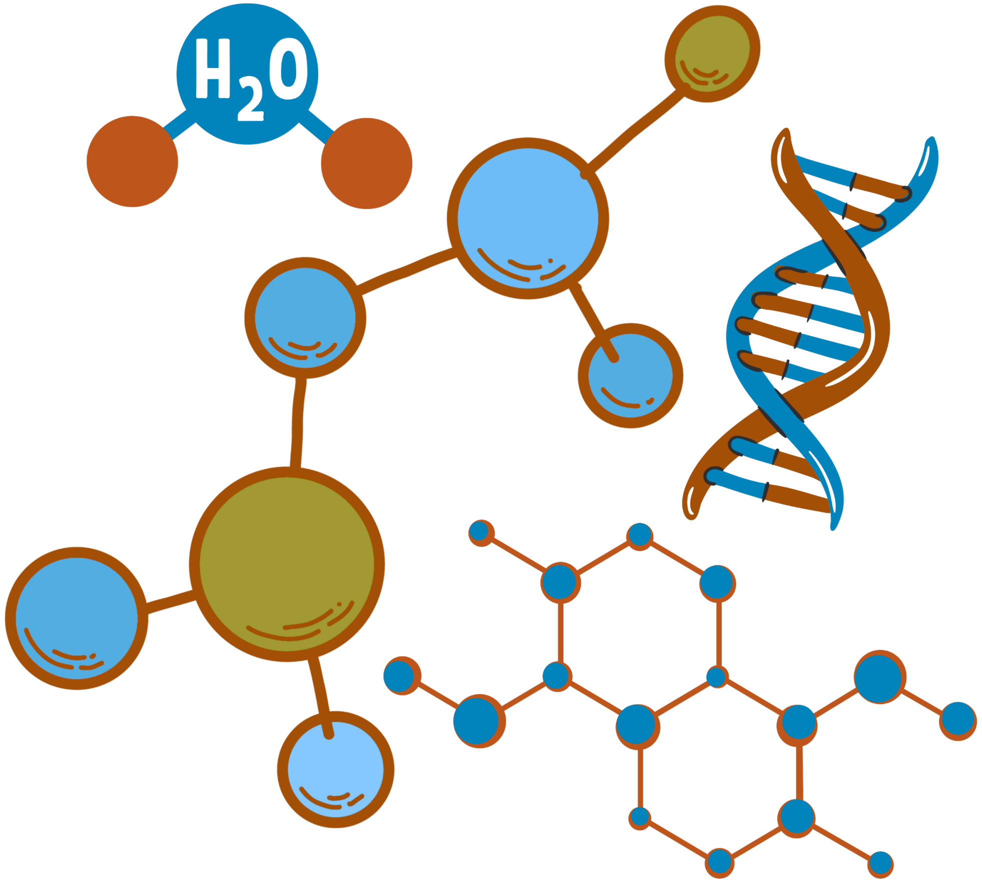
Introduction to Organic Chemistry
CHEM 109

جامعة الملك سعود
King Saud University
COLLEGE OF SCIENCES
CHEMISTRY DEPARTMENT

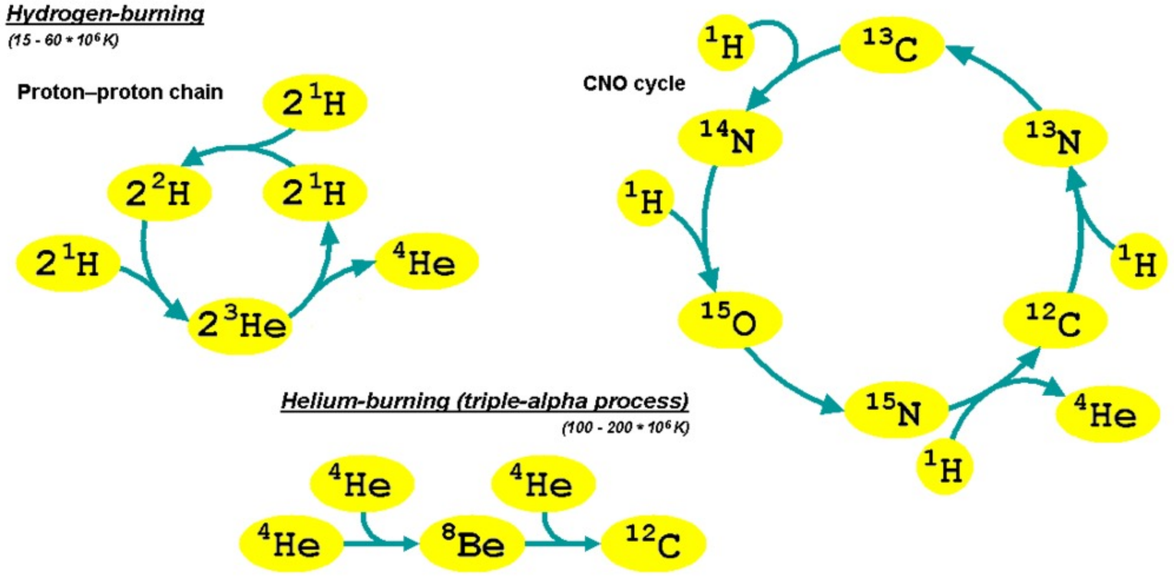
Chapter 1:
Introduction to Organic Chemistry



1. Origins and Scope of Organic Chemistry

1.1 Life and the Chemistry of Carbon Compounds.

- **Why Carbon?**
  - Basis of organic chemistry (carbon compounds).
  - Carbon forms strong and diverse bonds:
    - With itself → form long chains and rings.
    - With H, N, O, S → form wide variety of compounds.
    - Central to life's molecular structure compared with silicon-based life molecules (weaker bonds).
- **Origin of Carbon**
  - Heavier elements (like carbon) formed in stars through nuclear fusion and released during supernova explosions.



1. Origins and Scope of Organic Chemistry

1.2 Development of the Science of Organic Chemistry

- **The modern definition of *Organic Chemistry* is the study of carbon/hydrogen-based compounds and their corresponding derivatives.**
- **The development for the concept of organic chemistry has passed in different stages:**

1- Vitalism in the 19th Century:

- Claimed organic compounds only came from living organisms.
- Inorganic compounds = substances from nonliving sources.

2- Wöhler's Discovery (1828)

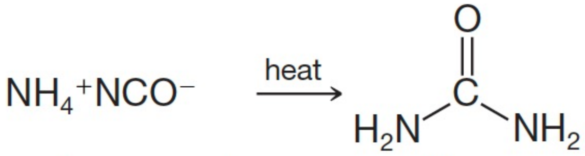
- Friedrich Wöhler synthesized urea (organic, from urine) from ammonium cyanate (inorganic).
- Proved that organic compounds can be synthesized from inorganic precursors.

3- Despite science rejecting vitalism, "organic" is still used in popular contexts:

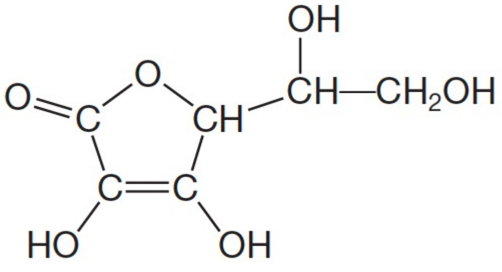
- Organic food → grown without synthetic fertilizers/pesticides.
- Organic vitamins → isolated from natural sources, not synthesized.
- Organic fertilizers → derived from natural materials.

4- Modern Terminology:

- In science, the study of compounds from living organisms is now called natural products chemistry.
- This field explores biologically derived molecules, often with pharmaceutical and industrial importance.



Ammonium cyanate **Urea**

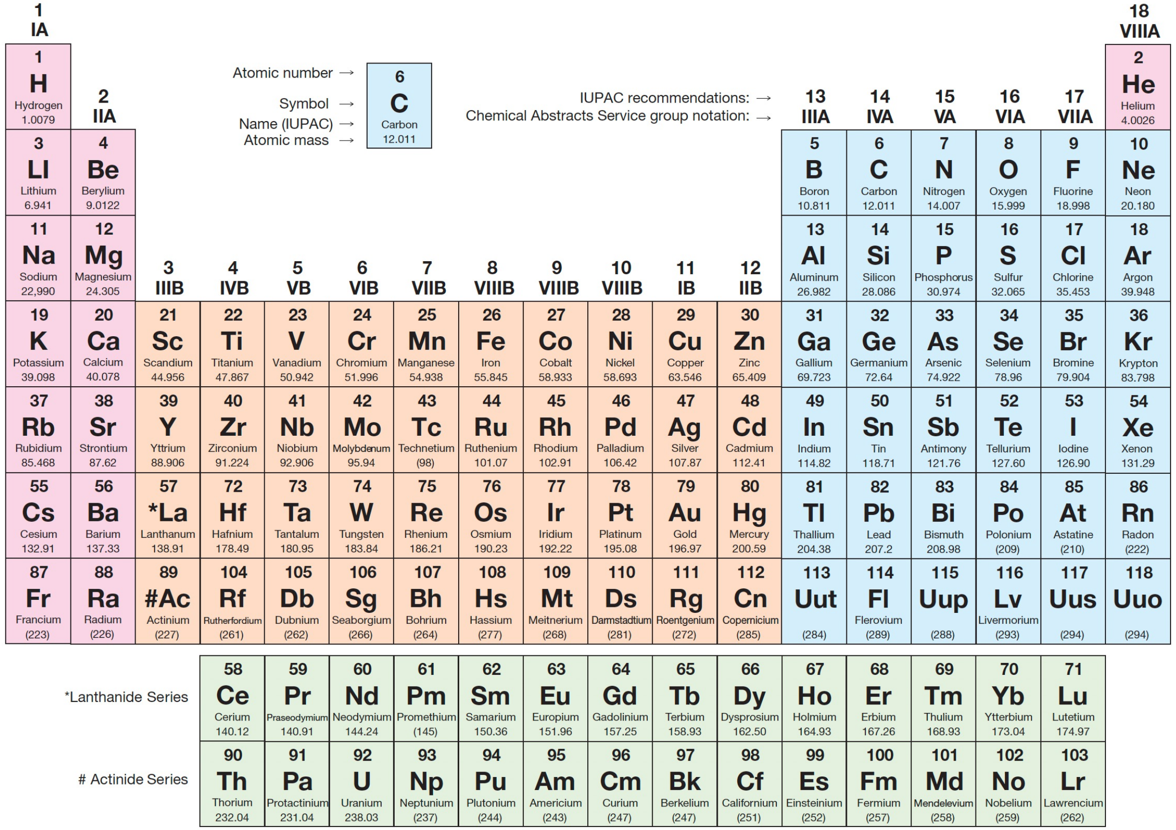


Vitamin C

2. Atomic structure, Electron Configuration, and Molecular Orbitals

2.1 Atomic Structure

- Compounds are made of elements combined in different proportions.
- An element is a pure chemical substance that cannot be broken down into simpler substances by ordinary chemical means.
- Each element is made up of only one kind of atom, which is the smallest unit that retains the element's properties.
- Atoms consist of three main particles: neutrons (neutral charge), protons (positively charged), and electrons (negatively charged).
  - Neutrons and protons are found in the nucleus.
  - Electrons are found outside the nucleus.



Atomic number →
Symbol →
Name (IUPAC) →
Atomic mass →

6
C
Carbon
12.011

IUPAC recommendations: →
Chemical Abstracts Service group notation: →

1 IA	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8 VIIIB	9 VIIIB	10 VIIIB	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
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19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.867	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.409	31 Ga Gallium 69.723	32 Ge Germanium 72.64	33 As Arsenic 74.922	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.798
37 Rb Rubidium 85.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.94	43 Tc Technetium (98)	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.91	46 Pd Palladium 106.42	47 Ag Silver 107.87	48 Cd Cadmium 112.41	49 In Indium 114.82	50 Sn Tin 118.71	51 Sb Antimony 121.76	52 Te Tellurium 127.60	53 I Iodine 126.90	54 Xe Xenon 131.29
55 Cs Cesium 132.91	56 Ba Barium 137.33	57 *La Lanthanum 138.91	72 Hf Hafnium 178.49	73 Ta Tantalum 180.95	74 W Tungsten 183.84	75 Re Rhenium 186.21	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.08	79 Au Gold 196.97	80 Hg Mercury 200.59	81 Tl Thallium 204.38	82 Pb Lead 207.2	83 Bi Bismuth 208.98	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)
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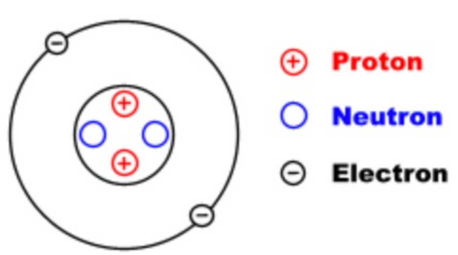
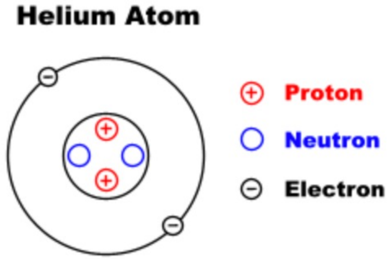
Helium Atom

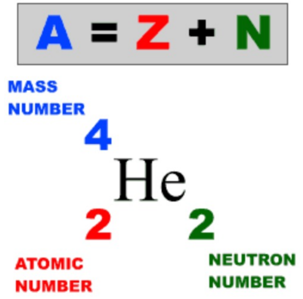


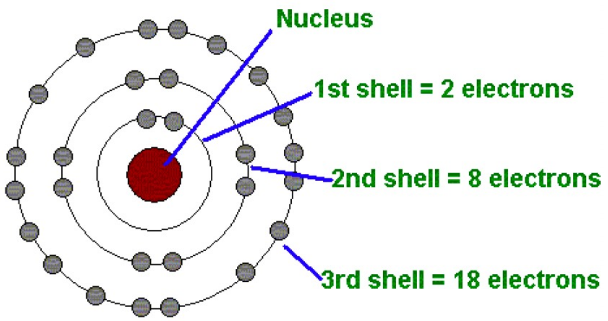
2. Atomic structure, Electron Configuration, and Molecular Orbitals

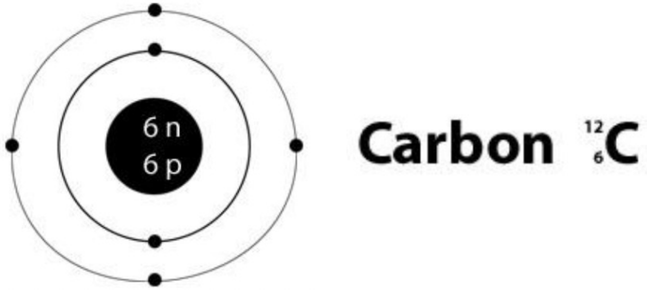
2.1 Atomic Structure

- Atom is electrically neutral:
  - Number of electrons = Number of protons
- The atomic number (Z) of an element is the number of protons.
- The atomic mass (A) is approximately equal to the sum of the number of protons and the number of neutrons in the nucleus.
- Electrons are distributed around the nucleus in successive shells (energy levels) that are designated by capital letters (*K*, *L*, *M*, *N*, ..) or whole numbers (*n*).
  - The maximum capacity of electrons in a shell= $2n^2$ electrons.
  - For example: carbon atom has an atomic number = 6 which means it has 6 electrons are distributed around its nucleus.







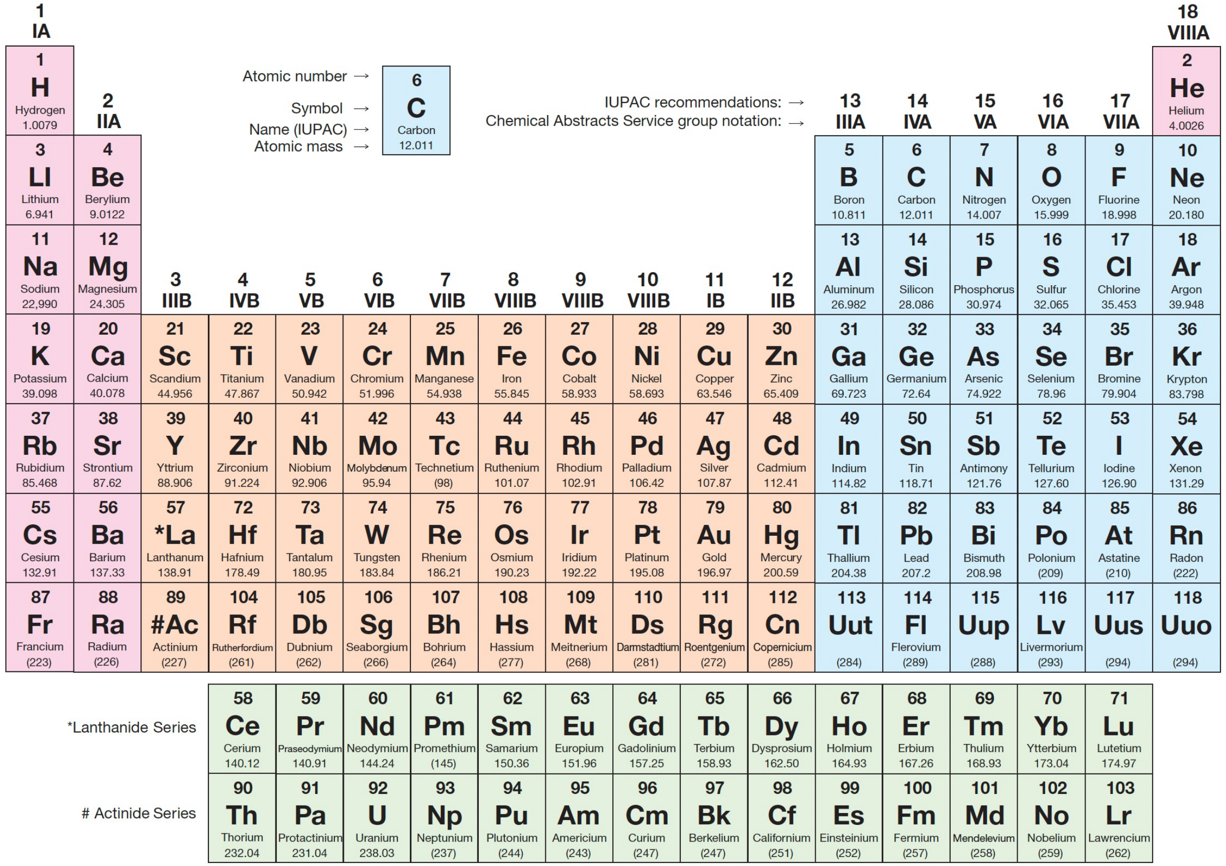


Shell	K	L	M	N
Number of electrons	2	4	0	0

2. Atomic structure, Electron Configuration, and Molecular Orbitals

2.1 Atomic Structure

- Valence Electrons
  - Electrons in general exist in shells of increasing energy and distance from the nucleus.
  - Valence electrons occupy the outmost shells (valence shells).
  - Valence electrons are involved in chemical bonding.
  - The number of valence electrons can be determined by the main group number of the element in the periodic table.
  - For examples:
    - Carbon ($_6C$) – group #4 = 4 valence electrons
    - Oxygen ($_8O$) – group #6 = 6 valence electrons
    - Halogens (X) – group #7 = 7 valence electrons



Atomic number → 6
Symbol → C
Name (IUPAC) → Carbon
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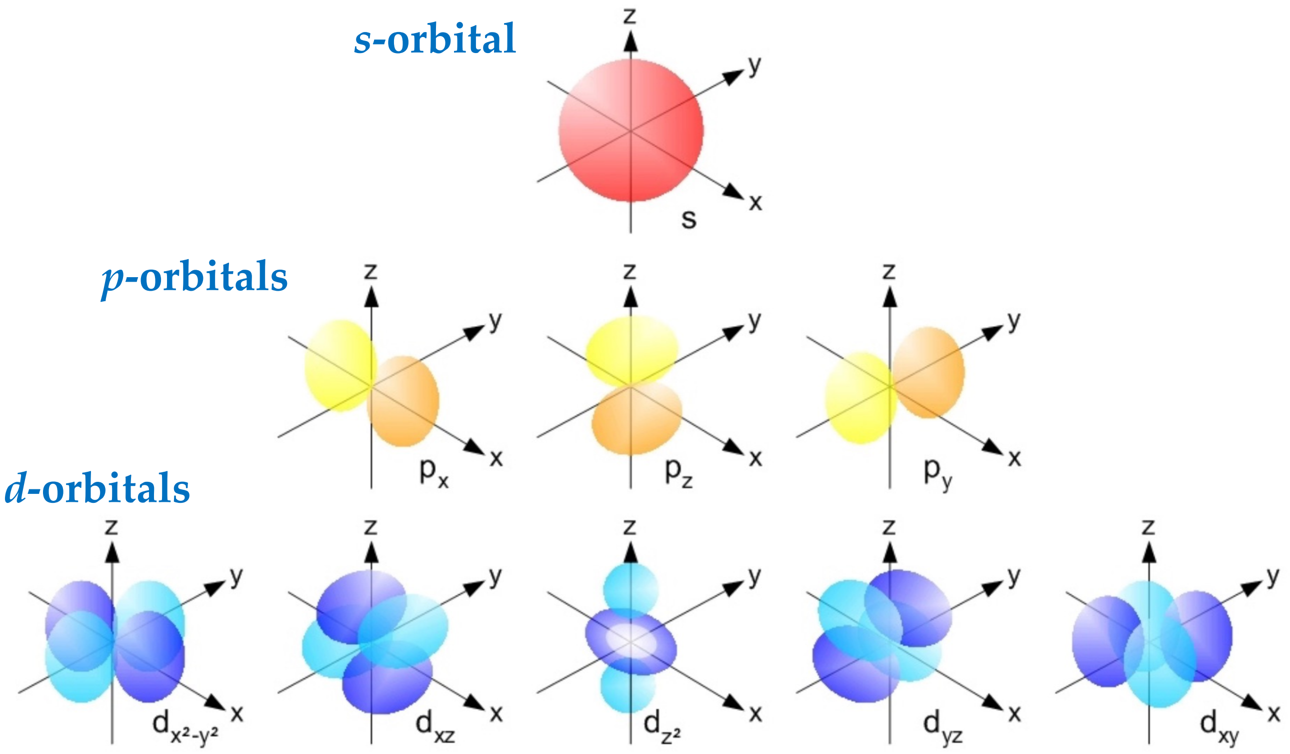
2. Atomic structure, Electron Configuration, and Molecular Orbitals

2.2 Atomic orbitals and electron configuration

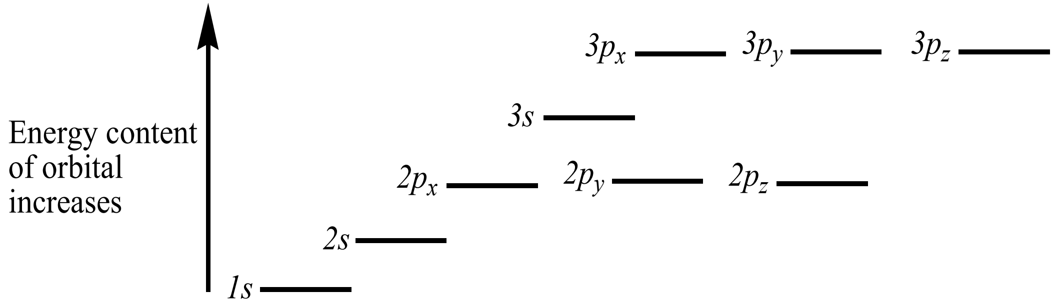
- Atomic Orbitals
  - Orbitals that represent a specific region in space of an atom in which an electron is mostly found.
  - These orbitals are arranged in the order to be filled and increasing their energy.
  - They are designated with letters (*s*, *p*, *d*, and f), and they have different shapes and orientations in space.
    - *s*-orbital: spherical shape.
    - *p*-orbital: dumbbell-shaped in three orientations.
    - *d*-orbital: clover-shaped in five orientations.
    - *f*-orbital: more complex shapes in seven orientations.



2. Atomic structure, Electron Configuration, and Molecular Orbitals

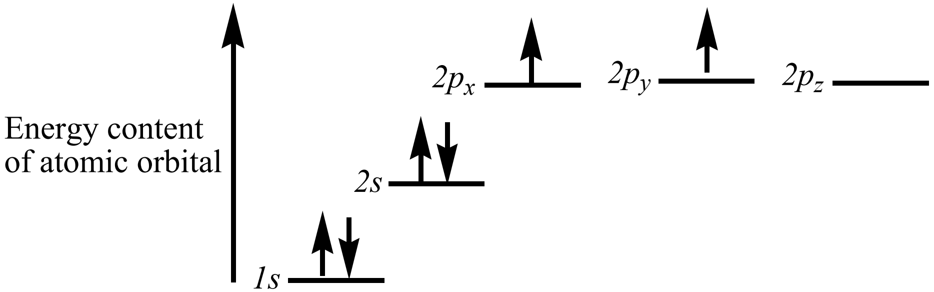
2.2 Atomic orbitals and electron configuration

- Atomic Orbitals
  - Each energy shell has specific numbers and types of the atomic orbitals. For example:
    - *K* shell has only one (1*s*) orbital.
    - L shell has one (2*s*) and three (2*p*) as ($2p_x$, $2p_y$, and $2p_z$).
  - The atomic orbitals are filled as follows:
    - An atomic orbital contains no more 2 electrons (*Aufbau Principle*).
    - Electrons fill orbitals of lower energy first (*Pauli Exclusion Principle*).
    - No sub-orbital is filled by 2 electrons until all the sub-orbitals of equal energy have at lease one electron (*Hund's Rule*).



- **Filling atomic orbitals of carbon atom ($_6$C):**

$1s^22s^22p1x2p1y$ **or** $1s^22s^22p^2$

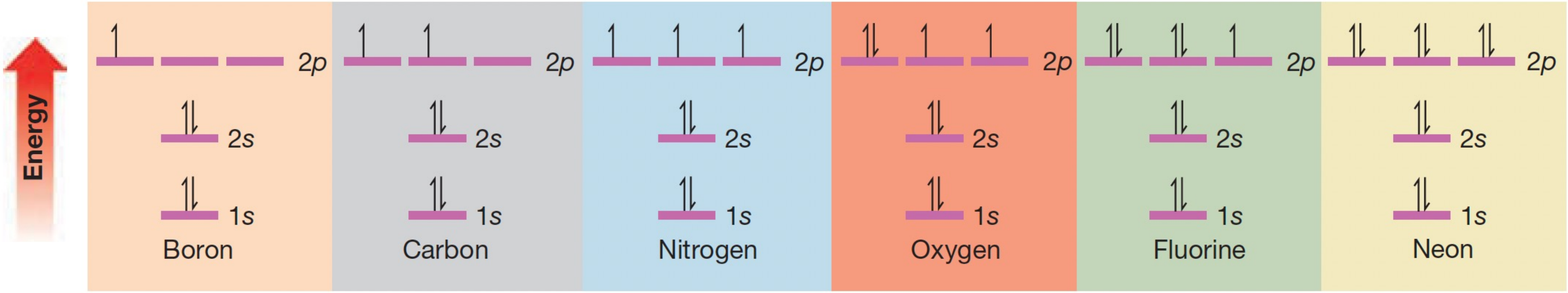


Energy level diagram for carbon.

2. Atomic structure, Electron Configuration, and Molecular Orbitals

2.2 Atomic orbitals and electron configuration

- **Electron configuration is a systematic arrangement of electrons in the orbitals of an atom.**
- **It shows that electrons are distributed among the energy levels (shells), and atomic orbitals (*s*, *p*, *d*, and f).**
- **The following figure shows the ground state electron configuration of some of the second-row elements.**

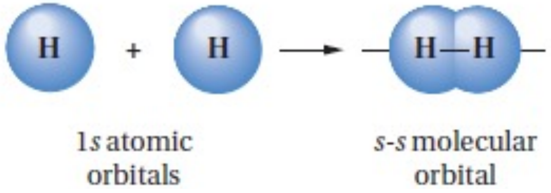


2. Atomic structure, Electron Configuration, and Molecular Orbitals

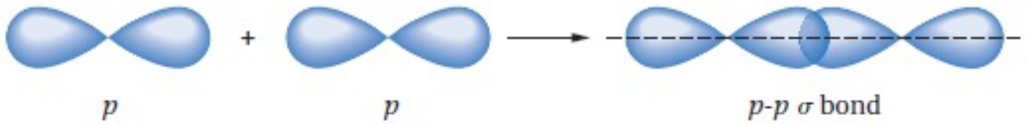
2.3 Molecular Orbitals (MOs)

- **Molecular orbitals are formed as a result of overlapping two atomic orbitals which then gives a bonding system called "covalent bond".**
- **They represent the region of space where one or two electrons of a molecule are likely to be found.**
- **There are two different covalent bonds based on the type of molecular atoms that are involved in the bond formation:**
  - **Sigma bonds (*σ* bonds) that can be formed via:**
    - **The overlap of two (*s*) atomic orbitals.**
    - **The end-on overlap of two (*p*) atomic orbitals.**
    - **The overlap of (*s*) atomic orbital with (*p*) orbital.**
  - **Pi bonds (*π* bonds) which can be formed from the side-side overlap between two (*p*) atomic orbitals.**

➢ **Two (*s*) atomic orbitals overlap:**

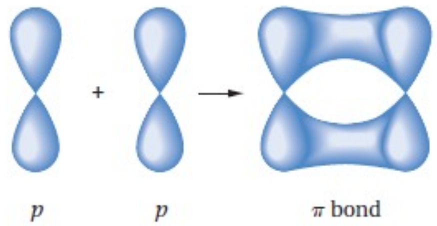


➢ **Two (*p*) atomic orbitals overlap to form (*σ* bond):**



➢ **(*s*) and (*p*) atomic orbitals overlap:**

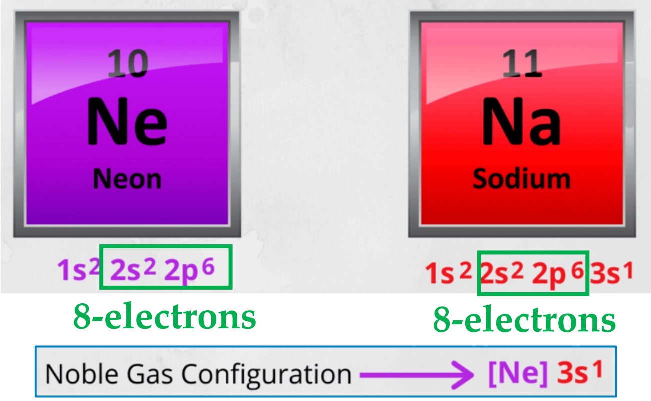
➢ **Two (*p*) atomic orbitals overlap to form (*π* bond):**



3. Chemical Bonding

3.1 Chemical Bonds: The Octet Rule

- **G. N. Lewis and W. Kossel introduced the first explanation for the nature of chemical bonds in 1916.**
- **They proposed that Nobel gases are stable elements and lack common chemical reactivity due to having their valence shells filled with electrons.**
  - **2 electrons in case of helium (exception).**
  - **8 electrons for the other gases.**
- **The Octet Rule can be defined as the trendy for an atom to achieve a configuration which its valence shell contains *eight electrons* alike to a Noble gas's configuration.**
- **According to Lewis, a greater degree of stability can be achieved when two atoms interact to each other by rearranging their valence electron to acquire the outer-shell structure of the nearest noble gas in the periodic table.**



$1s^2 \boxed{2s^2\, 2p^6}$

8-electrons

$1s^2 \boxed{2s^2\, 2p^6} 3s^1$

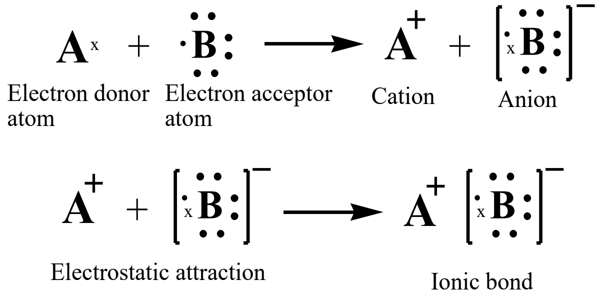
8-electrons

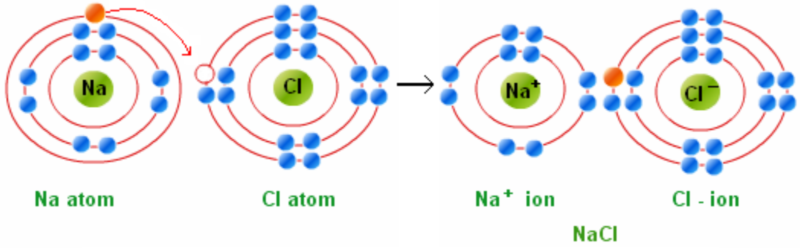
Noble Gas Configuration ⟶ $[Ne]\ 3s^1$

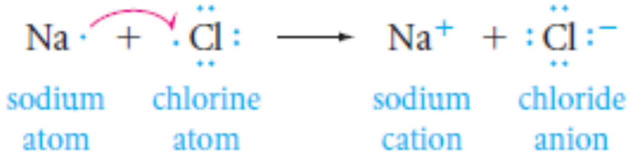
3. Chemical Bonding

3.2 Ionic Bonds

- **Ionic Bonds** (electrovalent bonds) are formed by transfer one or more electrons from one atom to another in order to create ions.
- The bond formation is resulted by the attractive forces between oppositely charged ions.
- Elements in the left side of the periodic table tend to donate their valance electrons and become positively charged ions +ve called (*cations*).
- Elements in the right side of the periodic table tend to gain the electrons and become negatively charged ions -ve called (*anions*).
- The attraction force between two atoms that form the ionic bond is due to the difference in electronegativity of these atoms (*Electronegativity is the measurement of the ability of an atom to attract electrons*).







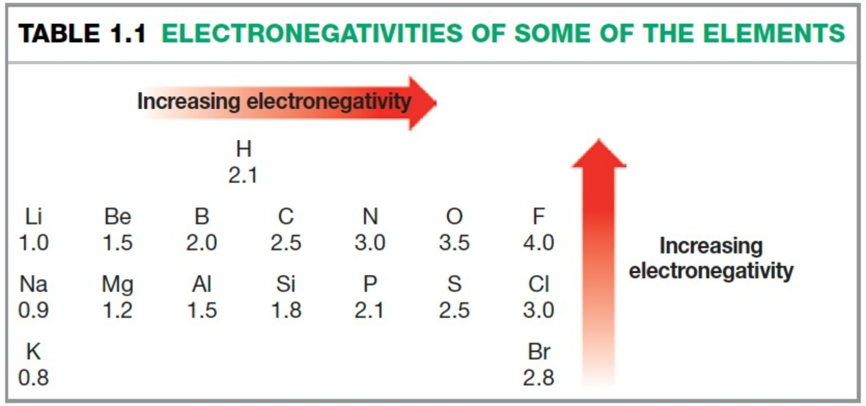


TABLE 1.1 ELECTRONEGATIVITIES OF SOME OF THE ELEMENTS

Increasing electronegativity

		H 2.1				
Li 1.0	Be 1.5	B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Na 0.9	Mg 1.2	Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0
K 0.8						Br 2.8

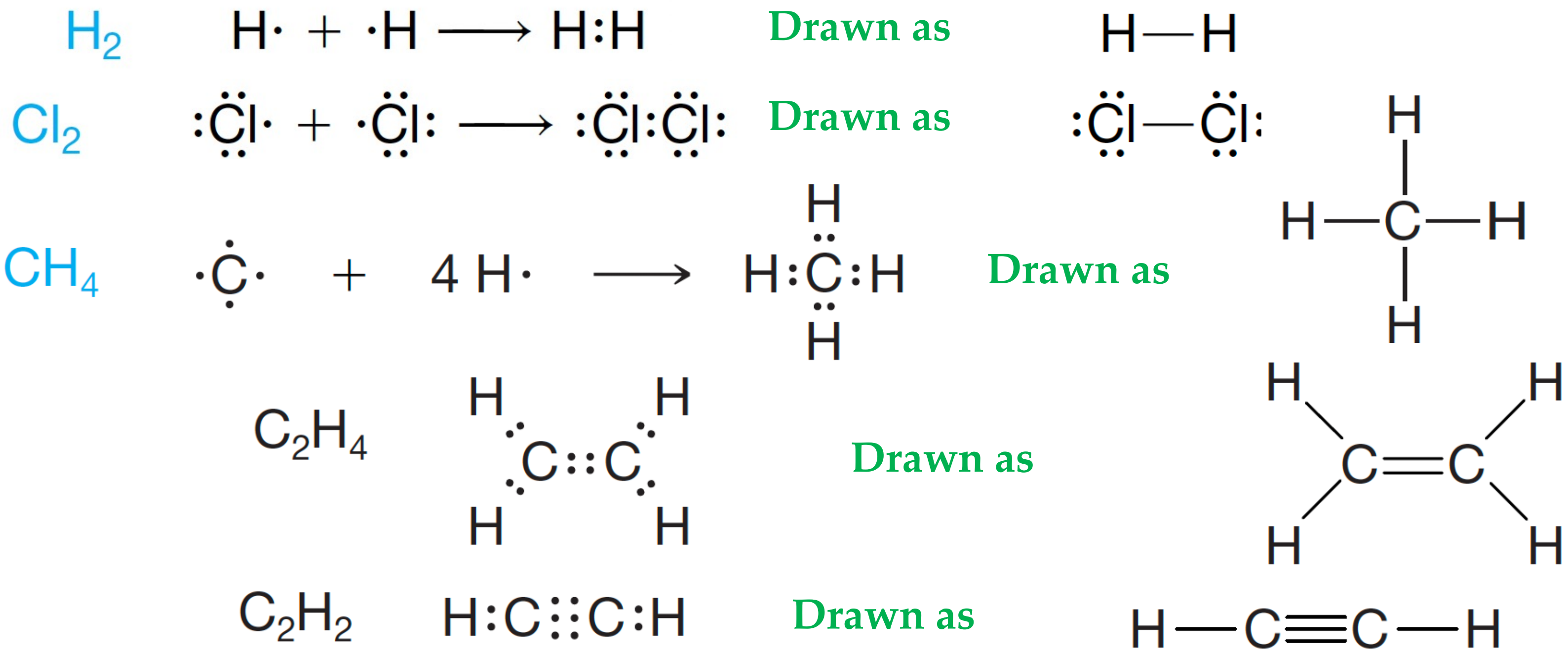
Increasing electronegativity

3. Chemical Bonding

3.3 Covalent Bonds

- **Covalent Bonds** are formed by sharing electrons between atoms that are similar or close in their electronegativities in order to achieve Nobel gases configurations.
- A shared electron pair between two atoms can be represented by a dash (–).
- When the atoms are identical or have equal electronegativities, the electron pairs are shared *equally*.

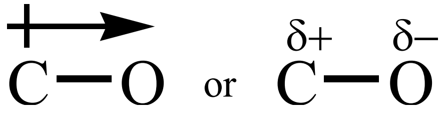
- Examples for representing covalent bonds in simple organic molecules:

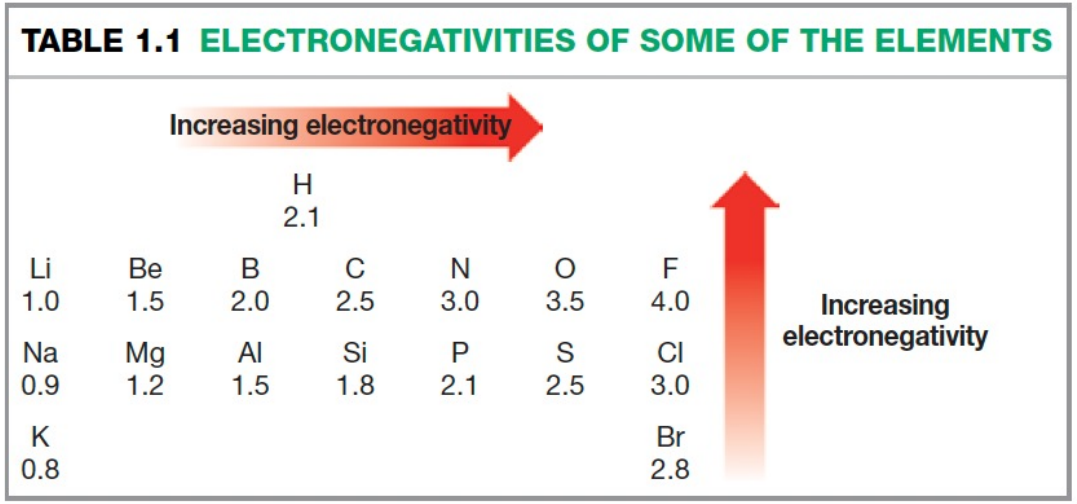


3. Chemical Bonding

3.3 Covalent Bonds

- **Polar Covalent Bonds**
  - **A type of covalent bonds in which the electron pair between two atoms is shared unequally due to the difference in their electronegativities.**
  - **The more electronegative atom assumes a partial negative charge (δ-), and the less electronegative atom assumes a partial positive charge (δ+).**
  - **Polar covalent bonds influence both physical properties and reactivity of molecules.**





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K 0.8						Br 2.8

3. Chemical Bonding

3.3 Covalent Bonds

- **Inductive Effect**
  - **It is defined as the permanent displacement of electrons forming a covalent bond (sigma *σ* bonds) towards the more electronegative element of group.**
  - **(+I) effect if the substituent is an electron-donating group.**
  - **(-I) effect if the substituent is an electron-withdrawing group.**

➢ **Electron-donating substituents (+I):**
$-CH_3$, $-C_2H_5$

➢ **Electron-withdrawing substituents (-I):**
$-NO_2$, $-NH_2$, $-OH$, $-OCH_3$

3. Chemical Bonding

3.4 Dipole Moment (*μ*)

- It is a quantitative measure of the separation of positive and negative charges in a molecule.
- It arises when two atoms in a molecule have wide different electronegativities, which creates a partial positive charge (δ+) on one atom and a partial negative charge (δ-) on the other atom.
- This physical property can be measured experimentally using the following equation:

$$\mu = e \text{ X } d$$

Where *μ*: dipole moment (measured in Debye units , D)

e: magnitude of separate charge (in esu)

d: distance between charges (in cm)

- Dipole moment of a molecule can affect other physical properties including polarity, solubility, and intermolecular forces.

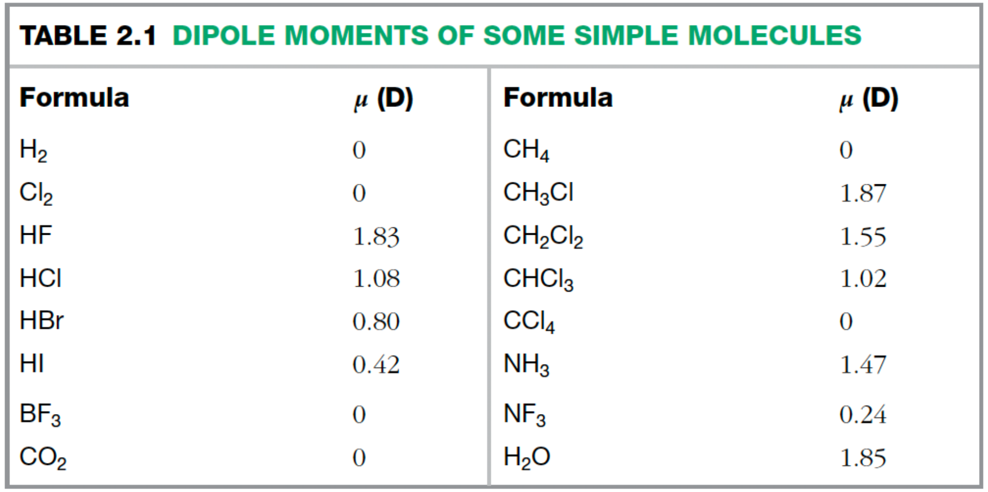
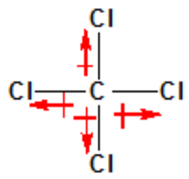


TABLE 2.1 DIPOLE MOMENTS OF SOME SIMPLE MOLECULES

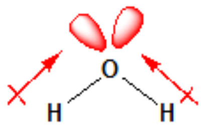
Formula	*μ* (D)	Formula	*μ* (D)
H_2	0	CH_4	0
Cl_2	0	CH_3Cl	1.87
HF	1.83	CH_2Cl_2	1.55
HCl	1.08	$CHCl_3$	1.02
HBr	0.80	CCl_4	0
HI	0.42	NH_3	1.47
BF_3	0	NF_3	0.24
CO_2	0	H_2O	1.85

CCl_4



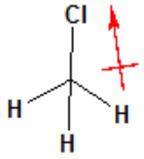
μ = zero

H_2O

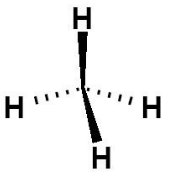


μ ≠ zero

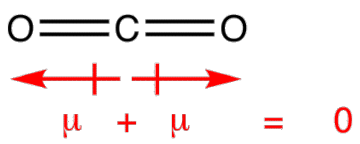
CH_3Cl



μ ≠ zero



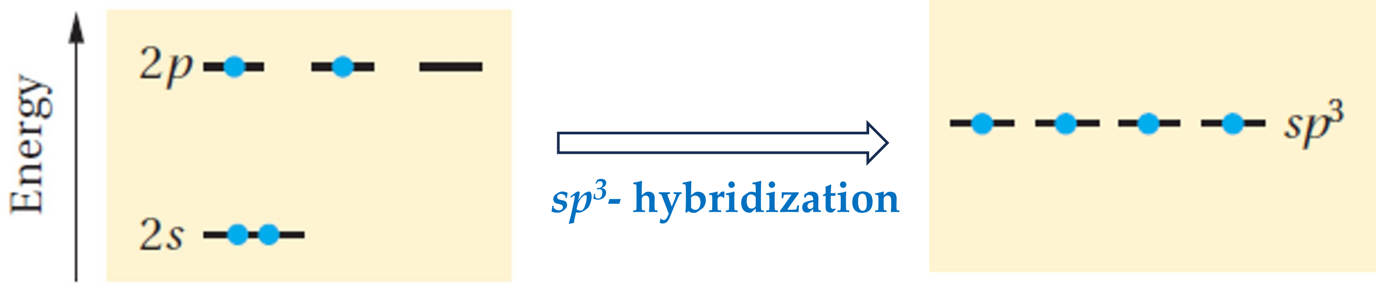
μ= 0D



4. Hybridization and Molecular Geometry

4.1 Orbitals Hybridization

- **Orbital hybridization describes how atomic orbitals mix to form new hybrid orbitals that are better suited for bonding in molecules having the same level of energy.**
- **It helps to explain shapes of molecules and their bond angles.**
- **In hydrocarbon organic molecules, there are three common types of hybridizations (sp^3, sp^2, and sp).**
- **sp^3- Hybridization (in alkanes):**
  - **The four atomic orbitals of the valence shell in the carbon atom are combined to form four identical hybrid orbitals, each has one valence electron having the same energy greater than the 2s orbital by lower than the 2p orbitals.**
  - **The four resulted hybrid orbitals are labeled (sp^3) because each one has on part of s-character and three parts of p-character.**



sp^3- hybridization

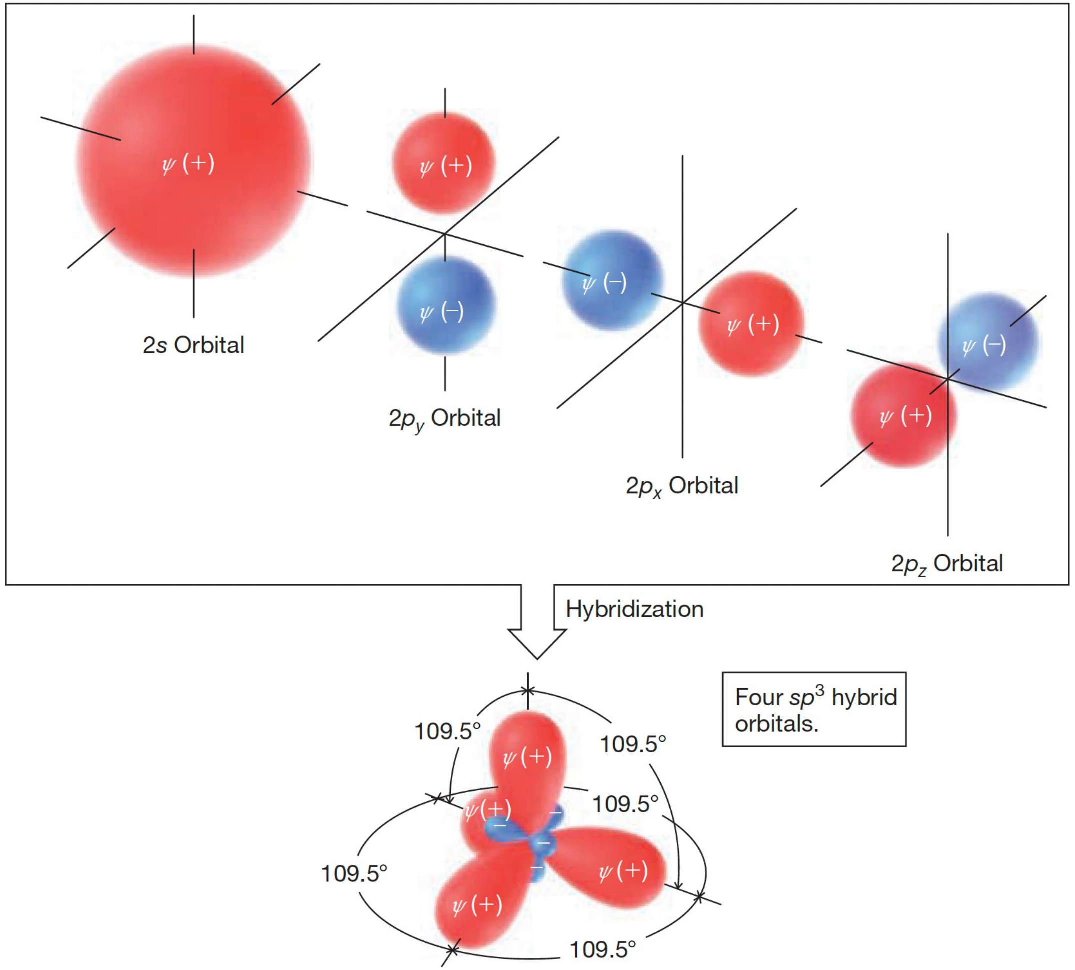
Ground state of carbon atom's atomic orbitals

Four equivalent sp^3 Hybrid orbitals

4. Hybridization and Molecular Geometry

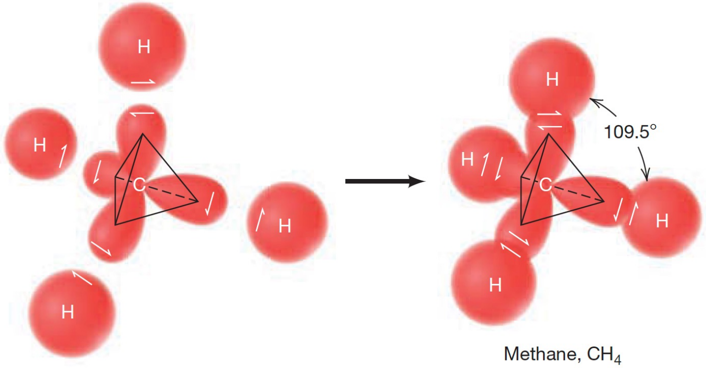
4.1 Orbitals Hybridization

- ***sp***^{3}**- Hybridization (in alkanes):**

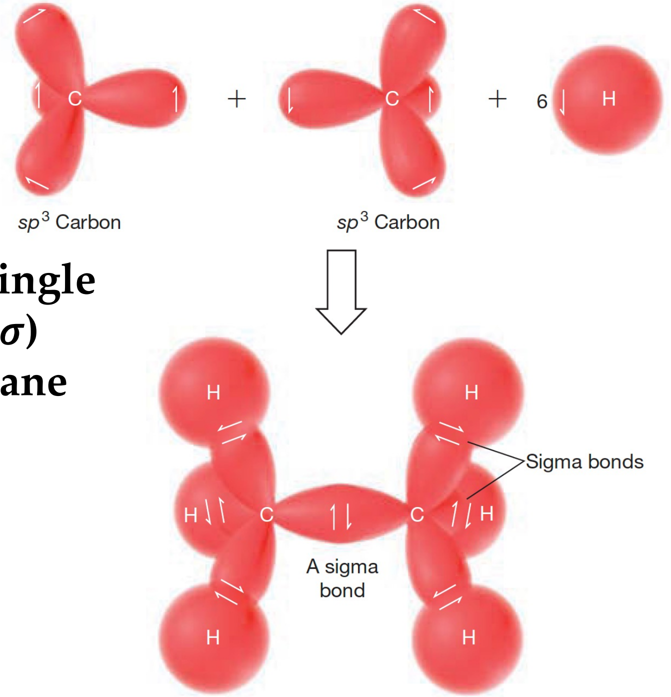


Four sp^3 hybrid orbitals.

- **Molecular Geometry of Methane (CH4):** *Tetrahedral*



Methane, CH_4



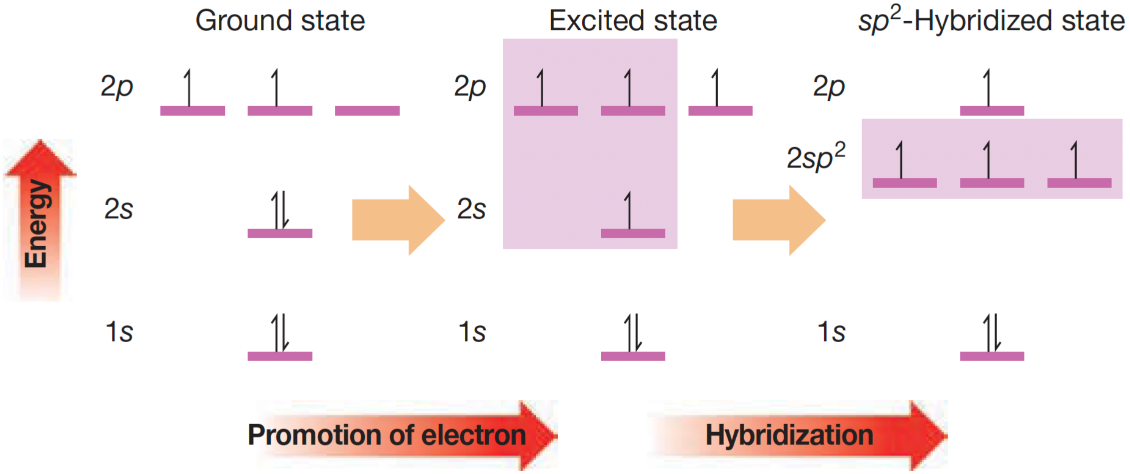
- **Forming single sigma (σ) bond in Ethane (C_2H_6)**

4. Hybridization and Molecular Geometry

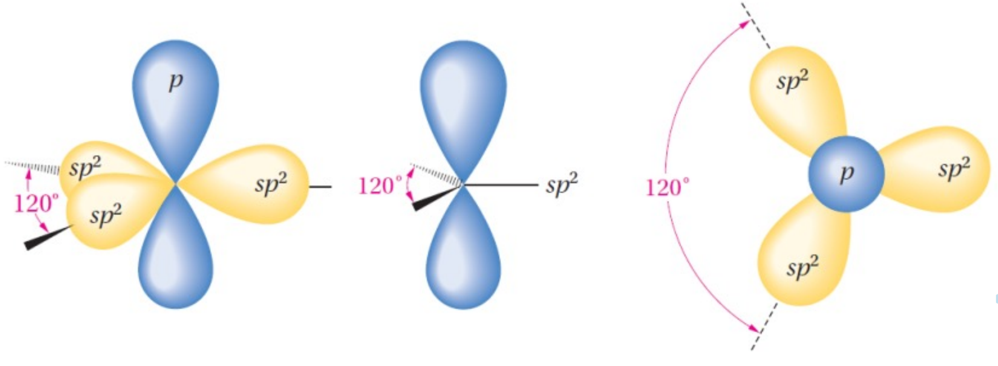
4.1 Orbitals Hybridization

- sp^2- Hybridization (in alkenes)
- **In this process, three of the atomic orbitals are mixed to produce three equivalent sp^2- hybridized orbitals.**
- **Each sp^2 hybridized orbital possesses one part of *s*-character and two parts of *p*-character.**
- **There are three valence electrons places in the three sp^2 hybridized orbitals. However, the fourth valence electron is placed in the remaining 2*p* orbital, whose axis is perpendicular to the plane formed by the three sp^2 hybridized orbitals.**
- **The molecular geometry resulted from sp^2- hybridization in alkenes is trigonal planar with bond angles of 120°.**

➢ sp^2- Hybridization Process in Carbon Atom:



➢ Molecular geometry and bond angles of sp^2- hybridization:



side view

side view with the sp^2 orbitals represented by lines

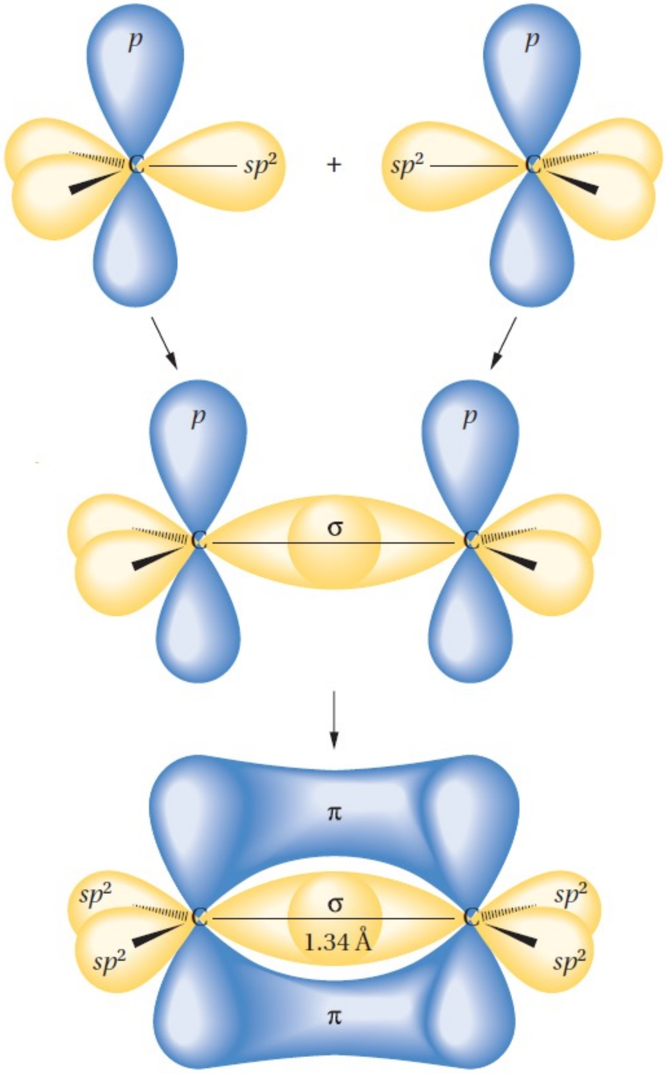
top view

4. Hybridization and Molecular Geometry

4.1 Orbitals Hybridization

- *sp*^{2}- Hybridization (in alkenes)
- **Schematic formation of a carbon–carbon double bond. Two *sp*2 carbons form a sigma (*s*) bond (end-on overlap of two sp2 orbitals) and a pi (*p*) bond (lateral overlap of two properly aligned *p* orbitals).**
- **The single sigma (*σ*) bond's length in unsaturated hydrocarbons (alkenes) is approximately equal to (1.34 °A).**

➢ *sp*^{2}- Hybridization Process in Carbon Atom:



two *sp*^{2}-hybridized carbons with *p* orbitals parallel

the σ bond is formed by two electrons in overlapping *sp*^{2} orbitals

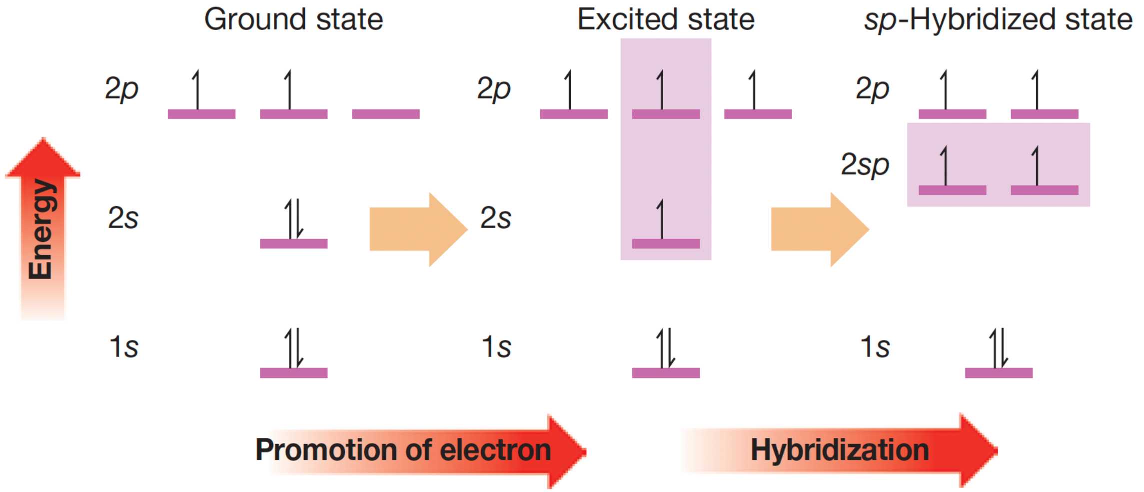
the π bond is formed by two electrons in overlapping parallel *p* orbitals

4. Hybridization and Molecular Geometry

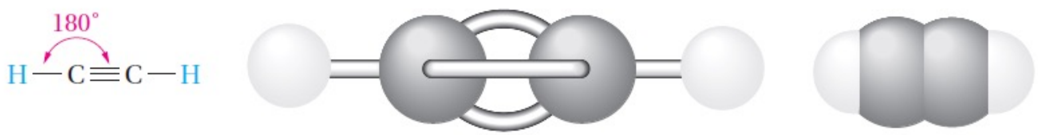
4.1 Orbitals Hybridization

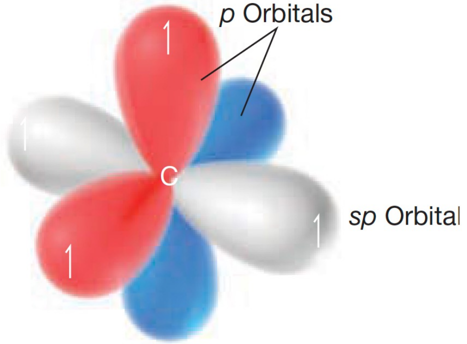
- *sp*- Hybridization (in alkynes)
- In this process, only two of the atomic orbitals are mixed to produce two equivalent *sp*-hybridized orbitals.
- Each *sp* hybridized orbital possesses one part of *s*-character and on part of *p*-character.
- There are two valence electrons places in the three *sp* hybridized orbitals, and the other two valence electrons are placed in the two remaining 2*p* orbitals.
- The molecular geometry resulted from *sp*-hybridization in alkynes is Linear with bond angles of 180°.

➢ ***sp*- Hybridization Process in Carbon Atom:**



➢ **Molecular geometry and bond angles of *sp*- hybridization:**



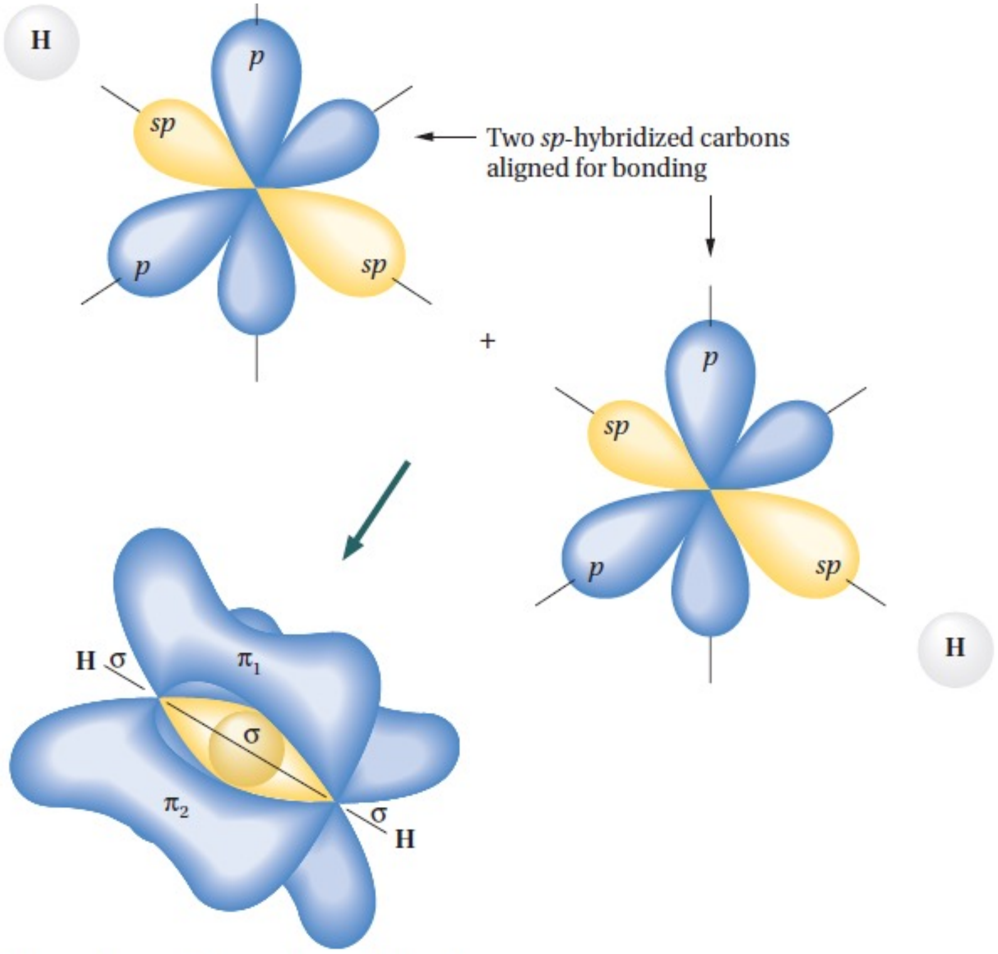


4. Hybridization and Molecular Geometry

4.1 Orbitals Hybridization

- *sp*- Hybridization (in alkynes)
- A triple bond consists of the end-on overlap of two *sp*-hybrid orbitals to form a sigma (σ) bond and the lateral overlap of two sets of parallel-oriented *p* orbitals to form two mutually perpendicular (π) bonds.
- The single sigma (*σ*) bond's length in unsaturated hydrocarbons (alkynes) is approximately equal to (1.20 °A).

➢ **Molecular geometry and bond angles of *sp*- hybridization:**

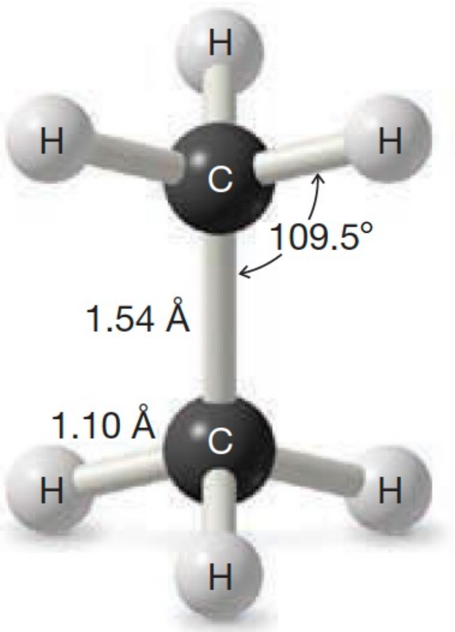


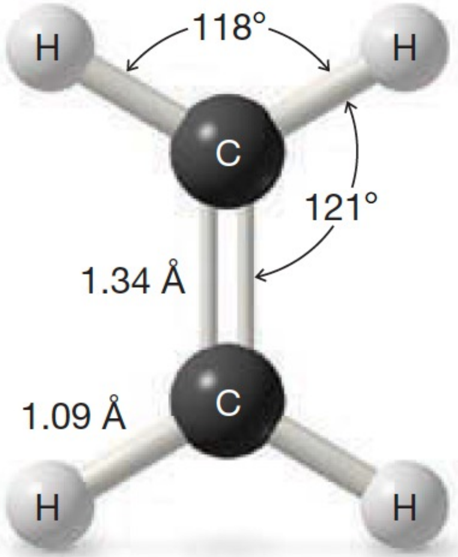
Two *sp*-hybridized carbons aligned for bonding

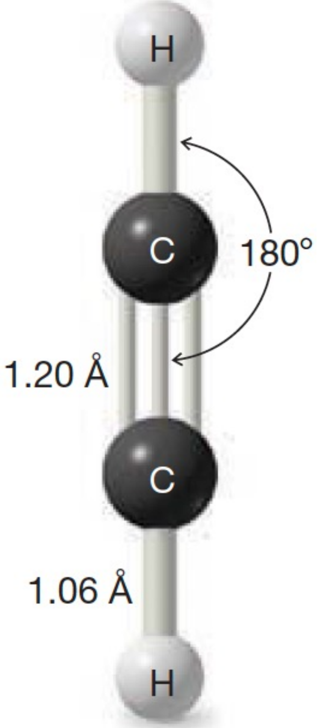
The resulting carbon–carbon triple bond, with a hydrogen atom attached to each remaining *sp* bond. (The orbitals involved in the C—H bonds are omitted for clarity.)

4. Hybridization and Molecular Geometry

4.2 Bond Lengths & Summary Slide







Molecule name: Ethane (Alkane)
Molecular formula: C_2H_6
Hybridization type: sp^3
Bond type: single sigma (σ) bond
Molecular geometry: Tetrahedral
Bond Angle: 109.5°
Bond Length: 1.54°A

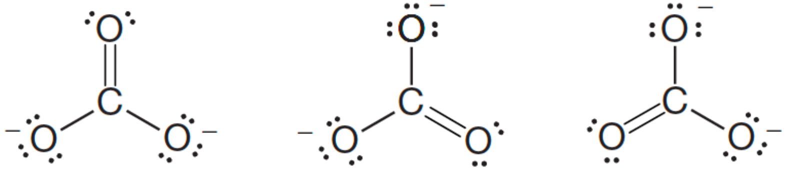
Molecule name: Ethene (Alkene)
Molecular formula: C_2H_4
Hybridization type: sp^2
Bond type: single sigma (σ) bond and one double (π)
Molecular geometry: trigonal planar
Bond Angle: 120°
Bond Length: 1.34°A

Molecule name: Ethyne (Alkyne)
Molecular formula: C_2H_2
Hybridization type: sp
Bond type: single sigma (σ) bond and two double (π)
Molecular geometry: Linear
Bond Angle: 180°
Bond Length: 1.20°A

5. Resonance and Delocalization

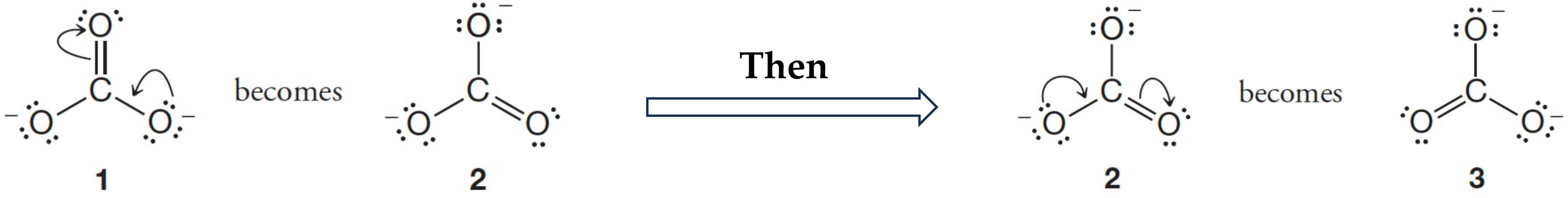
5.1 Resonance Theory

- **In chemistry, resonance is defined as a way of describing bonding in certain molecules or ions by the combination of several contributing structures or forms (commonly call resonance structures).**
- **It is especially useful for analyzing delocalized electrons in cases where bonding cannot be represented by a single Lewis structure.**
- **Resonance structures differ only in the arrangement of electrons (not atom positions).**
  - **Carbonate ion (CO_3^{-2}) can be drawn in three different, but equivalent structures:**



1 2 3

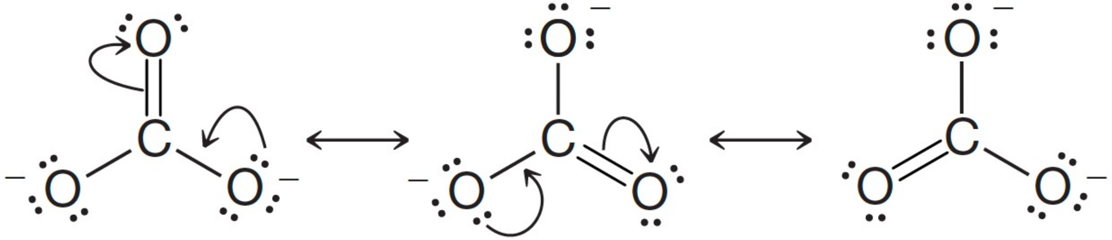
  - **The resonance structures of carbonate ion can be presented be delocalizing the electron pair of its atoms using the curved arrows, which emphasizes to move the electron pairs NOT the re-position its atoms:**



5. Resonance and Delocalization

5.2 The Use of Curved Arrows

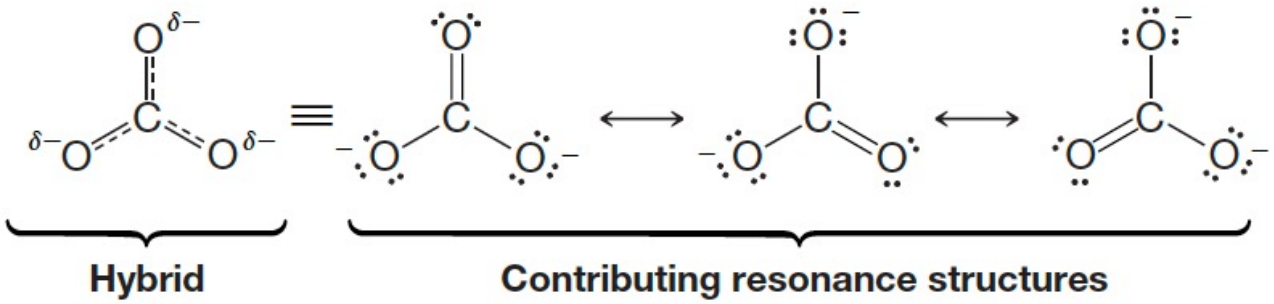
- **In organic chemistry, curved arrows (↷) are used to draw resonance structures as well as to illustrates reaction mechanisms.**
- **Important notes on the proper use of the curved arrows:**
  - **Curved arrows show the movement of both bonding and unshared electrons on atoms.**
  - **Each curved arrow represents a movement of two electrons only.**
  - **A curved arrow must originate at the electron source in the initial structure and end at the position where those electrons are represented in the resulting structure.**
  - **The new structure should show the result of the electron movement.**



5. Resonance and Delocalization

5.3 Contribution of Resonance Structures to Hybrid

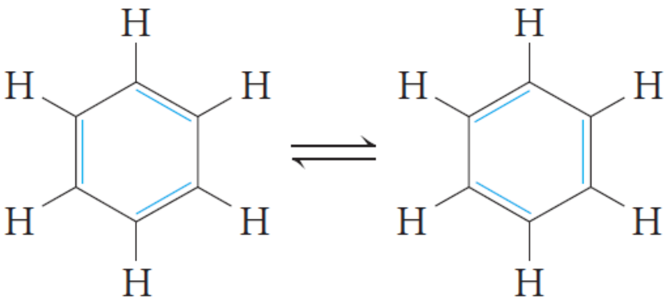
- A *Hybrid Structure* is defined as the actual electronic structure of a molecule that has more than one valid resonance structures.
- Electrons are delocalized across atoms rather than fixed in one bond or position.
- The solid and dashed lines in the hybrid structure indicates the alternation between single and double bonds as the electron pairs move across the molecules.
- The resulting hybrid structure is more stable than any individual contributing/resonance structures.



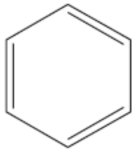
5. Resonance and Delocalization

5.4 The Resonance Explanation for the Structure of Benzene

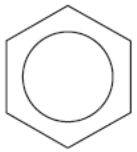
- **Benzene is an aromatic molecule that has the molecular formula of (C_6H_6) which a ratio of (1:1) between carbon and hydron atoms indicating a highly unsaturated structure.**
- **Kekule proposed that Benzene has six-carbon atoms that are located in the center of a regular hexagon one hydrogen atom attached to each carbon atom.**
- **His suggestion shows an alternation between single and double bonds through the ring via a conjugated system of doble bonds.**



the Kekulé structures for benzene



Kekulé



delocalized pi cloud

- **Resonance Model for Benzene:**