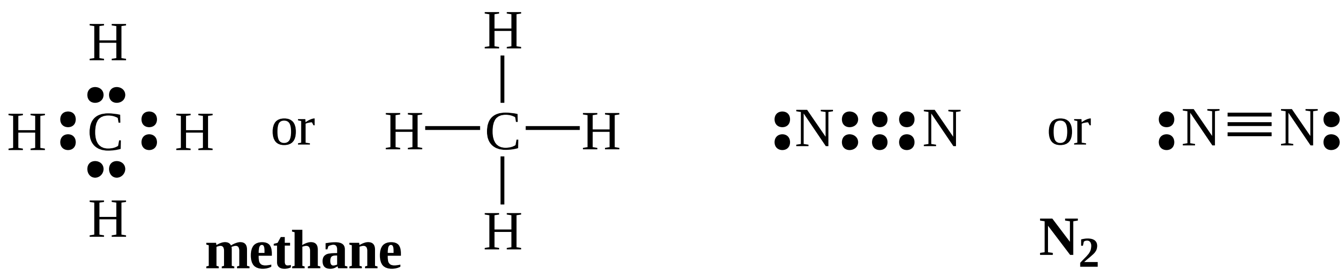
Covalent Bonds

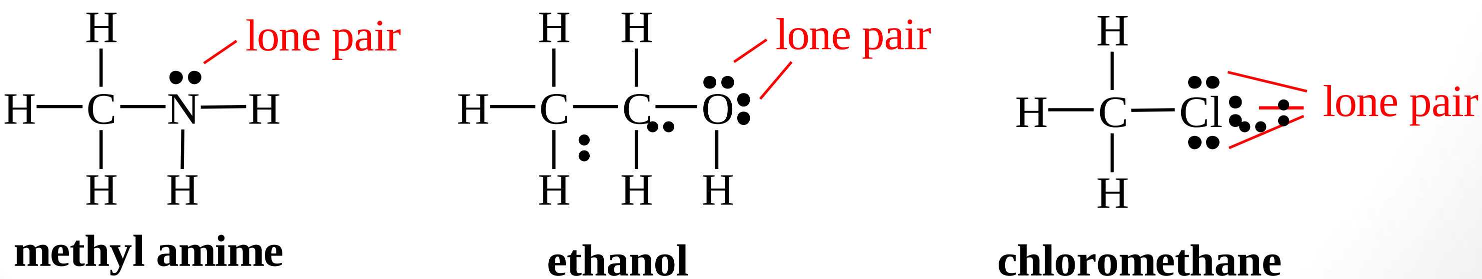
1. **Atoms achieve noble gas configurations by sharing electrons.**



each H shares two electrons (He configuration)







Chemical Bonding

B) Covalent Bonding

- **Elements that are close to each other in the periodic table attain the stable noble gas configuration**

  by sharing valence electrons between them.

- **Covalent bond**

  The chemical bond formed when two atoms share one pair of electrons.

- **A shared electron pair between two atoms or single covalent bond, will be represented by a dash (-).**

$$\mathbf{H}^{\times} + \cdot\mathbf{H} \longrightarrow \mathbf{H}^{\times}\cdot\mathbf{H} \qquad \mathrm{H-H}$$

A covalent bond

Chemical Bonding

B) Covalent Bonding

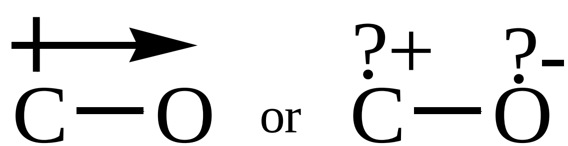
- **In molecules that consist of two like atoms;**
  the bonding electrons are shared equally
  (both atoms have the same electronegativity).

- **When two unlike atoms;**
  the bonding electrons are no longer shared equally
  (shared unequally).

> **A polar covalent bond**

A bond, in which an electron pair is shared unequally.

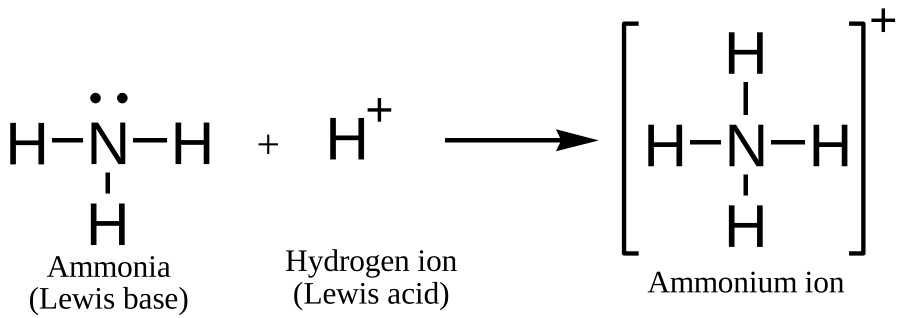
- **The more electronegative atom assumes a partial negative charge and the less electronegative atom assumes a partial positive charge.**



Chemical Bonding

C) Coordinate Covalent Bonding

- There are molecules in which one atom supplies both electrons to another atom in the formation of a covalent bond.
- For example;



- **Lewis base**

  The species that furnishes the electron pair to form a coordinate covalent bond.

- **Lewis acid**

  The species that accepts the electron pair to complete its valance shell.

How Many Bonds to an Atom? Covalence Number

- The number of covalent bonds that an atom can form with other atoms.
- i.e.

  the covalence number is equal to the number of electrons needed to fill its valance shell.

Element	Number of valence electrons	Number of electrons in filled valence shell	Covalence number
H	1	2	1
C	4	8	4
N	5	8	3
O	6	8	2
F, Cl, Br, I	7	8	1

Shapes of Organic Molecules: Orbital Picture of Covalent Bonds

Atomic Orbitals

- **An atomic orbital** *represents a specific region in space in which an electron is most likely to be found.*

- **Atomic orbitals are designated in the order in which they are filled by the letters** ***s, p, d,*** **and** ***f*****.**

- **Examples:**

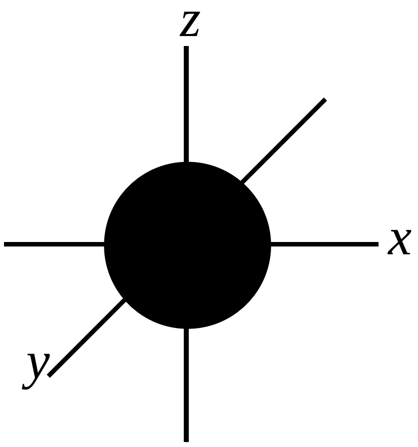
  K shell has only one 1s orbital.

  L shell has one 2s and three 2p ($2p_x$, $2p_y$ and $2p_z$).

Shapes of Organic Molecules: Orbital Picture of Covalent Bonds

Atomic Orbitals

- **An *s* orbital is spherically shaped electron cloud with the atom's nucleus and its center.**

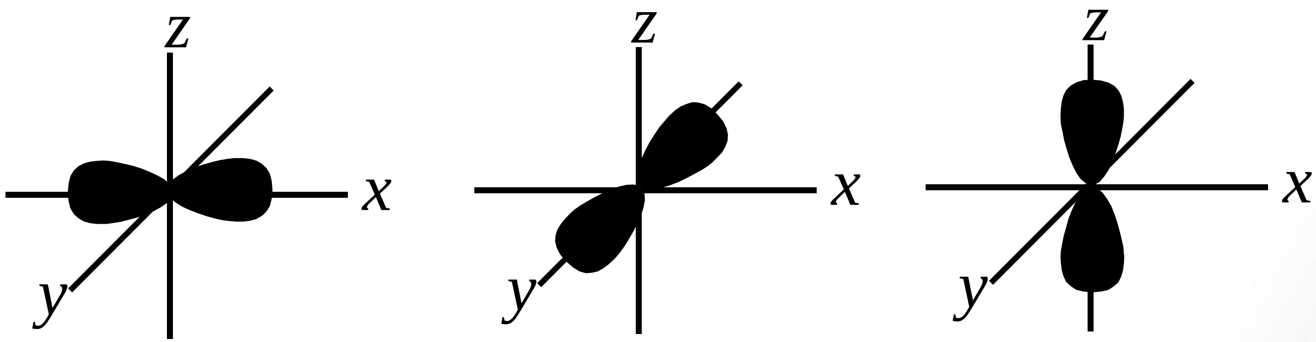


s orbital

Shapes of Organic Molecules: Orbital Picture of Covalent Bonds

Atomic Orbitals

- **A *p* orbital is a dumbbell-shaped electron cloud with the nucleus between the two lobes.**
- **Each *p* orbital is oriented along one of three perpendicular coordinate axes (in the *x*, *y*, or *z* direction).**

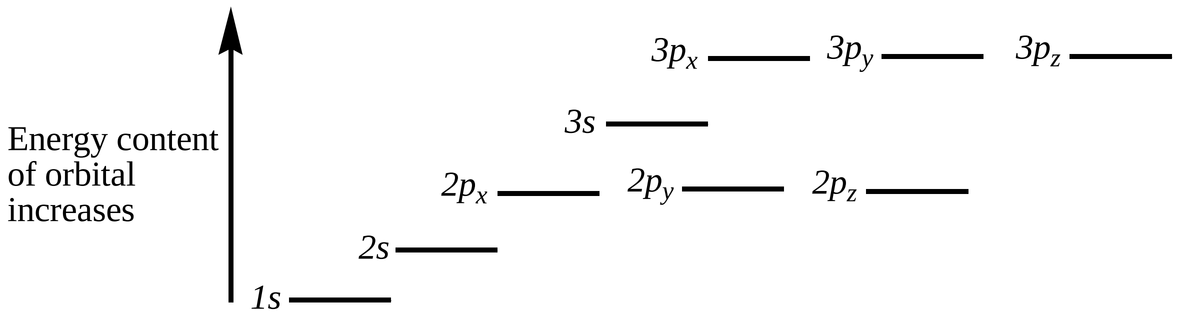


p_x orbital p_y orbital p_z orbital

Shapes of Organic Molecules: Orbital Picture of Covalent Bonds

Atomic Orbitals

- **An energy level diagram of atomic orbitals.**



- **When filling the atomic orbitals, keep in mind that**

  (1) An atomic orbital contain no more 2 electrons.

  (2) Electrons fill orbitals of lower energy first.

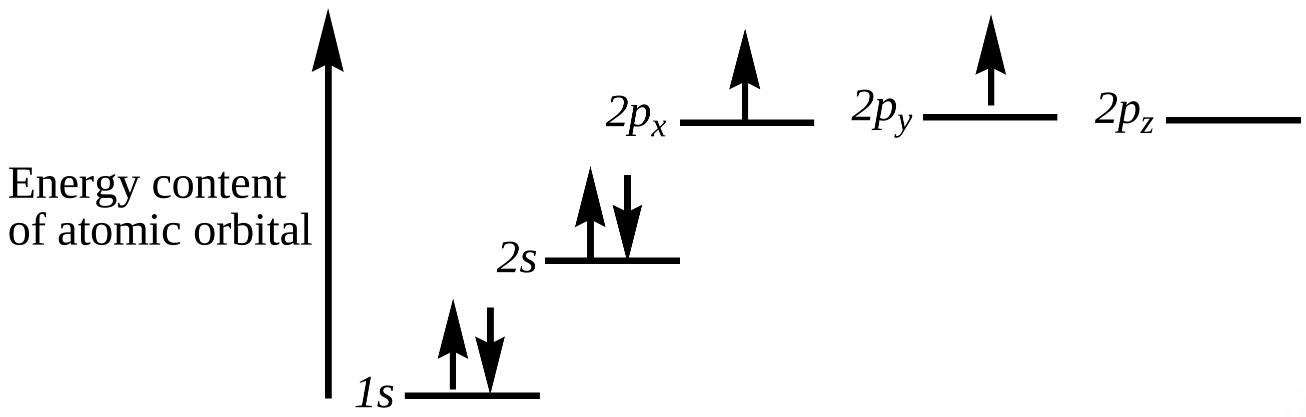
  (3) No orbital is filled by 2 electrons until all the orbitals of equal energy have at least one electron.

Shapes of Organic Molecules: Orbital Picture of Covalent Bonds

Atomic Orbitals

- The electronic configuration of carbon (atomic number 6) can be represented as

$1s^2 2s^2 sp^1{}_x 2p^1{}_y$ or $1s^2 2s^2 2p^2$

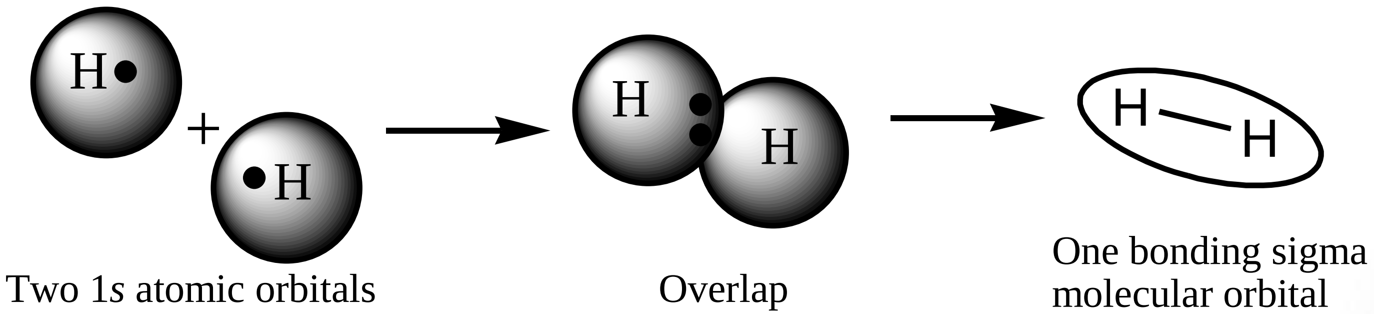


Energy level diagram for carbon.

Shapes of Organic Molecules: Orbital Picture of Covalent Bonds

Molecular Orbitals

- A covalent bond consists of the overlap between two atomic orbitals to form a **molecular orbital**.
- Example:
  - Molecular orbital of H_2



Sigma bonds (bond) can be formed from

Shapes of Organic Molecules: Orbital Picture of Covalent Bonds

Molecular Orbitals

- **Sigma bonds (σ bonds) can be formed from**
  - **The overlap of two *s* atomic orbitals.**
  - **The end-on overlap of two *p* atomic orbitals.**
  - **The overlap of two an *s* atomic orbital with a *p* atomic orbital.**

- **pi bonds (π bonds) can be formed from the side-side overlap between two *p* atomic orbitals.**

Bond Energy and Bond Length

- **A molecule is more stable than the isolated constituent atoms.**
  - **This stability is apparent in the release of energy during the formation of the molecular bond.**

- **Heat of formation (bond energy)**

  The amount of energy released when a bond is formed.

- **Bond dissociation energy**

  The amount of energy that must be absorbed to break a bond.

- **Bond length**

  The distance between nuclei in the molecular structure.

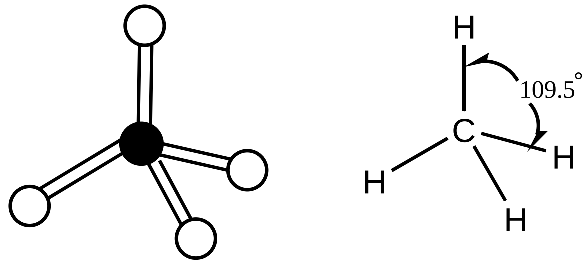
sp^3 Hybridization: the Tetrahedral Carbon
Shapes of Organic Molecules

Methane

- **Molecular formula CH_4.**
- **The four carbon-hydrogen bonds is identical.**

  The same strength, 101 kcal/mole, and length, 1.09 A.

- **Regular tetrahedron with all H-C-H bond angles of 109.5º.**



The tetrahedral structure of methane.

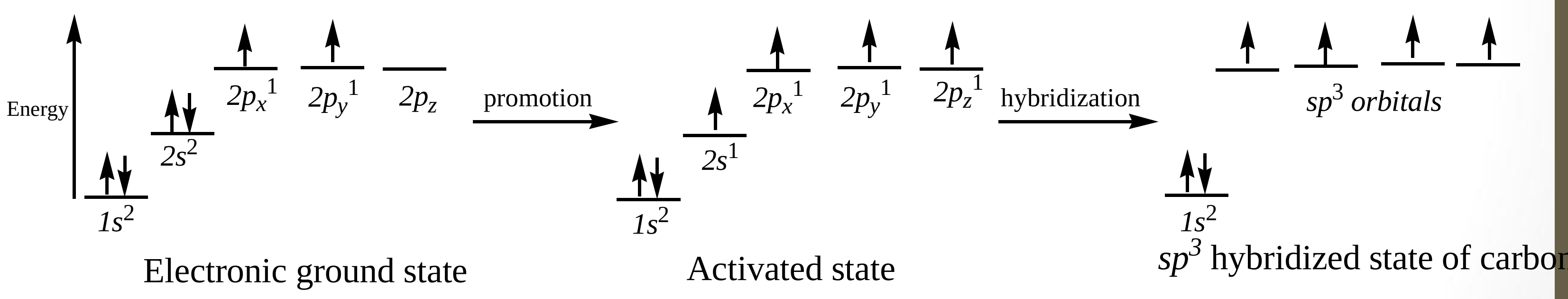
- **The tetrahedron is a pyramid-like structure with the carbon atom at the center and the four attached atoms located at a corner.**

sp^3 Hybridization: the Tetrahedral Carbon Shapes of Organic Molecules

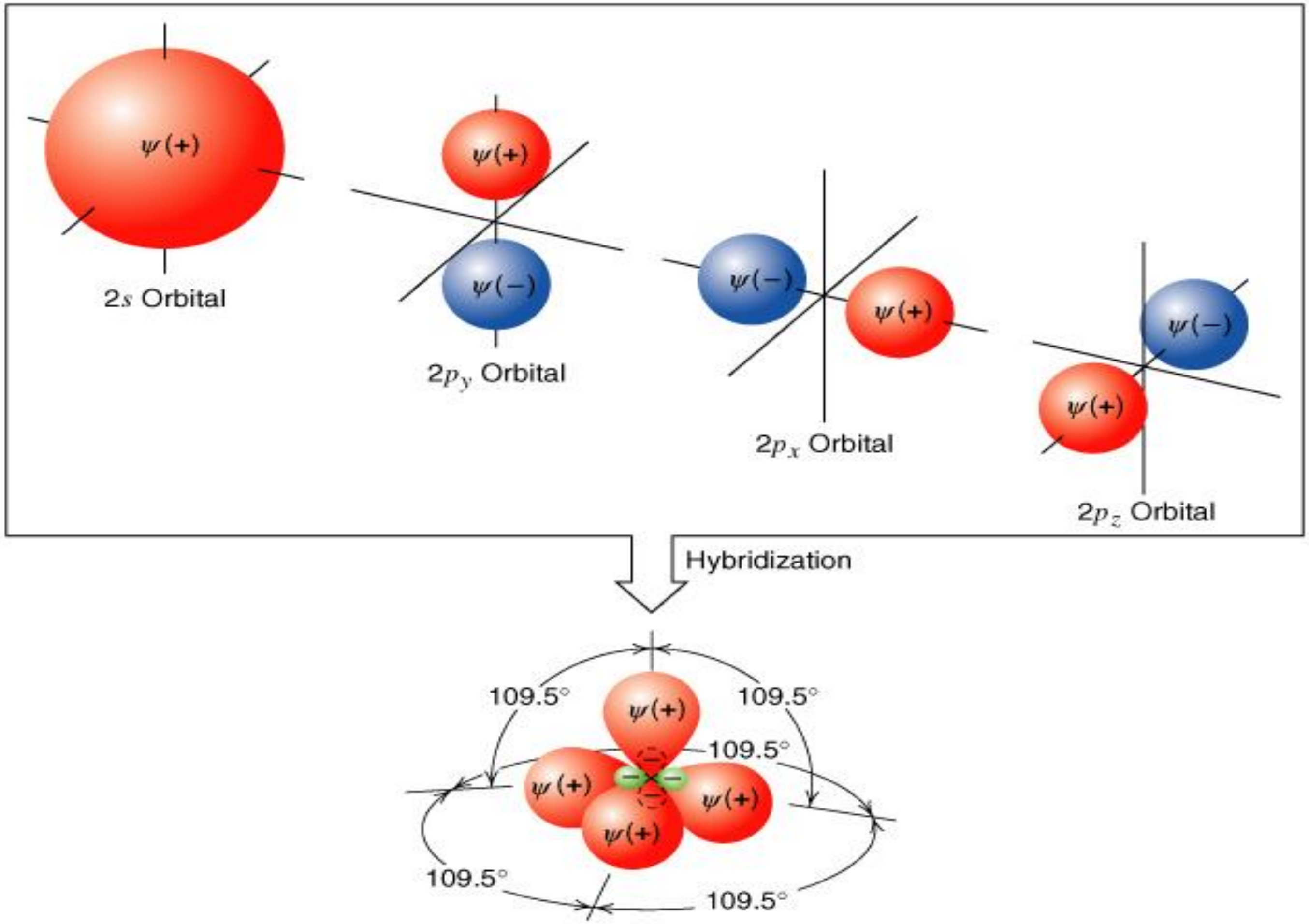
Methane

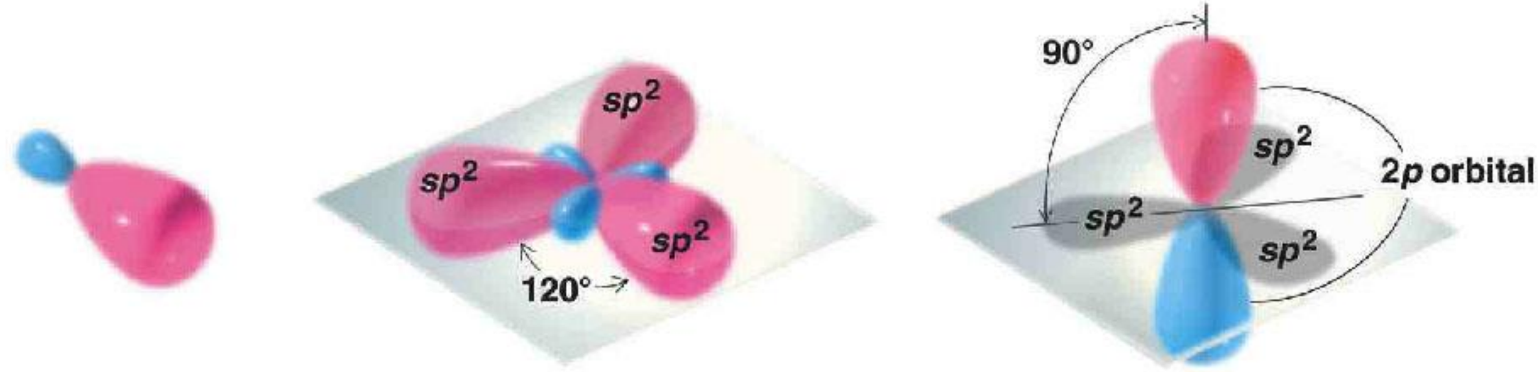
- **The electronic configuration of the isolated or ground-state carbon.**

$1s^2 2s^2 2p_x^{\,1} 2p_y^{\,1}$ *Equivalent to* $:\dot{C}\cdot$

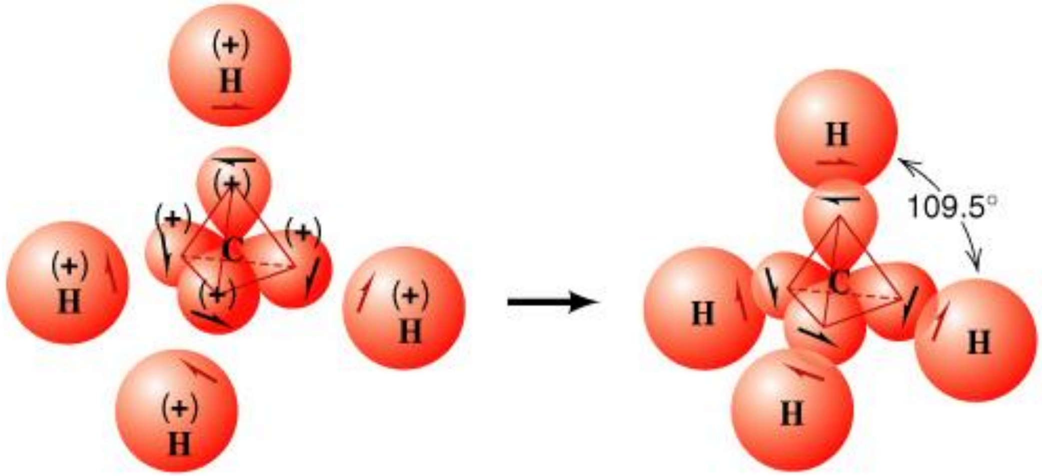


Hybridization of AOs of a carbon atom

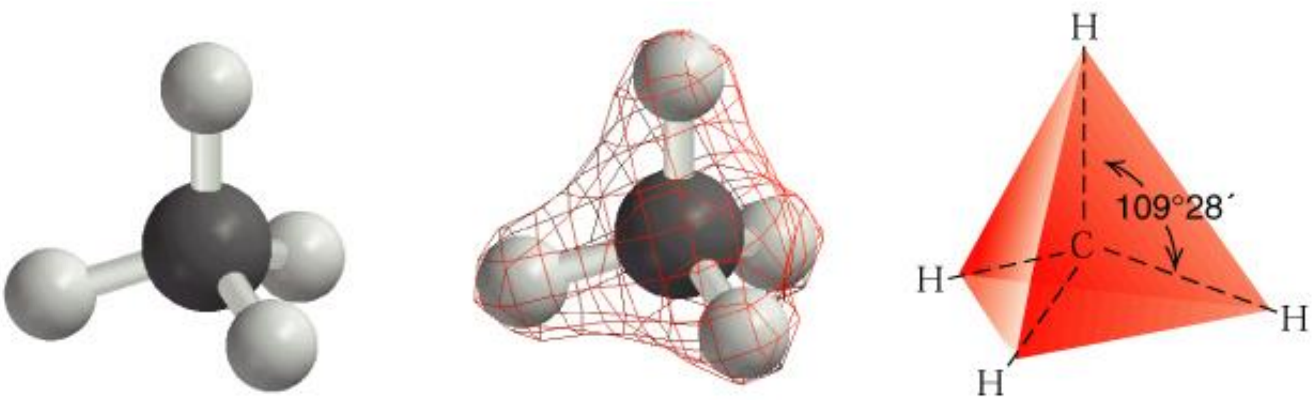




(a) An sp^2 orbital (b) Three sp^2 orbitals (c) Three sp^2 orbitals and an unhybridized 2*p* orbital



Methane, CH_4



(*a*) (*b*) (*c*)

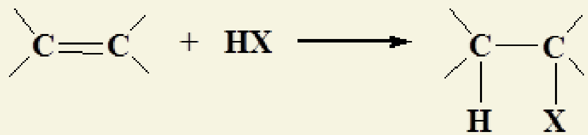
Types of Organic Reactions

Substitution reactions

$$CH_3(CH_2)_5CH_2OH + HBr \xrightarrow{120°C} CH_3(CH_2)_5CH_2Br + H_2O$$

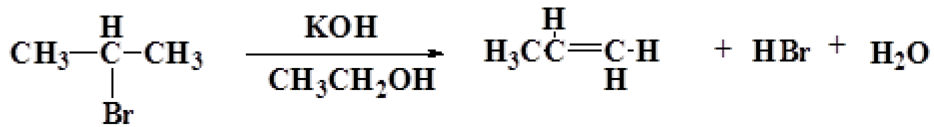
1-Heptanol; Hydrogen bromide; 1-Bromoheptane (87–90%); Water

Addition reactions

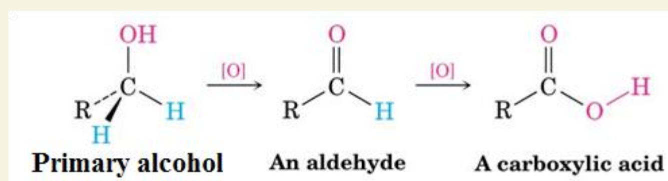


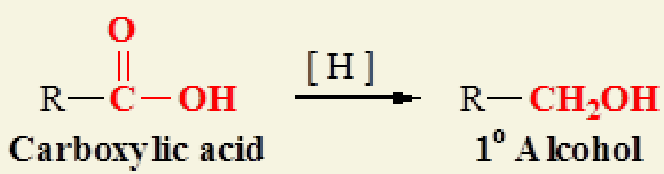
(X = Cl, Br)

Elimination reactions

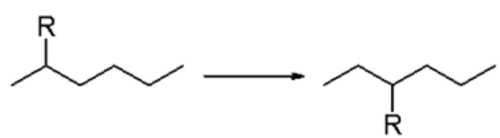


Oxidation-Reduction



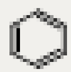
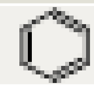
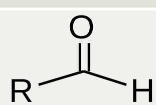
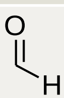
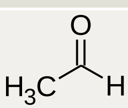
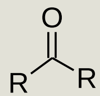
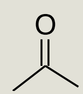
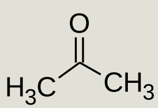
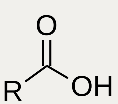
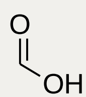
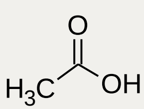


Rearrangement reactions



Functional Groups

is a reactive portion of an organic molecule, an atom, or a group of atoms that confers on the whole molecule its characteristic properties.

Class	General formula	Functional group	Specific
Alkane	RH	C – C (single bond)	**$H_3C – CH_3$**
Alkene	$R – CH = CH_2$	C = C (double bond)	**$H_2C = CH_2$**
Alkyne	R—C≡CH	(triple bond)	HC≡CH
Aromatic		Aromatic ring	
Alkyl halide	RX	-X (X = F, Cl, Br, I)	H_3C - Cl
Alcohol	R – OH	-OH	H_3C - OH
Ether	R – O –R'	- C- O – C -	$H_3C – O – CH_3$
Aldehyde			
Ketone			
Carboxylic acid			
Amines	$R-(CH_2)_nNH_2$	$-NH_2$	$CH_3-CH_2-NH_2$