Organic Chemistry
CHEM 145

2 Credit hrs

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BONDING, STRUCTURAL FORMULAS, AND MOLECULAR SHAPES

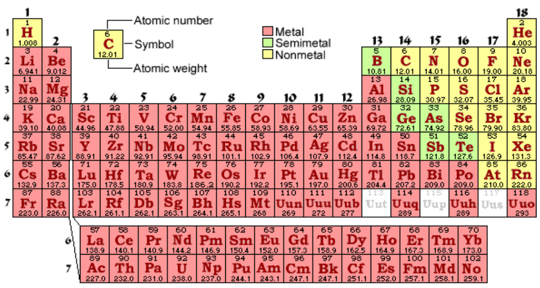
Organic Chemistry: Definition

- **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).**

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.**
- **The energy levels are designated by capital letters (*K, L, M, N, ..*).**
- **The maximum capacity of a shell = $2n^2$ electrons.**

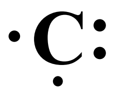
  n = number of the energy level.
- **For example, the element carbon (atomic number 6)**

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

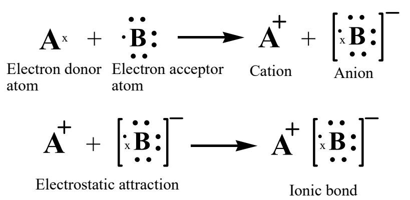
  A) Ionic Bonding
  through transfer of electrons between atoms.

  B) Covalent Bonding
  through sharing of electrons between atoms.

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.

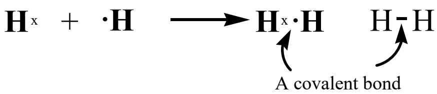


- **The majority of ionic compounds are** ***inorganic substances*****.**

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 (-).



- 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).

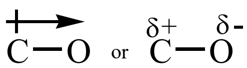
Chemical Bonding

B) Covalent Bonding

A polar covalent bond

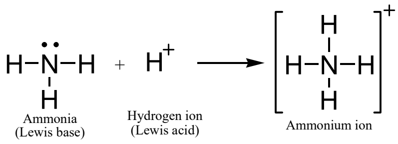
A bond, in which an electron pair is shared unequally.

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



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;



Chemical Bonding

- **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

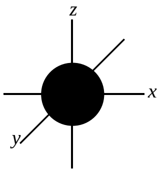
- **The number of covalent bonds that an atom can form with other atoms.**
- *i.e. the covalence number is equal to the number of electrons needed to fill its valance shell.*

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 $2p_z$).
- **An** *s* **orbital is spherically shaped electron cloud with the atom's nucleus and its center.**

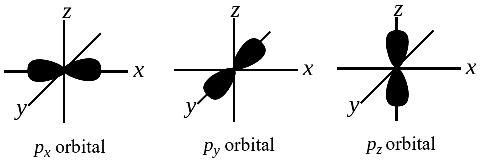


s orbital

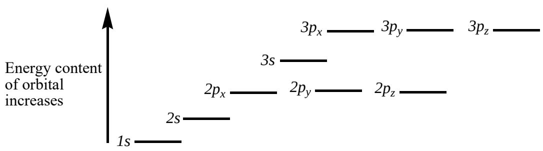
Shapes of Organic Molecules: Orbital Picture of Covalent Bonds

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).**



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

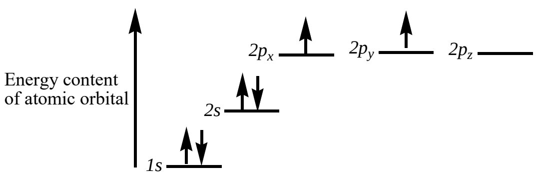


Shapes of Organic Molecules: Orbital Picture of Covalent Bonds

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

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

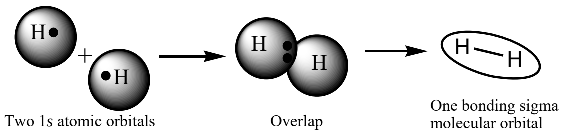


Energy level diagram for carbon.

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 (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.

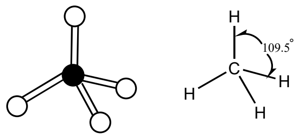
Bond Energy and Bond Length

- 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 109.5°.**



The tetrahedral structure of methane.

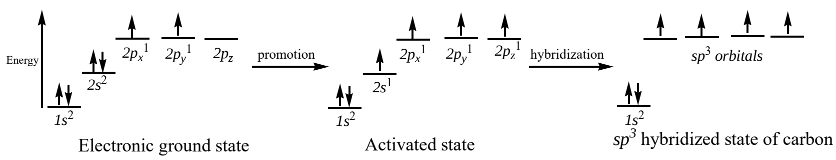
- **The *tetrahedron* is a pyramid-like structure with the carbon atom at the center and the four attached atoms located at a corner.**

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*** :Ċ·



Acid-Base Concept

- **In the Brønsted–Lowry definitions (1923), an acid is a species that donates a proton, and a base is a species that accepts a proton (or any compound possessing a lone pair).**
- **Example:**
  Hydrogen chloride (HCl) meets the Brønsted–Lowry definition of an acid because it donates a proton to water.
  Water meets the definition of a base because it accepts a proton from HCl.
  In the reverse reaction, H_3O^+ is an acid because it donates a proton to Cl^-, and Cl^- is a base because it accepts a proton from H_3O^+.

HCl	+	$H_2\ddot{O}:$	$\rightleftharpoons$	Cl^-	+	H_3O^+
an acid		a base		a base		an acid

Acid-Base rections are often called proton-transfer reactions.

- **When a compound loses a proton, the resulting species is called its conjugate base.**

  Thus, Cl^- is the conjugate base of HCl, and H_2O is the conjugate base of H_3O^+

  Thus, HCl is the conjugate acid of Cl^- and H_3O^+ is the conjugate acid of H_2O

- **Acidity** is a measure of the tendency of a compound to give up a proton.

  Basicity is a measure of a compound's affinity for a proton.

Lewis Acids and Bases

- In 1923, G. N. Lewis offered new definitions for the terms "acid" and "base." He defined an acid as a species that accepts a share in an electron pair and a base as a species that donates a share in an electron pair.

H^+	+	$:NH_3$	→	$H—NH_3$
an acid		a base		
accept a share in a pair of electron		donate a share in a pair of electron		

- **Lewis acid such as aluminum chloride ($AlCl_3$) boron trifluoride (BF_3) and borane (BH_3).**

The term "acid" is used to mean a proton-donating acid, and the term "Lewis acid" is used to refer to non-proton-donating acids such as $AlCl_3$ or BF_3.

- **All bases are Lewis bases because they have a pair of electrons that they can share, either with an atom such as aluminum or boron or with a proton.**

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	C≡C (triple bond)	HC≡CH
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	R—C(=O)—H	—C(=O)—H	H—C(=O)—H, H_3C—C(=O)—H
Ketone	R—C(=O)—R	—C—C(=O)—C—	H_3C—C(=O)—CH_3
Carboxylic acid	R—C(=O)—OH	—C(=O)—OH	H—C(=O)—OH, H_3C—C(=O)—OH
Ester	R—C(=O)—OR	—C(=O)—OR	H—C(=O)—OCH_3 H_3C—C(=O)—OCH_3
Amine	$R – NH_2$	—C—NH_2	$H_3C – NH_2$