

# **CHM-134 ORGANIC CHEMISTRY**

## **CHAPTER-I: BONDING & ISOMERISM**

**I.1** Introduction to Organic Chemistry

**I.2** Concepts of Bonding (Ionic-Covalent Bonding & Octet Rule)

**I.3** Valence

**I.4** The Shape of Molecules

**I.5** Resonance

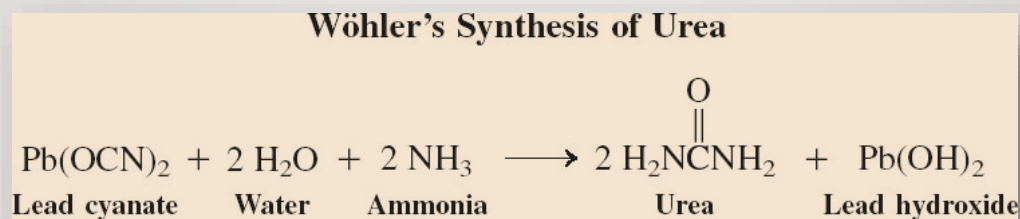
**I.6** Orbitals

**I.7** Oxidation State

**I.8** Classification of Organic Compounds According to Functional Groups

# I.1 INTRODUCTION TO ORGANIC CHEMISTRY

- In chemistry, organic and inorganic compound study is often divided. This is because reaction forms appear to be completely different between the two chemistry fields, and how they react.
- Indeed, they are so different that before the 1820s there was something fundamentally different between organic and inorganic compounds.
- They believed that only a «vital force» found in living creatures could make something organic. As Friedrich Wohler produced urea from non-organic compounds, the entire assumption was dissipated.

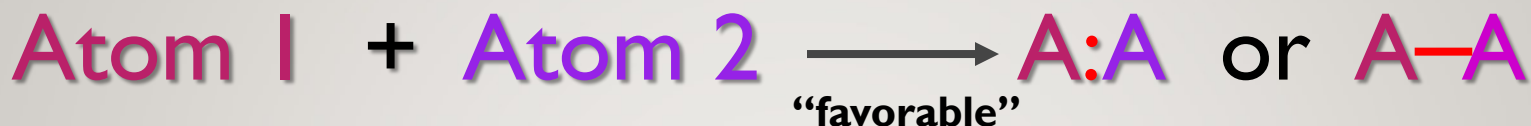


Organic synthesis: Preparation complex organic chemicals from simpler, more readily available ones.

- Reactants (Substrates) = Starting compounds
- Products
- Reaction Mechanism = Underlying details of a reaction
- Reaction Intermediate = Chemical species formed and then destroyed on the pathway between reactants and products.

## I.2 BONDING (IONIC AND COVALENT BONDING)

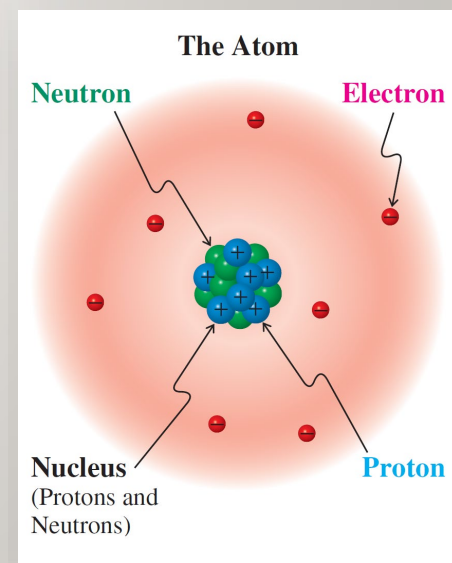
**Bonds** are made by simultaneous coulombic attraction and electron exchange.



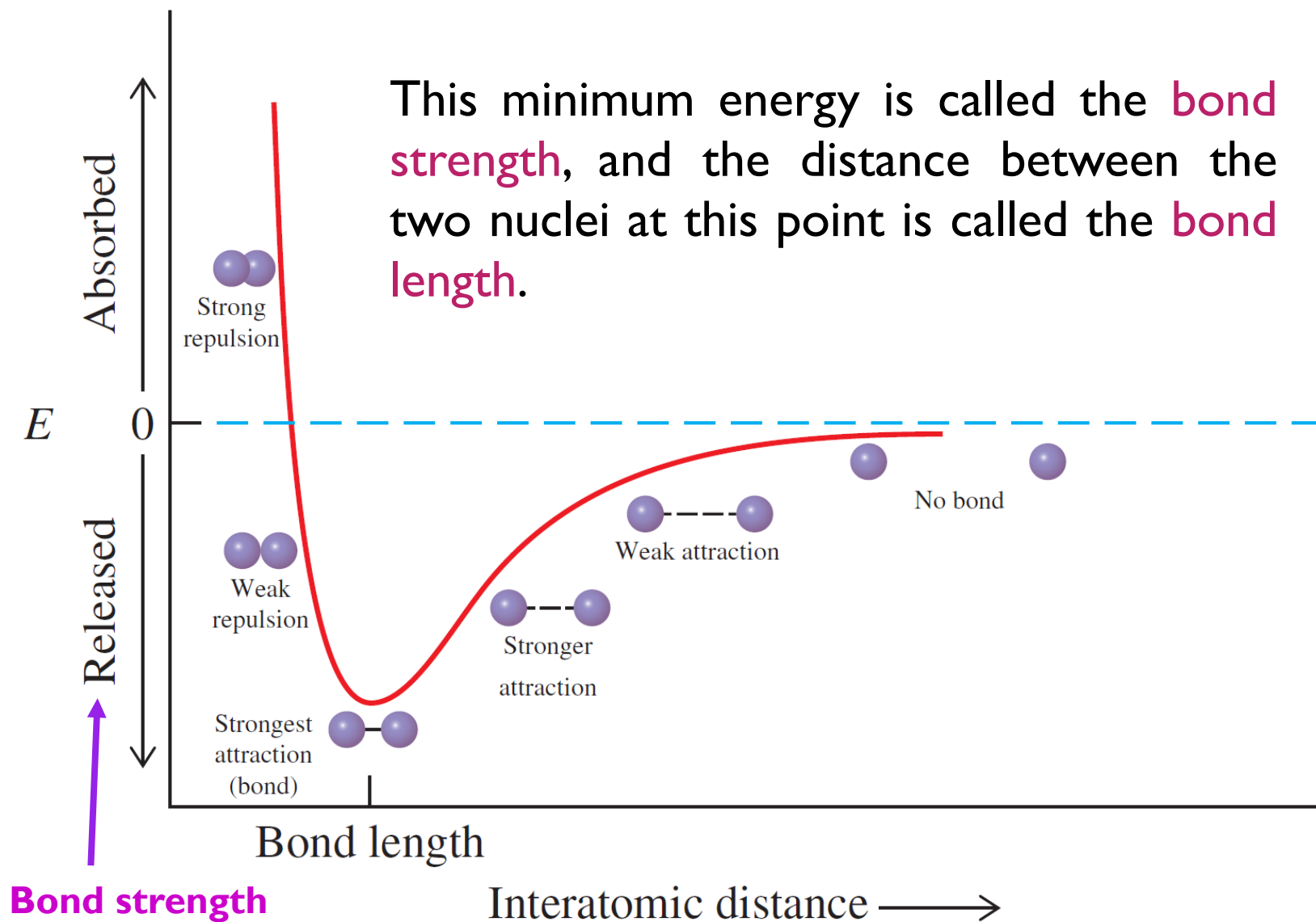
- ❑ Opposite charges attract each other (Coulomb's Law).

$$\text{Attracting force} = \text{constant} \times \frac{(+)\text{ charge} \times (-)\text{ charge}}{\text{distance}^2}$$

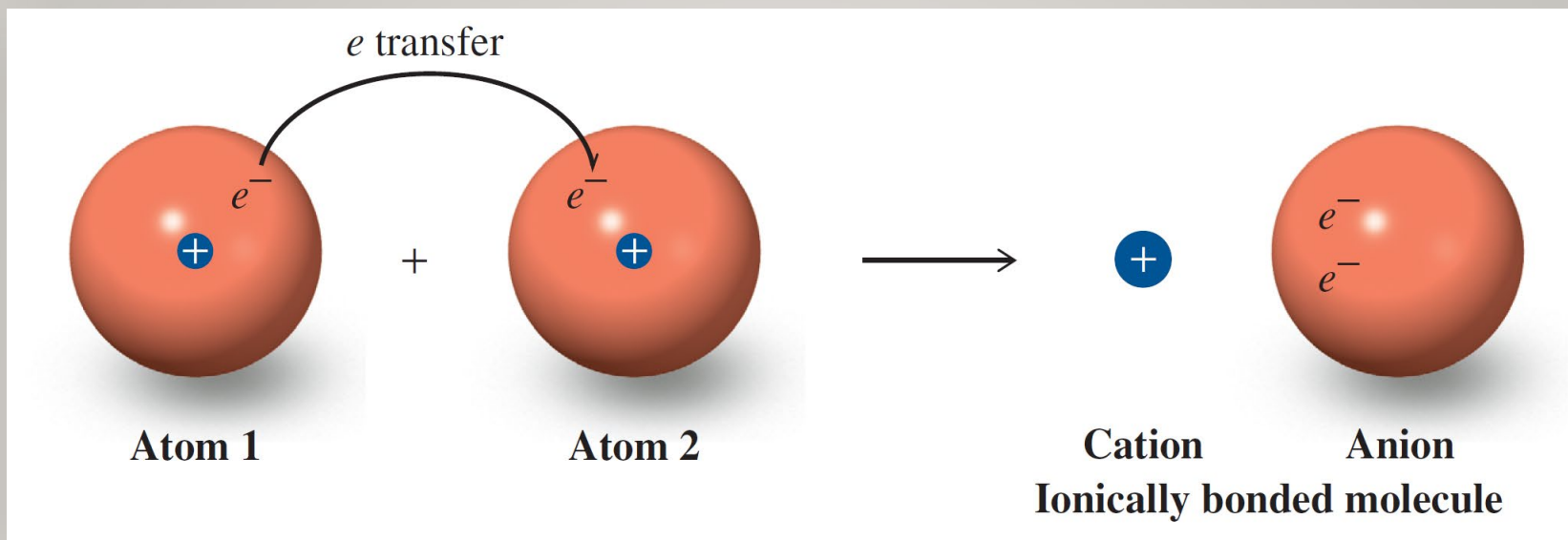
- ❑ Electrons spread out in space (delocalization).
- ❑ Noble gas configuration is desirable.



## I.2 BONDING (IONIC AND COVALENT BONDING)



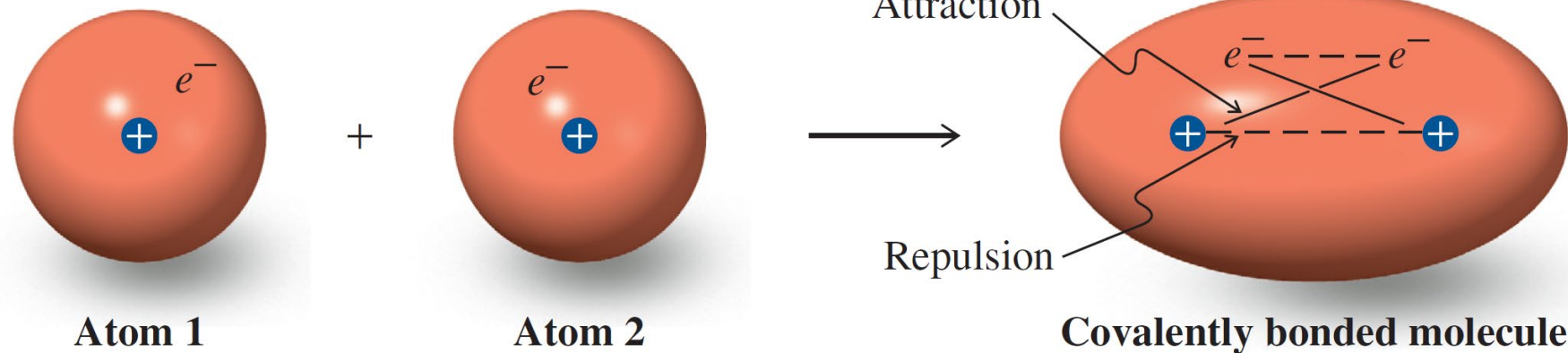
## I.2 ...IONIC BONDING



Ionic Bonds are based on the transfer of one or more electrons from atom to another. The resulting cation and anion are electrostatically attracted to each other.

## 1.2 ...COVALENT BONDING

Covalent Bonds are based on the sharing of electrons



### Dimensions:

Nuclear diameter  $\sim 10^{-15}$  m  
Electronic orbit  $\sim 10^{-10}$  m

} five orders of magnitude

Mass ratio proton/electron =  $\sim 1800$

If the electrons are not shared equally, a polar covalent (partially ionic) bond is formed, otherwise a pure covalent bond is formed.



## I.2 ...THE OCTET RULE

The periodic table underlies the octet rule.

Electrons in atoms occupy levels or shells of fixed capacity. The first has room for 2, the second 8, and the third 16. Noble gases have 8 valence electrons (Helium: 2) and are particularly stable.

Other elements lack octets in their outer electron shells and tend to form molecules in such a way as to create a stable octet arrangement.

Duet

TABLE 1-1 Partial Periodic Table								
Period							Halogens	Noble gases
First	H <sup>1</sup>							He <sup>2</sup>
Second	Li <sup>2,1</sup>	Be <sup>2,2</sup>	B <sup>2,3</sup>	C <sup>2,4</sup>	N <sup>2,5</sup>	O <sup>2,6</sup>	F <sup>2,7</sup>	Ne <sup>2,8</sup>
Third	Na <sup>2,8,1</sup>	Mg <sup>2,8,2</sup>	Al <sup>2,8,3</sup>	Si <sup>2,8,4</sup>	P <sup>2,8,5</sup>	S <sup>2,8,6</sup>	Cl <sup>2,8,7</sup>	Ar <sup>2,8,8</sup>
Fourth	K <sup>2,8,8,1</sup>						Br <sup>2,8,18,7</sup>	Kr <sup>2,8,18,8</sup>
Fifth							I <sup>2,8,18,18,7</sup>	Xe <sup>2,8,18,18,8</sup>
<i>Note:</i> The superscripts indicate the number of electrons in each principal shell of the atom.								

Valence electrons

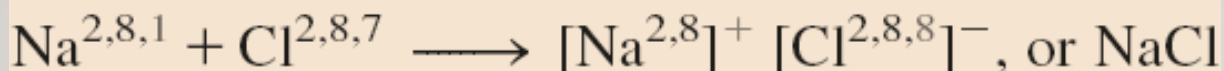
Octets

## I.2 ...THE OCTET RULE

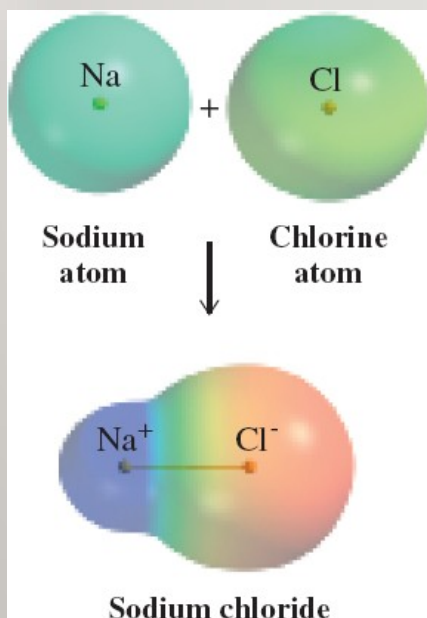
In pure ionic bonds, electron octets are formed by transfer of electrons.

Alkali metals react with halogens by the transfer of one electron from the alkali metal to the halogen.

### Formation of Ionic Bonds by Electron Transfer



Both atoms achieve a noble gas configuration: the alkali metal that of the preceding inert gas, the halogen that of the following inert gas.



$$IP_{\text{Na}} = +119 \text{ kcal mol}^{-1}$$

$$EA_{\text{Cl}} = -83 \text{ kcal mol}^{-1}$$

$$-LE = -120 \text{ kcal mol}^{-1}$$

$$\otimes E = -84 \text{ kcal mol}^{-1}$$

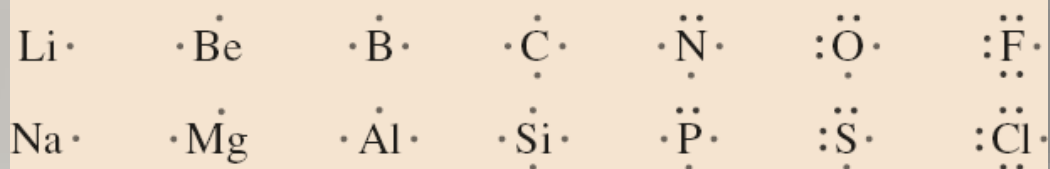


## I.3 VALENCE

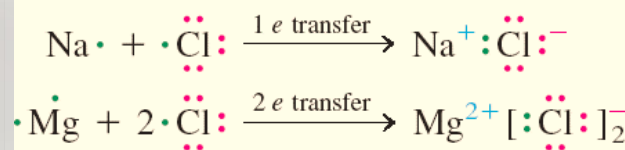
Valence electrons are conveniently indicated by placing dots around the symbol for an element.

(The letters represent the nucleus and the core electrons, and the dots represent the valence electrons)

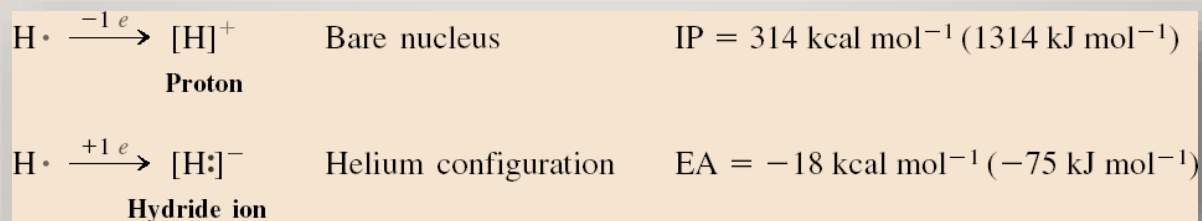
### Valence Electrons as Electron Dots



### Electron-Dot Picture of Salts



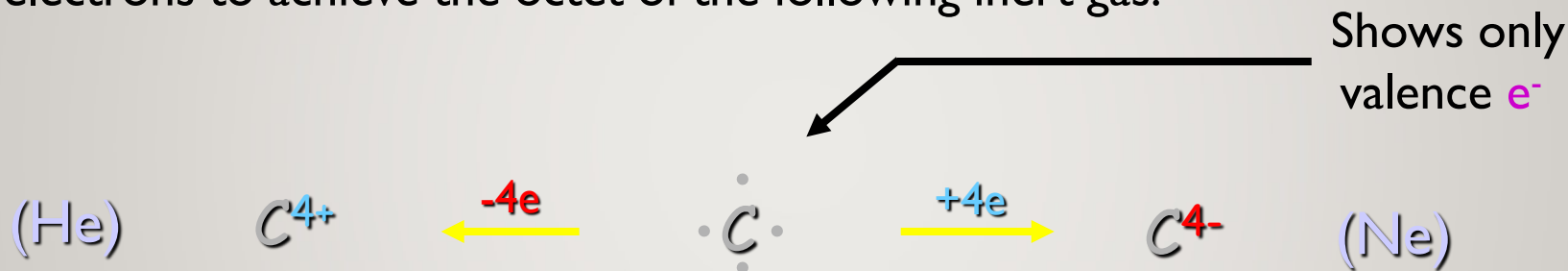
Hydrogen can either lose an electron to form an  $\text{H}^+$  ion, or gain an electron to form a  $\text{H}^-$ , or hydride, ion



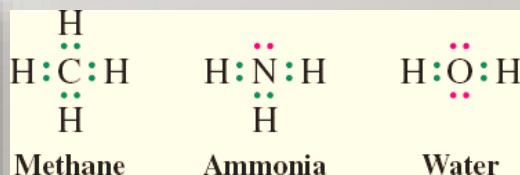
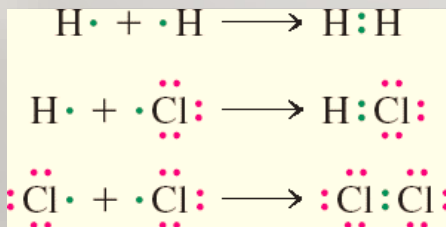
# 1.3 VALENCE

In covalent bonds, electrons are shared to achieve octet configurations

- ❑ Ionic bonds between identical atoms of the same element do not form.
- ❑ The high ionization potential of hydrogen prevents it from forming ionic bonds with halogens and other non-metallic elements.
- ❑ Ionic bonds are also unfeasible for carbon since it would require the loss of 4 electrons to achieve the octet of the preceding inert gas, or the gain of 4 electrons to achieve the octet of the following inert gas.

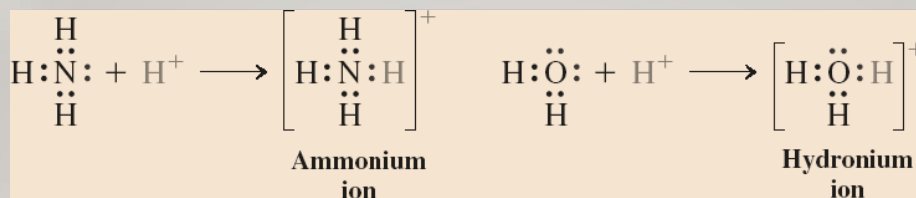


- ❑ In these and similar cases, covalent bonding occurs. Atoms share electrons to achieve a noble gas configuration.

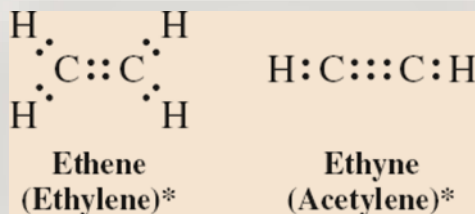


## 1.3 VALENCE

□ In certain cases, one atom supplies both of the electrons in the bond:



□ Often 4 electron (double) and 6 electron (triple) bonds are formed:



- ❖ In most organic bonds, the electrons are not shared equally: polar covalent bonds.
- ❖ Pure covalent bonds (perfect sharing of electrons) and ionic bonds (complete transfer of electrons) are two extreme types of bonding.
- ❖ Most bonds lie somewhere between these extremes and are called **polar covalent bonds**.
- ❖ Each element can be assigned an electronegativity value which represents its electron accepting ability when participating in a chemical bond.

# I.4 VALENCE

**Table 1-2** Electronegativities of Selected Elements

Increasing electronegativity →

			H 2.2				
Li 1.0	Be 1.6	B 2.0	C 2.6	N 3.0	O 3.4	F 4.0	
Na 0.9	Mg 1.3	Al 1.6	Si 1.9	P 2.2	S 2.6	Cl 3.2	
K 0.8						Br 3.0	
						I 2.7	

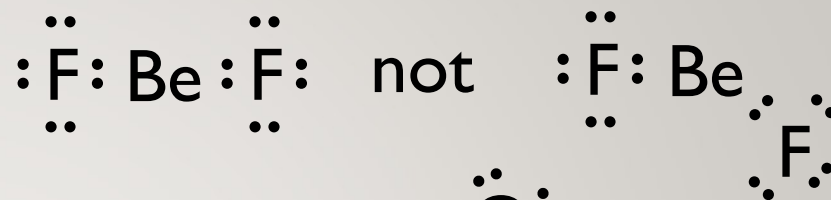
↑ Increasing electronegativity

# I.4 THE SHAPE OF MOLECULES

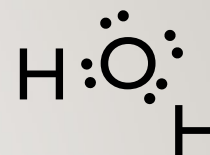
Diatomics: linear (of course), e.g.



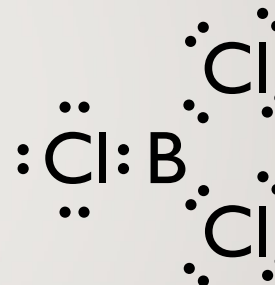
Triatomics: either linear, e.g.



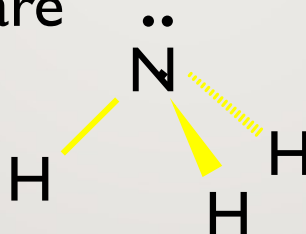
or bent, when there are lone e-pairs, e.g.



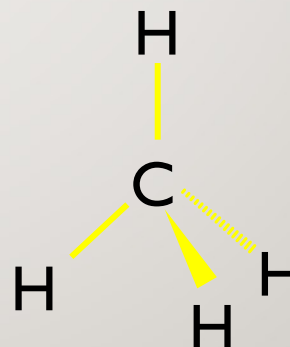
Tetraatomics: either trigonal, e.g.



or pyramidal, when there are lone e-pairs, e.g.



Pentaatomics: tetrahedral, e.g.



## I.5 RESONANCE

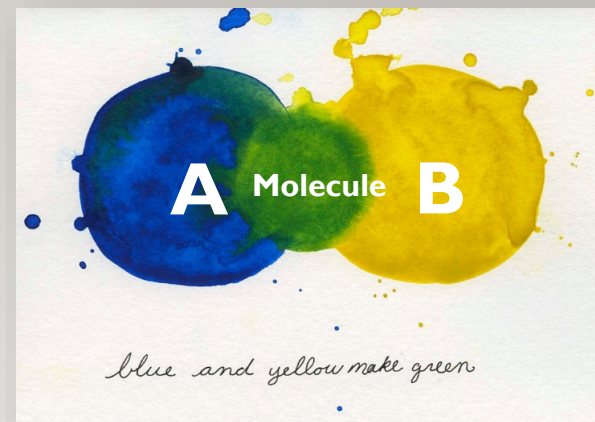
Often several octet structures are possible for a molecule:

Resonance forms



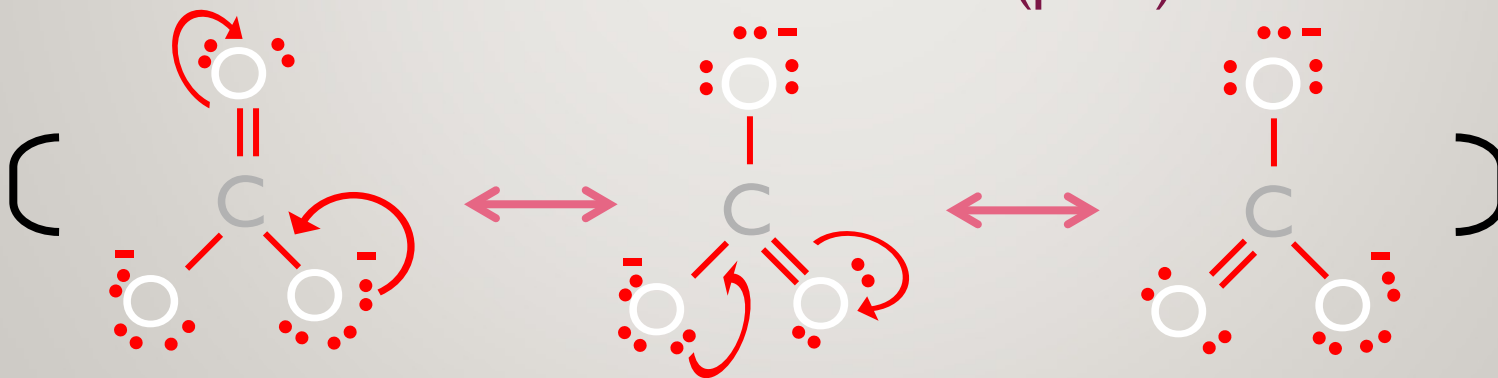
Octet

Non-octet



( Form A  $\longleftrightarrow$  Form B )

move  
electrons  
(pairs)



Carbonate,  $\text{CO}_3^{2-}$  (All forms are equivalent)

# I.6 ORBITALS

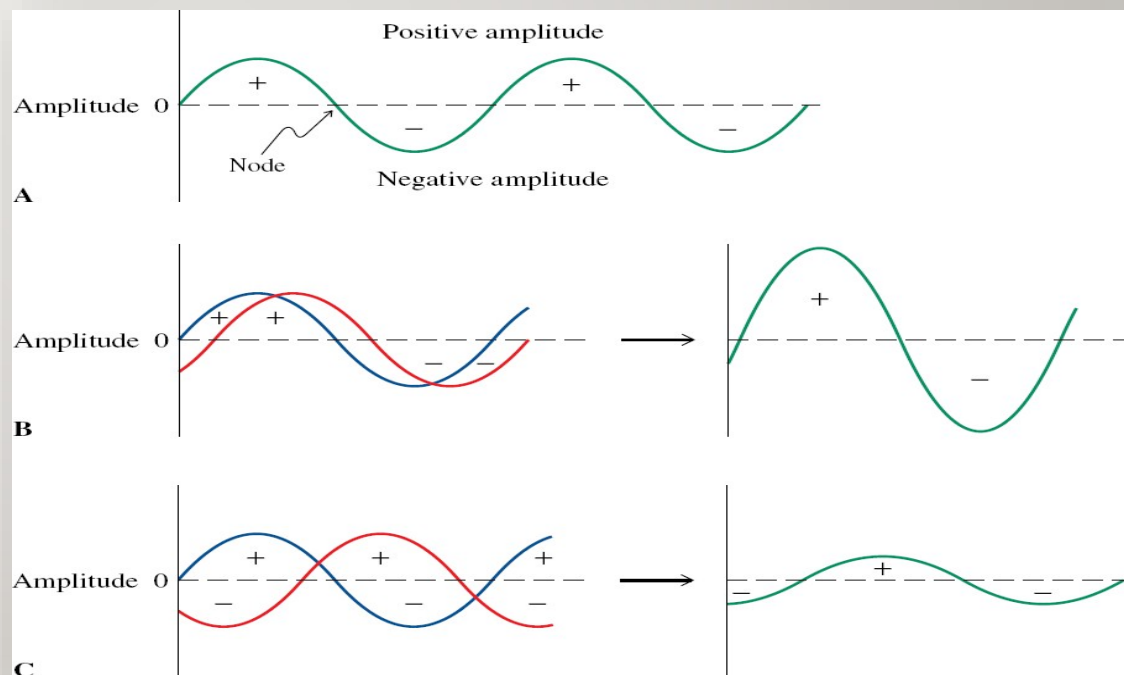
The electron is described by wave equations.

- ❑ An electron within an atom can have only certain definite energies called energy states.
- ❑ Moving particles such as electrons exhibit a wavelength determined by the de Broglie relation:

$$\lambda = \frac{h}{mv}$$

- ❑ Where  $h$  is Planck's constant,  $m$  is the mass of the electron in kg, and  $v$  is the velocity of the electron in m/s.

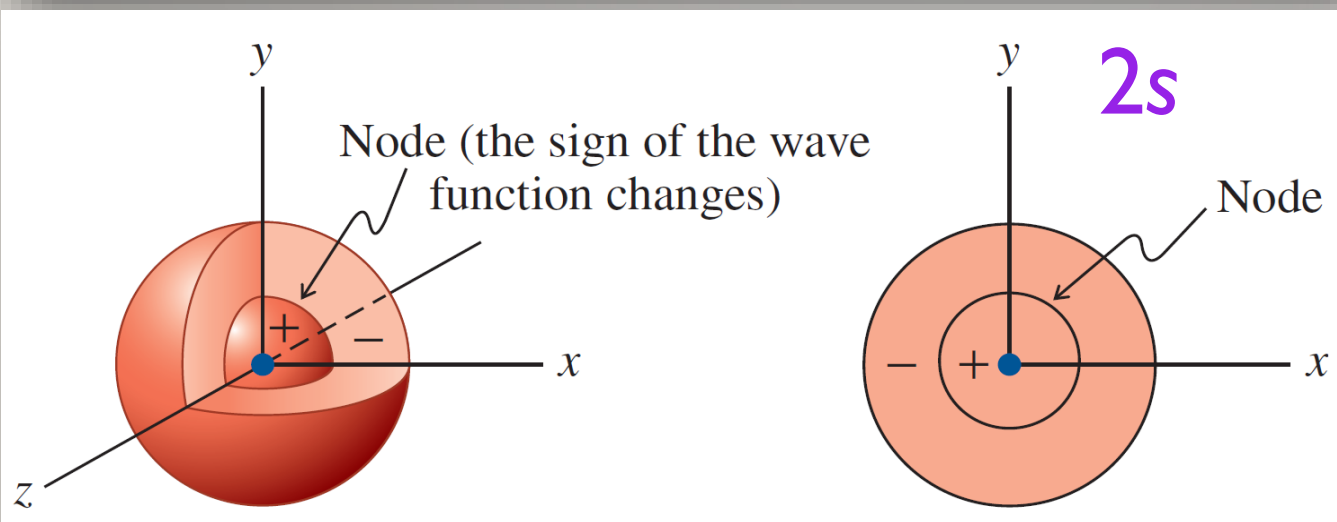
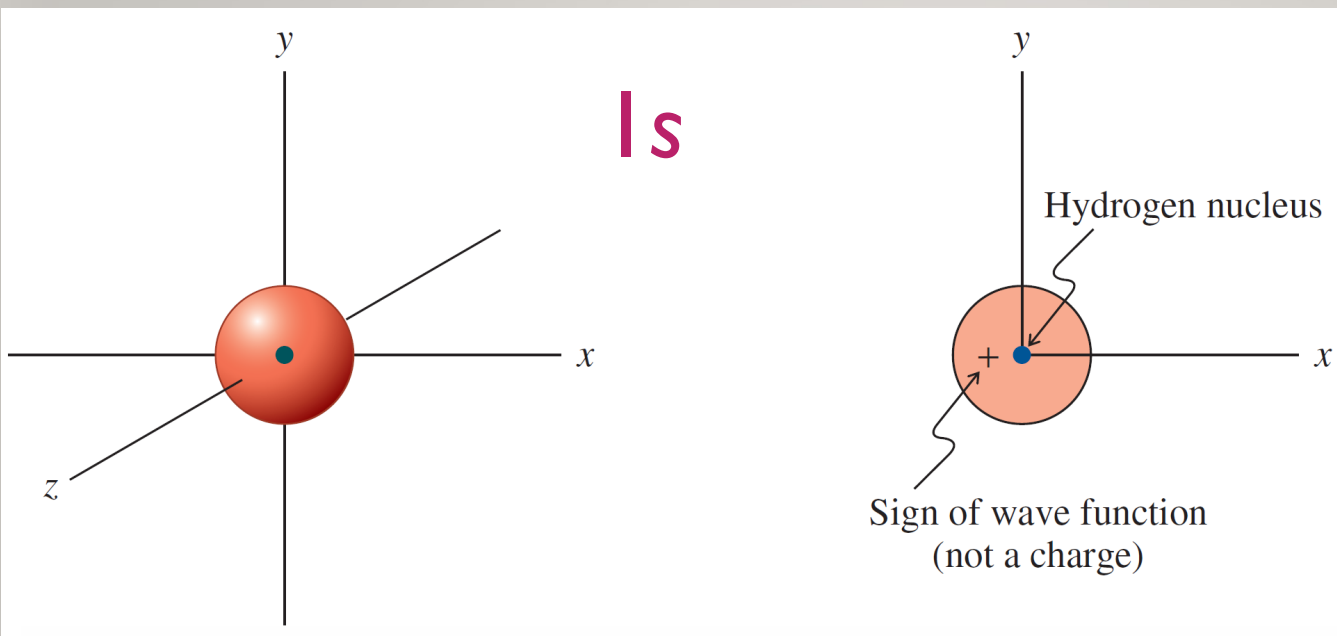
The electron waves contain nodes, where the amplitude of the wave changes sign, and can interact with each other, producing either constructive or destructive interference:





## 1.6.1 ATOMIC ORBITALS

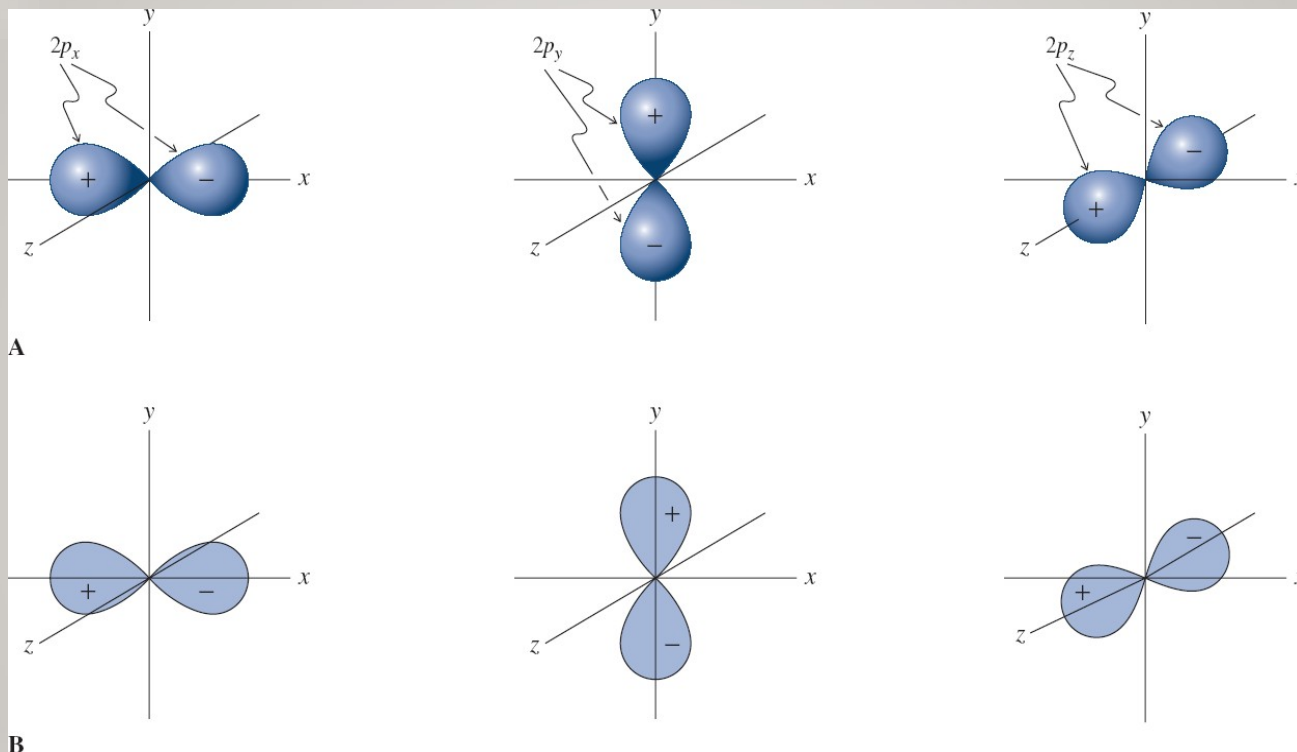
The simplest atomic orbitals are spherical in shape and are called s orbitals. The lowest energy s orbital is the 1s orbital.



For more details please study: *Organic Chemistry: Structure and Function Eighth Edition*. [K. Peter C. Vollhardt](#) (Author), [Neil E. Schore](#) (Author) **ISBN-10:** 1319079458

## I.6.1 ATOMIC ORBITALS

Of slightly higher energy than the 2s orbital are 3 degenerate 2p orbitals. These orbitals are shaped like a figure 8 and point along the 3 Cartesian axes.



## I.6.2 MOLECULAR ORBITALS

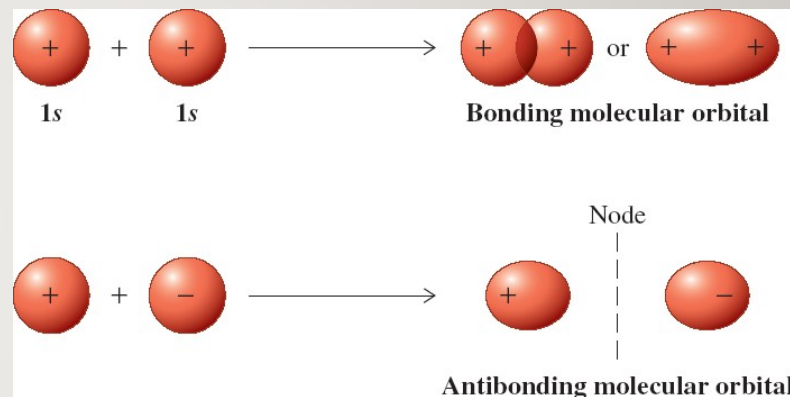
The bond in the hydrogen molecule is formed by the overlap of 1s atomic orbitals

Atomic orbitals on different atoms may overlap.

The overlap of electron waves represented by the atomic orbitals may result in constructive (in phase) or destructive (out of phase) interference.

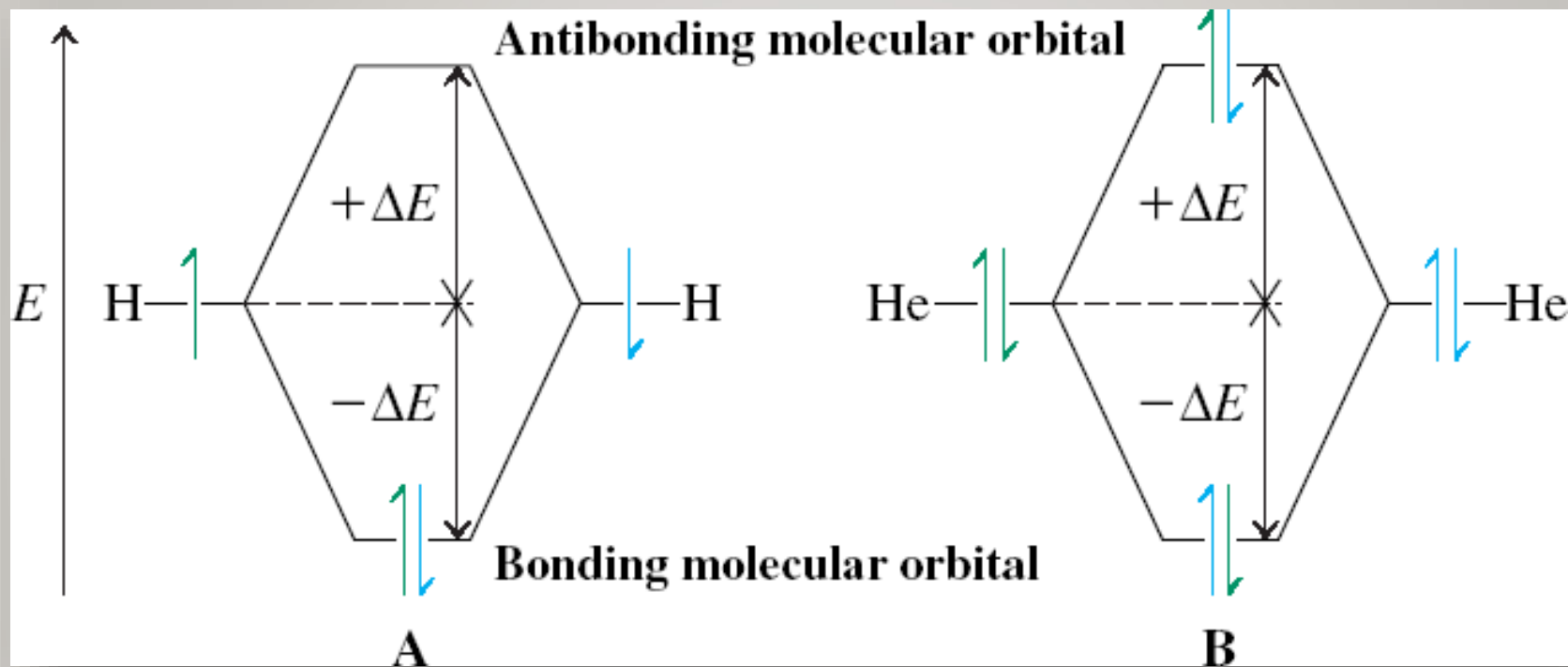
In phase overlap between two 1s orbitals results in a new orbital having lower energy than either of the s orbitals. This new orbital concentrates the electron probability between the two nuclei.

Out of phase overlap between two 1s orbitals results in a new orbital having higher energy than either of the s orbitals. This new orbital places most of the electron probability to the left and right of the two nuclei.



## I.6.2 MOLECULAR ORBITALS

An energy level diagram can now be made of the two overlapping orbitals, and the Aufbau process used to determine the electronic configurations of  $\text{H}_2$  and  $\text{He}_2$ :

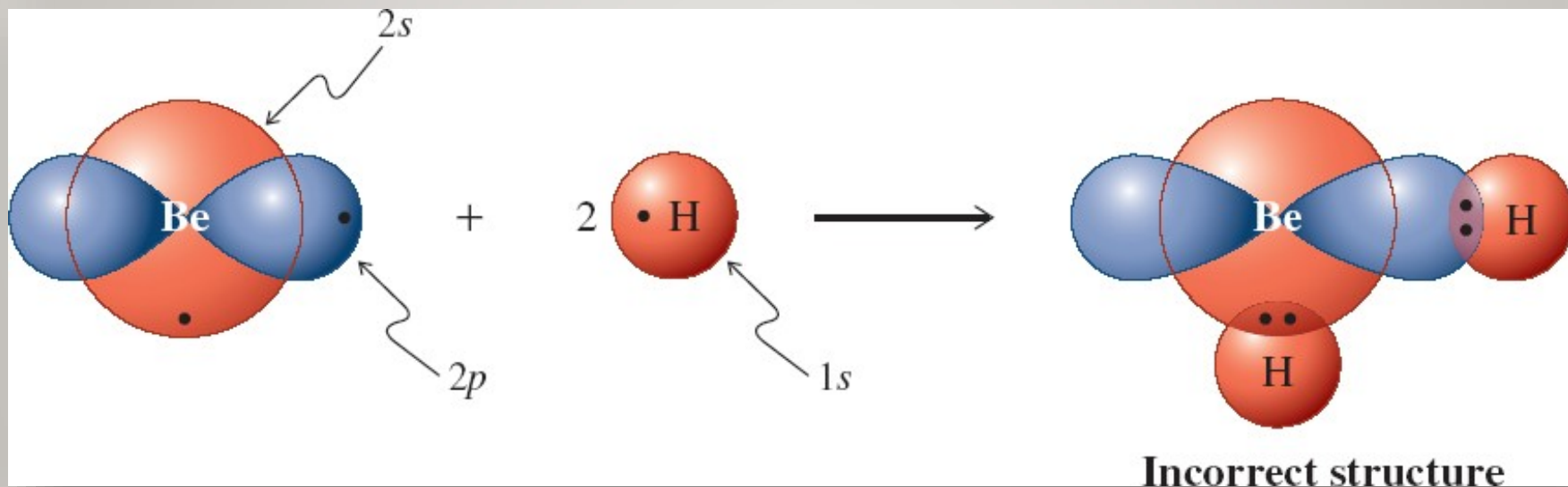


## I.6.3 HYBRID ORBITALS

Mixing of atomic orbitals from the same atom results in new atomic orbitals of different energy and directionality.

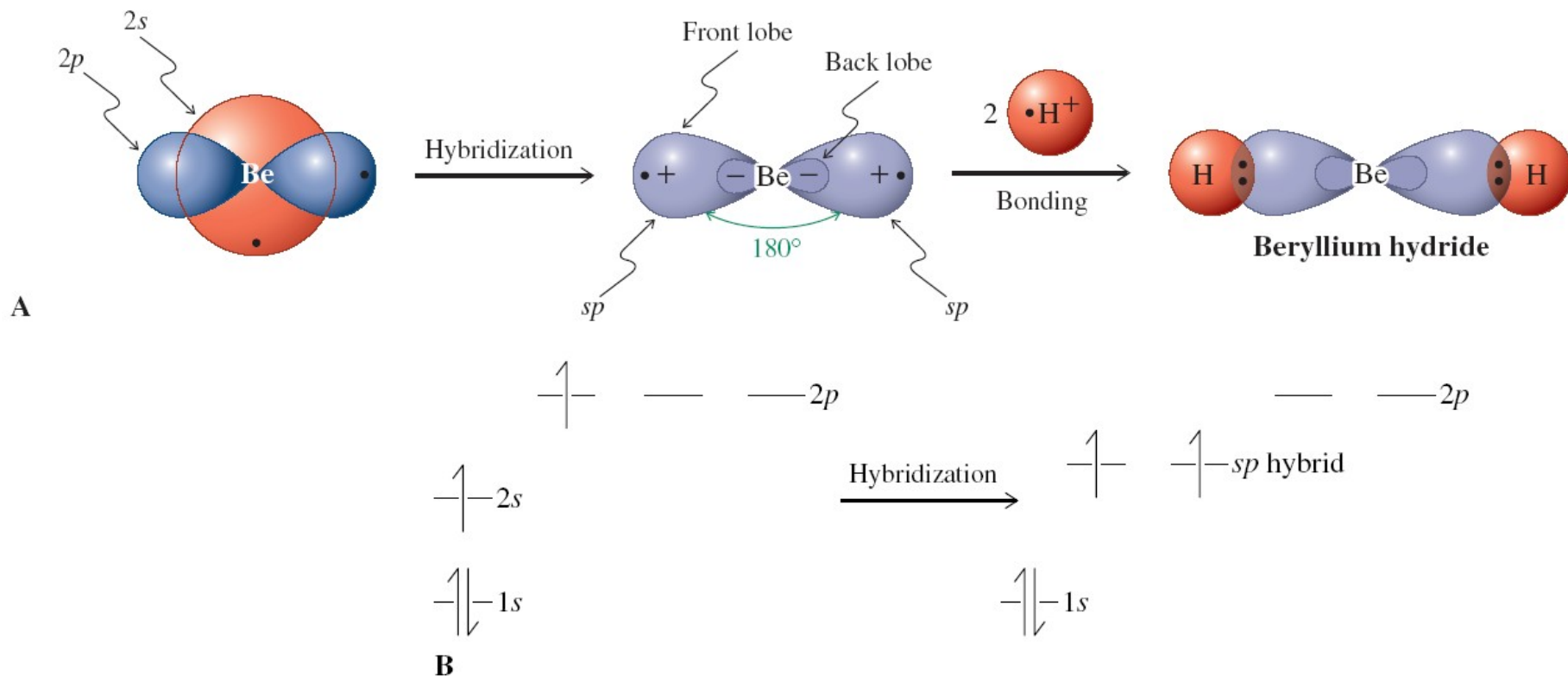
**sp Hybrids produce linear structures:**

An incorrect structure for  $\text{BeH}_2$  is predicted if 2s and 2p orbitals of Be are overlapped with the 1s orbitals of H:



## 1.6.3 HYBRID ORBITALS

Mixing the 2s orbital with one of the 2p orbitals of Be results in two new hybrid sp orbitals, each made up of 50% s and 50% p character. The resulting bond angle is  $180^\circ$  which corresponds with the observed bond angle in the  $\text{BeH}_2$  molecule



Hybridization does not change the number of orbitals on the atom. In this case two atomic orbitals are replaced by two new hybrid orbitals. The two unhybridized p orbitals are still available to hold electrons.

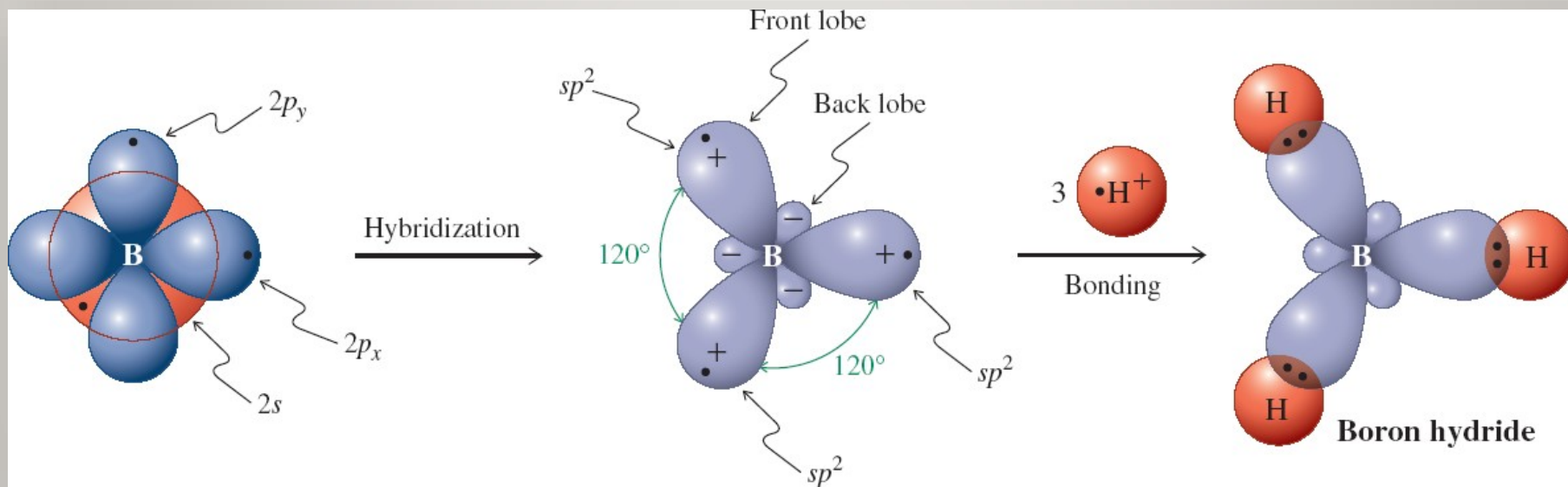
## I.6.3 HYBRID ORBITALS

$sp^2$  Hybrids create trigonal structures.

Hybridization of a 2s and two 2p orbitals results in three new hybrid orbitals that point to the corners of an equilateral triangle.

The remaining p orbital points up and down, perpendicular to each of the three hybrid orbitals.

Bond angles in molecules using  $sp^2$  hybridization are approximately  $120^\circ$



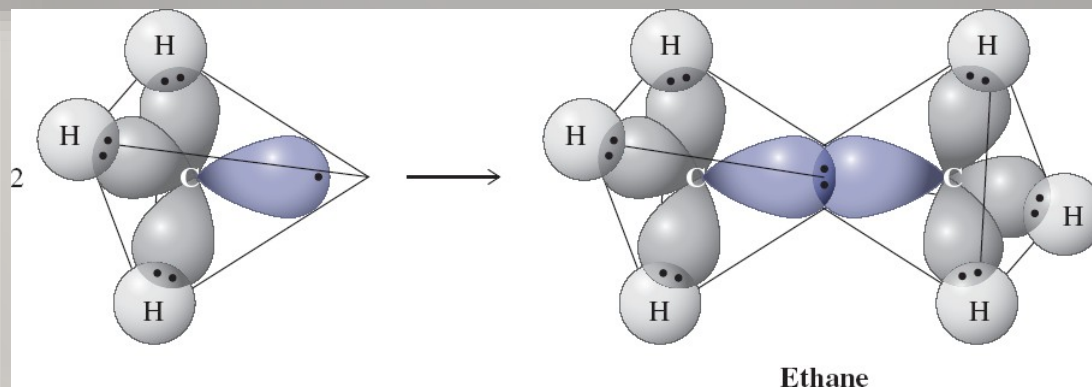
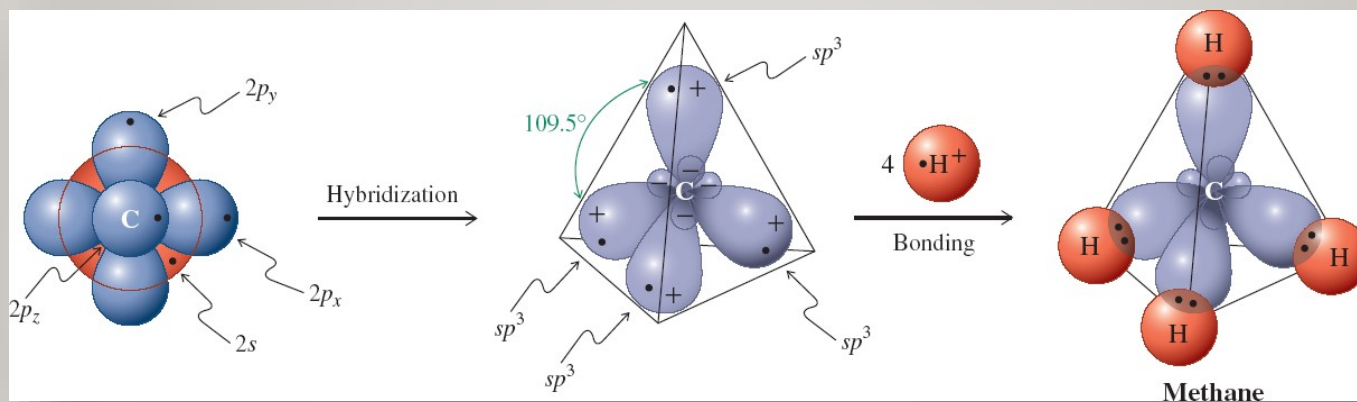


## I.6.3 HYBRID ORBITALS

$sp^3$  hybridization explains the shape of tetrahedral carbon compounds.

When the 2s and all three 2p orbitals are hybridized, four hybrid orbitals called  $sp^3$  orbitals are formed. These orbitals point to the corners of a regular tetrahedron.

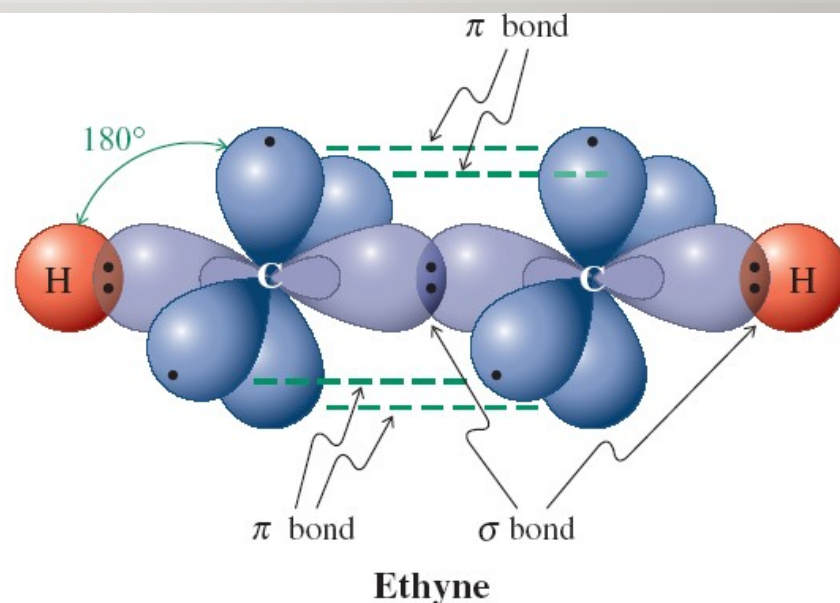
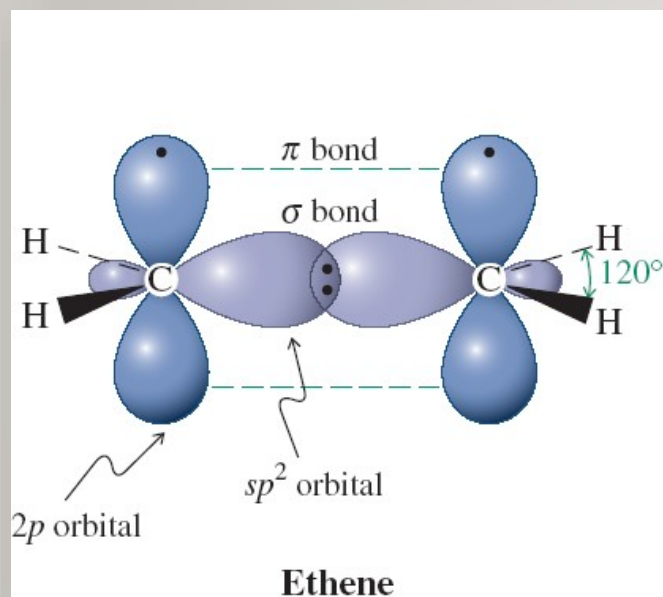
Bond angles in molecules using  $sp^3$  hybridization are approximately  $109.5^\circ$



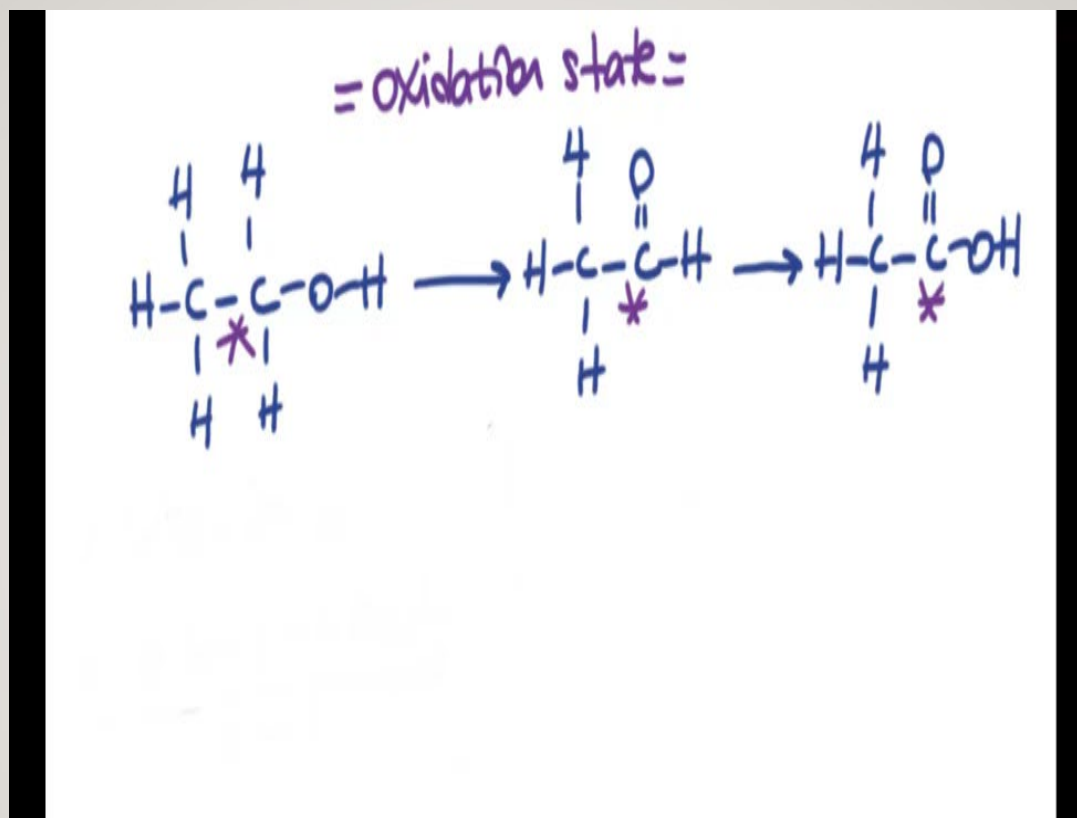
## I.6.3 HYBRID ORBITALS

Pi bonds are present in ethene (ethylene) and ethyne (acetylene).



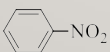
Molecules containing double or triple bonds contain unhybridized p orbitals that overlap lengthwise rather than end on.



## I.7 OXIDATION STATE



# I.8 CLASSIFICATION OF ORGANIC COMPOUNDS ACCORDING TO FUNCTIONAL GROUPS

Functional Group	Compound	Prefix/Suffix	Example	IUPAC Name (Common Name)
<b>Hydrocarbons</b>				
R-H	Alkane	-ane	CH <sub>3</sub> CH <sub>3</sub>	ethane
C=C	Alkene	-ene	H <sub>2</sub> C=CH <sub>2</sub>	ethene (ethylene)
C≡C	Alkyne	-yne	HC≡CH	ethyne (acetylene)
Ar-H	Arenes	-ene		benzene
<b>Halogen-Containing Compounds</b>				
R-X	Haloalkane	halo-	CH <sub>3</sub> Cl	chloromethane
Ar-X	Aryl halides	halo-		chlorobenzene
<b>Oxygen-Containing Compounds</b>				
R-OH	Alcohol	-ol (hydroxy-)	CH <sub>3</sub> OH	methanol
ArOH	Phenols	-ol		phenol
R-O-R	Ether	ether (alkoxy-)	CH <sub>3</sub> OCH <sub>3</sub>	dimethyl ether
RCOH	Aldehyde	-al	CH <sub>3</sub> CHO	ethanal (acetaldehyde)
RCOR	Ketone	-one	CH <sub>3</sub> COCH <sub>3</sub>	propanone (acetone)
RCOOH	Carboxylic acid	-oic acid	CH <sub>3</sub> COOH	ethanoic acid (acetic acid)
<b>Carboxylic Acid Derivatives</b>				
RCOOR	Ester	-oate	CH <sub>3</sub> COOCH <sub>3</sub>	methyl ethanoate (methyl acetate)
RCOOX	Acyl halides	-acyl	CH <sub>3</sub> COOCl	Acetyl chloride
RCONH <sub>2</sub>	Amide	-amide	CH <sub>3</sub> CONH <sub>2</sub>	ethanamide (acetamide)
RCOOCOR	Anhydride	-anhydride	CH <sub>3</sub> COOOCH <sub>3</sub>	Acetic anhydride
<b>Nitrogen-Containing Acid Derivatives</b>				
R-NH <sub>2</sub>	Amine	-amine (amino-)	CH <sub>3</sub> CH <sub>2</sub> NH <sub>2</sub>	ethylamine aminoethane
RC≡N	Nitriles	-nitrile (cyano)	CH <sub>3</sub> C≡N	acetonitril
ArNO <sub>2</sub>	Nitro compounds	-nitro		nitrobenzene

For more details please study: *Organic Chemistry: Structure and Function Eighth Edition* [K. Peter C. Vollhardt](#) (Author), [Neil E. Schore](#) (Author) **ISBN-10: 1319079458**